Entering Gaussian System, Link 0=g09

Initial command:

/apps/gaussian/g09d01/g09/l1.exe "/srv/scratch/z5105842/Gau-399324.inp" -scrdir="/srv/scratch/z5105842/"

Entering Link 1 = /apps/gaussian/g09d01/g09/l1.exe PID= 399344.

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Cite this work as:

Gaussian 09, Revision D.01,

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

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

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

26-Jul-2019

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

%nprocshared=12

Will use up to 12 processors via shared memory.

%mem=10GB

%chk=ZnTSPsim0.chk

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

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

d3bj

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

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

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

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

4//1;

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

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

7//1,2,3,16;

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

2/9=110/2;

99//99;

2/9=110/2;

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

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

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

7//1,2,3,16;

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

2/9=110/2;

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

99/9=1/99;

Leave Link 1 at Fri Jul 26 14:12:01 2019, MaxMem= 1342177280 cpu: 0.5

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

---------

ZnTSPsim0

---------

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C 0.68139 4.27875 -0.05521

C 1.10344 2.89397 -0.04677

N 0. 2.08942 -0.04264

C -1.10344 2.89397 -0.04677

C -0.68139 4.27875 -0.05521

C -2.44815 2.44815 -0.03857

C -2.89397 1.10344 -0.04677

N -2.08942 0. -0.04264

C -2.89397 -1.10344 -0.04677

C -4.27875 -0.68139 -0.05521

C -4.27875 0.68139 -0.05521

C 2.44815 2.44815 -0.03857

C 2.89397 1.10344 -0.04677

C 4.27875 0.68139 -0.05521

C 4.27875 -0.68139 -0.05521

C 2.89397 -1.10344 -0.04677

N 2.08942 0. -0.04264

C 2.44815 -2.44815 -0.03857

C 1.10344 -2.89397 -0.04677

C 0.68139 -4.27875 -0.05521

C -0.68139 -4.27875 -0.05521

C -1.10344 -2.89397 -0.04677

N 0. -2.08942 -0.04264

H 1.3383 5.13549 -0.0677

H -1.3383 5.13549 -0.0677

H -5.13549 -1.3383 -0.0677

H -5.13549 1.3383 -0.0677

H 5.13549 1.3383 -0.0677

H 5.13549 -1.3383 -0.0677

H 1.3383 -5.13549 -0.0677

H -1.3383 -5.13549 -0.0677

Zn 0. 0. 0.26816

C -2.44815 -2.44815 -0.03857

C -3.45725 -3.45725 -0.02147

C 3.45725 3.45725 -0.02147

C -4.30994 -4.30994 -0.00042

C 4.30994 4.30994 -0.00042

C -3.45725 3.45725 -0.02147

C -4.30994 4.30994 -0.00042

C 3.45725 -3.45725 -0.02147

C 4.30994 -4.30994 -0.00042

H 5.06464 -5.06464 0.01171

H -5.06464 -5.06464 0.01171

H -5.06464 5.06464 0.01171

H 5.06464 5.06464 0.01171

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 12 14 12 12 12 12 14 12 12

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

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

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

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

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

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

Atom 11 12 13 14 15 16 17 18 19 20

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

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

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

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

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

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

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

Atom 21 22 23 24 25 26 27 28 29 30

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

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

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

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

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

Atom 31 32 33 34 35 36 37 38 39 40

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

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

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

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

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

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

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

Atom 41 42 43 44 45

IAtWgt= 12 1 1 1 1

AtmWgt= 12.0000000 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 0 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= 0.0000000 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 6.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Leave Link 101 at Fri Jul 26 14:12:02 2019, MaxMem= 1342177280 cpu: 5.5

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Initialization pass.

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

! Initial Parameters !

! (Angstroms and Degrees) !

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

! Name Definition Value Derivative Info. !

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

! R1 R(1,2) 1.4477 estimate D2E/DX2 !

! R2 R(1,5) 1.3628 estimate D2E/DX2 !

! R3 R(1,24) 1.0797 estimate D2E/DX2 !

! R4 R(2,3) 1.3656 estimate D2E/DX2 !

! R5 R(2,12) 1.4167 estimate D2E/DX2 !

! R6 R(3,4) 1.3656 estimate D2E/DX2 !

! R7 R(3,32) 2.1124 estimate D2E/DX2 !

! R8 R(4,5) 1.4477 estimate D2E/DX2 !

! R9 R(4,6) 1.4167 estimate D2E/DX2 !

! R10 R(5,25) 1.0797 estimate D2E/DX2 !

! R11 R(6,7) 1.4167 estimate D2E/DX2 !

! R12 R(6,38) 1.4272 estimate D2E/DX2 !

! R13 R(7,8) 1.3656 estimate D2E/DX2 !

! R14 R(7,11) 1.4477 estimate D2E/DX2 !

! R15 R(8,9) 1.3656 estimate D2E/DX2 !

! R16 R(8,32) 2.1124 estimate D2E/DX2 !

! R17 R(9,10) 1.4477 estimate D2E/DX2 !

! R18 R(9,33) 1.4167 estimate D2E/DX2 !

! R19 R(10,11) 1.3628 estimate D2E/DX2 !

! R20 R(10,26) 1.0797 estimate D2E/DX2 !

! R21 R(11,27) 1.0797 estimate D2E/DX2 !

! R22 R(12,13) 1.4167 estimate D2E/DX2 !

! R23 R(12,35) 1.4272 estimate D2E/DX2 !

! R24 R(13,14) 1.4477 estimate D2E/DX2 !

! R25 R(13,17) 1.3656 estimate D2E/DX2 !

! R26 R(14,15) 1.3628 estimate D2E/DX2 !

! R27 R(14,28) 1.0797 estimate D2E/DX2 !

! R28 R(15,16) 1.4477 estimate D2E/DX2 !

! R29 R(15,29) 1.0797 estimate D2E/DX2 !

! R30 R(16,17) 1.3656 estimate D2E/DX2 !

! R31 R(16,18) 1.4167 estimate D2E/DX2 !

! R32 R(17,32) 2.1124 estimate D2E/DX2 !

! R33 R(18,19) 1.4167 estimate D2E/DX2 !

! R34 R(18,40) 1.4272 estimate D2E/DX2 !

! R35 R(19,20) 1.4477 estimate D2E/DX2 !

! R36 R(19,23) 1.3656 estimate D2E/DX2 !

! R37 R(20,21) 1.3628 estimate D2E/DX2 !

! R38 R(20,30) 1.0797 estimate D2E/DX2 !

! R39 R(21,22) 1.4477 estimate D2E/DX2 !

! R40 R(21,31) 1.0797 estimate D2E/DX2 !

! R41 R(22,23) 1.3656 estimate D2E/DX2 !

! R42 R(22,33) 1.4167 estimate D2E/DX2 !

! R43 R(23,32) 2.1124 estimate D2E/DX2 !

! R44 R(33,34) 1.4272 estimate D2E/DX2 !

! R45 R(34,36) 1.2061 estimate D2E/DX2 !

! R46 R(35,37) 1.2061 estimate D2E/DX2 !

! R47 R(36,43) 1.0674 estimate D2E/DX2 !

! R48 R(37,45) 1.0674 estimate D2E/DX2 !

! R49 R(38,39) 1.2061 estimate D2E/DX2 !

! R50 R(39,44) 1.0674 estimate D2E/DX2 !

! R51 R(40,41) 1.2061 estimate D2E/DX2 !

! R52 R(41,42) 1.0674 estimate D2E/DX2 !

! A1 A(2,1,5) 106.9498 estimate D2E/DX2 !

! A2 A(2,1,24) 125.5719 estimate D2E/DX2 !

! A3 A(5,1,24) 127.4763 estimate D2E/DX2 !

! A4 A(1,2,3) 109.1475 estimate D2E/DX2 !

! A5 A(1,2,12) 125.2934 estimate D2E/DX2 !

! A6 A(3,2,12) 125.5586 estimate D2E/DX2 !

! A7 A(2,3,4) 107.8054 estimate D2E/DX2 !

! A8 A(2,3,32) 125.6749 estimate D2E/DX2 !

! A9 A(4,3,32) 125.6749 estimate D2E/DX2 !

! A10 A(3,4,5) 109.1475 estimate D2E/DX2 !

! A11 A(3,4,6) 125.5586 estimate D2E/DX2 !

! A12 A(5,4,6) 125.2934 estimate D2E/DX2 !

! A13 A(1,5,4) 106.9498 estimate D2E/DX2 !

! A14 A(1,5,25) 127.4763 estimate D2E/DX2 !

! A15 A(4,5,25) 125.5719 estimate D2E/DX2 !

! A16 A(4,6,7) 126.6808 estimate D2E/DX2 !

! A17 A(4,6,38) 116.6596 estimate D2E/DX2 !

! A18 A(7,6,38) 116.6596 estimate D2E/DX2 !

! A19 A(6,7,8) 125.5586 estimate D2E/DX2 !

! A20 A(6,7,11) 125.2934 estimate D2E/DX2 !

! A21 A(8,7,11) 109.1475 estimate D2E/DX2 !

! A22 A(7,8,9) 107.8054 estimate D2E/DX2 !

! A23 A(7,8,32) 125.6749 estimate D2E/DX2 !

! A24 A(9,8,32) 125.6749 estimate D2E/DX2 !

! A25 A(8,9,10) 109.1475 estimate D2E/DX2 !

! A26 A(8,9,33) 125.5586 estimate D2E/DX2 !

! A27 A(10,9,33) 125.2934 estimate D2E/DX2 !

! A28 A(9,10,11) 106.9498 estimate D2E/DX2 !

! A29 A(9,10,26) 125.5719 estimate D2E/DX2 !

! A30 A(11,10,26) 127.4763 estimate D2E/DX2 !

! A31 A(7,11,10) 106.9498 estimate D2E/DX2 !

! A32 A(7,11,27) 125.5719 estimate D2E/DX2 !

! A33 A(10,11,27) 127.4763 estimate D2E/DX2 !

! A34 A(2,12,13) 126.6808 estimate D2E/DX2 !

! A35 A(2,12,35) 116.6596 estimate D2E/DX2 !

! A36 A(13,12,35) 116.6596 estimate D2E/DX2 !

! A37 A(12,13,14) 125.2934 estimate D2E/DX2 !

! A38 A(12,13,17) 125.5586 estimate D2E/DX2 !

! A39 A(14,13,17) 109.1475 estimate D2E/DX2 !

! A40 A(13,14,15) 106.9498 estimate D2E/DX2 !

! A41 A(13,14,28) 125.5719 estimate D2E/DX2 !

! A42 A(15,14,28) 127.4763 estimate D2E/DX2 !

! A43 A(14,15,16) 106.9498 estimate D2E/DX2 !

! A44 A(14,15,29) 127.4763 estimate D2E/DX2 !

! A45 A(16,15,29) 125.5719 estimate D2E/DX2 !

! A46 A(15,16,17) 109.1475 estimate D2E/DX2 !

! A47 A(15,16,18) 125.2934 estimate D2E/DX2 !

! A48 A(17,16,18) 125.5586 estimate D2E/DX2 !

! A49 A(13,17,16) 107.8054 estimate D2E/DX2 !

! A50 A(13,17,32) 125.6749 estimate D2E/DX2 !

! A51 A(16,17,32) 125.6749 estimate D2E/DX2 !

! A52 A(16,18,19) 126.6808 estimate D2E/DX2 !

! A53 A(16,18,40) 116.6596 estimate D2E/DX2 !

! A54 A(19,18,40) 116.6596 estimate D2E/DX2 !

! A55 A(18,19,20) 125.2934 estimate D2E/DX2 !

! A56 A(18,19,23) 125.5586 estimate D2E/DX2 !

! A57 A(20,19,23) 109.1475 estimate D2E/DX2 !

! A58 A(19,20,21) 106.9498 estimate D2E/DX2 !

! A59 A(19,20,30) 125.5719 estimate D2E/DX2 !

! A60 A(21,20,30) 127.4763 estimate D2E/DX2 !

! A61 A(20,21,22) 106.9498 estimate D2E/DX2 !

! A62 A(20,21,31) 127.4763 estimate D2E/DX2 !

! A63 A(22,21,31) 125.5719 estimate D2E/DX2 !

! A64 A(21,22,23) 109.1475 estimate D2E/DX2 !

! A65 A(21,22,33) 125.2934 estimate D2E/DX2 !

! A66 A(23,22,33) 125.5586 estimate D2E/DX2 !

! A67 A(19,23,22) 107.8054 estimate D2E/DX2 !

! A68 A(19,23,32) 125.6749 estimate D2E/DX2 !

! A69 A(22,23,32) 125.6749 estimate D2E/DX2 !

! A70 A(3,32,8) 88.7596 estimate D2E/DX2 !

! A71 A(3,32,17) 88.7596 estimate D2E/DX2 !

! A72 A(3,32,23) 163.0786 estimate D2E/DX2 !

! A73 A(8,32,17) 163.0786 estimate D2E/DX2 !

! A74 A(8,32,23) 88.7596 estimate D2E/DX2 !

! A75 A(17,32,23) 88.7596 estimate D2E/DX2 !

! A76 A(9,33,22) 126.6808 estimate D2E/DX2 !

! A77 A(9,33,34) 116.6596 estimate D2E/DX2 !

! A78 A(22,33,34) 116.6596 estimate D2E/DX2 !

! A79 L(33,34,36,26,-1) 180.0049 estimate D2E/DX2 !

! A80 L(12,35,37,24,-1) 180.0049 estimate D2E/DX2 !

! A81 L(34,36,43,26,-1) 179.9941 estimate D2E/DX2 !

! A82 L(35,37,45,24,-1) 179.9941 estimate D2E/DX2 !

! A83 L(6,38,39,25,-1) 180.0049 estimate D2E/DX2 !

! A84 L(38,39,44,25,-1) 179.9941 estimate D2E/DX2 !

! A85 L(18,40,41,29,-1) 180.0049 estimate D2E/DX2 !

! A86 L(40,41,42,29,-1) 179.9941 estimate D2E/DX2 !

! A87 L(33,34,36,26,-2) 180.3162 estimate D2E/DX2 !

! A88 L(12,35,37,24,-2) 179.6838 estimate D2E/DX2 !

! A89 L(34,36,43,26,-2) 179.5984 estimate D2E/DX2 !

! A90 L(35,37,45,24,-2) 180.4016 estimate D2E/DX2 !

! A91 L(6,38,39,25,-2) 180.3162 estimate D2E/DX2 !

! A92 L(38,39,44,25,-2) 179.5984 estimate D2E/DX2 !

! A93 L(18,40,41,29,-2) 179.6838 estimate D2E/DX2 !

! A94 L(40,41,42,29,-2) 180.4016 estimate D2E/DX2 !

! D1 D(5,1,2,3) 0.0339 estimate D2E/DX2 !

! D2 D(5,1,2,12) -179.7279 estimate D2E/DX2 !

! D3 D(24,1,2,3) -179.4915 estimate D2E/DX2 !

! D4 D(24,1,2,12) 0.7467 estimate D2E/DX2 !

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

! D6 D(2,1,5,25) -179.5136 estimate D2E/DX2 !

! D7 D(24,1,5,4) 179.5136 estimate D2E/DX2 !

! D8 D(24,1,5,25) 0.0 estimate D2E/DX2 !

! D9 D(1,2,3,4) -0.055 estimate D2E/DX2 !

! D10 D(1,2,3,32) -169.9848 estimate D2E/DX2 !

! D11 D(12,2,3,4) 179.7059 estimate D2E/DX2 !

! D12 D(12,2,3,32) 9.7762 estimate D2E/DX2 !

! D13 D(1,2,12,13) -179.1648 estimate D2E/DX2 !

! D14 D(1,2,12,35) 0.7752 estimate D2E/DX2 !

! D15 D(3,2,12,13) 1.1119 estimate D2E/DX2 !

! D16 D(3,2,12,35) -178.9481 estimate D2E/DX2 !

! D17 D(2,3,4,5) 0.055 estimate D2E/DX2 !

! D18 D(2,3,4,6) -179.7059 estimate D2E/DX2 !

! D19 D(32,3,4,5) 169.9848 estimate D2E/DX2 !

! D20 D(32,3,4,6) -9.7762 estimate D2E/DX2 !

! D21 D(2,3,32,8) -177.543 estimate D2E/DX2 !

! D22 D(2,3,32,17) -14.2829 estimate D2E/DX2 !

! D23 D(2,3,32,23) -95.913 estimate D2E/DX2 !

! D24 D(4,3,32,8) 14.2829 estimate D2E/DX2 !

! D25 D(4,3,32,17) 177.543 estimate D2E/DX2 !

! D26 D(4,3,32,23) 95.913 estimate D2E/DX2 !

! D27 D(3,4,5,1) -0.0339 estimate D2E/DX2 !

! D28 D(3,4,5,25) 179.4915 estimate D2E/DX2 !

! D29 D(6,4,5,1) 179.7279 estimate D2E/DX2 !

! D30 D(6,4,5,25) -0.7467 estimate D2E/DX2 !

! D31 D(3,4,6,7) -1.1119 estimate D2E/DX2 !

! D32 D(3,4,6,38) 178.9481 estimate D2E/DX2 !

! D33 D(5,4,6,7) 179.1648 estimate D2E/DX2 !

! D34 D(5,4,6,38) -0.7752 estimate D2E/DX2 !

! D35 D(4,6,7,8) 1.1119 estimate D2E/DX2 !

! D36 D(4,6,7,11) -179.1648 estimate D2E/DX2 !

! D37 D(38,6,7,8) -178.9481 estimate D2E/DX2 !

! D38 D(38,6,7,11) 0.7752 estimate D2E/DX2 !

! D39 D(6,7,8,9) 179.7059 estimate D2E/DX2 !

! D40 D(6,7,8,32) 9.7762 estimate D2E/DX2 !

! D41 D(11,7,8,9) -0.055 estimate D2E/DX2 !

! D42 D(11,7,8,32) -169.9848 estimate D2E/DX2 !

! D43 D(6,7,11,10) -179.7279 estimate D2E/DX2 !

! D44 D(6,7,11,27) 0.7467 estimate D2E/DX2 !

! D45 D(8,7,11,10) 0.0339 estimate D2E/DX2 !

! D46 D(8,7,11,27) -179.4915 estimate D2E/DX2 !

! D47 D(7,8,9,10) 0.055 estimate D2E/DX2 !

! D48 D(7,8,9,33) -179.7059 estimate D2E/DX2 !

! D49 D(32,8,9,10) 169.9848 estimate D2E/DX2 !

! D50 D(32,8,9,33) -9.7762 estimate D2E/DX2 !

! D51 D(7,8,32,3) -14.2829 estimate D2E/DX2 !

! D52 D(7,8,32,17) -95.913 estimate D2E/DX2 !

! D53 D(7,8,32,23) -177.543 estimate D2E/DX2 !

! D54 D(9,8,32,3) 177.543 estimate D2E/DX2 !

! D55 D(9,8,32,17) 95.913 estimate D2E/DX2 !

! D56 D(9,8,32,23) 14.2829 estimate D2E/DX2 !

! D57 D(8,9,10,11) -0.0339 estimate D2E/DX2 !

! D58 D(8,9,10,26) 179.4915 estimate D2E/DX2 !

! D59 D(33,9,10,11) 179.7279 estimate D2E/DX2 !

! D60 D(33,9,10,26) -0.7467 estimate D2E/DX2 !

! D61 D(8,9,33,22) -1.1119 estimate D2E/DX2 !

! D62 D(8,9,33,34) 178.9481 estimate D2E/DX2 !

! D63 D(10,9,33,22) 179.1648 estimate D2E/DX2 !

! D64 D(10,9,33,34) -0.7752 estimate D2E/DX2 !

! D65 D(9,10,11,7) 0.0 estimate D2E/DX2 !

! D66 D(9,10,11,27) 179.5136 estimate D2E/DX2 !

! D67 D(26,10,11,7) -179.5136 estimate D2E/DX2 !

! D68 D(26,10,11,27) 0.0 estimate D2E/DX2 !

! D69 D(2,12,13,14) 179.1648 estimate D2E/DX2 !

! D70 D(2,12,13,17) -1.1119 estimate D2E/DX2 !

! D71 D(35,12,13,14) -0.7752 estimate D2E/DX2 !

! D72 D(35,12,13,17) 178.9481 estimate D2E/DX2 !

! D73 D(12,13,14,15) 179.7279 estimate D2E/DX2 !

! D74 D(12,13,14,28) -0.7467 estimate D2E/DX2 !

! D75 D(17,13,14,15) -0.0339 estimate D2E/DX2 !

! D76 D(17,13,14,28) 179.4915 estimate D2E/DX2 !

! D77 D(12,13,17,16) -179.7059 estimate D2E/DX2 !

! D78 D(12,13,17,32) -9.7762 estimate D2E/DX2 !

! D79 D(14,13,17,16) 0.055 estimate D2E/DX2 !

! D80 D(14,13,17,32) 169.9848 estimate D2E/DX2 !

! D81 D(13,14,15,16) 0.0 estimate D2E/DX2 !

! D82 D(13,14,15,29) 179.5136 estimate D2E/DX2 !

! D83 D(28,14,15,16) -179.5136 estimate D2E/DX2 !

! D84 D(28,14,15,29) 0.0 estimate D2E/DX2 !

! D85 D(14,15,16,17) 0.0339 estimate D2E/DX2 !

! D86 D(14,15,16,18) -179.7279 estimate D2E/DX2 !

! D87 D(29,15,16,17) -179.4915 estimate D2E/DX2 !

! D88 D(29,15,16,18) 0.7467 estimate D2E/DX2 !

! D89 D(15,16,17,13) -0.055 estimate D2E/DX2 !

! D90 D(15,16,17,32) -169.9848 estimate D2E/DX2 !

! D91 D(18,16,17,13) 179.7059 estimate D2E/DX2 !

! D92 D(18,16,17,32) 9.7762 estimate D2E/DX2 !

! D93 D(15,16,18,19) -179.1648 estimate D2E/DX2 !

! D94 D(15,16,18,40) 0.7752 estimate D2E/DX2 !

! D95 D(17,16,18,19) 1.1119 estimate D2E/DX2 !

! D96 D(17,16,18,40) -178.9481 estimate D2E/DX2 !

! D97 D(13,17,32,3) 14.2829 estimate D2E/DX2 !

! D98 D(13,17,32,8) 95.913 estimate D2E/DX2 !

! D99 D(13,17,32,23) 177.543 estimate D2E/DX2 !

! D100 D(16,17,32,3) -177.543 estimate D2E/DX2 !

! D101 D(16,17,32,8) -95.913 estimate D2E/DX2 !

! D102 D(16,17,32,23) -14.2829 estimate D2E/DX2 !

! D103 D(16,18,19,20) 179.1648 estimate D2E/DX2 !

! D104 D(16,18,19,23) -1.1119 estimate D2E/DX2 !

! D105 D(40,18,19,20) -0.7752 estimate D2E/DX2 !

! D106 D(40,18,19,23) 178.9481 estimate D2E/DX2 !

! D107 D(18,19,20,21) 179.7279 estimate D2E/DX2 !

! D108 D(18,19,20,30) -0.7467 estimate D2E/DX2 !

! D109 D(23,19,20,21) -0.0339 estimate D2E/DX2 !

! D110 D(23,19,20,30) 179.4915 estimate D2E/DX2 !

! D111 D(18,19,23,22) -179.7059 estimate D2E/DX2 !

! D112 D(18,19,23,32) -9.7762 estimate D2E/DX2 !

! D113 D(20,19,23,22) 0.055 estimate D2E/DX2 !

! D114 D(20,19,23,32) 169.9848 estimate D2E/DX2 !

! D115 D(19,20,21,22) 0.0 estimate D2E/DX2 !

! D116 D(19,20,21,31) 179.5136 estimate D2E/DX2 !

! D117 D(30,20,21,22) -179.5136 estimate D2E/DX2 !

! D118 D(30,20,21,31) 0.0 estimate D2E/DX2 !

! D119 D(20,21,22,23) 0.0339 estimate D2E/DX2 !

! D120 D(20,21,22,33) -179.7279 estimate D2E/DX2 !

! D121 D(31,21,22,23) -179.4915 estimate D2E/DX2 !

! D122 D(31,21,22,33) 0.7467 estimate D2E/DX2 !

! D123 D(21,22,23,19) -0.055 estimate D2E/DX2 !

! D124 D(21,22,23,32) -169.9848 estimate D2E/DX2 !

! D125 D(33,22,23,19) 179.7059 estimate D2E/DX2 !

! D126 D(33,22,23,32) 9.7762 estimate D2E/DX2 !

! D127 D(21,22,33,9) -179.1648 estimate D2E/DX2 !

! D128 D(21,22,33,34) 0.7752 estimate D2E/DX2 !

! D129 D(23,22,33,9) 1.1119 estimate D2E/DX2 !

! D130 D(23,22,33,34) -178.9481 estimate D2E/DX2 !

! D131 D(19,23,32,3) 95.913 estimate D2E/DX2 !

! D132 D(19,23,32,8) 177.543 estimate D2E/DX2 !

! D133 D(19,23,32,17) 14.2829 estimate D2E/DX2 !

! D134 D(22,23,32,3) -95.913 estimate D2E/DX2 !

! D135 D(22,23,32,8) -14.2829 estimate D2E/DX2 !

! D136 D(22,23,32,17) -177.543 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 Fri Jul 26 14:12:02 2019, MaxMem= 1342177280 cpu: 0.1

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.681394 4.278747 -0.055208

2 6 0 1.103444 2.893972 -0.046773

3 7 0 0.000000 2.089417 -0.042635

4 6 0 -1.103444 2.893972 -0.046773

5 6 0 -0.681394 4.278747 -0.055208

6 6 0 -2.448151 2.448151 -0.038565

7 6 0 -2.893972 1.103444 -0.046773

8 7 0 -2.089417 0.000000 -0.042635

9 6 0 -2.893972 -1.103444 -0.046773

10 6 0 -4.278747 -0.681394 -0.055208

11 6 0 -4.278747 0.681394 -0.055208

12 6 0 2.448151 2.448151 -0.038565

13 6 0 2.893972 1.103444 -0.046773

14 6 0 4.278747 0.681394 -0.055208

15 6 0 4.278747 -0.681394 -0.055208

16 6 0 2.893972 -1.103444 -0.046773

17 7 0 2.089417 0.000000 -0.042635

18 6 0 2.448151 -2.448151 -0.038565

19 6 0 1.103444 -2.893972 -0.046773

20 6 0 0.681394 -4.278747 -0.055208

21 6 0 -0.681394 -4.278747 -0.055208

22 6 0 -1.103444 -2.893972 -0.046773

23 7 0 0.000000 -2.089417 -0.042635

24 1 0 1.338301 5.135487 -0.067701

25 1 0 -1.338301 5.135487 -0.067701

26 1 0 -5.135487 -1.338301 -0.067701

27 1 0 -5.135487 1.338301 -0.067701

28 1 0 5.135487 1.338301 -0.067701

29 1 0 5.135487 -1.338301 -0.067701

30 1 0 1.338301 -5.135487 -0.067701

31 1 0 -1.338301 -5.135487 -0.067701

32 30 0 0.000000 0.000000 0.268165

33 6 0 -2.448151 -2.448151 -0.038565

34 6 0 -3.457249 -3.457249 -0.021472

35 6 0 3.457249 3.457249 -0.021472

36 6 0 -4.309940 -4.309940 -0.000415

37 6 0 4.309940 4.309940 -0.000415

38 6 0 -3.457249 3.457249 -0.021472

39 6 0 -4.309940 4.309940 -0.000415

40 6 0 3.457249 -3.457249 -0.021472

41 6 0 4.309940 -4.309940 -0.000415

42 1 0 5.064642 -5.064642 0.011707

43 1 0 -5.064642 -5.064642 0.011707

44 1 0 -5.064642 5.064642 0.011707

45 1 0 5.064642 5.064642 0.011707

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.447687 0.000000

3 N 2.292950 1.365619 0.000000

4 C 2.259052 2.206887 1.365619 0.000000

5 C 1.362787 2.259052 2.292950 1.447687 0.000000

6 C 3.625660 3.579476 2.474298 1.416708 2.544168

7 C 4.781826 4.380106 3.057325 2.532190 3.870159

8 N 5.097571 4.309229 2.954882 3.057325 4.504483

9 C 6.461524 5.653200 4.309229 4.380106 5.819240

10 C 7.014698 6.461524 5.097571 4.781826 6.127311

11 C 6.127311 5.819240 4.504483 3.870159 5.087426

12 C 2.544168 1.416708 2.474298 3.579476 3.625660

13 C 3.870159 2.532190 3.057325 4.380106 4.781826

14 C 5.087426 3.870159 4.504483 5.819240 6.127311

15 C 6.127311 4.781826 5.097571 6.461524 7.014698

16 C 5.819240 4.380106 4.309229 5.653200 6.461524

17 N 4.504483 3.057325 2.954882 4.309229 5.097571

18 C 6.955060 5.508773 5.155869 6.414996 7.419264

19 C 7.185131 5.787945 5.104094 6.194405 7.391456

20 C 8.557494 7.185131 6.404527 7.391456 8.665327

21 C 8.665327 7.391456 6.404527 7.185131 8.557494

22 C 7.391456 6.194405 5.104094 5.787945 7.185131

23 N 6.404527 5.104094 4.178834 5.104094 6.404527

24 H 1.079670 2.253882 3.327195 3.314656 2.193930

25 H 2.193930 3.314656 3.327195 2.253882 1.079670

26 H 8.086253 7.539021 6.174392 5.845507 7.168706

27 H 6.517859 6.429993 5.190186 4.321797 5.337165

28 H 5.337165 4.321797 5.190186 6.429993 6.517859

29 H 7.168706 5.845507 6.174392 7.539021 8.086253

30 H 9.437134 8.032921 7.347852 8.392543 9.628454

31 H 9.628454 8.392543 7.347852 8.032921 9.437134

32 Zn 4.344714 3.113174 2.112406 3.113174 4.344714

33 C 7.419264 6.414996 5.155869 5.508773 6.955060

34 C 8.773548 7.819116 6.535941 6.773408 8.219012

35 C 2.895060 2.420397 3.718062 4.595415 4.219522

36 C 9.933880 9.011284 7.715513 7.885438 9.323889

37 C 3.629094 3.505529 4.848514 5.595698 4.991732

38 C 4.219522 4.595415 3.718062 2.420397 2.895060

39 C 4.991732 5.595698 4.848514 3.505529 3.629094

40 C 8.219012 6.773408 6.535941 7.819116 8.773548

41 C 9.323889 7.885438 7.715513 9.011284 9.933880

42 H 10.320671 8.890110 8.765507 10.069173 10.969062

43 H 10.969062 10.069173 8.765507 8.890110 10.320671

44 H 5.799916 6.539152 5.874139 4.517335 4.453647

45 H 4.453647 4.517335 5.874139 6.539152 5.799916

6 7 8 9 10

6 C 0.000000

7 C 1.416708 0.000000

8 N 2.474298 1.365619 0.000000

9 C 3.579476 2.206887 1.365619 0.000000

10 C 3.625660 2.259052 2.292950 1.447687 0.000000

11 C 2.544168 1.447687 2.292950 2.259052 1.362787

12 C 4.896302 5.508773 5.155869 6.414996 7.419264

13 C 5.508773 5.787945 5.104094 6.194405 7.391456

14 C 6.955060 7.185131 6.404527 7.391456 8.665327

15 C 7.419264 7.391456 6.404527 7.185131 8.557494

16 C 6.414996 6.194405 5.104094 5.787945 7.185131

17 N 5.155869 5.104094 4.178834 5.104094 6.404527

18 C 6.924416 6.414996 5.155869 5.508773 6.955060

19 C 6.414996 5.653200 4.309229 4.380106 5.819240

20 C 7.419264 6.461524 5.097571 4.781826 6.127311

21 C 6.955060 5.819240 4.504483 3.870159 5.087426

22 C 5.508773 4.380106 3.057325 2.532190 3.870159

23 N 5.155869 4.309229 2.954882 3.057325 4.504483

24 H 4.643258 5.845507 6.174392 7.539021 8.086253

25 H 2.907644 4.321797 5.190186 6.429993 6.517859

26 H 4.643258 3.314656 3.327195 2.253882 1.079670

27 H 2.907644 2.253882 3.327195 3.314656 2.193930

28 H 7.664475 8.032921 7.347852 8.392543 9.628454

29 H 8.476417 8.392543 7.347852 8.032921 9.437134

30 H 8.476417 7.539021 6.174392 5.845507 7.168706

31 H 7.664475 6.429993 5.190186 4.321797 5.337165

32 Zn 3.475769 3.113174 2.112406 3.113174 4.344714

33 C 4.896302 3.579476 2.474298 1.416708 2.544168

34 C 5.991020 4.595415 3.718062 2.420397 2.895060

35 C 5.991020 6.773408 6.535941 7.819116 8.773548

36 C 7.009958 5.595698 4.848514 3.505529 3.629094

37 C 7.009958 7.885438 7.715513 9.011284 9.933880

38 C 1.427183 2.420397 3.718062 4.595415 4.219522

39 C 2.633244 3.505529 4.848514 5.595698 4.991732

40 C 8.351514 7.819116 6.535941 6.773408 8.219012

41 C 9.557460 9.011284 7.715513 7.885438 9.323889

42 H 10.624812 10.069173 8.765507 8.890110 10.320671

43 H 7.955539 6.539152 5.874139 4.517335 4.453647

44 H 3.700618 4.517335 5.874139 6.539152 5.799916

45 H 7.955539 8.890110 8.765507 10.069173 10.969062

11 12 13 14 15

11 C 0.000000

12 C 6.955060 0.000000

13 C 7.185131 1.416708 0.000000

14 C 8.557494 2.544168 1.447687 0.000000

15 C 8.665327 3.625660 2.259052 1.362787 0.000000

16 C 7.391456 3.579476 2.206887 2.259052 1.447687

17 N 6.404527 2.474298 1.365619 2.292950 2.292950

18 C 7.419264 4.896302 3.579476 3.625660 2.544168

19 C 6.461524 5.508773 4.380106 4.781826 3.870159

20 C 7.014698 6.955060 5.819240 6.127311 5.087426

21 C 6.127311 7.419264 6.461524 7.014698 6.127311

22 C 4.781826 6.414996 5.653200 6.461524 5.819240

23 N 5.097571 5.155869 4.309229 5.097571 4.504483

24 H 7.168706 2.907644 4.321797 5.337165 6.517859

25 H 5.337165 4.643258 5.845507 7.168706 8.086253

26 H 2.193930 8.476417 8.392543 9.628454 9.437134

27 H 1.079670 7.664475 8.032921 9.437134 9.628454

28 H 9.437134 2.907644 2.253882 1.079670 2.193930

29 H 9.628454 4.643258 3.314656 2.193930 1.079670

30 H 8.086253 7.664475 6.429993 6.517859 5.337165

31 H 6.517859 8.476417 7.539021 8.086253 7.168706

32 Zn 4.344714 3.475769 3.113174 4.344714 4.344714

33 C 3.625660 6.924416 6.414996 7.419264 6.955060

34 C 4.219522 8.351514 7.819116 8.773548 8.219012

35 C 8.219012 1.427183 2.420397 2.895060 4.219522

36 C 4.991732 9.557460 9.011284 9.933880 9.323889

37 C 9.323889 2.633244 3.505529 3.629094 4.991732

38 C 2.895060 5.991020 6.773408 8.219012 8.773548

39 C 3.629094 7.009958 7.885438 9.323889 9.933880

40 C 8.773548 5.991020 4.595415 4.219522 2.895060

41 C 9.933880 7.009958 5.595698 4.991732 3.629094

42 H 10.969062 7.955539 6.539152 5.799916 4.453647

43 H 5.799916 10.624812 10.069173 10.969062 10.320671

44 H 4.453647 7.955539 8.890110 10.320671 10.969062

45 H 10.320671 3.700618 4.517335 4.453647 5.799916

16 17 18 19 20

16 C 0.000000

17 N 1.365619 0.000000

18 C 1.416708 2.474298 0.000000

19 C 2.532190 3.057325 1.416708 0.000000

20 C 3.870159 4.504483 2.544168 1.447687 0.000000

21 C 4.781826 5.097571 3.625660 2.259052 1.362787

22 C 4.380106 4.309229 3.579476 2.206887 2.259052

23 N 3.057325 2.954882 2.474298 1.365619 2.292950

24 H 6.429993 5.190186 7.664475 8.032921 9.437134

25 H 7.539021 6.174392 8.476417 8.392543 9.628454

26 H 8.032921 7.347852 7.664475 6.429993 6.517859

27 H 8.392543 7.347852 8.476417 7.539021 8.086253

28 H 3.314656 3.327195 4.643258 5.845507 7.168706

29 H 2.253882 3.327195 2.907644 4.321797 5.337165

30 H 4.321797 5.190186 2.907644 2.253882 1.079670

31 H 5.845507 6.174392 4.643258 3.314656 2.193930

32 Zn 3.113174 2.112406 3.475769 3.113174 4.344714

33 C 5.508773 5.155869 4.896302 3.579476 3.625660

34 C 6.773408 6.535941 5.991020 4.595415 4.219522

35 C 4.595415 3.718062 5.991020 6.773408 8.219012

36 C 7.885438 7.715513 7.009958 5.595698 4.991732

37 C 5.595698 4.848514 7.009958 7.885438 9.323889

38 C 7.819116 6.535941 8.351514 7.819116 8.773548

39 C 9.011284 7.715513 9.557460 9.011284 9.933880

40 C 2.420397 3.718062 1.427183 2.420397 2.895060

41 C 3.505529 4.848514 2.633244 3.505529 3.629094

42 H 4.517335 5.874139 3.700618 4.517335 4.453647

43 H 8.890110 8.765507 7.955539 6.539152 5.799916

44 H 10.069173 8.765507 10.624812 10.069173 10.969062

45 H 6.539152 5.874139 7.955539 8.890110 10.320671

21 22 23 24 25

21 C 0.000000

22 C 1.447687 0.000000

23 N 2.292950 1.365619 0.000000

24 H 9.628454 8.392543 7.347852 0.000000

25 H 9.437134 8.032921 7.347852 2.676603 0.000000

26 H 5.337165 4.321797 5.190186 9.155320 7.505236

27 H 7.168706 5.845507 6.174392 7.505236 5.370032

28 H 8.086253 7.539021 6.174392 5.370032 7.505236

29 H 6.517859 6.429993 5.190186 7.505236 9.155320

30 H 2.193930 3.314656 3.327195 10.270975 10.614006

31 H 1.079670 2.253882 3.327195 10.614006 10.270975

32 Zn 4.344714 3.113174 2.112406 5.317621 5.317621

33 C 2.544168 1.416708 2.474298 8.476417 7.664475

34 C 2.895060 2.420397 3.718062 9.840456 8.850266

35 C 8.773548 7.819116 6.535941 2.703435 5.080938

36 C 3.629094 3.505529 4.848514 11.005602 9.902084

37 C 9.933880 9.011284 7.715513 3.084914 5.708650

38 C 8.219012 6.773408 6.535941 5.080938 2.703435

39 C 9.323889 7.885438 7.715513 5.708650 3.084914

40 C 4.219522 4.595415 3.718062 8.850266 9.840456

41 C 4.991732 5.595698 4.848514 9.902084 11.005602

42 H 5.799916 6.539152 5.874139 10.859768 12.043530

43 H 4.453647 4.517335 5.874139 12.043530 10.859768

44 H 10.320671 8.890110 8.765507 6.403827 3.727860

45 H 10.969062 10.069173 8.765507 3.727860 6.403827

26 27 28 29 30

26 H 0.000000

27 H 2.676603 0.000000

28 H 10.614006 10.270975 0.000000

29 H 10.270975 10.614006 2.676603 0.000000

30 H 7.505236 9.155320 7.505236 5.370032 0.000000

31 H 5.370032 7.505236 9.155320 7.505236 2.676603

32 Zn 5.317621 5.317621 5.317621 5.317621 5.317621

33 C 2.907644 4.643258 8.476417 7.664475 4.643258

34 C 2.703435 5.080938 9.840456 8.850266 5.080938

35 C 9.840456 8.850266 2.703435 5.080938 8.850266

36 C 3.084914 5.708650 11.005602 9.902084 5.708650

37 C 11.005602 9.902084 3.084914 5.708650 9.902084

38 C 5.080938 2.703435 8.850266 9.840456 9.840456

39 C 5.708650 3.084914 9.902084 11.005602 11.005602

40 C 8.850266 9.840456 5.080938 2.703435 2.703435

41 C 9.902084 11.005602 5.708650 3.084914 3.084914

42 H 10.859768 12.043530 6.403827 3.727860 3.727860

43 H 3.727860 6.403827 12.043530 10.859768 6.403827

44 H 6.403827 3.727860 10.859768 12.043530 12.043530

45 H 12.043530 10.859768 3.727860 6.403827 10.859768

31 32 33 34 35

31 H 0.000000

32 Zn 5.317621 0.000000

33 C 2.907644 3.475769 0.000000

34 C 2.703435 4.897860 1.427183 0.000000

35 C 9.840456 4.897860 8.351514 9.778578 0.000000

36 C 3.084914 6.101091 2.633244 1.206071 10.984485

37 C 11.005602 6.101091 9.557460 10.984485 1.206071

38 C 8.850266 4.897860 5.991020 6.914499 6.914499

39 C 9.902084 6.101091 7.009958 7.813883 7.813883

40 C 5.080938 4.897860 5.991020 6.914499 6.914499

41 C 5.708650 6.101091 7.009958 7.813883 7.813883

42 H 6.403827 7.167075 7.955539 8.672222 8.672222

43 H 3.727860 7.167075 3.700618 2.273438 12.051820

44 H 10.859768 7.167075 7.955539 8.672222 8.672222

45 H 12.043530 7.167075 10.624812 12.051820 2.273438

36 37 38 39 40

36 C 0.000000

37 C 12.190352 0.000000

38 C 7.813883 7.813883 0.000000

39 C 8.619881 8.619881 1.206071 0.000000

40 C 7.813883 7.813883 9.778578 10.984485 0.000000

41 C 8.619881 8.619881 10.984485 12.190352 1.206071

42 H 9.404919 9.404919 12.051820 13.257667 2.273438

43 H 1.067378 13.257667 8.672222 9.404919 8.672222

44 H 9.404919 9.404919 2.273438 1.067378 12.051820

45 H 13.257667 1.067378 8.672222 9.404919 8.672222

41 42 43 44 45

41 C 0.000000

42 H 1.067378 0.000000

43 H 9.404919 10.129283 0.000000

44 H 13.257667 14.324970 10.129283 0.000000

45 H 9.404919 10.129283 14.324970 10.129283 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(C6H2),2SGD(N2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 2.543713 -3.507349 -0.055252

2 6 0 1.266095 -2.826600 -0.046817

3 7 0 1.477441 -1.477441 -0.042679

4 6 0 2.826600 -1.266095 -0.046817

5 6 0 3.507349 -2.543713 -0.055252

6 6 0 3.462208 0.000000 -0.038609

7 6 0 2.826600 1.266095 -0.046817

8 7 0 1.477441 1.477441 -0.042679

9 6 0 1.266095 2.826600 -0.046817

10 6 0 2.543713 3.507349 -0.055252

11 6 0 3.507349 2.543713 -0.055252

12 6 0 0.000000 -3.462208 -0.038609

13 6 0 -1.266095 -2.826600 -0.046817

14 6 0 -2.543713 -3.507349 -0.055252

15 6 0 -3.507349 -2.543713 -0.055252

16 6 0 -2.826600 -1.266095 -0.046817

17 7 0 -1.477441 -1.477441 -0.042679

18 6 0 -3.462208 0.000000 -0.038609

19 6 0 -2.826600 1.266095 -0.046817

20 6 0 -3.507349 2.543713 -0.055252

21 6 0 -2.543713 3.507349 -0.055252

22 6 0 -1.266095 2.826600 -0.046817

23 7 0 -1.477441 1.477441 -0.042679

24 1 0 2.685016 -4.577660 -0.067745

25 1 0 4.577660 -2.685016 -0.067745

26 1 0 2.685016 4.577660 -0.067745

27 1 0 4.577660 2.685016 -0.067745

28 1 0 -2.685016 -4.577660 -0.067745

29 1 0 -4.577660 -2.685016 -0.067745

30 1 0 -4.577660 2.685016 -0.067745

31 1 0 -2.685016 4.577660 -0.067745

32 30 0 0.000000 0.000000 0.268121

33 6 0 0.000000 3.462208 -0.038609

34 6 0 0.000000 4.889289 -0.021516

35 6 0 0.000000 -4.889289 -0.021516

36 6 0 0.000000 6.095176 -0.000459

37 6 0 0.000000 -6.095176 -0.000459

38 6 0 4.889289 0.000000 -0.021516

39 6 0 6.095176 0.000000 -0.000459

40 6 0 -4.889289 0.000000 -0.021516

41 6 0 -6.095176 0.000000 -0.000459

42 1 0 -7.162485 0.000000 0.011663

43 1 0 0.000000 7.162485 0.011663

44 1 0 7.162485 0.000000 0.011663

45 1 0 0.000000 -7.162485 0.011663

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

Rotational constants (GHZ): 0.1461023 0.1461023 0.0731638

Leave Link 202 at Fri Jul 26 14:12:02 2019, MaxMem= 1342177280 cpu: 0.1

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

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

Centers: 32

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: 24 25 26 27 28 29 30 31 42 43

Centers: 44 45 1 2 4 5 6 7 9 10

Centers: 11 12 13 14 15 16 18 19 20 21

Centers: 22 33 34 35 36 37 38 39 40 41

Centers: 3 8 17 23

6-311G\*

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

Pseudopotential Parameters

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

Center Atomic Valence Angular Power

Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

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

1 6

No pseudopotential on this center.

2 6

No pseudopotential on this center.

3 7

No pseudopotential on this center.

4 6

No pseudopotential on this center.

5 6

No pseudopotential on this center.

6 6

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 6

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 6

No pseudopotential on this center.

17 7

No pseudopotential on this center.

18 6

No pseudopotential on this center.

19 6

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 7

No pseudopotential on this center.

24 1

No pseudopotential on this center.

25 1

No pseudopotential on this center.

26 1

No pseudopotential on this center.

27 1

No pseudopotential on this center.

28 1

No pseudopotential on this center.

29 1

No pseudopotential on this center.

30 1

No pseudopotential on this center.

31 1

No pseudopotential on this center.

32 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

33 6

No pseudopotential on this center.

34 6

No pseudopotential on this center.

35 6

No pseudopotential on this center.

36 6

No pseudopotential on this center.

37 6

No pseudopotential on this center.

38 6

No pseudopotential on this center.

39 6

No pseudopotential on this center.

40 6

No pseudopotential on this center.

41 6

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 205 symmetry adapted cartesian basis functions of A1 symmetry.

There are 134 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 191 symmetry adapted basis functions of A1 symmetry.

There are 129 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3056.5064699504 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= 9 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= -0.1303756707 Hartrees.

Nuclear repulsion after empirical dispersion term = 3056.3760942797 Hartrees.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3898

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.11D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 224

GePol: Fraction of low-weight points (<1% of avg) = 5.75%

GePol: Cavity surface area = 415.284 Ang\*\*2

GePol: Cavity volume = 420.587 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0082802908 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3056.3843745705 Hartrees.

Leave Link 301 at Fri Jul 26 14:12:02 2019, MaxMem= 1342177280 cpu: 1.1

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16207 LenP2D= 44776.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 5.10D-05 NBF= 191 129 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 191 129 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:12:03 2019, MaxMem= 1342177280 cpu: 6.6

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:12:03 2019, MaxMem= 1342177280 cpu: 0.8

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

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1359.45139599129

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

Occupied (E) (E) (A1) (B1) (B2) (E) (E) (A1) (B2) (E) (E)

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

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

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

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

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

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

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

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

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

(E) (E) (A2) (A1)

Virtual (E) (E) (B2) (B1) (E) (E) (B1) (A2) (B2) (A1)

(E) (E) (E) (E) (A2) (A1) (A1) (A1) (E) (E) (B2)

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

(B2) (E) (E) (E) (E) (A2) (B2) (B2) (E) (E) (A1)

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

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

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

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(B2) (E) (E) (E) (E) (B2) (E) (E) (B1) (A2) (B1)

(B2) (A2) (E) (E) (A1) (B2) (A1) (E) (E) (A2)

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

(E) (B2) (A2) (B2) (E) (E) (A1) (B2) (E) (E) (A1)

(B2) (B1) (E) (E) (B1) (A2) (E) (E) (B1) (A2)

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

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

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

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

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

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

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

(E) (E) (B2) (A1) (E) (E) (B2) (A2) (B2) (E) (E)

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

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

(E) (E) (A2) (B2) (E) (E) (A2) (E) (E) (A1) (B2)

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

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

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

(A1) (E) (E)

The electronic state of the initial guess is 1-A1.

Leave Link 401 at Fri Jul 26 14:12:04 2019, MaxMem= 1342177280 cpu: 11.9

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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= 660000000 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= 0 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= 45583212.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.22D-15 for 309.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.28D-15 for 2582 487.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.33D-15 for 649.

Iteration 1 A^-1\*A deviation from orthogonality is 6.22D-11 for 1794 1792.

E= -1358.34707076729

DIIS: error= 8.78D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1358.34707076729 IErMin= 1 ErrMin= 8.78D-02

ErrMax= 8.78D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.46D-01 BMatP= 9.46D-01

IDIUse=3 WtCom= 1.22D-01 WtEn= 8.78D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.095 Goal= None Shift= 0.000

GapD= 0.095 DampG=0.500 DampE=0.250 DampFc=0.1250 IDamp=-1.

Damping current iteration by 1.25D-01

RMSDP=2.76D-03 MaxDP=1.16D-01 OVMax= 1.66D-01

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.43D-04 CP: 9.96D-01

E= -1358.49312013499 Delta-E= -0.146049367690 Rises=F Damp=T

DIIS: error= 6.27D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1358.49312013499 IErMin= 2 ErrMin= 6.27D-02

ErrMax= 6.27D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.51D-01 BMatP= 9.46D-01

IDIUse=3 WtCom= 3.73D-01 WtEn= 6.27D-01

Coeff-Com: -0.299D+01 0.399D+01

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

Coeff: -0.112D+01 0.212D+01

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=1.59D-03 MaxDP=6.67D-02 DE=-1.46D-01 OVMax= 4.37D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 9.46D-04 CP: 9.64D-01 3.00D+00

E= -1358.94097692917 Delta-E= -0.447856794183 Rises=F Damp=F

DIIS: error= 4.10D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1358.94097692917 IErMin= 3 ErrMin= 4.10D-02

ErrMax= 4.10D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.56D-01 BMatP= 5.51D-01

IDIUse=3 WtCom= 5.90D-01 WtEn= 4.10D-01

Coeff-Com: 0.163D+01-0.163D+01 0.100D+01

Coeff-En: 0.299D-01 0.000D+00 0.970D+00

Coeff: 0.974D+00-0.963D+00 0.988D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=8.34D-04 MaxDP=3.81D-02 DE=-4.48D-01 OVMax= 4.67D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.72D-04 CP: 9.70D-01 3.00D+00 3.61D-01

E= -1359.04107536257 Delta-E= -0.100098433398 Rises=F Damp=F

DIIS: error= 1.80D-02 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.04107536257 IErMin= 4 ErrMin= 1.80D-02

ErrMax= 1.80D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.75D-02 BMatP= 1.56D-01

IDIUse=3 WtCom= 8.20D-01 WtEn= 1.80D-01

Coeff-Com: -0.160D+00 0.228D+00 0.288D+00 0.644D+00

Coeff-En: 0.000D+00 0.000D+00 0.708D-01 0.929D+00

Coeff: -0.131D+00 0.187D+00 0.249D+00 0.695D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=2.65D-04 MaxDP=1.03D-02 DE=-1.00D-01 OVMax= 2.30D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 8.79D-05 CP: 9.69D-01 3.00D+00 5.26D-01 6.59D-01

E= -1359.05954270851 Delta-E= -0.018467345942 Rises=F Damp=F

DIIS: error= 2.95D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.05954270851 IErMin= 5 ErrMin= 2.95D-03

ErrMax= 2.95D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.88D-03 BMatP= 2.75D-02

IDIUse=3 WtCom= 9.71D-01 WtEn= 2.95D-02

Coeff-Com: -0.204D+00 0.239D+00 0.933D-01 0.439D+00 0.433D+00

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

Coeff: -0.198D+00 0.232D+00 0.906D-01 0.426D+00 0.450D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=6.10D-05 MaxDP=2.77D-03 DE=-1.85D-02 OVMax= 7.43D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.18D-05 CP: 9.69D-01 3.00D+00 5.20D-01 7.28D-01 5.39D-01

E= -1359.06114867889 Delta-E= -0.001605970378 Rises=F Damp=F

DIIS: error= 5.90D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.06114867889 IErMin= 6 ErrMin= 5.90D-04

ErrMax= 5.90D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.25D-05 BMatP= 1.88D-03

IDIUse=3 WtCom= 9.94D-01 WtEn= 5.90D-03

Coeff-Com: -0.778D-01 0.893D-01 0.261D-01 0.151D+00 0.211D+00 0.600D+00

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

Coeff: -0.774D-01 0.888D-01 0.259D-01 0.150D+00 0.210D+00 0.603D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=8.48D-06 MaxDP=3.54D-04 DE=-1.61D-03 OVMax= 9.92D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 6.04D-06 CP: 9.69D-01 3.00D+00 5.22D-01 7.27D-01 5.50D-01

CP: 7.44D-01

E= -1359.06117085410 Delta-E= -0.000022175216 Rises=F Damp=F

DIIS: error= 9.70D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.06117085410 IErMin= 7 ErrMin= 9.70D-05

ErrMax= 9.70D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.60D-06 BMatP= 3.25D-05

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

Coeff-Com: -0.336D-01 0.382D-01 0.728D-02 0.540D-01 0.853D-01 0.315D+00

Coeff-Com: 0.534D+00

Coeff: -0.336D-01 0.382D-01 0.728D-02 0.540D-01 0.853D-01 0.315D+00

Coeff: 0.534D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=2.48D-06 MaxDP=1.01D-04 DE=-2.22D-05 OVMax= 4.02D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.89D-06 CP: 9.69D-01 3.00D+00 5.22D-01 7.27D-01 5.58D-01

CP: 7.49D-01 7.68D-01

E= -1359.06117314518 Delta-E= -0.000002291073 Rises=F Damp=F

DIIS: error= 2.98D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.06117314518 IErMin= 8 ErrMin= 2.98D-05

ErrMax= 2.98D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.48D-07 BMatP= 2.60D-06

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

Coeff-Com: -0.592D-02 0.662D-02 0.944D-03 0.852D-02 0.165D-01 0.717D-01

Coeff-Com: 0.271D+00 0.631D+00

Coeff: -0.592D-02 0.662D-02 0.944D-03 0.852D-02 0.165D-01 0.717D-01

Coeff: 0.271D+00 0.631D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=7.81D-07 MaxDP=3.62D-05 DE=-2.29D-06 OVMax= 1.18D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 5.02D-07 CP: 9.69D-01 3.00D+00 5.22D-01 7.27D-01 5.57D-01

CP: 7.52D-01 8.35D-01 8.18D-01

E= -1359.06117334207 Delta-E= -0.000000196896 Rises=F Damp=F

DIIS: error= 1.24D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1359.06117334207 IErMin= 9 ErrMin= 1.24D-05

ErrMax= 1.24D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.00D-08 BMatP= 2.48D-07

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

Coeff-Com: 0.153D-02-0.183D-02-0.357D-03-0.261D-02-0.176D-02 0.240D-02

Coeff-Com: 0.111D+00 0.399D+00 0.493D+00

Coeff: 0.153D-02-0.183D-02-0.357D-03-0.261D-02-0.176D-02 0.240D-02

Coeff: 0.111D+00 0.399D+00 0.493D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=3.25D-07 MaxDP=1.53D-05 DE=-1.97D-07 OVMax= 5.02D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.40D-07 CP: 9.69D-01 3.00D+00 5.22D-01 7.27D-01 5.58D-01

CP: 7.55D-01 8.29D-01 8.30D-01 7.05D-01

E= -1359.06117338110 Delta-E= -0.000000039030 Rises=F Damp=F

DIIS: error= 4.04D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1359.06117338110 IErMin=10 ErrMin= 4.04D-06

ErrMax= 4.04D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.23D-09 BMatP= 5.00D-08

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

Coeff-Com: 0.808D-03-0.934D-03-0.834D-04-0.988D-03-0.129D-02-0.343D-02

Coeff-Com: 0.554D-02 0.448D-01 0.164D+00 0.792D+00

Coeff: 0.808D-03-0.934D-03-0.834D-04-0.988D-03-0.129D-02-0.343D-02

Coeff: 0.554D-02 0.448D-01 0.164D+00 0.792D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=8.16D-08 MaxDP=2.98D-06 DE=-3.90D-08 OVMax= 7.26D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.08D-08 CP: 9.69D-01 3.00D+00 5.22D-01 7.27D-01 5.58D-01

CP: 7.56D-01 8.30D-01 8.35D-01 7.58D-01 9.62D-01

E= -1359.06117338195 Delta-E= -0.000000000849 Rises=F Damp=F

DIIS: error= 4.16D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1359.06117338195 IErMin=11 ErrMin= 4.16D-07

ErrMax= 4.16D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.28D-11 BMatP= 1.23D-09

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

Coeff-Com: 0.114D-03-0.130D-03-0.228D-04-0.171D-03-0.277D-03-0.635D-03

Coeff-Com: -0.192D-02 0.459D-02 0.381D-01 0.221D+00 0.739D+00

Coeff: 0.114D-03-0.130D-03-0.228D-04-0.171D-03-0.277D-03-0.635D-03

Coeff: -0.192D-02 0.459D-02 0.381D-01 0.221D+00 0.739D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=1.82D-08 MaxDP=9.69D-07 DE=-8.49D-10 OVMax= 1.86D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.38D-08 CP: 9.69D-01 3.00D+00 5.22D-01 7.27D-01 5.58D-01

CP: 7.56D-01 8.29D-01 8.36D-01 7.59D-01 9.72D-01

CP: 9.39D-01

E= -1359.06117338189 Delta-E= 0.000000000055 Rises=F Damp=F

DIIS: error= 2.10D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=11 EnMin= -1359.06117338195 IErMin=12 ErrMin= 2.10D-07

ErrMax= 2.10D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.11D-11 BMatP= 6.28D-11

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

Coeff-Com: -0.379D-04 0.449D-04-0.891D-05 0.280D-05-0.334D-04-0.297D-04

Coeff-Com: -0.167D-02-0.189D-02-0.112D-02 0.252D-03 0.337D+00 0.667D+00

Coeff: -0.379D-04 0.449D-04-0.891D-05 0.280D-05-0.334D-04-0.297D-04

Coeff: -0.167D-02-0.189D-02-0.112D-02 0.252D-03 0.337D+00 0.667D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=7.33D-09 MaxDP=3.01D-07 DE= 5.46D-11 OVMax= 6.86D-07

Error on total polarization charges = 0.06219

SCF Done: E(RB3LYP) = -1359.06117338 A.U. after 12 cycles

NFock= 12 Conv=0.73D-08 -V/T= 1.9682

KE= 1.403669532524D+03 PE=-9.354832583184D+03 EE= 3.535717502708D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.20

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:12:48 2019, MaxMem= 1342177280 cpu: 500.7

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

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

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Population analysis using the SCF density.

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

Orbital symmetries:

Occupied (E) (E) (B1) (A1) (E) (E) (B2) (A1) (B1) (E) (E)

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

(E) (E) (A1) (A2) (E) (E) (B2) (B2) (E) (E) (A1)

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

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

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

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

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

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

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

(E) (E) (A2) (A1)

Virtual (E) (E) (B2) (A1) (B1) (E) (E) (B1) (B2) (A2)

(E) (E) (A1) (E) (E) (A1) (E) (E) (A2) (A1) (E)

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(A1) (E) (E) (B2) (E) (E) (A1) (B2) (A1) (E) (E)

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

(A2) (B2) (E) (E) (B2) (E) (E) (E) (E) (B1) (A2)

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

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

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

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

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

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

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(E) (A1) (B1) (E) (E) (A2) (A2) (A1) (A2) (E)

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

(B1) (B2) (E) (E) (B2) (E) (E) (A2) (E) (E) (B1)

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

(A2) (A1) (E) (E) (B2) (E) (E) (A1) (A2) (B2)

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

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

(E) (E) (B1) (E) (E) (A2) (B2) (E) (E) (A2) (E)

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

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

(B2) (E) (E) (A1) (B2) (E) (E) (A2) (B2) (A1)

(E) (E) (B1) (A1) (E) (E)

The electronic state is 1-A1.

Alpha occ. eigenvalues -- -14.31344 -14.31344 -14.31343 -14.31343 -10.22129

Alpha occ. eigenvalues -- -10.22129 -10.22129 -10.22128 -10.22121 -10.22121

Alpha occ. eigenvalues -- -10.22121 -10.22121 -10.22002 -10.22002 -10.22002

Alpha occ. eigenvalues -- -10.22001 -10.18483 -10.18483 -10.18483 -10.18483

Alpha occ. eigenvalues -- -10.17615 -10.17615 -10.17615 -10.17614 -10.17548

Alpha occ. eigenvalues -- -10.17548 -10.17548 -10.17548 -10.17339 -10.17339

Alpha occ. eigenvalues -- -10.17339 -10.17339 -0.97546 -0.96712 -0.96712

Alpha occ. eigenvalues -- -0.95818 -0.85113 -0.83097 -0.83097 -0.81086

Alpha occ. eigenvalues -- -0.77527 -0.77499 -0.77499 -0.76974 -0.75425

Alpha occ. eigenvalues -- -0.74786 -0.74786 -0.73047 -0.73004 -0.67761

Alpha occ. eigenvalues -- -0.67761 -0.62763 -0.60244 -0.59961 -0.59145

Alpha occ. eigenvalues -- -0.59145 -0.58271 -0.57391 -0.56587 -0.56587

Alpha occ. eigenvalues -- -0.56231 -0.55771 -0.55252 -0.55024 -0.55024

Alpha occ. eigenvalues -- -0.53389 -0.52380 -0.52380 -0.52253 -0.51472

Alpha occ. eigenvalues -- -0.51472 -0.50683 -0.49332 -0.46117 -0.45048

Alpha occ. eigenvalues -- -0.45048 -0.44309 -0.43352 -0.42985 -0.42852

Alpha occ. eigenvalues -- -0.42852 -0.41443 -0.41443 -0.40219 -0.40022

Alpha occ. eigenvalues -- -0.39159 -0.38488 -0.38488 -0.38164 -0.37807

Alpha occ. eigenvalues -- -0.37490 -0.34131 -0.34131 -0.32432 -0.32281

Alpha occ. eigenvalues -- -0.32281 -0.29689 -0.29371 -0.29371 -0.29050

Alpha occ. eigenvalues -- -0.27617 -0.27006 -0.26945 -0.26945 -0.26805

Alpha occ. eigenvalues -- -0.25553 -0.25255 -0.25255 -0.21136 -0.19922

Alpha virt. eigenvalues -- -0.10794 -0.10794 -0.05758 0.01699 0.02798

Alpha virt. eigenvalues -- 0.03134 0.03134 0.03241 0.03565 0.03713

Alpha virt. eigenvalues -- 0.04164 0.04164 0.04667 0.04971 0.04971

Alpha virt. eigenvalues -- 0.05651 0.05675 0.05675 0.06434 0.07828

Alpha virt. eigenvalues -- 0.08472 0.08472 0.08533 0.09691 0.09858

Alpha virt. eigenvalues -- 0.09865 0.09865 0.11480 0.12490 0.12490

Alpha virt. eigenvalues -- 0.13617 0.14315 0.15234 0.16365 0.16365

Alpha virt. eigenvalues -- 0.16379 0.17351 0.17351 0.19077 0.19855

Alpha virt. eigenvalues -- 0.22168 0.23092 0.23092 0.23567 0.24250

Alpha virt. eigenvalues -- 0.24305 0.24887 0.24887 0.25550 0.25550

Alpha virt. eigenvalues -- 0.26455 0.26471 0.26743 0.27948 0.29705

Alpha virt. eigenvalues -- 0.29705 0.31016 0.31191 0.32439 0.32447

Alpha virt. eigenvalues -- 0.32447 0.34535 0.34535 0.35097 0.35230

Alpha virt. eigenvalues -- 0.35669 0.35669 0.35992 0.35992 0.36460

Alpha virt. eigenvalues -- 0.36596 0.36962 0.37960 0.38488 0.39525

Alpha virt. eigenvalues -- 0.39991 0.40224 0.40224 0.40352 0.40968

Alpha virt. eigenvalues -- 0.40968 0.41450 0.41871 0.41871 0.43214

Alpha virt. eigenvalues -- 0.43357 0.43357 0.43550 0.44366 0.44544

Alpha virt. eigenvalues -- 0.45227 0.46022 0.46022 0.47242 0.47242

Alpha virt. eigenvalues -- 0.47765 0.48103 0.48854 0.48854 0.49366

Alpha virt. eigenvalues -- 0.49366 0.50674 0.51132 0.51221 0.51345

Alpha virt. eigenvalues -- 0.51722 0.51942 0.51942 0.51994 0.54971

Alpha virt. eigenvalues -- 0.55658 0.55658 0.57199 0.57199 0.57586

Alpha virt. eigenvalues -- 0.57726 0.57726 0.57728 0.58185 0.58647

Alpha virt. eigenvalues -- 0.58647 0.61305 0.62034 0.62078 0.62190

Alpha virt. eigenvalues -- 0.62295 0.62295 0.63307 0.63307 0.63362

Alpha virt. eigenvalues -- 0.63936 0.64380 0.64833 0.65158 0.65158

Alpha virt. eigenvalues -- 0.65358 0.68109 0.68109 0.68938 0.68945

Alpha virt. eigenvalues -- 0.69846 0.69986 0.69986 0.70161 0.71870

Alpha virt. eigenvalues -- 0.71870 0.72964 0.72964 0.73602 0.74322

Alpha virt. eigenvalues -- 0.74470 0.74470 0.74631 0.74818 0.75144

Alpha virt. eigenvalues -- 0.75144 0.77023 0.77648 0.79217 0.81403

Alpha virt. eigenvalues -- 0.81403 0.81696 0.82322 0.83088 0.84192

Alpha virt. eigenvalues -- 0.84192 0.85196 0.85913 0.85913 0.88232

Alpha virt. eigenvalues -- 0.89939 0.90657 0.91047 0.91237 0.92505

Alpha virt. eigenvalues -- 0.92505 0.94768 0.95616 0.95616 0.96087

Alpha virt. eigenvalues -- 0.96961 0.96961 0.99662 1.00093 1.00093

Alpha virt. eigenvalues -- 1.00835 1.01398 1.01419 1.02137 1.02137

Alpha virt. eigenvalues -- 1.03699 1.03699 1.03883 1.05234 1.05963

Alpha virt. eigenvalues -- 1.06967 1.07160 1.08705 1.08705 1.11631

Alpha virt. eigenvalues -- 1.12359 1.12376 1.12376 1.12481 1.13472

Alpha virt. eigenvalues -- 1.13472 1.13680 1.13700 1.14046 1.14982

Alpha virt. eigenvalues -- 1.14982 1.15772 1.15772 1.16803 1.17318

Alpha virt. eigenvalues -- 1.18304 1.18654 1.18654 1.19281 1.20094

Alpha virt. eigenvalues -- 1.20120 1.20120 1.21013 1.21106 1.21983

Alpha virt. eigenvalues -- 1.23613 1.24538 1.24538 1.25094 1.25568

Alpha virt. eigenvalues -- 1.25568 1.28291 1.28765 1.29597 1.29597

Alpha virt. eigenvalues -- 1.30708 1.32175 1.33828 1.33828 1.34054

Alpha virt. eigenvalues -- 1.37350 1.40053 1.40053 1.42154 1.46655

Alpha virt. eigenvalues -- 1.47819 1.48962 1.48962 1.49436 1.51114

Alpha virt. eigenvalues -- 1.51114 1.52867 1.55045 1.55045 1.55300

Alpha virt. eigenvalues -- 1.55398 1.55409 1.55409 1.56856 1.57591

Alpha virt. eigenvalues -- 1.58275 1.58485 1.58485 1.59437 1.59437

Alpha virt. eigenvalues -- 1.59453 1.61039 1.61539 1.61539 1.63121

Alpha virt. eigenvalues -- 1.63273 1.63273 1.64498 1.64934 1.65610

Alpha virt. eigenvalues -- 1.66229 1.68896 1.68896 1.70552 1.70552

Alpha virt. eigenvalues -- 1.71989 1.72168 1.73659 1.74962 1.75734

Alpha virt. eigenvalues -- 1.77250 1.77250 1.78637 1.78637 1.78776

Alpha virt. eigenvalues -- 1.79936 1.79936 1.79947 1.80060 1.80718

Alpha virt. eigenvalues -- 1.83986 1.83986 1.84830 1.86135 1.87705

Alpha virt. eigenvalues -- 1.87705 1.88275 1.88921 1.89384 1.89384

Alpha virt. eigenvalues -- 1.89621 1.89765 1.90074 1.92946 1.93708

Alpha virt. eigenvalues -- 1.94518 1.94631 1.94631 1.94819 1.95584

Alpha virt. eigenvalues -- 1.95584 1.97185 1.97185 1.98222 1.99779

Alpha virt. eigenvalues -- 2.00592 2.03051 2.03051 2.04204 2.04248

Alpha virt. eigenvalues -- 2.04248 2.09203 2.09203 2.11308 2.11659

Alpha virt. eigenvalues -- 2.13564 2.17873 2.19659 2.25355 2.27475

Alpha virt. eigenvalues -- 2.27698 2.27698 2.28406 2.31322 2.31322

Alpha virt. eigenvalues -- 2.33372 2.33372 2.34526 2.36034 2.36278

Alpha virt. eigenvalues -- 2.36531 2.36531 2.37604 2.40168 2.40168

Alpha virt. eigenvalues -- 2.40732 2.40732 2.40898 2.40989 2.43127

Alpha virt. eigenvalues -- 2.45423 2.48282 2.48282 2.48989 2.49902

Alpha virt. eigenvalues -- 2.52856 2.53472 2.53980 2.53980 2.56345

Alpha virt. eigenvalues -- 2.56345 2.56994 2.57451 2.57708 2.57924

Alpha virt. eigenvalues -- 2.57924 2.59457 2.59937 2.61790 2.62491

Alpha virt. eigenvalues -- 2.62491 2.64294 2.64294 2.64564 2.66591

Alpha virt. eigenvalues -- 2.66826 2.71073 2.71073 2.73417 2.76566

Alpha virt. eigenvalues -- 2.78784 2.78784 2.79868 2.81139 2.82750

Alpha virt. eigenvalues -- 2.82750 2.83403 2.83925 2.87190 2.87190

Alpha virt. eigenvalues -- 2.88536 2.88577 2.88577 2.88615 2.91608

Alpha virt. eigenvalues -- 2.95123 2.95491 2.95491 2.96025 2.96025

Alpha virt. eigenvalues -- 2.96932 2.97555 2.98855 2.98855 2.99946

Alpha virt. eigenvalues -- 3.00127 3.01217 3.02931 3.03792 3.03792

Alpha virt. eigenvalues -- 3.03998 3.04321 3.05421 3.05421 3.06890

Alpha virt. eigenvalues -- 3.07905 3.08118 3.08118 3.09101 3.16844

Alpha virt. eigenvalues -- 3.17390 3.17394 3.17922 3.17922 3.21091

Alpha virt. eigenvalues -- 3.21446 3.21446 3.23963 3.25603 3.25603

Alpha virt. eigenvalues -- 3.28476 3.29882 3.30668 3.31509 3.32229

Alpha virt. eigenvalues -- 3.32229 3.33046 3.33046 3.35275 3.35556

Alpha virt. eigenvalues -- 3.36927 3.36927 3.44222 3.48265 3.52033

Alpha virt. eigenvalues -- 3.52033 3.52879 3.56877 3.56877 3.57075

Alpha virt. eigenvalues -- 3.57450 3.58477 3.62762 3.65179 3.65179

Alpha virt. eigenvalues -- 3.80640 3.80640 3.82002 3.84226 3.85964

Alpha virt. eigenvalues -- 3.87615 3.87615 3.89352 3.93158 3.93158

Alpha virt. eigenvalues -- 3.96624 3.99534 4.11418 4.18383 4.18383

Alpha virt. eigenvalues -- 4.32079 4.33835 4.46869 4.49627 4.49627

Alpha virt. eigenvalues -- 4.61393 4.63731 4.63731 4.65539 5.14438

Alpha virt. eigenvalues -- 5.19612 5.19612 5.32054 7.81619 7.81619

Alpha virt. eigenvalues -- 7.84667 7.90153 8.09361 11.07390 23.26882

Alpha virt. eigenvalues -- 23.32149 23.32149 23.35086 23.51534 23.54644

Alpha virt. eigenvalues -- 23.54644 23.56749 23.74639 23.76288 23.76288

Alpha virt. eigenvalues -- 23.78039 23.90561 23.92804 23.92804 23.95755

Alpha virt. eigenvalues -- 23.99883 24.01419 24.01419 24.02474 24.12413

Alpha virt. eigenvalues -- 24.12877 24.12877 24.13556 24.93962 24.94012

Alpha virt. eigenvalues -- 24.94314 24.94314 35.62575 35.63903 35.65134

Alpha virt. eigenvalues -- 35.65134

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 5.149772 0.402825 -0.078868 -0.061982 0.533980 0.013880

2 C 0.402825 4.877123 0.436037 -0.145451 -0.061982 -0.001255

3 N -0.078868 0.436037 6.932151 0.436037 -0.078868 -0.019846

4 C -0.061982 -0.145451 0.436037 4.877123 0.402825 0.405967

5 C 0.533980 -0.061982 -0.078868 0.402825 5.149772 -0.073908

6 C 0.013880 -0.001255 -0.019846 0.405967 -0.073908 5.213339

7 C -0.001167 -0.000390 -0.019216 -0.105863 0.012854 0.405967

8 N 0.000051 0.000341 -0.013576 -0.019216 -0.000348 -0.019846

9 C -0.000005 0.000007 0.000341 -0.000390 0.000045 -0.001255

10 C 0.000001 -0.000005 0.000051 -0.001167 -0.000006 0.013880

11 C -0.000006 0.000045 -0.000348 0.012854 -0.000139 -0.073908

12 C -0.073908 0.405967 -0.019846 -0.001255 0.013880 -0.002313

13 C 0.012854 -0.105863 -0.019216 -0.000390 -0.001167 0.000198

14 C -0.000139 0.012854 -0.000348 0.000045 -0.000006 0.000001

15 C -0.000006 -0.001167 0.000051 -0.000005 0.000001 0.000000

16 C 0.000045 -0.000390 0.000341 0.000007 -0.000005 0.000001

17 N -0.000348 -0.019216 -0.013576 0.000341 0.000051 -0.000136

18 C 0.000001 0.000198 -0.000136 0.000001 0.000000 0.000002

19 C 0.000000 -0.000054 0.000135 -0.000003 0.000000 0.000001

20 C 0.000000 0.000000 0.000001 0.000000 0.000000 0.000000

21 C 0.000000 0.000000 0.000001 0.000000 0.000000 0.000001

22 C 0.000000 -0.000003 0.000135 -0.000054 0.000000 0.000198

23 N 0.000001 0.000135 -0.001352 0.000135 0.000001 -0.000136

24 H 0.388059 -0.038071 0.005172 0.005584 -0.033082 -0.000162

25 H -0.033082 0.005584 0.005172 -0.038071 0.388059 -0.005196

26 H 0.000000 0.000000 0.000002 0.000009 0.000000 -0.000162

27 H 0.000000 0.000001 -0.000002 -0.000026 0.000005 -0.005196

28 H 0.000005 -0.000026 -0.000002 0.000001 0.000000 0.000000

29 H 0.000000 0.000009 0.000002 0.000000 0.000000 0.000000

30 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

31 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

32 Zn 0.002131 -0.013488 0.134795 -0.013488 0.002131 -0.011933

33 C 0.000000 0.000001 -0.000136 0.000198 0.000001 -0.002313

34 C 0.000000 0.000000 0.000000 0.000002 0.000000 -0.000054

35 C -0.015092 -0.075652 0.004263 -0.000524 0.002562 -0.000054

36 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

37 C -0.000653 -0.005147 -0.000045 -0.000052 0.000353 -0.000002

38 C 0.002562 -0.000524 0.004263 -0.075652 -0.015092 0.542415

39 C 0.000353 -0.000052 -0.000045 -0.005147 -0.000653 -0.104310

40 C 0.000000 0.000002 0.000000 0.000000 0.000000 0.000000

41 C 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 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000002 0.000000 0.000001 -0.000034 0.000093 0.001814

45 H 0.000093 -0.000034 0.000001 0.000000 0.000002 0.000000

7 8 9 10 11 12

1 C -0.001167 0.000051 -0.000005 0.000001 -0.000006 -0.073908

2 C -0.000390 0.000341 0.000007 -0.000005 0.000045 0.405967

3 N -0.019216 -0.013576 0.000341 0.000051 -0.000348 -0.019846

4 C -0.105863 -0.019216 -0.000390 -0.001167 0.012854 -0.001255

5 C 0.012854 -0.000348 0.000045 -0.000006 -0.000139 0.013880

6 C 0.405967 -0.019846 -0.001255 0.013880 -0.073908 -0.002313

7 C 4.877123 0.436037 -0.145451 -0.061982 0.402825 0.000198

8 N 0.436037 6.932151 0.436037 -0.078868 -0.078868 -0.000136

9 C -0.145451 0.436037 4.877123 0.402825 -0.061982 0.000001

10 C -0.061982 -0.078868 0.402825 5.149772 0.533980 0.000000

11 C 0.402825 -0.078868 -0.061982 0.533980 5.149772 0.000001

12 C 0.000198 -0.000136 0.000001 0.000000 0.000001 5.213339

13 C -0.000054 0.000135 -0.000003 0.000000 0.000000 0.405967

14 C 0.000000 0.000001 0.000000 0.000000 0.000000 -0.073908

15 C 0.000000 0.000001 0.000000 0.000000 0.000000 0.013880

16 C -0.000003 0.000135 -0.000054 0.000000 0.000000 -0.001255

17 N 0.000135 -0.001352 0.000135 0.000001 0.000001 -0.019846

18 C 0.000001 -0.000136 0.000198 0.000001 0.000000 -0.002313

19 C 0.000007 0.000341 -0.000390 0.000045 -0.000005 0.000198

20 C -0.000005 0.000051 -0.001167 -0.000006 0.000001 0.000001

21 C 0.000045 -0.000348 0.012854 -0.000139 -0.000006 0.000000

22 C -0.000390 -0.019216 -0.105863 0.012854 -0.001167 0.000001

23 N 0.000341 -0.013576 -0.019216 -0.000348 0.000051 -0.000136

24 H 0.000009 0.000002 0.000000 0.000000 0.000000 -0.005196

25 H -0.000026 -0.000002 0.000001 0.000000 0.000005 -0.000162

26 H 0.005584 0.005172 -0.038071 0.388059 -0.033082 0.000000

27 H -0.038071 0.005172 0.005584 -0.033082 0.388059 0.000000

28 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.005196

29 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000162

30 H 0.000000 0.000002 0.000009 0.000000 0.000000 0.000000

31 H 0.000001 -0.000002 -0.000026 0.000005 0.000000 0.000000

32 Zn -0.013488 0.134795 -0.013488 0.002131 0.002131 -0.011933

33 C -0.001255 -0.019846 0.405967 -0.073908 0.013880 0.000002

34 C -0.000524 0.004263 -0.075652 -0.015092 0.002562 0.000000

35 C 0.000002 0.000000 0.000000 0.000000 0.000000 0.542415

36 C -0.000052 -0.000045 -0.005147 -0.000653 0.000353 0.000000

37 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.104310

38 C -0.075652 0.004263 -0.000524 0.002562 -0.015092 -0.000054

39 C -0.005147 -0.000045 -0.000052 0.000353 -0.000653 -0.000002

40 C 0.000000 0.000000 0.000002 0.000000 0.000000 -0.000054

41 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

43 H 0.000000 0.000001 -0.000034 0.000093 0.000002 0.000000

44 H -0.000034 0.000001 0.000000 0.000002 0.000093 0.000000

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.001814

13 14 15 16 17 18

1 C 0.012854 -0.000139 -0.000006 0.000045 -0.000348 0.000001

2 C -0.105863 0.012854 -0.001167 -0.000390 -0.019216 0.000198

3 N -0.019216 -0.000348 0.000051 0.000341 -0.013576 -0.000136

4 C -0.000390 0.000045 -0.000005 0.000007 0.000341 0.000001

5 C -0.001167 -0.000006 0.000001 -0.000005 0.000051 0.000000

6 C 0.000198 0.000001 0.000000 0.000001 -0.000136 0.000002

7 C -0.000054 0.000000 0.000000 -0.000003 0.000135 0.000001

8 N 0.000135 0.000001 0.000001 0.000135 -0.001352 -0.000136

9 C -0.000003 0.000000 0.000000 -0.000054 0.000135 0.000198

10 C 0.000000 0.000000 0.000000 0.000000 0.000001 0.000001

11 C 0.000000 0.000000 0.000000 0.000000 0.000001 0.000000

12 C 0.405967 -0.073908 0.013880 -0.001255 -0.019846 -0.002313

13 C 4.877123 0.402825 -0.061982 -0.145451 0.436037 -0.001255

14 C 0.402825 5.149772 0.533980 -0.061982 -0.078868 0.013880

15 C -0.061982 0.533980 5.149772 0.402825 -0.078868 -0.073908

16 C -0.145451 -0.061982 0.402825 4.877123 0.436037 0.405967

17 N 0.436037 -0.078868 -0.078868 0.436037 6.932151 -0.019846

18 C -0.001255 0.013880 -0.073908 0.405967 -0.019846 5.213339

19 C -0.000390 -0.001167 0.012854 -0.105863 -0.019216 0.405967

20 C 0.000045 -0.000006 -0.000139 0.012854 -0.000348 -0.073908

21 C -0.000005 0.000001 -0.000006 -0.001167 0.000051 0.013880

22 C 0.000007 -0.000005 0.000045 -0.000390 0.000341 -0.001255

23 N 0.000341 0.000051 -0.000348 -0.019216 -0.013576 -0.019846

24 H -0.000026 0.000005 0.000000 0.000001 -0.000002 0.000000

25 H 0.000009 0.000000 0.000000 0.000000 0.000002 0.000000

26 H 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 H -0.038071 0.388059 -0.033082 0.005584 0.005172 -0.000162

29 H 0.005584 -0.033082 0.388059 -0.038071 0.005172 -0.005196

30 H 0.000001 0.000000 0.000005 -0.000026 -0.000002 -0.005196

31 H 0.000000 0.000000 0.000000 0.000009 0.000002 -0.000162

32 Zn -0.013488 0.002131 0.002131 -0.013488 0.134795 -0.011933

33 C 0.000001 0.000000 0.000001 0.000198 -0.000136 -0.002313

34 C 0.000000 0.000000 0.000000 0.000002 0.000000 -0.000054

35 C -0.075652 -0.015092 0.002562 -0.000524 0.004263 -0.000054

36 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

37 C -0.005147 -0.000653 0.000353 -0.000052 -0.000045 -0.000002

38 C 0.000002 0.000000 0.000000 0.000000 0.000000 0.000000

39 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

40 C -0.000524 0.002562 -0.015092 -0.075652 0.004263 0.542415

41 C -0.000052 0.000353 -0.000653 -0.005147 -0.000045 -0.104310

42 H 0.000000 0.000002 0.000093 -0.000034 0.000001 0.001814

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 -0.000034 0.000093 0.000002 0.000000 0.000001 0.000000

19 20 21 22 23 24

1 C 0.000000 0.000000 0.000000 0.000000 0.000001 0.388059

2 C -0.000054 0.000000 0.000000 -0.000003 0.000135 -0.038071

3 N 0.000135 0.000001 0.000001 0.000135 -0.001352 0.005172

4 C -0.000003 0.000000 0.000000 -0.000054 0.000135 0.005584

5 C 0.000000 0.000000 0.000000 0.000000 0.000001 -0.033082

6 C 0.000001 0.000000 0.000001 0.000198 -0.000136 -0.000162

7 C 0.000007 -0.000005 0.000045 -0.000390 0.000341 0.000009

8 N 0.000341 0.000051 -0.000348 -0.019216 -0.013576 0.000002

9 C -0.000390 -0.001167 0.012854 -0.105863 -0.019216 0.000000

10 C 0.000045 -0.000006 -0.000139 0.012854 -0.000348 0.000000

11 C -0.000005 0.000001 -0.000006 -0.001167 0.000051 0.000000

12 C 0.000198 0.000001 0.000000 0.000001 -0.000136 -0.005196

13 C -0.000390 0.000045 -0.000005 0.000007 0.000341 -0.000026

14 C -0.001167 -0.000006 0.000001 -0.000005 0.000051 0.000005

15 C 0.012854 -0.000139 -0.000006 0.000045 -0.000348 0.000000

16 C -0.105863 0.012854 -0.001167 -0.000390 -0.019216 0.000001

17 N -0.019216 -0.000348 0.000051 0.000341 -0.013576 -0.000002

18 C 0.405967 -0.073908 0.013880 -0.001255 -0.019846 0.000000

19 C 4.877123 0.402825 -0.061982 -0.145451 0.436037 0.000000

20 C 0.402825 5.149772 0.533980 -0.061982 -0.078868 0.000000

21 C -0.061982 0.533980 5.149772 0.402825 -0.078868 0.000000

22 C -0.145451 -0.061982 0.402825 4.877123 0.436037 0.000000

23 N 0.436037 -0.078868 -0.078868 0.436037 6.932151 0.000000

24 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.427868

25 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.002187

26 H 0.000001 0.000000 0.000005 -0.000026 -0.000002 0.000000

27 H 0.000000 0.000000 0.000000 0.000009 0.000002 0.000000

28 H 0.000009 0.000000 0.000000 0.000000 0.000002 -0.000006

29 H -0.000026 0.000005 0.000000 0.000001 -0.000002 0.000000

30 H -0.038071 0.388059 -0.033082 0.005584 0.005172 0.000000

31 H 0.005584 -0.033082 0.388059 -0.038071 0.005172 0.000000

32 Zn -0.013488 0.002131 0.002131 -0.013488 0.134795 -0.000345

33 C -0.001255 0.013880 -0.073908 0.405967 -0.019846 0.000000

34 C -0.000524 0.002562 -0.015092 -0.075652 0.004263 0.000000

35 C 0.000002 0.000000 0.000000 0.000000 0.000000 0.006445

36 C -0.000052 0.000353 -0.000653 -0.005147 -0.000045 0.000000

37 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.003317

38 C 0.000000 0.000000 0.000000 0.000002 0.000000 -0.000081

39 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000008

40 C -0.075652 -0.015092 0.002562 -0.000524 0.004263 0.000000

41 C -0.005147 -0.000653 0.000353 -0.000052 -0.000045 0.000000

42 H -0.000034 0.000093 0.000002 0.000000 0.000001 0.000000

43 H 0.000000 0.000002 0.000093 -0.000034 0.000001 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 0.000055

25 26 27 28 29 30

1 C -0.033082 0.000000 0.000000 0.000005 0.000000 0.000000

2 C 0.005584 0.000000 0.000001 -0.000026 0.000009 0.000000

3 N 0.005172 0.000002 -0.000002 -0.000002 0.000002 0.000000

4 C -0.038071 0.000009 -0.000026 0.000001 0.000000 0.000000

5 C 0.388059 0.000000 0.000005 0.000000 0.000000 0.000000

6 C -0.005196 -0.000162 -0.005196 0.000000 0.000000 0.000000

7 C -0.000026 0.005584 -0.038071 0.000000 0.000000 0.000000

8 N -0.000002 0.005172 0.005172 0.000000 0.000000 0.000002

9 C 0.000001 -0.038071 0.005584 0.000000 0.000000 0.000009

10 C 0.000000 0.388059 -0.033082 0.000000 0.000000 0.000000

11 C 0.000005 -0.033082 0.388059 0.000000 0.000000 0.000000

12 C -0.000162 0.000000 0.000000 -0.005196 -0.000162 0.000000

13 C 0.000009 0.000000 0.000000 -0.038071 0.005584 0.000001

14 C 0.000000 0.000000 0.000000 0.388059 -0.033082 0.000000

15 C 0.000000 0.000000 0.000000 -0.033082 0.388059 0.000005

16 C 0.000000 0.000000 0.000000 0.005584 -0.038071 -0.000026

17 N 0.000002 0.000000 0.000000 0.005172 0.005172 -0.000002

18 C 0.000000 0.000000 0.000000 -0.000162 -0.005196 -0.005196

19 C 0.000000 0.000001 0.000000 0.000009 -0.000026 -0.038071

20 C 0.000000 0.000000 0.000000 0.000000 0.000005 0.388059

21 C 0.000000 0.000005 0.000000 0.000000 0.000000 -0.033082

22 C 0.000000 -0.000026 0.000009 0.000000 0.000001 0.005584

23 N 0.000000 -0.000002 0.000002 0.000002 -0.000002 0.005172

24 H -0.002187 0.000000 0.000000 -0.000006 0.000000 0.000000

25 H 0.427868 0.000000 -0.000006 0.000000 0.000000 0.000000

26 H 0.000000 0.427868 -0.002187 0.000000 0.000000 0.000000

27 H -0.000006 -0.002187 0.427868 0.000000 0.000000 0.000000

28 H 0.000000 0.000000 0.000000 0.427868 -0.002187 0.000000

29 H 0.000000 0.000000 0.000000 -0.002187 0.427868 -0.000006

30 H 0.000000 0.000000 0.000000 0.000000 -0.000006 0.427868

31 H 0.000000 -0.000006 0.000000 0.000000 0.000000 -0.002187

32 Zn -0.000345 -0.000345 -0.000345 -0.000345 -0.000345 -0.000345

33 C 0.000000 -0.005196 -0.000162 0.000000 0.000000 -0.000162

34 C 0.000000 0.006445 -0.000081 0.000000 0.000000 -0.000081

35 C -0.000081 0.000000 0.000000 0.006445 -0.000081 0.000000

36 C 0.000000 0.003317 -0.000008 0.000000 0.000000 -0.000008

37 C -0.000008 0.000000 0.000000 0.003317 -0.000008 0.000000

38 C 0.006445 -0.000081 0.006445 0.000000 0.000000 0.000000

39 C 0.003317 -0.000008 0.003317 0.000000 0.000000 0.000000

40 C 0.000000 0.000000 0.000000 -0.000081 0.006445 0.006445

41 C 0.000000 0.000000 0.000000 -0.000008 0.003317 0.003317

42 H 0.000000 0.000000 0.000000 0.000000 0.000055 0.000055

43 H 0.000000 0.000055 0.000000 0.000000 0.000000 0.000000

44 H 0.000055 0.000000 0.000055 0.000000 0.000000 0.000000

45 H 0.000000 0.000000 0.000000 0.000055 0.000000 0.000000

31 32 33 34 35 36

1 C 0.000000 0.002131 0.000000 0.000000 -0.015092 0.000000

2 C 0.000000 -0.013488 0.000001 0.000000 -0.075652 0.000000

3 N 0.000000 0.134795 -0.000136 0.000000 0.004263 0.000000

4 C 0.000000 -0.013488 0.000198 0.000002 -0.000524 0.000000

5 C 0.000000 0.002131 0.000001 0.000000 0.002562 0.000000

6 C 0.000000 -0.011933 -0.002313 -0.000054 -0.000054 -0.000002

7 C 0.000001 -0.013488 -0.001255 -0.000524 0.000002 -0.000052

8 N -0.000002 0.134795 -0.019846 0.004263 0.000000 -0.000045

9 C -0.000026 -0.013488 0.405967 -0.075652 0.000000 -0.005147

10 C 0.000005 0.002131 -0.073908 -0.015092 0.000000 -0.000653

11 C 0.000000 0.002131 0.013880 0.002562 0.000000 0.000353

12 C 0.000000 -0.011933 0.000002 0.000000 0.542415 0.000000

13 C 0.000000 -0.013488 0.000001 0.000000 -0.075652 0.000000

14 C 0.000000 0.002131 0.000000 0.000000 -0.015092 0.000000

15 C 0.000000 0.002131 0.000001 0.000000 0.002562 0.000000

16 C 0.000009 -0.013488 0.000198 0.000002 -0.000524 0.000000

17 N 0.000002 0.134795 -0.000136 0.000000 0.004263 0.000000

18 C -0.000162 -0.011933 -0.002313 -0.000054 -0.000054 -0.000002

19 C 0.005584 -0.013488 -0.001255 -0.000524 0.000002 -0.000052

20 C -0.033082 0.002131 0.013880 0.002562 0.000000 0.000353

21 C 0.388059 0.002131 -0.073908 -0.015092 0.000000 -0.000653

22 C -0.038071 -0.013488 0.405967 -0.075652 0.000000 -0.005147

23 N 0.005172 0.134795 -0.019846 0.004263 0.000000 -0.000045

24 H 0.000000 -0.000345 0.000000 0.000000 0.006445 0.000000

25 H 0.000000 -0.000345 0.000000 0.000000 -0.000081 0.000000

26 H -0.000006 -0.000345 -0.005196 0.006445 0.000000 0.003317

27 H 0.000000 -0.000345 -0.000162 -0.000081 0.000000 -0.000008

28 H 0.000000 -0.000345 0.000000 0.000000 0.006445 0.000000

29 H 0.000000 -0.000345 0.000000 0.000000 -0.000081 0.000000

30 H -0.002187 -0.000345 -0.000162 -0.000081 0.000000 -0.000008

31 H 0.427868 -0.000345 -0.005196 0.006445 0.000000 0.003317

32 Zn -0.000345 10.230077 -0.011933 -0.000701 -0.000701 -0.000052

33 C -0.005196 -0.011933 5.213339 0.542415 0.000000 -0.104310

34 C 0.006445 -0.000701 0.542415 4.812635 0.000000 0.856742

35 C 0.000000 -0.000701 0.000000 0.000000 4.812635 0.000000

36 C 0.003317 -0.000052 -0.104310 0.856742 0.000000 5.177224

37 C 0.000000 -0.000052 0.000000 0.000000 0.856742 0.000000

38 C 0.000000 -0.000701 -0.000054 -0.000001 -0.000001 0.000000

39 C 0.000000 -0.000052 -0.000002 0.000000 0.000000 0.000000

40 C -0.000081 -0.000701 -0.000054 -0.000001 -0.000001 0.000000

41 C -0.000008 -0.000052 -0.000002 0.000000 0.000000 0.000000

42 H 0.000000 -0.000004 0.000000 0.000000 0.000000 0.000000

43 H 0.000055 -0.000004 0.001814 -0.019631 0.000000 0.370700

44 H 0.000000 -0.000004 0.000000 0.000000 0.000000 0.000000

45 H 0.000000 -0.000004 0.000000 0.000000 -0.019631 0.000000

37 38 39 40 41 42

1 C -0.000653 0.002562 0.000353 0.000000 0.000000 0.000000

2 C -0.005147 -0.000524 -0.000052 0.000002 0.000000 0.000000

3 N -0.000045 0.004263 -0.000045 0.000000 0.000000 0.000000

4 C -0.000052 -0.075652 -0.005147 0.000000 0.000000 0.000000

5 C 0.000353 -0.015092 -0.000653 0.000000 0.000000 0.000000

6 C -0.000002 0.542415 -0.104310 0.000000 0.000000 0.000000

7 C 0.000000 -0.075652 -0.005147 0.000000 0.000000 0.000000

8 N 0.000000 0.004263 -0.000045 0.000000 0.000000 0.000000

9 C 0.000000 -0.000524 -0.000052 0.000002 0.000000 0.000000

10 C 0.000000 0.002562 0.000353 0.000000 0.000000 0.000000

11 C 0.000000 -0.015092 -0.000653 0.000000 0.000000 0.000000

12 C -0.104310 -0.000054 -0.000002 -0.000054 -0.000002 0.000000

13 C -0.005147 0.000002 0.000000 -0.000524 -0.000052 0.000000

14 C -0.000653 0.000000 0.000000 0.002562 0.000353 0.000002

15 C 0.000353 0.000000 0.000000 -0.015092 -0.000653 0.000093

16 C -0.000052 0.000000 0.000000 -0.075652 -0.005147 -0.000034

17 N -0.000045 0.000000 0.000000 0.004263 -0.000045 0.000001

18 C -0.000002 0.000000 0.000000 0.542415 -0.104310 0.001814

19 C 0.000000 0.000000 0.000000 -0.075652 -0.005147 -0.000034

20 C 0.000000 0.000000 0.000000 -0.015092 -0.000653 0.000093

21 C 0.000000 0.000000 0.000000 0.002562 0.000353 0.000002

22 C 0.000000 0.000002 0.000000 -0.000524 -0.000052 0.000000

23 N 0.000000 0.000000 0.000000 0.004263 -0.000045 0.000001

24 H 0.003317 -0.000081 -0.000008 0.000000 0.000000 0.000000

25 H -0.000008 0.006445 0.003317 0.000000 0.000000 0.000000

26 H 0.000000 -0.000081 -0.000008 0.000000 0.000000 0.000000

27 H 0.000000 0.006445 0.003317 0.000000 0.000000 0.000000

28 H 0.003317 0.000000 0.000000 -0.000081 -0.000008 0.000000

29 H -0.000008 0.000000 0.000000 0.006445 0.003317 0.000055

30 H 0.000000 0.000000 0.000000 0.006445 0.003317 0.000055

31 H 0.000000 0.000000 0.000000 -0.000081 -0.000008 0.000000

32 Zn -0.000052 -0.000701 -0.000052 -0.000701 -0.000052 -0.000004

33 C 0.000000 -0.000054 -0.000002 -0.000054 -0.000002 0.000000

34 C 0.000000 -0.000001 0.000000 -0.000001 0.000000 0.000000

35 C 0.856742 -0.000001 0.000000 -0.000001 0.000000 0.000000

36 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 C 5.177224 0.000000 0.000000 0.000000 0.000000 0.000000

38 C 0.000000 4.812635 0.856742 0.000000 0.000000 0.000000

39 C 0.000000 0.856742 5.177224 0.000000 0.000000 0.000000

40 C 0.000000 0.000000 0.000000 4.812635 0.856742 -0.019631

41 C 0.000000 0.000000 0.000000 0.856742 5.177224 0.370700

42 H 0.000000 0.000000 0.000000 -0.019631 0.370700 0.348293

43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 -0.019631 0.370700 0.000000 0.000000 0.000000

45 H 0.370700 0.000000 0.000000 0.000000 0.000000 0.000000

43 44 45

1 C 0.000000 0.000002 0.000093

2 C 0.000000 0.000000 -0.000034

3 N 0.000000 0.000001 0.000001

4 C 0.000000 -0.000034 0.000000

5 C 0.000000 0.000093 0.000002

6 C 0.000000 0.001814 0.000000

7 C 0.000000 -0.000034 0.000000

8 N 0.000001 0.000001 0.000000

9 C -0.000034 0.000000 0.000000

10 C 0.000093 0.000002 0.000000

11 C 0.000002 0.000093 0.000000

12 C 0.000000 0.000000 0.001814

13 C 0.000000 0.000000 -0.000034

14 C 0.000000 0.000000 0.000093

15 C 0.000000 0.000000 0.000002

16 C 0.000000 0.000000 0.000000

17 N 0.000000 0.000000 0.000001

18 C 0.000000 0.000000 0.000000

19 C 0.000000 0.000000 0.000000

20 C 0.000002 0.000000 0.000000

21 C 0.000093 0.000000 0.000000

22 C -0.000034 0.000000 0.000000

23 N 0.000001 0.000000 0.000000

24 H 0.000000 0.000000 0.000055

25 H 0.000000 0.000055 0.000000

26 H 0.000055 0.000000 0.000000

27 H 0.000000 0.000055 0.000000

28 H 0.000000 0.000000 0.000055

29 H 0.000000 0.000000 0.000000

30 H 0.000000 0.000000 0.000000

31 H 0.000055 0.000000 0.000000

32 Zn -0.000004 -0.000004 -0.000004

33 C 0.001814 0.000000 0.000000

34 C -0.019631 0.000000 0.000000

35 C 0.000000 0.000000 -0.019631

36 C 0.370700 0.000000 0.000000

37 C 0.000000 0.000000 0.370700

38 C 0.000000 -0.019631 0.000000

39 C 0.000000 0.370700 0.000000

40 C 0.000000 0.000000 0.000000

41 C 0.000000 0.000000 0.000000

42 H 0.000000 0.000000 0.000000

43 H 0.348293 0.000000 0.000000

44 H 0.000000 0.348293 0.000000

45 H 0.000000 0.000000 0.348293

Mulliken charges:

1

1 C -0.241358

2 C 0.327640

3 N -0.693529

4 C 0.327640

5 C -0.241358

6 C -0.275679

7 C 0.327640

8 N -0.693529

9 C 0.327640

10 C -0.241358

11 C -0.241358

12 C -0.275679

13 C 0.327640

14 C -0.241358

15 C -0.241358

16 C 0.327640

17 N -0.693529

18 C -0.275679

19 C 0.327640

20 C -0.241358

21 C -0.241358

22 C 0.327640

23 N -0.693529

24 H 0.242650

25 H 0.242650

26 H 0.242650

27 H 0.242650

28 H 0.242650

29 H 0.242650

30 H 0.242650

31 H 0.242650

32 Zn 1.375111

33 C -0.275679

34 C -0.035195

35 C -0.035195

36 C -0.295832

37 C -0.295832

38 C -0.035195

39 C -0.295832

40 C -0.035195

41 C -0.295832

42 H 0.298595

43 H 0.298595

44 H 0.298595

45 H 0.298595

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 C 0.001292

2 C 0.327640

3 N -0.693529

4 C 0.327640

5 C 0.001292

6 C -0.275679

7 C 0.327640

8 N -0.693529

9 C 0.327640

10 C 0.001292

11 C 0.001292

12 C -0.275679

13 C 0.327640

14 C 0.001292

15 C 0.001292

16 C 0.327640

17 N -0.693529

18 C -0.275679

19 C 0.327640

20 C 0.001292

21 C 0.001292

22 C 0.327640

23 N -0.693529

32 Zn 1.375111

33 C -0.275679

34 C -0.035195

35 C -0.035195

36 C 0.002763

37 C 0.002763

38 C -0.035195

39 C 0.002763

40 C -0.035195

41 C 0.002763

Electronic spatial extent (au): <R\*\*2>= 13485.1096

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0000 Y= 0.0000 Z= 1.9484 Tot= 1.9484

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

XX= -158.6180 YY= -158.6180 ZZ= -199.9187

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XX= 13.7669 YY= 13.7669 ZZ= -27.5338

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XXX= 0.0000 YYY= 0.0000 ZZZ= 17.5833 XYY= 0.0000

XXY= 0.0000 XXZ= 4.0866 XZZ= 0.0000 YZZ= 0.0000

YYZ= 4.0866 XYZ= 0.0000

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

XXXX= -6752.1745 YYYY= -6752.1745 ZZZZ= -227.7881 XXXY= 0.0000

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

ZZZY= 0.0000 XXYY= -3047.5218 XXZZ= -1805.4677 YYZZ= -1805.4677

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 3.056384374570D+03 E-N=-9.354832642545D+03 KE= 1.403669532524D+03

Symmetry A1 KE= 4.737419412520D+02

Symmetry A2 KE= 2.409315557033D+02

Symmetry B1 KE= 3.444980177842D+02

Symmetry B2 KE= 3.444980177842D+02

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Fri Jul 26 14:12:50 2019, MaxMem= 1342177280 cpu: 12.9

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16207 LenP2D= 44776.

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 = 260

Leave Link 701 at Fri Jul 26 14:12:54 2019, MaxMem= 1342177280 cpu: 43.5

(Enter /apps/gaussian/g09d01/g09/l702.exe)

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

Leave Link 702 at Fri Jul 26 14:12:54 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Fri Jul 26 14:12:57 2019, MaxMem= 1342177280 cpu: 42.6

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-3.73034936D-14-3.73034936D-14 7.66578381D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000095730 0.000132184 -0.000494582

2 6 -0.000245993 -0.000101583 0.000723010

3 7 0.000000000 -0.005375032 0.000471825

4 6 0.000245993 -0.000101583 0.000723010

5 6 -0.000095730 0.000132184 -0.000494582

6 6 -0.000065761 0.000065761 -0.000443596

7 6 0.000101583 -0.000245993 0.000723010

8 7 0.005375032 0.000000000 0.000471825

9 6 0.000101583 0.000245993 0.000723010

10 6 -0.000132184 -0.000095730 -0.000494582

11 6 -0.000132184 0.000095730 -0.000494582

12 6 0.000065761 0.000065761 -0.000443596

13 6 -0.000101583 -0.000245993 0.000723010

14 6 0.000132184 0.000095730 -0.000494582

15 6 0.000132184 -0.000095730 -0.000494582

16 6 -0.000101583 0.000245993 0.000723010

17 7 -0.005375032 0.000000000 0.000471825

18 6 0.000065761 -0.000065761 -0.000443596

19 6 -0.000245993 0.000101583 0.000723010

20 6 0.000095730 -0.000132184 -0.000494582

21 6 -0.000095730 -0.000132184 -0.000494582

22 6 0.000245993 0.000101583 0.000723010

23 7 0.000000000 0.005375032 0.000471825

24 1 -0.000013019 0.000002045 0.000027782

25 1 0.000013019 0.000002045 0.000027782

26 1 -0.000002045 0.000013019 0.000027782

27 1 -0.000002045 -0.000013019 0.000027782

28 1 0.000002045 -0.000013019 0.000027782

29 1 0.000002045 0.000013019 0.000027782

30 1 -0.000013019 -0.000002045 0.000027782

31 1 0.000013019 -0.000002045 0.000027782

32 30 0.000000000 0.000000000 -0.001650945

33 6 -0.000065761 -0.000065761 -0.000443596

34 6 -0.000160420 -0.000160420 -0.000019413

35 6 0.000160420 0.000160420 -0.000019413

36 6 0.000181890 0.000181890 -0.000192874

37 6 -0.000181890 -0.000181890 -0.000192874

38 6 -0.000160420 0.000160420 -0.000019413

39 6 0.000181890 -0.000181890 -0.000192874

40 6 0.000160420 -0.000160420 -0.000019413

41 6 -0.000181890 0.000181890 -0.000192874

42 1 -0.000042316 0.000042316 0.000084372

43 1 0.000042316 0.000042316 0.000084372

44 1 0.000042316 -0.000042316 0.000084372

45 1 -0.000042316 -0.000042316 0.000084372

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

Cartesian Forces: Max 0.005375032 RMS 0.000972174

Leave Link 716 at Fri Jul 26 14:12:57 2019, MaxMem= 1342177280 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.003715870 RMS 0.000561747

Search for a local minimum.

Step number 1 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .56175D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Second derivative matrix not updated -- first step.

ITU= 0

Eigenvalues --- 0.00534 0.00534 0.00534 0.00534 0.00534

Eigenvalues --- 0.00534 0.00534 0.00534 0.01205 0.01369

Eigenvalues --- 0.01369 0.01447 0.01677 0.01677 0.01679

Eigenvalues --- 0.01683 0.01800 0.01805 0.01805 0.01826

Eigenvalues --- 0.01830 0.01858 0.01858 0.01863 0.01868

Eigenvalues --- 0.01868 0.01868 0.01868 0.01910 0.01922

Eigenvalues --- 0.01923 0.01923 0.01934 0.01954 0.01954

Eigenvalues --- 0.01973 0.02174 0.02174 0.02177 0.02180

Eigenvalues --- 0.02579 0.02579 0.03337 0.04654 0.04654

Eigenvalues --- 0.04654 0.04654 0.04654 0.04654 0.04654

Eigenvalues --- 0.04654 0.06856 0.13804 0.15096 0.15096

Eigenvalues --- 0.15999 0.15999 0.15999 0.15999 0.15999

Eigenvalues --- 0.15999 0.15999 0.15999 0.16262 0.22770

Eigenvalues --- 0.22862 0.22862 0.22863 0.24132 0.24285

Eigenvalues --- 0.24474 0.24474 0.24606 0.24908 0.24929

Eigenvalues --- 0.24929 0.24987 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.35067 0.35067 0.35417 0.35505

Eigenvalues --- 0.35983 0.36034 0.36034 0.36034 0.36034

Eigenvalues --- 0.36034 0.36034 0.36034 0.36034 0.36759

Eigenvalues --- 0.36839 0.36839 0.37563 0.37563 0.37563

Eigenvalues --- 0.37563 0.38610 0.38936 0.38936 0.39549

Eigenvalues --- 0.41397 0.41397 0.41397 0.41397 0.41416

Eigenvalues --- 0.41416 0.41728 0.42441 0.43497 0.43761

Eigenvalues --- 0.43761 0.45083 0.47694 0.49060 0.49060

Eigenvalues --- 0.50140 0.51394 0.51893 0.51893 0.52080

Eigenvalues --- 1.01831 1.01831 1.01831 1.01831

RFO step: Lambda=-7.35459249D-04 EMin= 5.34077952D-03

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.01980011 RMS(Int)= 0.00014617

Iteration 2 RMS(Cart)= 0.00029869 RMS(Int)= 0.00003614

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00003614

ITry= 1 IFail=0 DXMaxC= 7.74D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.19D-04 for atom 45.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73573 -0.00003 0.00000 -0.00042 -0.00044 2.73529

R2 2.57529 -0.00048 0.00000 -0.00177 -0.00183 2.57347

R3 2.04028 -0.00001 0.00000 -0.00002 -0.00002 2.04026

R4 2.58065 0.00010 0.00000 0.00059 0.00063 2.58128

R5 2.67719 -0.00102 0.00000 -0.00445 -0.00448 2.67271

R6 2.58065 0.00010 0.00000 0.00059 0.00063 2.58128

R7 3.99187 -0.00372 0.00000 -0.02120 -0.02112 3.97075

R8 2.73573 -0.00003 0.00000 -0.00042 -0.00044 2.73529

R9 2.67719 -0.00102 0.00000 -0.00445 -0.00448 2.67271

R10 2.04028 -0.00001 0.00000 -0.00002 -0.00002 2.04026

R11 2.67719 -0.00102 0.00000 -0.00445 -0.00448 2.67271

R12 2.69699 -0.00009 0.00000 -0.00022 -0.00025 2.69674

R13 2.58065 0.00010 0.00000 0.00059 0.00063 2.58128

R14 2.73573 -0.00003 0.00000 -0.00042 -0.00044 2.73529

R15 2.58065 0.00010 0.00000 0.00059 0.00063 2.58128

R16 3.99187 -0.00372 0.00000 -0.02120 -0.02112 3.97075

R17 2.73573 -0.00003 0.00000 -0.00042 -0.00044 2.73529

R18 2.67719 -0.00102 0.00000 -0.00445 -0.00448 2.67271

R19 2.57529 -0.00048 0.00000 -0.00177 -0.00183 2.57347

R20 2.04028 -0.00001 0.00000 -0.00002 -0.00002 2.04026

R21 2.04028 -0.00001 0.00000 -0.00002 -0.00002 2.04026

R22 2.67719 -0.00102 0.00000 -0.00445 -0.00448 2.67271

R23 2.69699 -0.00009 0.00000 -0.00022 -0.00025 2.69674

R24 2.73573 -0.00003 0.00000 -0.00042 -0.00044 2.73529

R25 2.58065 0.00010 0.00000 0.00059 0.00063 2.58128

R26 2.57529 -0.00048 0.00000 -0.00177 -0.00183 2.57347

R27 2.04028 -0.00001 0.00000 -0.00002 -0.00002 2.04026

R28 2.73573 -0.00003 0.00000 -0.00042 -0.00044 2.73529

R29 2.04028 -0.00001 0.00000 -0.00002 -0.00002 2.04026

R30 2.58065 0.00010 0.00000 0.00059 0.00063 2.58128

R31 2.67719 -0.00102 0.00000 -0.00445 -0.00448 2.67271

R32 3.99187 -0.00372 0.00000 -0.02120 -0.02112 3.97075

R33 2.67719 -0.00102 0.00000 -0.00445 -0.00448 2.67271

R34 2.69699 -0.00009 0.00000 -0.00022 -0.00025 2.69674

R35 2.73573 -0.00003 0.00000 -0.00042 -0.00044 2.73529

R36 2.58065 0.00010 0.00000 0.00059 0.00063 2.58128

R37 2.57529 -0.00048 0.00000 -0.00177 -0.00183 2.57347

R38 2.04028 -0.00001 0.00000 -0.00002 -0.00002 2.04026

R39 2.73573 -0.00003 0.00000 -0.00042 -0.00044 2.73529

R40 2.04028 -0.00001 0.00000 -0.00002 -0.00002 2.04026

R41 2.58065 0.00010 0.00000 0.00059 0.00063 2.58128

R42 2.67719 -0.00102 0.00000 -0.00445 -0.00448 2.67271

R43 3.99187 -0.00372 0.00000 -0.02120 -0.02112 3.97075

R44 2.69699 -0.00009 0.00000 -0.00022 -0.00025 2.69674

R45 2.27914 -0.00032 0.00000 -0.00031 -0.00031 2.27883

R46 2.27914 -0.00032 0.00000 -0.00031 -0.00031 2.27883

R47 2.01705 -0.00006 0.00000 -0.00016 -0.00016 2.01690

R48 2.01705 -0.00006 0.00000 -0.00016 -0.00016 2.01690

R49 2.27914 -0.00032 0.00000 -0.00031 -0.00031 2.27883

R50 2.01705 -0.00006 0.00000 -0.00016 -0.00016 2.01690

R51 2.27914 -0.00032 0.00000 -0.00031 -0.00031 2.27883

R52 2.01705 -0.00006 0.00000 -0.00016 -0.00016 2.01690

A1 1.86663 -0.00019 0.00000 -0.00149 -0.00148 1.86514

A2 2.19164 0.00011 0.00000 0.00081 0.00081 2.19245

A3 2.22488 0.00008 0.00000 0.00066 0.00066 2.22554

A4 1.90498 0.00073 0.00000 0.00503 0.00504 1.91003

A5 2.18678 -0.00054 0.00000 -0.00395 -0.00408 2.18270

A6 2.19141 -0.00019 0.00000 -0.00102 -0.00103 2.19039

A7 1.88156 -0.00108 0.00000 -0.00708 -0.00713 1.87442

A8 2.19344 0.00056 0.00000 0.00470 0.00468 2.19812

A9 2.19344 0.00056 0.00000 0.00470 0.00468 2.19812

A10 1.90498 0.00073 0.00000 0.00503 0.00504 1.91003

A11 2.19141 -0.00019 0.00000 -0.00102 -0.00103 2.19039

A12 2.18678 -0.00054 0.00000 -0.00395 -0.00408 2.18270

A13 1.86663 -0.00019 0.00000 -0.00149 -0.00148 1.86514

A14 2.22488 0.00008 0.00000 0.00066 0.00066 2.22554

A15 2.19164 0.00011 0.00000 0.00081 0.00081 2.19245

A16 2.21100 -0.00070 0.00000 -0.00493 -0.00489 2.20611

A17 2.03609 0.00035 0.00000 0.00246 0.00242 2.03851

A18 2.03609 0.00035 0.00000 0.00246 0.00242 2.03851

A19 2.19141 -0.00019 0.00000 -0.00102 -0.00103 2.19039

A20 2.18678 -0.00054 0.00000 -0.00395 -0.00408 2.18270

A21 1.90498 0.00073 0.00000 0.00503 0.00504 1.91003

A22 1.88156 -0.00108 0.00000 -0.00708 -0.00713 1.87442

A23 2.19344 0.00056 0.00000 0.00470 0.00468 2.19812

A24 2.19344 0.00056 0.00000 0.00470 0.00468 2.19812

A25 1.90498 0.00073 0.00000 0.00503 0.00504 1.91003

A26 2.19141 -0.00019 0.00000 -0.00102 -0.00103 2.19039

A27 2.18678 -0.00054 0.00000 -0.00395 -0.00408 2.18270

A28 1.86663 -0.00019 0.00000 -0.00149 -0.00148 1.86514

A29 2.19164 0.00011 0.00000 0.00081 0.00081 2.19245

A30 2.22488 0.00008 0.00000 0.00066 0.00066 2.22554

A31 1.86663 -0.00019 0.00000 -0.00149 -0.00148 1.86514

A32 2.19164 0.00011 0.00000 0.00081 0.00081 2.19245

A33 2.22488 0.00008 0.00000 0.00066 0.00066 2.22554

A34 2.21100 -0.00070 0.00000 -0.00493 -0.00489 2.20611

A35 2.03609 0.00035 0.00000 0.00246 0.00242 2.03851

A36 2.03609 0.00035 0.00000 0.00246 0.00242 2.03851

A37 2.18678 -0.00054 0.00000 -0.00395 -0.00408 2.18270

A38 2.19141 -0.00019 0.00000 -0.00102 -0.00103 2.19039

A39 1.90498 0.00073 0.00000 0.00503 0.00504 1.91003

A40 1.86663 -0.00019 0.00000 -0.00149 -0.00148 1.86514

A41 2.19164 0.00011 0.00000 0.00081 0.00081 2.19245

A42 2.22488 0.00008 0.00000 0.00066 0.00066 2.22554

A43 1.86663 -0.00019 0.00000 -0.00149 -0.00148 1.86514

A44 2.22488 0.00008 0.00000 0.00066 0.00066 2.22554

A45 2.19164 0.00011 0.00000 0.00081 0.00081 2.19245

A46 1.90498 0.00073 0.00000 0.00503 0.00504 1.91003

A47 2.18678 -0.00054 0.00000 -0.00395 -0.00408 2.18270

A48 2.19141 -0.00019 0.00000 -0.00102 -0.00103 2.19039

A49 1.88156 -0.00108 0.00000 -0.00708 -0.00713 1.87442

A50 2.19344 0.00056 0.00000 0.00470 0.00468 2.19812

A51 2.19344 0.00056 0.00000 0.00470 0.00468 2.19812

A52 2.21100 -0.00070 0.00000 -0.00493 -0.00489 2.20611

A53 2.03609 0.00035 0.00000 0.00246 0.00242 2.03851

A54 2.03609 0.00035 0.00000 0.00246 0.00242 2.03851

A55 2.18678 -0.00054 0.00000 -0.00395 -0.00408 2.18270

A56 2.19141 -0.00019 0.00000 -0.00102 -0.00103 2.19039

A57 1.90498 0.00073 0.00000 0.00503 0.00504 1.91003

A58 1.86663 -0.00019 0.00000 -0.00149 -0.00148 1.86514

A59 2.19164 0.00011 0.00000 0.00081 0.00081 2.19245

A60 2.22488 0.00008 0.00000 0.00066 0.00066 2.22554

A61 1.86663 -0.00019 0.00000 -0.00149 -0.00148 1.86514

A62 2.22488 0.00008 0.00000 0.00066 0.00066 2.22554

A63 2.19164 0.00011 0.00000 0.00081 0.00081 2.19245

A64 1.90498 0.00073 0.00000 0.00503 0.00504 1.91003

A65 2.18678 -0.00054 0.00000 -0.00395 -0.00408 2.18270

A66 2.19141 -0.00019 0.00000 -0.00102 -0.00103 2.19039

A67 1.88156 -0.00108 0.00000 -0.00708 -0.00713 1.87442

A68 2.19344 0.00056 0.00000 0.00470 0.00468 2.19812

A69 2.19344 0.00056 0.00000 0.00470 0.00468 2.19812

A70 1.54915 -0.00007 0.00000 -0.00068 -0.00069 1.54845

A71 1.54915 -0.00007 0.00000 -0.00068 -0.00069 1.54845

A72 2.84626 -0.00046 0.00000 -0.00468 -0.00474 2.84152

A73 2.84626 -0.00046 0.00000 -0.00468 -0.00474 2.84152

A74 1.54915 -0.00007 0.00000 -0.00068 -0.00069 1.54845

A75 1.54915 -0.00007 0.00000 -0.00068 -0.00069 1.54845

A76 2.21100 -0.00070 0.00000 -0.00493 -0.00489 2.20611

A77 2.03609 0.00035 0.00000 0.00246 0.00242 2.03851

A78 2.03609 0.00035 0.00000 0.00246 0.00242 2.03851

A79 3.14168 0.00000 0.00000 -0.00001 0.00000 3.14168

A80 3.14168 0.00000 0.00000 -0.00001 0.00000 3.14168

A81 3.14149 0.00000 0.00000 0.00053 0.00034 3.14183

A82 3.14149 0.00000 0.00000 0.00053 0.00034 3.14183

A83 3.14168 0.00000 0.00000 -0.00001 0.00000 3.14168

A84 3.14149 0.00000 0.00000 0.00053 0.00034 3.14183

A85 3.14168 0.00000 0.00000 -0.00001 0.00000 3.14168

A86 3.14149 0.00000 0.00000 0.00053 0.00034 3.14183

A87 3.14711 -0.00006 0.00000 -0.00133 -0.00133 3.14579

A88 3.13607 0.00006 0.00000 0.00133 0.00133 3.13740

A89 3.13458 0.00015 0.00000 0.02457 0.02457 3.15916

A90 3.14860 -0.00015 0.00000 -0.02457 -0.02457 3.12403

A91 3.14711 -0.00006 0.00000 -0.00133 -0.00133 3.14579

A92 3.13458 0.00015 0.00000 0.02457 0.02457 3.15916

A93 3.13607 0.00006 0.00000 0.00133 0.00133 3.13740

A94 3.14860 -0.00015 0.00000 -0.02457 -0.02457 3.12403

D1 0.00059 0.00001 0.00000 0.00273 0.00277 0.00336

D2 -3.13684 -0.00033 0.00000 -0.01356 -0.01352 3.13282

D3 -3.13272 0.00010 0.00000 0.00480 0.00481 -3.12791

D4 0.01303 -0.00024 0.00000 -0.01150 -0.01148 0.00155

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13310 0.00009 0.00000 0.00211 0.00209 -3.13101

D7 3.13310 -0.00009 0.00000 -0.00211 -0.00209 3.13101

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 -0.00096 -0.00001 0.00000 -0.00443 -0.00448 -0.00544

D10 -2.96679 -0.00025 0.00000 -0.01838 -0.01841 -2.98521

D11 3.13646 0.00033 0.00000 0.01191 0.01190 -3.13483

D12 0.17063 0.00008 0.00000 -0.00205 -0.00204 0.16859

D13 -3.12701 0.00042 0.00000 0.01484 0.01479 -3.11222

D14 0.01353 0.00011 0.00000 0.00480 0.00477 0.01830

D15 0.01941 0.00003 0.00000 -0.00409 -0.00409 0.01531

D16 -3.12323 -0.00029 0.00000 -0.01414 -0.01411 -3.13735

D17 0.00096 0.00001 0.00000 0.00443 0.00448 0.00544

D18 -3.13646 -0.00033 0.00000 -0.01191 -0.01190 3.13483

D19 2.96679 0.00025 0.00000 0.01838 0.01841 2.98521

D20 -0.17063 -0.00008 0.00000 0.00205 0.00204 -0.16859

D21 -3.09871 0.00029 0.00000 0.00990 0.00996 -3.08875

D22 -0.24928 -0.00016 0.00000 0.00537 0.00538 -0.24391

D23 -1.67400 0.00006 0.00000 0.00763 0.00767 -1.66633

D24 0.24928 0.00016 0.00000 -0.00537 -0.00538 0.24391

D25 3.09871 -0.00029 0.00000 -0.00990 -0.00996 3.08875

D26 1.67400 -0.00006 0.00000 -0.00763 -0.00767 1.66633

D27 -0.00059 -0.00001 0.00000 -0.00273 -0.00277 -0.00336

D28 3.13272 -0.00010 0.00000 -0.00480 -0.00481 3.12791

D29 3.13684 0.00033 0.00000 0.01356 0.01352 -3.13282

D30 -0.01303 0.00024 0.00000 0.01150 0.01148 -0.00155

D31 -0.01941 -0.00003 0.00000 0.00409 0.00409 -0.01531

D32 3.12323 0.00029 0.00000 0.01414 0.01411 3.13735

D33 3.12701 -0.00042 0.00000 -0.01484 -0.01479 3.11222

D34 -0.01353 -0.00011 0.00000 -0.00480 -0.00477 -0.01830

D35 0.01941 0.00003 0.00000 -0.00409 -0.00409 0.01531

D36 -3.12701 0.00042 0.00000 0.01484 0.01479 -3.11222

D37 -3.12323 -0.00029 0.00000 -0.01414 -0.01411 -3.13735

D38 0.01353 0.00011 0.00000 0.00480 0.00477 0.01830

D39 3.13646 0.00033 0.00000 0.01191 0.01190 -3.13483

D40 0.17063 0.00008 0.00000 -0.00205 -0.00204 0.16859

D41 -0.00096 -0.00001 0.00000 -0.00443 -0.00448 -0.00544

D42 -2.96679 -0.00025 0.00000 -0.01838 -0.01841 -2.98521

D43 -3.13684 -0.00033 0.00000 -0.01356 -0.01352 3.13282

D44 0.01303 -0.00024 0.00000 -0.01150 -0.01148 0.00155

D45 0.00059 0.00001 0.00000 0.00273 0.00277 0.00336

D46 -3.13272 0.00010 0.00000 0.00480 0.00481 -3.12791

D47 0.00096 0.00001 0.00000 0.00443 0.00448 0.00544

D48 -3.13646 -0.00033 0.00000 -0.01191 -0.01190 3.13483

D49 2.96679 0.00025 0.00000 0.01838 0.01841 2.98521

D50 -0.17063 -0.00008 0.00000 0.00205 0.00204 -0.16859

D51 -0.24928 -0.00016 0.00000 0.00537 0.00538 -0.24391

D52 -1.67400 0.00006 0.00000 0.00763 0.00767 -1.66633

D53 -3.09871 0.00029 0.00000 0.00990 0.00996 -3.08875

D54 3.09871 -0.00029 0.00000 -0.00990 -0.00996 3.08875

D55 1.67400 -0.00006 0.00000 -0.00763 -0.00767 1.66633

D56 0.24928 0.00016 0.00000 -0.00537 -0.00538 0.24391

D57 -0.00059 -0.00001 0.00000 -0.00273 -0.00277 -0.00336

D58 3.13272 -0.00010 0.00000 -0.00480 -0.00481 3.12791

D59 3.13684 0.00033 0.00000 0.01356 0.01352 -3.13282

D60 -0.01303 0.00024 0.00000 0.01150 0.01148 -0.00155

D61 -0.01941 -0.00003 0.00000 0.00409 0.00409 -0.01531

D62 3.12323 0.00029 0.00000 0.01414 0.01411 3.13735

D63 3.12701 -0.00042 0.00000 -0.01484 -0.01479 3.11222

D64 -0.01353 -0.00011 0.00000 -0.00480 -0.00477 -0.01830

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13310 -0.00009 0.00000 -0.00211 -0.00209 3.13101

D67 -3.13310 0.00009 0.00000 0.00211 0.00209 -3.13101

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.12701 -0.00042 0.00000 -0.01484 -0.01479 3.11222

D70 -0.01941 -0.00003 0.00000 0.00409 0.00409 -0.01531

D71 -0.01353 -0.00011 0.00000 -0.00480 -0.00477 -0.01830

D72 3.12323 0.00029 0.00000 0.01414 0.01411 3.13735

D73 3.13684 0.00033 0.00000 0.01356 0.01352 -3.13282

D74 -0.01303 0.00024 0.00000 0.01150 0.01148 -0.00155

D75 -0.00059 -0.00001 0.00000 -0.00273 -0.00277 -0.00336

D76 3.13272 -0.00010 0.00000 -0.00480 -0.00481 3.12791

D77 -3.13646 -0.00033 0.00000 -0.01191 -0.01190 3.13483

D78 -0.17063 -0.00008 0.00000 0.00205 0.00204 -0.16859

D79 0.00096 0.00001 0.00000 0.00443 0.00448 0.00544

D80 2.96679 0.00025 0.00000 0.01838 0.01841 2.98521

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 3.13310 -0.00009 0.00000 -0.00211 -0.00209 3.13101

D83 -3.13310 0.00009 0.00000 0.00211 0.00209 -3.13101

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 0.00059 0.00001 0.00000 0.00273 0.00277 0.00336

D86 -3.13684 -0.00033 0.00000 -0.01356 -0.01352 3.13282

D87 -3.13272 0.00010 0.00000 0.00480 0.00481 -3.12791

D88 0.01303 -0.00024 0.00000 -0.01150 -0.01148 0.00155

D89 -0.00096 -0.00001 0.00000 -0.00443 -0.00448 -0.00544

D90 -2.96679 -0.00025 0.00000 -0.01838 -0.01841 -2.98521

D91 3.13646 0.00033 0.00000 0.01191 0.01190 -3.13483

D92 0.17063 0.00008 0.00000 -0.00205 -0.00204 0.16859

D93 -3.12701 0.00042 0.00000 0.01484 0.01479 -3.11222

D94 0.01353 0.00011 0.00000 0.00480 0.00477 0.01830

D95 0.01941 0.00003 0.00000 -0.00409 -0.00409 0.01531

D96 -3.12323 -0.00029 0.00000 -0.01414 -0.01411 -3.13735

D97 0.24928 0.00016 0.00000 -0.00537 -0.00538 0.24391

D98 1.67400 -0.00006 0.00000 -0.00763 -0.00767 1.66633

D99 3.09871 -0.00029 0.00000 -0.00990 -0.00996 3.08875

D100 -3.09871 0.00029 0.00000 0.00990 0.00996 -3.08875

D101 -1.67400 0.00006 0.00000 0.00763 0.00767 -1.66633

D102 -0.24928 -0.00016 0.00000 0.00537 0.00538 -0.24391

D103 3.12701 -0.00042 0.00000 -0.01484 -0.01479 3.11222

D104 -0.01941 -0.00003 0.00000 0.00409 0.00409 -0.01531

D105 -0.01353 -0.00011 0.00000 -0.00480 -0.00477 -0.01830

D106 3.12323 0.00029 0.00000 0.01414 0.01411 3.13735

D107 3.13684 0.00033 0.00000 0.01356 0.01352 -3.13282

D108 -0.01303 0.00024 0.00000 0.01150 0.01148 -0.00155

D109 -0.00059 -0.00001 0.00000 -0.00273 -0.00277 -0.00336

D110 3.13272 -0.00010 0.00000 -0.00480 -0.00481 3.12791

D111 -3.13646 -0.00033 0.00000 -0.01191 -0.01190 3.13483

D112 -0.17063 -0.00008 0.00000 0.00205 0.00204 -0.16859

D113 0.00096 0.00001 0.00000 0.00443 0.00448 0.00544

D114 2.96679 0.00025 0.00000 0.01838 0.01841 2.98521

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.13310 -0.00009 0.00000 -0.00211 -0.00209 3.13101

D117 -3.13310 0.00009 0.00000 0.00211 0.00209 -3.13101

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 0.00059 0.00001 0.00000 0.00273 0.00277 0.00336

D120 -3.13684 -0.00033 0.00000 -0.01356 -0.01352 3.13282

D121 -3.13272 0.00010 0.00000 0.00480 0.00481 -3.12791

D122 0.01303 -0.00024 0.00000 -0.01150 -0.01148 0.00155

D123 -0.00096 -0.00001 0.00000 -0.00443 -0.00448 -0.00544

D124 -2.96679 -0.00025 0.00000 -0.01838 -0.01841 -2.98521

D125 3.13646 0.00033 0.00000 0.01191 0.01190 -3.13483

D126 0.17063 0.00008 0.00000 -0.00205 -0.00204 0.16859

D127 -3.12701 0.00042 0.00000 0.01484 0.01479 -3.11222

D128 0.01353 0.00011 0.00000 0.00480 0.00477 0.01830

D129 0.01941 0.00003 0.00000 -0.00409 -0.00409 0.01531

D130 -3.12323 -0.00029 0.00000 -0.01414 -0.01411 -3.13735

D131 1.67400 -0.00006 0.00000 -0.00763 -0.00767 1.66633

D132 3.09871 -0.00029 0.00000 -0.00990 -0.00996 3.08875

D133 0.24928 0.00016 0.00000 -0.00537 -0.00538 0.24391

D134 -1.67400 0.00006 0.00000 0.00763 0.00767 -1.66633

D135 -0.24928 -0.00016 0.00000 0.00537 0.00538 -0.24391

D136 -3.09871 0.00029 0.00000 0.00990 0.00996 -3.08875

Item Value Threshold Converged?

Maximum Force 0.003716 0.000450 NO

RMS Force 0.000562 0.000300 NO

Maximum Displacement 0.077370 0.001800 NO

RMS Displacement 0.019864 0.001200 NO

Predicted change in Energy=-3.726427D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:12:57 2019, MaxMem= 1342177280 cpu: 1.3

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.680910 4.270955 -0.054556

2 6 0 1.100836 2.886171 -0.020514

3 7 0 0.000000 2.077625 -0.004970

4 6 0 -1.100836 2.886171 -0.020514

5 6 0 -0.680910 4.270955 -0.054556

6 6 0 -2.444414 2.444414 -0.019813

7 6 0 -2.886171 1.100836 -0.020514

8 7 0 -2.077625 0.000000 -0.004970

9 6 0 -2.886171 -1.100836 -0.020514

10 6 0 -4.270955 -0.680910 -0.054556

11 6 0 -4.270955 0.680910 -0.054556

12 6 0 2.444414 2.444414 -0.019813

13 6 0 2.886171 1.100836 -0.020514

14 6 0 4.270955 0.680910 -0.054556

15 6 0 4.270955 -0.680910 -0.054556

16 6 0 2.886171 -1.100836 -0.020514

17 7 0 2.077625 0.000000 -0.004970

18 6 0 2.444414 -2.444414 -0.019813

19 6 0 1.100836 -2.886171 -0.020514

20 6 0 0.680910 -4.270955 -0.054556

21 6 0 -0.680910 -4.270955 -0.054556

22 6 0 -1.100836 -2.886171 -0.020514

23 7 0 0.000000 -2.077625 -0.004970

24 1 0 1.338375 5.126817 -0.084657

25 1 0 -1.338375 5.126817 -0.084657

26 1 0 -5.126817 -1.338375 -0.084657

27 1 0 -5.126817 1.338375 -0.084657

28 1 0 5.126817 1.338375 -0.084657

29 1 0 5.126817 -1.338375 -0.084657

30 1 0 1.338375 -5.126817 -0.084657

31 1 0 -1.338375 -5.126817 -0.084657

32 30 0 0.000000 0.000000 0.309107

33 6 0 -2.444414 -2.444414 -0.019813

34 6 0 -3.453453 -3.453453 -0.032339

35 6 0 3.453453 3.453453 -0.032339

36 6 0 -4.306148 -4.306148 -0.037899

37 6 0 4.306148 4.306148 -0.037899

38 6 0 -3.453453 3.453453 -0.032339

39 6 0 -4.306148 4.306148 -0.037899

40 6 0 3.453453 -3.453453 -0.032339

41 6 0 4.306148 -4.306148 -0.037899

42 1 0 5.060797 -5.060797 -0.026510

43 1 0 -5.060797 -5.060797 -0.026510

44 1 0 -5.060797 5.060797 -0.026510

45 1 0 5.060797 5.060797 -0.026510

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.447454 0.000000

3 N 2.297127 1.365953 0.000000

4 C 2.256857 2.201672 1.365953 0.000000

5 C 1.361820 2.256857 2.297127 1.447454 0.000000

6 C 3.620098 3.572667 2.471824 1.414338 2.539174

7 C 4.772304 4.368483 3.047022 2.524845 3.861864

8 N 5.084588 4.293348 2.938206 3.047022 4.493810

9 C 6.448361 5.638479 4.293348 4.368483 5.806933

10 C 7.002995 6.448361 5.084588 4.772304 6.116322

11 C 6.116322 5.806933 4.493810 3.861864 5.077090

12 C 2.539174 1.414338 2.471824 3.572667 3.620098

13 C 3.861864 2.524845 3.047022 4.368483 4.772304

14 C 5.077090 3.861864 4.493810 5.806933 6.116322

15 C 6.116322 4.772304 5.084588 6.448361 7.002995

16 C 5.806933 4.368483 4.293348 5.638479 6.448361

17 N 4.493810 3.047022 2.938206 4.293348 5.084588

18 C 6.943151 5.497303 5.140450 6.401870 7.407094

19 C 7.169515 5.772342 5.084423 6.177968 7.375651

20 C 8.541910 7.169515 6.385184 7.375651 8.649785

21 C 8.649785 7.375651 6.385184 7.169515 8.541910

22 C 7.375651 6.177968 5.084423 5.772342 7.169515

23 N 6.385184 5.084423 4.155251 5.084423 6.385184

24 H 1.079661 2.254115 3.330941 3.312757 2.193381

25 H 2.193381 3.312757 3.330941 2.254115 1.079661

26 H 8.074354 7.525594 6.161142 5.836046 7.157624

27 H 6.506199 6.417433 5.180453 4.313735 5.326070

28 H 5.326070 4.313735 5.180453 6.417433 6.506199

29 H 7.157624 5.836046 6.161142 7.525594 8.074354

30 H 9.420790 8.016765 7.328137 8.376267 9.612312

31 H 9.612312 8.376267 7.328137 8.016765 9.420790

32 Zn 4.340155 3.106521 2.101231 3.106521 4.340155

33 C 7.407094 6.401870 5.140450 5.497303 6.943151

34 C 8.761275 7.805929 6.520730 6.762085 8.206947

35 C 2.890640 2.420074 3.717525 4.589499 4.214471

36 C 9.921579 8.998068 7.700426 7.874248 9.311784

37 C 3.625447 3.505804 4.848743 5.590359 4.987210

38 C 4.214471 4.589499 3.717525 2.420074 2.890640

39 C 4.987210 5.590359 4.848743 3.505804 3.625447

40 C 8.206947 6.762085 6.520730 7.805929 8.761275

41 C 9.311784 7.874248 7.700426 8.998068 9.921579

42 H 10.308529 8.878943 8.750382 10.055846 10.956714

43 H 10.956714 10.055846 8.750382 8.878943 10.308529

44 H 5.795846 6.534122 5.874644 4.517778 4.450623

45 H 4.450623 4.517778 5.874644 6.534122 5.795846

6 7 8 9 10

6 C 0.000000

7 C 1.414338 0.000000

8 N 2.471824 1.365953 0.000000

9 C 3.572667 2.201672 1.365953 0.000000

10 C 3.620098 2.256857 2.297127 1.447454 0.000000

11 C 2.539174 1.447454 2.297127 2.256857 1.361820

12 C 4.888829 5.497303 5.140450 6.401870 7.407094

13 C 5.497303 5.772342 5.084423 6.177968 7.375651

14 C 6.943151 7.169515 6.385184 7.375651 8.649785

15 C 7.407094 7.375651 6.385184 7.169515 8.541910

16 C 6.401870 6.177968 5.084423 5.772342 7.169515

17 N 5.140450 5.084423 4.155251 5.084423 6.385184

18 C 6.913848 6.401870 5.140450 5.497303 6.943151

19 C 6.401870 5.638479 4.293348 4.368483 5.806933

20 C 7.407094 6.448361 5.084588 4.772304 6.116322

21 C 6.943151 5.806933 4.493810 3.861864 5.077090

22 C 5.497303 4.368483 3.047022 2.524845 3.861864

23 N 5.140450 4.293348 2.938206 3.047022 4.493810

24 H 4.637778 5.836046 6.161142 7.525594 8.074354

25 H 2.902208 4.313735 5.180453 6.417433 6.506199

26 H 4.637778 3.312757 3.330941 2.254115 1.079661

27 H 2.902208 2.254115 3.330941 3.312757 2.193381

28 H 7.651867 8.016765 7.328137 8.376267 9.612312

29 H 8.463879 8.376267 7.328137 8.016765 9.420790

30 H 8.463879 7.525594 6.161142 5.836046 7.157624

31 H 7.651867 6.417433 5.180453 4.313735 5.326070

32 Zn 3.472537 3.106521 2.101231 3.106521 4.340155

33 C 4.888829 3.572667 2.471824 1.414338 2.539174

34 C 5.983574 4.589499 3.717525 2.420074 2.890640

35 C 5.983574 6.762085 6.520730 7.805929 8.761275

36 C 7.002605 5.590359 4.848743 3.505804 3.625447

37 C 7.002605 7.874248 7.700426 8.998068 9.921579

38 C 1.427052 2.420074 3.717525 4.589499 4.214471

39 C 2.632951 3.505804 4.848743 5.590359 4.987210

40 C 8.340854 7.805929 6.520730 6.762085 8.206947

41 C 9.546754 8.998068 7.700426 7.874248 9.311784

42 H 10.613973 10.055846 8.750382 8.878943 10.308529

43 H 7.948188 6.534122 5.874644 4.517778 4.450623

44 H 3.700129 4.517778 5.874644 6.534122 5.795846

45 H 7.948188 8.878943 8.750382 10.055846 10.956714

11 12 13 14 15

11 C 0.000000

12 C 6.943151 0.000000

13 C 7.169515 1.414338 0.000000

14 C 8.541910 2.539174 1.447454 0.000000

15 C 8.649785 3.620098 2.256857 1.361820 0.000000

16 C 7.375651 3.572667 2.201672 2.256857 1.447454

17 N 6.385184 2.471824 1.365953 2.297127 2.297127

18 C 7.407094 4.888829 3.572667 3.620098 2.539174

19 C 6.448361 5.497303 4.368483 4.772304 3.861864

20 C 7.002995 6.943151 5.806933 6.116322 5.077090

21 C 6.116322 7.407094 6.448361 7.002995 6.116322

22 C 4.772304 6.401870 5.638479 6.448361 5.806933

23 N 5.084588 5.140450 4.293348 5.084588 4.493810

24 H 7.157624 2.902208 4.313735 5.326070 6.506199

25 H 5.326070 4.637778 5.836046 7.157624 8.074354

26 H 2.193381 8.463879 8.376267 9.612312 9.420790

27 H 1.079661 7.651867 8.016765 9.420790 9.612312

28 H 9.420790 2.902208 2.254115 1.079661 2.193381

29 H 9.612312 4.637778 3.312757 2.193381 1.079661

30 H 8.074354 7.651867 6.417433 6.506199 5.326070

31 H 6.506199 8.463879 7.525594 8.074354 7.157624

32 Zn 4.340155 3.472537 3.106521 4.340155 4.340155

33 C 3.620098 6.913848 6.401870 7.407094 6.943151

34 C 4.214471 8.340854 7.805929 8.761275 8.206947

35 C 8.206947 1.427052 2.420074 2.890640 4.214471

36 C 4.987210 9.546754 8.998068 9.921579 9.311784

37 C 9.311784 2.632951 3.505804 3.625447 4.987210

38 C 2.890640 5.983574 6.762085 8.206947 8.761275

39 C 3.625447 7.002605 7.874248 9.311784 9.921579

40 C 8.761275 5.983574 4.589499 4.214471 2.890640

41 C 9.921579 7.002605 5.590359 4.987210 3.625447

42 H 10.956714 7.948188 6.534122 5.795846 4.450623

43 H 5.795846 10.613973 10.055846 10.956714 10.308529

44 H 4.450623 7.948188 8.878943 10.308529 10.956714

45 H 10.308529 3.700129 4.517778 4.450623 5.795846

16 17 18 19 20

16 C 0.000000

17 N 1.365953 0.000000

18 C 1.414338 2.471824 0.000000

19 C 2.524845 3.047022 1.414338 0.000000

20 C 3.861864 4.493810 2.539174 1.447454 0.000000

21 C 4.772304 5.084588 3.620098 2.256857 1.361820

22 C 4.368483 4.293348 3.572667 2.201672 2.256857

23 N 3.047022 2.938206 2.471824 1.365953 2.297127

24 H 6.417433 5.180453 7.651867 8.016765 9.420790

25 H 7.525594 6.161142 8.463879 8.376267 9.612312

26 H 8.016765 7.328137 7.651867 6.417433 6.506199

27 H 8.376267 7.328137 8.463879 7.525594 8.074354

28 H 3.312757 3.330941 4.637778 5.836046 7.157624

29 H 2.254115 3.330941 2.902208 4.313735 5.326070

30 H 4.313735 5.180453 2.902208 2.254115 1.079661

31 H 5.836046 6.161142 4.637778 3.312757 2.193381

32 Zn 3.106521 2.101231 3.472537 3.106521 4.340155

33 C 5.497303 5.140450 4.888829 3.572667 3.620098

34 C 6.762085 6.520730 5.983574 4.589499 4.214471

35 C 4.589499 3.717525 5.983574 6.762085 8.206947

36 C 7.874248 7.700426 7.002605 5.590359 4.987210

37 C 5.590359 4.848743 7.002605 7.874248 9.311784

38 C 7.805929 6.520730 8.340854 7.805929 8.761275

39 C 8.998068 7.700426 9.546754 8.998068 9.921579

40 C 2.420074 3.717525 1.427052 2.420074 2.890640

41 C 3.505804 4.848743 2.632951 3.505804 3.625447

42 H 4.517778 5.874644 3.700129 4.517778 4.450623

43 H 8.878943 8.750382 7.948188 6.534122 5.795846

44 H 10.055846 8.750382 10.613973 10.055846 10.956714

45 H 6.534122 5.874644 7.948188 8.878943 10.308529

21 22 23 24 25

21 C 0.000000

22 C 1.447454 0.000000

23 N 2.297127 1.365953 0.000000

24 H 9.612312 8.376267 7.328137 0.000000

25 H 9.420790 8.016765 7.328137 2.676751 0.000000

26 H 5.326070 4.313735 5.180453 9.143163 7.493398

27 H 7.157624 5.836046 6.161142 7.493398 5.357666

28 H 8.074354 7.525594 6.161142 5.357666 7.493398

29 H 6.506199 6.417433 5.180453 7.493398 9.143163

30 H 2.193381 3.312757 3.330941 10.253635 10.597265

31 H 1.079661 2.254115 3.330941 10.597265 10.253635

32 Zn 4.340155 3.106521 2.101231 5.313243 5.313243

33 C 2.539174 1.414338 2.471824 8.463879 7.651867

34 C 2.890640 2.420074 3.717525 9.827787 8.837270

35 C 8.761275 7.805929 6.520730 2.697487 5.075875

36 C 3.625447 3.505804 4.848743 10.992892 9.888918

37 C 9.921579 8.998068 7.700426 3.079506 5.704063

38 C 8.206947 6.762085 6.520730 5.075875 2.697487

39 C 9.311784 7.874248 7.700426 5.704063 3.079506

40 C 4.214471 4.589499 3.717525 8.837270 9.827787

41 C 4.987210 5.590359 4.848743 9.888918 10.992892

42 H 5.795846 6.534122 5.874644 10.846533 12.030805

43 H 4.450623 4.517778 5.874644 12.030805 10.846533

44 H 10.308529 8.878943 8.750382 6.399777 3.723461

45 H 10.956714 10.055846 8.750382 3.723461 6.399777

26 27 28 29 30

26 H 0.000000

27 H 2.676751 0.000000

28 H 10.597265 10.253635 0.000000

29 H 10.253635 10.597265 2.676751 0.000000

30 H 7.493398 9.143163 7.493398 5.357666 0.000000

31 H 5.357666 7.493398 9.143163 7.493398 2.676751

32 Zn 5.313243 5.313243 5.313243 5.313243 5.313243

33 C 2.902208 4.637778 8.463879 7.651867 4.637778

34 C 2.697487 5.075875 9.827787 8.837270 5.075875

35 C 9.827787 8.837270 2.697487 5.075875 8.837270

36 C 3.079506 5.704063 10.992892 9.888918 5.704063

37 C 10.992892 9.888918 3.079506 5.704063 9.888918

38 C 5.075875 2.697487 8.837270 9.827787 9.827787

39 C 5.704063 3.079506 9.888918 10.992892 10.992892

40 C 8.837270 9.827787 5.075875 2.697487 2.697487

41 C 9.888918 10.992892 5.704063 3.079506 3.079506

42 H 10.846533 12.030805 6.399777 3.723461 3.723461

43 H 3.723461 6.399777 12.030805 10.846533 6.399777

44 H 6.399777 3.723461 10.846533 12.030805 12.030805

45 H 12.030805 10.846533 3.723461 6.399777 10.846533

31 32 33 34 35

31 H 0.000000

32 Zn 5.313243 0.000000

33 C 2.902208 3.472537 0.000000

34 C 2.697487 4.895842 1.427052 0.000000

35 C 9.827787 4.895842 8.340854 9.767841 0.000000

36 C 3.079506 6.099691 2.632951 1.205905 10.973735

37 C 10.992892 6.099691 9.546754 10.973735 1.205905

38 C 8.837270 4.895842 5.983574 6.906907 6.906907

39 C 9.888918 6.099691 7.002605 7.806314 7.806314

40 C 5.075875 4.895842 5.983574 6.906907 6.906907

41 C 5.704063 6.099691 7.002605 7.806314 7.806314

42 H 6.399777 7.164912 7.948188 8.664643 8.664643

43 H 3.723461 7.164912 3.700129 2.273134 12.040969

44 H 10.846533 7.164912 7.948188 8.664643 8.664643

45 H 12.030805 7.164912 10.613973 12.040969 2.273134

36 37 38 39 40

36 C 0.000000

37 C 12.179626 0.000000

38 C 7.806314 7.806314 0.000000

39 C 8.612296 8.612296 1.205905 0.000000

40 C 7.806314 7.806314 9.767841 10.973735 0.000000

41 C 8.612296 8.612296 10.973735 12.179626 1.205905

42 H 9.397302 9.397302 12.040969 13.246865 2.273134

43 H 1.067295 13.246865 8.664643 9.397302 8.664643

44 H 9.397302 9.397302 2.273134 1.067295 12.040969

45 H 13.246865 1.067295 8.664643 9.397302 8.664643

41 42 43 44 45

41 C 0.000000

42 H 1.067295 0.000000

43 H 9.397302 10.121593 0.000000

44 H 13.246865 14.314094 10.121593 0.000000

45 H 9.397302 10.121593 14.314094 10.121593 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

Omega: Change in point group or standard orientation.

Old FWG=C04V [C4(Zn1),2SGV(C6H2),2SGD(N2),X(C16H8)]

New FWG=C04V [C4(Zn1),2SGV(N2),2SGD(C6H2),X(C16H8)]

RotChk: IX=3 Diff= 1.08D+00

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.680910 -4.270955 -0.065422

2 6 0 -1.100836 -2.886171 -0.031380

3 7 0 0.000000 -2.077625 -0.015836

4 6 0 1.100836 -2.886171 -0.031380

5 6 0 0.680910 -4.270955 -0.065422

6 6 0 2.444414 -2.444414 -0.030679

7 6 0 2.886171 -1.100836 -0.031380

8 7 0 2.077625 0.000000 -0.015836

9 6 0 2.886171 1.100836 -0.031380

10 6 0 4.270955 0.680910 -0.065422

11 6 0 4.270955 -0.680910 -0.065422

12 6 0 -2.444414 -2.444414 -0.030679

13 6 0 -2.886171 -1.100836 -0.031380

14 6 0 -4.270955 -0.680910 -0.065422

15 6 0 -4.270955 0.680910 -0.065422

16 6 0 -2.886171 1.100836 -0.031380

17 7 0 -2.077625 0.000000 -0.015836

18 6 0 -2.444414 2.444414 -0.030679

19 6 0 -1.100836 2.886171 -0.031380

20 6 0 -0.680910 4.270955 -0.065422

21 6 0 0.680910 4.270955 -0.065422

22 6 0 1.100836 2.886171 -0.031380

23 7 0 0.000000 2.077625 -0.015836

24 1 0 -1.338375 -5.126817 -0.095523

25 1 0 1.338375 -5.126817 -0.095523

26 1 0 5.126817 1.338375 -0.095523

27 1 0 5.126817 -1.338375 -0.095523

28 1 0 -5.126817 -1.338375 -0.095523

29 1 0 -5.126817 1.338375 -0.095523

30 1 0 -1.338375 5.126817 -0.095523

31 1 0 1.338375 5.126817 -0.095523

32 30 0 0.000000 0.000000 0.298241

33 6 0 2.444414 2.444414 -0.030679

34 6 0 3.453453 3.453453 -0.043205

35 6 0 -3.453453 -3.453453 -0.043205

36 6 0 4.306148 4.306148 -0.048766

37 6 0 -4.306148 -4.306148 -0.048766

38 6 0 3.453453 -3.453453 -0.043205

39 6 0 4.306148 -4.306148 -0.048766

40 6 0 -3.453453 3.453453 -0.043205

41 6 0 -4.306148 4.306148 -0.048766

42 1 0 -5.060797 5.060797 -0.037376

43 1 0 5.060797 5.060797 -0.037376

44 1 0 5.060797 -5.060797 -0.037376

45 1 0 -5.060797 -5.060797 -0.037376

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

Rotational constants (GHZ): 0.1465288 0.1465288 0.0734033

Leave Link 202 at Fri Jul 26 14:12:58 2019, MaxMem= 1342177280 cpu: 0.1

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 184 symmetry adapted cartesian basis functions of A1 symmetry.

There are 155 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3060.9225390603 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= 9 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= -0.1304908461 Hartrees.

Nuclear repulsion after empirical dispersion term = 3060.7920482142 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: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3890

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.45D-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) = 3.19%

GePol: Cavity surface area = 414.867 Ang\*\*2

GePol: Cavity volume = 419.624 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0084853542 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3060.8005335684 Hartrees.

Leave Link 301 at Fri Jul 26 14:12:58 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44832.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.39D-05 NBF= 172 148 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 172 148 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:12:58 2019, MaxMem= 1342177280 cpu: 6.6

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:12:58 2019, MaxMem= 1342177280 cpu: 0.8

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

Initial guess from the checkpoint file: "ZnTSPsim0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.923880 0.000000 0.000000 0.382683 Ang= 45.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Occupied (E) (E) (B2) (A1) (E) (E) (B1) (A1) (B2) (E) (E)

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

(E) (E) (A1) (A2) (E) (E) (B1) (B1) (E) (E) (A1)

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

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

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

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(E) (E) (A2) (A1)

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(E) (E) (E)

The electronic state of the initial guess is 1-A1.

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= -1359.45268647259

Leave Link 401 at Fri Jul 26 14:13:00 2019, MaxMem= 1342177280 cpu: 21.0

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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.

An orbital has undefined symmetry, so N\*\*3 symmetry is turned off.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 660000000 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= 0 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= 45396300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.22D-15 for 637.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.84D-15 for 3437 3216.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.44D-15 for 974.

Iteration 1 A^-1\*A deviation from orthogonality is 1.34D-14 for 2311 2259.

E= -1359.05776442171

DIIS: error= 2.08D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.05776442171 IErMin= 1 ErrMin= 2.08D-03

ErrMax= 2.08D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.24D-03 BMatP= 2.24D-03

IDIUse=3 WtCom= 9.79D-01 WtEn= 2.08D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 3.198 Goal= None Shift= 0.000

GapD= 3.198 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.64D-04 MaxDP=6.28D-03 OVMax= 9.39D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.64D-04 CP: 1.00D+00

E= -1359.06103130049 Delta-E= -0.003266878779 Rises=F Damp=F

DIIS: error= 2.50D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.06103130049 IErMin= 2 ErrMin= 2.50D-04

ErrMax= 2.50D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.37D-05 BMatP= 2.24D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.50D-03

Coeff-Com: -0.473D-01 0.105D+01

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

Coeff: -0.472D-01 0.105D+01

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=1.75D-05 MaxDP=4.29D-04 DE=-3.27D-03 OVMax= 1.49D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.64D-05 CP: 1.00D+00 1.04D+00

E= -1359.06106093774 Delta-E= -0.000029637253 Rises=F Damp=F

DIIS: error= 3.36D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.06106093774 IErMin= 2 ErrMin= 2.50D-04

ErrMax= 3.36D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.15D-05 BMatP= 2.37D-05

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.36D-03

Coeff-Com: -0.301D-01 0.545D+00 0.485D+00

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

Coeff: -0.300D-01 0.543D+00 0.487D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=8.48D-06 MaxDP=3.91D-04 DE=-2.96D-05 OVMax= 1.34D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.08D-06 CP: 1.00D+00 1.05D+00 6.59D-01

E= -1359.06107513723 Delta-E= -0.000014199489 Rises=F Damp=F

DIIS: error= 1.01D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.06107513723 IErMin= 4 ErrMin= 1.01D-04

ErrMax= 1.01D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.91D-06 BMatP= 2.15D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.01D-03

Coeff-Com: -0.716D-02 0.959D-01 0.273D+00 0.638D+00

Coeff-En: 0.000D+00 0.000D+00 0.126D+00 0.874D+00

Coeff: -0.715D-02 0.958D-01 0.273D+00 0.638D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=2.76D-06 MaxDP=1.29D-04 DE=-1.42D-05 OVMax= 4.16D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.14D-06 CP: 1.00D+00 1.05D+00 7.12D-01 7.52D-01

E= -1359.06107744633 Delta-E= -0.000002309093 Rises=F Damp=F

DIIS: error= 5.00D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.06107744633 IErMin= 5 ErrMin= 5.00D-05

ErrMax= 5.00D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.89D-07 BMatP= 2.91D-06

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

Coeff-Com: -0.108D-02 0.116D-02 0.988D-01 0.335D+00 0.566D+00

Coeff: -0.108D-02 0.116D-02 0.988D-01 0.335D+00 0.566D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=9.18D-07 MaxDP=3.24D-05 DE=-2.31D-06 OVMax= 9.03D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.15D-07 CP: 1.00D+00 1.05D+00 7.23D-01 8.26D-01 7.78D-01

E= -1359.06107764466 Delta-E= -0.000000198330 Rises=F Damp=F

DIIS: error= 1.62D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.06107764466 IErMin= 6 ErrMin= 1.62D-05

ErrMax= 1.62D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.19D-08 BMatP= 2.89D-07

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

Coeff-Com: 0.384D-03-0.137D-01 0.160D-01 0.916D-01 0.297D+00 0.609D+00

Coeff: 0.384D-03-0.137D-01 0.160D-01 0.916D-01 0.297D+00 0.609D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.95D-07 MaxDP=8.73D-06 DE=-1.98D-07 OVMax= 2.90D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.32D-07 CP: 1.00D+00 1.05D+00 7.31D-01 8.26D-01 7.88D-01

CP: 6.19D-01

E= -1359.06107766628 Delta-E= -0.000000021623 Rises=F Damp=F

DIIS: error= 3.80D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.06107766628 IErMin= 7 ErrMin= 3.80D-06

ErrMax= 3.80D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.94D-09 BMatP= 3.19D-08

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

Coeff-Com: 0.293D-03-0.854D-02 0.477D-02 0.386D-01 0.152D+00 0.371D+00

Coeff-Com: 0.442D+00

Coeff: 0.293D-03-0.854D-02 0.477D-02 0.386D-01 0.152D+00 0.371D+00

Coeff: 0.442D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=8.41D-08 MaxDP=5.02D-06 DE=-2.16D-08 OVMax= 1.34D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.43D-08 CP: 1.00D+00 1.05D+00 7.32D-01 8.24D-01 7.89D-01

CP: 6.05D-01 6.17D-01

E= -1359.06107766967 Delta-E= -0.000000003391 Rises=F Damp=F

DIIS: error= 1.02D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.06107766967 IErMin= 8 ErrMin= 1.02D-06

ErrMax= 1.02D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.82D-10 BMatP= 3.94D-09

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

Coeff-Com: 0.982D-04-0.253D-02 0.288D-03 0.699D-02 0.366D-01 0.109D+00

Coeff-Com: 0.244D+00 0.606D+00

Coeff: 0.982D-04-0.253D-02 0.288D-03 0.699D-02 0.366D-01 0.109D+00

Coeff: 0.244D+00 0.606D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.53D-08 MaxDP=1.20D-06 DE=-3.39D-09 OVMax= 3.74D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.25D-08 CP: 1.00D+00 1.05D+00 7.32D-01 8.25D-01 7.88D-01

CP: 6.04D-01 6.54D-01 8.50D-01

E= -1359.06107766997 Delta-E= -0.000000000302 Rises=F Damp=F

DIIS: error= 1.89D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1359.06107766997 IErMin= 9 ErrMin= 1.89D-07

ErrMax= 1.89D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.21D-11 BMatP= 2.82D-10

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

Coeff-Com: 0.637D-05-0.954D-05-0.458D-03-0.192D-02-0.321D-02 0.309D-02

Coeff-Com: 0.554D-01 0.281D+00 0.666D+00

Coeff: 0.637D-05-0.954D-05-0.458D-03-0.192D-02-0.321D-02 0.309D-02

Coeff: 0.554D-01 0.281D+00 0.666D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=8.84D-09 MaxDP=3.51D-07 DE=-3.02D-10 OVMax= 1.07D-06

Error on total polarization charges = 0.06223

SCF Done: E(RB3LYP) = -1359.06107767 A.U. after 9 cycles

NFock= 9 Conv=0.88D-08 -V/T= 1.9682

KE= 1.403750414238D+03 PE=-9.363768233852D+03 EE= 3.540156208375D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.32

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:13:38 2019, MaxMem= 1342177280 cpu: 426.8

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44832.

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 Fri Jul 26 14:13:42 2019, MaxMem= 1342177280 cpu: 43.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

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

Leave Link 702 at Fri Jul 26 14:13:42 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Fri Jul 26 14:13:46 2019, MaxMem= 1342177280 cpu: 43.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 4.97379915D-14 3.23296945D-13 7.39396026D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000132572 -0.000287176 -0.000157789

2 6 0.000377686 0.000590572 -0.000352656

3 7 0.000000000 -0.001683887 0.003606650

4 6 -0.000377686 0.000590572 -0.000352656

5 6 -0.000132572 -0.000287176 -0.000157789

6 6 -0.000302754 0.000302754 -0.000523703

7 6 -0.000590572 0.000377686 -0.000352656

8 7 0.001683887 0.000000000 0.003606650

9 6 -0.000590572 -0.000377686 -0.000352656

10 6 0.000287176 -0.000132572 -0.000157789

11 6 0.000287176 0.000132572 -0.000157789

12 6 0.000302754 0.000302754 -0.000523703

13 6 0.000590572 0.000377686 -0.000352656

14 6 -0.000287176 0.000132572 -0.000157789

15 6 -0.000287176 -0.000132572 -0.000157789

16 6 0.000590572 -0.000377686 -0.000352656

17 7 -0.001683887 0.000000000 0.003606650

18 6 0.000302754 -0.000302754 -0.000523703

19 6 0.000377686 -0.000590572 -0.000352656

20 6 0.000132572 0.000287176 -0.000157789

21 6 -0.000132572 0.000287176 -0.000157789

22 6 -0.000377686 -0.000590572 -0.000352656

23 7 0.000000000 0.001683887 0.003606650

24 1 0.000180018 -0.000074815 0.000114360

25 1 -0.000180018 -0.000074815 0.000114360

26 1 0.000074815 -0.000180018 0.000114360

27 1 0.000074815 0.000180018 0.000114360

28 1 -0.000074815 0.000180018 0.000114360

29 1 -0.000074815 -0.000180018 0.000114360

30 1 0.000180018 0.000074815 0.000114360

31 1 -0.000180018 0.000074815 0.000114360

32 30 0.000000000 0.000000000 -0.010330430

33 6 -0.000302754 -0.000302754 -0.000523703

34 6 -0.000165785 -0.000165785 0.000223980

35 6 0.000165785 0.000165785 0.000223980

36 6 0.000168457 0.000168457 0.000471798

37 6 -0.000168457 -0.000168457 0.000471798

38 6 -0.000165785 0.000165785 0.000223980

39 6 0.000168457 -0.000168457 0.000471798

40 6 0.000165785 -0.000165785 0.000223980

41 6 -0.000168457 0.000168457 0.000471798

42 1 0.000029998 -0.000029998 -0.000403948

43 1 -0.000029998 -0.000029998 -0.000403948

44 1 -0.000029998 0.000029998 -0.000403948

45 1 0.000029998 0.000029998 -0.000403948

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

Cartesian Forces: Max 0.010330430 RMS 0.001156156

Leave Link 716 at Fri Jul 26 14:13:46 2019, MaxMem= 1342177280 cpu: 0.6

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001906973 RMS 0.000421334

Search for a local minimum.

Step number 2 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .42133D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2

DE= 9.57D-05 DEPred=-3.73D-04 R=-2.57D-01

Trust test=-2.57D-01 RLast= 1.32D-01 DXMaxT set to 1.50D-01

ITU= -1 0

Eigenvalues --- 0.00534 0.00534 0.00534 0.00534 0.00534

Eigenvalues --- 0.00534 0.00534 0.00594 0.01009 0.01199

Eigenvalues --- 0.01360 0.01360 0.01673 0.01674 0.01674

Eigenvalues --- 0.01681 0.01788 0.01805 0.01805 0.01826

Eigenvalues --- 0.01830 0.01840 0.01858 0.01858 0.01868

Eigenvalues --- 0.01868 0.01868 0.01873 0.01910 0.01920

Eigenvalues --- 0.01922 0.01922 0.01933 0.01954 0.01954

Eigenvalues --- 0.01979 0.02175 0.02175 0.02177 0.02180

Eigenvalues --- 0.02621 0.02621 0.03330 0.04648 0.04654

Eigenvalues --- 0.04654 0.04654 0.04654 0.04654 0.04654

Eigenvalues --- 0.04654 0.07221 0.13826 0.15125 0.15125

Eigenvalues --- 0.15688 0.15998 0.15998 0.15998 0.15998

Eigenvalues --- 0.15999 0.15999 0.15999 0.18935 0.22779

Eigenvalues --- 0.22864 0.22864 0.22864 0.24244 0.24375

Eigenvalues --- 0.24518 0.24518 0.24630 0.24937 0.24937

Eigenvalues --- 0.24991 0.24999 0.24999 0.24999 0.24999

Eigenvalues --- 0.25017 0.35056 0.35056 0.35403 0.35491

Eigenvalues --- 0.35814 0.36034 0.36034 0.36034 0.36034

Eigenvalues --- 0.36034 0.36034 0.36034 0.36039 0.36771

Eigenvalues --- 0.36856 0.36856 0.37563 0.37563 0.37563

Eigenvalues --- 0.37566 0.38949 0.38949 0.39289 0.39535

Eigenvalues --- 0.41397 0.41397 0.41397 0.41403 0.41416

Eigenvalues --- 0.41416 0.41737 0.42436 0.43509 0.43774

Eigenvalues --- 0.43774 0.45336 0.47671 0.49048 0.49048

Eigenvalues --- 0.50125 0.51391 0.51892 0.51892 0.52961

Eigenvalues --- 1.01787 1.01831 1.01831 1.01831

En-DIIS/RFO-DIIS IScMMF= 0 using points: 2 1

RFO step: Lambda=-1.97036484D-04.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= -9.57D-05 SmlDif= 1.00D-05

RMS Error= 0.2038426811D-02 NUsed= 2 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.05449 -0.05449

Maximum step size ( 0.150) exceeded in Quadratic search.

-- Step size scaled by 0.643

Iteration 1 RMS(Cart)= 0.03691749 RMS(Int)= 0.00094475

Iteration 2 RMS(Cart)= 0.00126052 RMS(Int)= 0.00005789

Iteration 3 RMS(Cart)= 0.00000116 RMS(Int)= 0.00005789

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00005789

ITry= 1 IFail=0 DXMaxC= 2.55D-01 DCOld= 1.00D+10 DXMaxT= 1.50D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.15D-03 for atom 45.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73529 -0.00035 -0.00002 -0.00108 -0.00112 2.73417

R2 2.57347 0.00030 -0.00006 -0.00149 -0.00164 2.57183

R3 2.04026 0.00005 0.00000 0.00007 0.00007 2.04033

R4 2.58128 0.00068 0.00002 0.00154 0.00163 2.58290

R5 2.67271 0.00005 -0.00016 -0.00450 -0.00462 2.66810

R6 2.58128 0.00068 0.00002 0.00154 0.00163 2.58290

R7 3.97075 -0.00118 -0.00074 -0.02775 -0.02824 3.94251

R8 2.73529 -0.00035 -0.00002 -0.00108 -0.00112 2.73417

R9 2.67271 0.00005 -0.00016 -0.00450 -0.00462 2.66810

R10 2.04026 0.00005 0.00000 0.00007 0.00007 2.04033

R11 2.67271 0.00005 -0.00016 -0.00450 -0.00462 2.66810

R12 2.69674 0.00004 -0.00001 -0.00019 -0.00043 2.69631

R13 2.58128 0.00067 0.00002 0.00154 0.00163 2.58290

R14 2.73529 -0.00035 -0.00002 -0.00108 -0.00112 2.73417

R15 2.58128 0.00068 0.00002 0.00154 0.00163 2.58290

R16 3.97075 -0.00118 -0.00074 -0.02775 -0.02824 3.94251

R17 2.73529 -0.00035 -0.00002 -0.00108 -0.00112 2.73417

R18 2.67271 0.00005 -0.00016 -0.00450 -0.00462 2.66810

R19 2.57347 0.00030 -0.00006 -0.00149 -0.00164 2.57183

R20 2.04026 0.00005 0.00000 0.00007 0.00007 2.04033

R21 2.04026 0.00005 0.00000 0.00007 0.00007 2.04033

R22 2.67271 0.00005 -0.00016 -0.00450 -0.00462 2.66810

R23 2.69674 0.00004 -0.00001 -0.00019 -0.00043 2.69631

R24 2.73529 -0.00035 -0.00002 -0.00108 -0.00112 2.73417

R25 2.58128 0.00067 0.00002 0.00154 0.00163 2.58290

R26 2.57347 0.00030 -0.00006 -0.00149 -0.00164 2.57183

R27 2.04026 0.00005 0.00000 0.00007 0.00007 2.04033

R28 2.73529 -0.00035 -0.00002 -0.00108 -0.00112 2.73417

R29 2.04026 0.00005 0.00000 0.00007 0.00007 2.04033

R30 2.58128 0.00068 0.00002 0.00154 0.00163 2.58290

R31 2.67271 0.00005 -0.00016 -0.00450 -0.00462 2.66810

R32 3.97075 -0.00118 -0.00074 -0.02775 -0.02824 3.94251

R33 2.67271 0.00005 -0.00016 -0.00450 -0.00462 2.66810

R34 2.69674 0.00004 -0.00001 -0.00019 -0.00043 2.69631

R35 2.73529 -0.00035 -0.00002 -0.00107 -0.00112 2.73417

R36 2.58128 0.00067 0.00002 0.00154 0.00163 2.58290

R37 2.57347 0.00030 -0.00006 -0.00149 -0.00164 2.57183

R38 2.04026 0.00005 0.00000 0.00007 0.00007 2.04033

R39 2.73529 -0.00035 -0.00002 -0.00107 -0.00112 2.73417

R40 2.04026 0.00005 0.00000 0.00007 0.00007 2.04033

R41 2.58128 0.00067 0.00002 0.00154 0.00163 2.58290

R42 2.67271 0.00005 -0.00016 -0.00450 -0.00462 2.66810

R43 3.97075 -0.00118 -0.00074 -0.02775 -0.02824 3.94251

R44 2.69674 0.00004 -0.00001 -0.00019 -0.00043 2.69631

R45 2.27883 -0.00020 -0.00001 -0.00044 -0.00045 2.27838

R46 2.27883 -0.00020 -0.00001 -0.00044 -0.00045 2.27838

R47 2.01690 0.00004 -0.00001 -0.00009 -0.00009 2.01680

R48 2.01690 0.00004 -0.00001 -0.00009 -0.00009 2.01680

R49 2.27883 -0.00020 -0.00001 -0.00044 -0.00045 2.27838

R50 2.01690 0.00004 -0.00001 -0.00009 -0.00009 2.01680

R51 2.27883 -0.00020 -0.00001 -0.00044 -0.00045 2.27838

R52 2.01690 0.00004 -0.00001 -0.00009 -0.00009 2.01680

A1 1.86514 0.00011 -0.00005 -0.00129 -0.00134 1.86380

A2 2.19245 -0.00025 0.00003 -0.00011 -0.00008 2.19237

A3 2.22554 0.00014 0.00002 0.00139 0.00141 2.22695

A4 1.91003 0.00003 0.00018 0.00500 0.00524 1.91526

A5 2.18270 -0.00006 -0.00014 -0.00448 -0.00476 2.17795

A6 2.19039 0.00003 -0.00004 -0.00069 -0.00078 2.18961

A7 1.87442 -0.00028 -0.00025 -0.00742 -0.00779 1.86663

A8 2.19812 0.00017 0.00016 0.00585 0.00588 2.20400

A9 2.19812 0.00017 0.00016 0.00585 0.00588 2.20400

A10 1.91003 0.00003 0.00018 0.00500 0.00524 1.91526

A11 2.19039 0.00003 -0.00004 -0.00069 -0.00078 2.18961

A12 2.18270 -0.00006 -0.00014 -0.00448 -0.00476 2.17795

A13 1.86514 0.00011 -0.00005 -0.00129 -0.00134 1.86380

A14 2.22554 0.00014 0.00002 0.00139 0.00141 2.22695

A15 2.19245 -0.00025 0.00003 -0.00011 -0.00008 2.19237

A16 2.20611 -0.00034 -0.00017 -0.00569 -0.00579 2.20032

A17 2.03851 0.00018 0.00008 0.00283 0.00287 2.04139

A18 2.03851 0.00017 0.00008 0.00282 0.00287 2.04139

A19 2.19039 0.00003 -0.00004 -0.00069 -0.00078 2.18961

A20 2.18270 -0.00006 -0.00014 -0.00448 -0.00476 2.17795

A21 1.91003 0.00003 0.00018 0.00500 0.00524 1.91526

A22 1.87442 -0.00028 -0.00025 -0.00742 -0.00779 1.86663

A23 2.19812 0.00017 0.00016 0.00585 0.00588 2.20400

A24 2.19812 0.00017 0.00016 0.00585 0.00588 2.20400

A25 1.91003 0.00003 0.00018 0.00500 0.00524 1.91526

A26 2.19039 0.00003 -0.00004 -0.00069 -0.00078 2.18961

A27 2.18270 -0.00006 -0.00014 -0.00448 -0.00476 2.17795

A28 1.86514 0.00011 -0.00005 -0.00129 -0.00134 1.86380

A29 2.19245 -0.00025 0.00003 -0.00011 -0.00008 2.19237

A30 2.22554 0.00014 0.00002 0.00139 0.00141 2.22695

A31 1.86514 0.00011 -0.00005 -0.00129 -0.00134 1.86380

A32 2.19245 -0.00025 0.00003 -0.00011 -0.00008 2.19237

A33 2.22554 0.00014 0.00002 0.00139 0.00141 2.22695

A34 2.20611 -0.00034 -0.00017 -0.00569 -0.00579 2.20032

A35 2.03851 0.00018 0.00008 0.00283 0.00287 2.04139

A36 2.03851 0.00017 0.00008 0.00282 0.00287 2.04139

A37 2.18270 -0.00006 -0.00014 -0.00448 -0.00476 2.17795

A38 2.19039 0.00003 -0.00004 -0.00069 -0.00078 2.18961

A39 1.91003 0.00003 0.00018 0.00500 0.00524 1.91526

A40 1.86514 0.00011 -0.00005 -0.00129 -0.00134 1.86380

A41 2.19245 -0.00025 0.00003 -0.00011 -0.00008 2.19237

A42 2.22554 0.00014 0.00002 0.00139 0.00141 2.22695

A43 1.86514 0.00011 -0.00005 -0.00129 -0.00134 1.86380

A44 2.22554 0.00014 0.00002 0.00139 0.00141 2.22695

A45 2.19245 -0.00025 0.00003 -0.00011 -0.00008 2.19237

A46 1.91003 0.00003 0.00018 0.00500 0.00524 1.91526

A47 2.18270 -0.00006 -0.00014 -0.00448 -0.00476 2.17795

A48 2.19039 0.00003 -0.00004 -0.00069 -0.00078 2.18961

A49 1.87442 -0.00028 -0.00025 -0.00742 -0.00779 1.86663

A50 2.19812 0.00017 0.00016 0.00585 0.00588 2.20400

A51 2.19812 0.00017 0.00016 0.00585 0.00588 2.20400

A52 2.20611 -0.00034 -0.00017 -0.00569 -0.00579 2.20032

A53 2.03851 0.00018 0.00008 0.00283 0.00287 2.04139

A54 2.03851 0.00017 0.00008 0.00282 0.00287 2.04139

A55 2.18270 -0.00006 -0.00014 -0.00448 -0.00476 2.17795

A56 2.19039 0.00003 -0.00004 -0.00069 -0.00078 2.18961

A57 1.91003 0.00003 0.00018 0.00500 0.00524 1.91526

A58 1.86514 0.00011 -0.00005 -0.00129 -0.00134 1.86380

A59 2.19245 -0.00025 0.00003 -0.00011 -0.00008 2.19237

A60 2.22554 0.00014 0.00002 0.00139 0.00141 2.22695

A61 1.86514 0.00011 -0.00005 -0.00129 -0.00134 1.86380

A62 2.22554 0.00014 0.00002 0.00139 0.00141 2.22695

A63 2.19245 -0.00025 0.00003 -0.00011 -0.00008 2.19237

A64 1.91003 0.00003 0.00018 0.00500 0.00524 1.91526

A65 2.18270 -0.00006 -0.00014 -0.00448 -0.00476 2.17795

A66 2.19039 0.00003 -0.00004 -0.00069 -0.00078 2.18961

A67 1.87442 -0.00028 -0.00025 -0.00742 -0.00779 1.86663

A68 2.19812 0.00017 0.00016 0.00585 0.00588 2.20400

A69 2.19812 0.00017 0.00016 0.00585 0.00588 2.20400

A70 1.54845 0.00028 -0.00002 0.00215 0.00206 1.55051

A71 1.54845 0.00028 -0.00002 0.00215 0.00206 1.55051

A72 2.84152 0.00191 -0.00017 0.01452 0.01427 2.85579

A73 2.84152 0.00191 -0.00017 0.01452 0.01427 2.85579

A74 1.54845 0.00028 -0.00002 0.00215 0.00206 1.55051

A75 1.54845 0.00028 -0.00002 0.00215 0.00206 1.55051

A76 2.20611 -0.00034 -0.00017 -0.00569 -0.00579 2.20032

A77 2.03851 0.00018 0.00008 0.00283 0.00287 2.04139

A78 2.03851 0.00017 0.00008 0.00282 0.00287 2.04139

A79 3.14168 -0.00001 0.00000 -0.00011 -0.00024 3.14144

A80 3.14168 -0.00001 0.00000 -0.00011 -0.00024 3.14144

A81 3.14183 -0.00001 0.00001 -0.00085 -0.00166 3.14018

A82 3.14183 -0.00001 0.00001 -0.00085 -0.00166 3.14018

A83 3.14168 -0.00001 0.00000 -0.00011 -0.00024 3.14144

A84 3.14183 -0.00001 0.00001 -0.00085 -0.00166 3.14018

A85 3.14168 -0.00001 0.00000 -0.00011 -0.00024 3.14144

A86 3.14183 -0.00001 0.00001 -0.00085 -0.00166 3.14018

A87 3.14579 -0.00066 -0.00005 -0.01091 -0.01095 3.13484

A88 3.13740 0.00066 0.00005 0.01091 0.01095 3.14835

A89 3.15916 -0.00071 0.00086 -0.06556 -0.06465 3.09451

A90 3.12403 0.00071 -0.00086 0.06556 0.06465 3.18868

A91 3.14579 -0.00066 -0.00005 -0.01091 -0.01095 3.13484

A92 3.15916 -0.00071 0.00086 -0.06556 -0.06465 3.09451

A93 3.13740 0.00066 0.00005 0.01091 0.01095 3.14835

A94 3.12403 0.00071 -0.00086 0.06556 0.06465 3.18868

D1 0.00336 0.00008 0.00010 0.00017 0.00032 0.00368

D2 3.13282 0.00019 -0.00047 -0.01487 -0.01528 3.11754

D3 -3.12791 -0.00007 0.00017 0.00097 0.00116 -3.12675

D4 0.00155 0.00004 -0.00040 -0.01406 -0.01444 -0.01290

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13101 -0.00015 0.00007 0.00084 0.00087 -3.13014

D7 3.13101 0.00015 -0.00007 -0.00084 -0.00087 3.13014

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 -0.00544 -0.00013 -0.00016 -0.00025 -0.00049 -0.00592

D10 -2.98521 -0.00056 -0.00065 -0.02802 -0.02870 -3.01390

D11 -3.13483 -0.00024 0.00042 0.01490 0.01528 -3.11955

D12 0.16859 -0.00067 -0.00007 -0.01287 -0.01293 0.15566

D13 -3.11222 -0.00053 0.00052 0.00921 0.00965 -3.10258

D14 0.01830 -0.00004 0.00017 0.00505 0.00518 0.02349

D15 0.01531 -0.00040 -0.00014 -0.00818 -0.00835 0.00696

D16 -3.13735 0.00009 -0.00049 -0.01234 -0.01281 3.13303

D17 0.00544 0.00013 0.00016 0.00025 0.00049 0.00592

D18 3.13483 0.00024 -0.00042 -0.01490 -0.01528 3.11955

D19 2.98521 0.00056 0.00065 0.02802 0.02870 3.01390

D20 -0.16859 0.00067 0.00007 0.01287 0.01293 -0.15566

D21 -3.08875 -0.00068 0.00035 0.00880 0.00925 -3.07950

D22 -0.24391 0.00116 0.00019 0.02284 0.02308 -0.22083

D23 -1.66633 0.00024 0.00027 0.01582 0.01616 -1.65017

D24 0.24391 -0.00116 -0.00019 -0.02284 -0.02308 0.22083

D25 3.08875 0.00068 -0.00035 -0.00880 -0.00925 3.07950

D26 1.66633 -0.00024 -0.00027 -0.01582 -0.01616 1.65017

D27 -0.00336 -0.00008 -0.00010 -0.00017 -0.00032 -0.00368

D28 3.12791 0.00007 -0.00017 -0.00097 -0.00116 3.12675

D29 -3.13282 -0.00019 0.00047 0.01487 0.01528 -3.11754

D30 -0.00155 -0.00004 0.00040 0.01406 0.01444 0.01290

D31 -0.01531 0.00040 0.00014 0.00818 0.00835 -0.00696

D32 3.13735 -0.00009 0.00049 0.01234 0.01281 -3.13303

D33 3.11222 0.00053 -0.00052 -0.00921 -0.00965 3.10258

D34 -0.01830 0.00004 -0.00017 -0.00505 -0.00518 -0.02349

D35 0.01531 -0.00040 -0.00014 -0.00818 -0.00835 0.00696

D36 -3.11222 -0.00053 0.00052 0.00921 0.00965 -3.10258

D37 -3.13735 0.00009 -0.00049 -0.01234 -0.01281 3.13303

D38 0.01830 -0.00004 0.00017 0.00505 0.00518 0.02349

D39 -3.13483 -0.00024 0.00042 0.01490 0.01528 -3.11955

D40 0.16859 -0.00067 -0.00007 -0.01287 -0.01293 0.15566

D41 -0.00544 -0.00013 -0.00016 -0.00025 -0.00049 -0.00592

D42 -2.98521 -0.00056 -0.00065 -0.02802 -0.02870 -3.01390

D43 3.13282 0.00019 -0.00047 -0.01487 -0.01528 3.11754

D44 0.00155 0.00004 -0.00040 -0.01406 -0.01444 -0.01290

D45 0.00336 0.00008 0.00010 0.00017 0.00032 0.00368

D46 -3.12791 -0.00007 0.00017 0.00097 0.00116 -3.12675

D47 0.00544 0.00013 0.00016 0.00025 0.00049 0.00592

D48 3.13483 0.00024 -0.00042 -0.01490 -0.01528 3.11955

D49 2.98521 0.00056 0.00065 0.02802 0.02870 3.01390

D50 -0.16859 0.00067 0.00007 0.01287 0.01293 -0.15566

D51 -0.24391 0.00116 0.00019 0.02284 0.02308 -0.22083

D52 -1.66633 0.00024 0.00027 0.01582 0.01616 -1.65017

D53 -3.08875 -0.00068 0.00035 0.00880 0.00925 -3.07950

D54 3.08875 0.00068 -0.00035 -0.00880 -0.00925 3.07950

D55 1.66633 -0.00024 -0.00027 -0.01582 -0.01616 1.65017

D56 0.24391 -0.00116 -0.00019 -0.02284 -0.02308 0.22083

D57 -0.00336 -0.00008 -0.00010 -0.00017 -0.00032 -0.00368

D58 3.12791 0.00007 -0.00017 -0.00097 -0.00116 3.12675

D59 -3.13282 -0.00019 0.00047 0.01487 0.01528 -3.11754

D60 -0.00155 -0.00004 0.00040 0.01406 0.01444 0.01290

D61 -0.01531 0.00040 0.00014 0.00818 0.00835 -0.00696

D62 3.13735 -0.00009 0.00049 0.01234 0.01281 -3.13303

D63 3.11222 0.00053 -0.00052 -0.00921 -0.00965 3.10258

D64 -0.01830 0.00004 -0.00017 -0.00505 -0.00518 -0.02349

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13101 0.00015 -0.00007 -0.00084 -0.00087 3.13014

D67 -3.13101 -0.00015 0.00007 0.00084 0.00087 -3.13014

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.11222 0.00053 -0.00052 -0.00921 -0.00965 3.10258

D70 -0.01531 0.00040 0.00014 0.00818 0.00835 -0.00696

D71 -0.01830 0.00004 -0.00017 -0.00505 -0.00518 -0.02349

D72 3.13735 -0.00009 0.00049 0.01234 0.01281 -3.13303

D73 -3.13282 -0.00019 0.00047 0.01487 0.01528 -3.11754

D74 -0.00155 -0.00004 0.00040 0.01406 0.01444 0.01290

D75 -0.00336 -0.00008 -0.00010 -0.00017 -0.00032 -0.00368

D76 3.12791 0.00007 -0.00017 -0.00097 -0.00116 3.12675

D77 3.13483 0.00024 -0.00042 -0.01490 -0.01528 3.11955

D78 -0.16859 0.00067 0.00007 0.01287 0.01293 -0.15566

D79 0.00544 0.00013 0.00016 0.00025 0.00049 0.00592

D80 2.98521 0.00056 0.00065 0.02802 0.02870 3.01390

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 3.13101 0.00015 -0.00007 -0.00084 -0.00087 3.13014

D83 -3.13101 -0.00015 0.00007 0.00084 0.00087 -3.13014

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 0.00336 0.00008 0.00010 0.00017 0.00032 0.00368

D86 3.13282 0.00019 -0.00047 -0.01487 -0.01528 3.11754

D87 -3.12791 -0.00007 0.00017 0.00097 0.00116 -3.12675

D88 0.00155 0.00004 -0.00040 -0.01406 -0.01444 -0.01290

D89 -0.00544 -0.00013 -0.00016 -0.00025 -0.00049 -0.00592

D90 -2.98521 -0.00056 -0.00065 -0.02802 -0.02870 -3.01390

D91 -3.13483 -0.00024 0.00042 0.01490 0.01528 -3.11955

D92 0.16859 -0.00067 -0.00007 -0.01287 -0.01293 0.15566

D93 -3.11222 -0.00053 0.00052 0.00921 0.00965 -3.10258

D94 0.01830 -0.00004 0.00017 0.00505 0.00518 0.02349

D95 0.01531 -0.00040 -0.00014 -0.00818 -0.00835 0.00696

D96 -3.13735 0.00009 -0.00049 -0.01234 -0.01281 3.13303

D97 0.24391 -0.00116 -0.00019 -0.02284 -0.02308 0.22083

D98 1.66633 -0.00024 -0.00027 -0.01582 -0.01616 1.65017

D99 3.08875 0.00068 -0.00035 -0.00880 -0.00925 3.07950

D100 -3.08875 -0.00068 0.00035 0.00880 0.00925 -3.07950

D101 -1.66633 0.00024 0.00027 0.01582 0.01616 -1.65017

D102 -0.24391 0.00116 0.00019 0.02284 0.02308 -0.22083

D103 3.11222 0.00053 -0.00052 -0.00921 -0.00965 3.10258

D104 -0.01531 0.00040 0.00014 0.00818 0.00835 -0.00696

D105 -0.01830 0.00004 -0.00017 -0.00505 -0.00518 -0.02349

D106 3.13735 -0.00009 0.00049 0.01234 0.01281 -3.13303

D107 -3.13282 -0.00019 0.00047 0.01487 0.01528 -3.11754

D108 -0.00155 -0.00004 0.00040 0.01406 0.01444 0.01290

D109 -0.00336 -0.00008 -0.00010 -0.00017 -0.00032 -0.00368

D110 3.12791 0.00007 -0.00017 -0.00097 -0.00116 3.12675

D111 3.13483 0.00024 -0.00042 -0.01490 -0.01528 3.11955

D112 -0.16859 0.00067 0.00007 0.01287 0.01293 -0.15566

D113 0.00544 0.00013 0.00016 0.00025 0.00049 0.00592

D114 2.98521 0.00056 0.00065 0.02802 0.02870 3.01390

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.13101 0.00015 -0.00007 -0.00084 -0.00087 3.13014

D117 -3.13101 -0.00015 0.00007 0.00084 0.00087 -3.13014

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 0.00336 0.00008 0.00010 0.00017 0.00032 0.00368

D120 3.13282 0.00019 -0.00047 -0.01487 -0.01528 3.11754

D121 -3.12791 -0.00007 0.00017 0.00097 0.00116 -3.12675

D122 0.00155 0.00004 -0.00040 -0.01406 -0.01444 -0.01290

D123 -0.00544 -0.00013 -0.00016 -0.00025 -0.00049 -0.00592

D124 -2.98521 -0.00056 -0.00065 -0.02802 -0.02870 -3.01390

D125 -3.13483 -0.00024 0.00042 0.01490 0.01528 -3.11955

D126 0.16859 -0.00067 -0.00007 -0.01287 -0.01293 0.15566

D127 -3.11222 -0.00053 0.00052 0.00921 0.00965 -3.10258

D128 0.01830 -0.00004 0.00017 0.00505 0.00518 0.02349

D129 0.01531 -0.00040 -0.00014 -0.00818 -0.00835 0.00696

D130 -3.13735 0.00009 -0.00049 -0.01234 -0.01281 3.13303

D131 1.66633 -0.00024 -0.00027 -0.01582 -0.01616 1.65017

D132 3.08875 0.00068 -0.00035 -0.00880 -0.00925 3.07950

D133 0.24391 -0.00116 -0.00019 -0.02284 -0.02308 0.22083

D134 -1.66633 0.00024 0.00027 0.01582 0.01616 -1.65017

D135 -0.24391 0.00116 0.00019 0.02284 0.02308 -0.22083

D136 -3.08875 -0.00068 0.00035 0.00880 0.00925 -3.07950

Item Value Threshold Converged?

Maximum Force 0.001907 0.000450 NO

RMS Force 0.000421 0.000300 NO

Maximum Displacement 0.255217 0.001800 NO

RMS Displacement 0.037157 0.001200 NO

Predicted change in Energy=-5.135429D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:13:46 2019, MaxMem= 1342177280 cpu: 1.3

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.680476 4.262034 -0.041105

2 6 0 1.098369 2.878006 0.015844

3 7 0 0.000000 2.065023 0.044555

4 6 0 -1.098369 2.878006 0.015844

5 6 0 -0.680476 4.262034 -0.041105

6 6 0 -2.440845 2.440845 0.005917

7 6 0 -2.878006 1.098369 0.015844

8 7 0 -2.065023 0.000000 0.044555

9 6 0 -2.878006 -1.098369 0.015844

10 6 0 -4.262034 -0.680476 -0.041105

11 6 0 -4.262034 0.680476 -0.041105

12 6 0 2.440845 2.440845 0.005917

13 6 0 2.878006 1.098369 0.015844

14 6 0 4.262034 0.680476 -0.041105

15 6 0 4.262034 -0.680476 -0.041105

16 6 0 2.878006 -1.098369 0.015844

17 7 0 2.065023 0.000000 0.044555

18 6 0 2.440845 -2.440845 0.005917

19 6 0 1.098369 -2.878006 0.015844

20 6 0 0.680476 -4.262034 -0.041105

21 6 0 -0.680476 -4.262034 -0.041105

22 6 0 -1.098369 -2.878006 0.015844

23 7 0 0.000000 -2.065023 0.044555

24 1 0 1.339172 5.116342 -0.086061

25 1 0 -1.339172 5.116342 -0.086061

26 1 0 -5.116342 -1.339172 -0.086061

27 1 0 -5.116342 1.339172 -0.086061

28 1 0 5.116342 1.339172 -0.086061

29 1 0 5.116342 -1.339172 -0.086061

30 1 0 1.339172 -5.116342 -0.086061

31 1 0 -1.339172 -5.116342 -0.086061

32 30 0 0.000000 0.000000 0.341671

33 6 0 -2.440845 -2.440845 0.005917

34 6 0 -3.449328 -3.449328 -0.035952

35 6 0 3.449328 3.449328 -0.035952

36 6 0 -4.301308 -4.301308 -0.079419

37 6 0 4.301308 4.301308 -0.079419

38 6 0 -3.449328 3.449328 -0.035952

39 6 0 -4.301308 4.301308 -0.079419

40 6 0 3.449328 -3.449328 -0.035952

41 6 0 4.301308 -4.301308 -0.079419

42 1 0 5.053726 -5.053726 -0.161565

43 1 0 -5.053726 -5.053726 -0.161565

44 1 0 -5.053726 5.053726 -0.161565

45 1 0 5.053726 5.053726 -0.161565

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.446863 0.000000

3 N 2.301574 1.366814 0.000000

4 C 2.254566 2.196738 1.366814 0.000000

5 C 1.360953 2.254566 2.301574 1.446863 0.000000

6 C 3.614082 3.566124 2.469910 1.411895 2.533345

7 C 4.761808 4.356451 3.036143 2.516786 3.852422

8 N 5.070507 4.276774 2.920384 3.036143 4.482102

9 C 6.434280 5.623443 4.276774 4.356451 5.793643

10 C 6.989765 6.434280 5.070507 4.761808 6.103766

11 C 6.103766 5.793643 4.482102 3.852422 5.065087

12 C 2.533345 1.411895 2.469910 3.566124 3.614082

13 C 3.852422 2.516786 3.036143 4.356451 4.761808

14 C 5.065087 3.852422 4.482102 5.793643 6.103766

15 C 6.103766 4.761808 5.070507 6.434280 6.989765

16 C 5.793643 4.356451 4.276774 5.623443 6.434280

17 N 4.482102 3.036143 2.920384 4.276774 5.070507

18 C 6.930345 5.485664 5.124652 6.388764 7.394149

19 C 7.152485 5.756011 5.063672 6.160952 7.358512

20 C 8.524068 7.152485 6.364121 7.358512 8.632029

21 C 8.632029 7.358512 6.364121 7.152485 8.524068

22 C 7.358512 6.160952 5.063672 5.756011 7.152485

23 N 6.364121 5.063672 4.130047 5.063672 6.364121

24 H 1.079696 2.253557 3.334815 3.310913 2.193364

25 H 2.193364 3.310913 3.334815 2.253557 1.079696

26 H 8.060933 7.511166 6.146752 5.825726 7.145099

27 H 6.492168 6.403204 5.169224 4.303777 5.312442

28 H 5.312442 4.303777 5.169224 6.403204 6.492168

29 H 7.145099 5.825726 6.146752 7.511166 8.060933

30 H 9.401587 7.998623 7.306330 8.358325 9.593484

31 H 9.593484 8.358325 7.306330 7.998623 9.401587

32 Zn 4.332955 3.097660 2.086288 3.097660 4.332955

33 C 7.394149 6.388764 5.124652 5.485664 6.930345

34 C 8.747595 7.792265 6.504800 6.750174 8.193392

35 C 2.885664 2.419938 3.717613 4.583737 4.209015

36 C 9.907092 8.983771 7.684192 7.861962 9.297458

37 C 3.621248 3.506235 4.849494 5.584925 4.982087

38 C 4.209015 4.583737 3.717613 2.419938 2.885664

39 C 4.982087 5.584925 4.849494 3.506235 3.621248

40 C 8.193392 6.750174 6.504800 7.792265 8.747595

41 C 9.297458 7.861962 7.684192 8.983771 9.907092

42 H 10.291900 8.865027 8.732653 10.039528 10.939789

43 H 10.939789 10.039528 8.732653 8.865027 10.291900

44 H 5.789850 6.527903 5.874945 4.517752 4.445965

45 H 4.445965 4.517752 5.874945 6.527903 5.789850

6 7 8 9 10

6 C 0.000000

7 C 1.411895 0.000000

8 N 2.469910 1.366814 0.000000

9 C 3.566124 2.196738 1.366814 0.000000

10 C 3.614082 2.254566 2.301574 1.446863 0.000000

11 C 2.533345 1.446863 2.301574 2.254566 1.360953

12 C 4.881689 5.485664 5.124652 6.388764 7.394149

13 C 5.485664 5.756011 5.063672 6.160952 7.358512

14 C 6.930345 7.152485 6.364121 7.358512 8.632029

15 C 7.394149 7.358512 6.364121 7.152485 8.524068

16 C 6.388764 6.160952 5.063672 5.756011 7.152485

17 N 5.124652 5.063672 4.130047 5.063672 6.364121

18 C 6.903751 6.388764 5.124652 5.485664 6.930345

19 C 6.388764 5.623443 4.276774 4.356451 5.793643

20 C 7.394149 6.434280 5.070507 4.761808 6.103766

21 C 6.930345 5.793643 4.482102 3.852422 5.065087

22 C 5.485664 4.356451 3.036143 2.516786 3.852422

23 N 5.124652 4.276774 2.920384 3.036143 4.482102

24 H 4.631984 5.825726 6.146752 7.511166 8.060933

25 H 2.894897 4.303777 5.169224 6.403204 6.492168

26 H 4.631984 3.310913 3.334815 2.253557 1.079696

27 H 2.894897 2.253557 3.334815 3.310913 2.193364

28 H 7.637618 7.998623 7.306330 8.358325 9.593484

29 H 8.450329 8.358325 7.306330 7.998623 9.401587

30 H 8.450329 7.511166 6.146752 5.825726 7.145099

31 H 7.637618 6.403204 5.169224 4.303777 5.312442

32 Zn 3.468166 3.097660 2.086288 3.097660 4.332955

33 C 4.881689 3.566124 2.469910 1.411895 2.533345

34 C 5.976030 4.583737 3.717613 2.419938 2.885664

35 C 5.976030 6.750174 6.504800 7.792265 8.747595

36 C 6.994658 5.584925 4.849494 3.506235 3.621248

37 C 6.994658 7.861962 7.684192 8.983771 9.907092

38 C 1.426826 2.419938 3.717613 4.583737 4.209015

39 C 2.632477 3.506235 4.849494 5.584925 4.982087

40 C 8.330068 7.792265 6.504800 6.750174 8.193392

41 C 9.535226 8.983771 7.684192 7.861962 9.297458

42 H 10.600247 10.039528 8.732653 8.865027 10.291900

43 H 7.938753 6.527903 5.874945 4.517752 4.445965

44 H 3.698966 4.517752 5.874945 6.527903 5.789850

45 H 7.938753 8.865027 8.732653 10.039528 10.939789

11 12 13 14 15

11 C 0.000000

12 C 6.930345 0.000000

13 C 7.152485 1.411895 0.000000

14 C 8.524068 2.533345 1.446863 0.000000

15 C 8.632029 3.614082 2.254566 1.360953 0.000000

16 C 7.358512 3.566124 2.196738 2.254566 1.446863

17 N 6.364121 2.469910 1.366814 2.301574 2.301574

18 C 7.394149 4.881689 3.566124 3.614082 2.533345

19 C 6.434280 5.485664 4.356451 4.761808 3.852422

20 C 6.989765 6.930345 5.793643 6.103766 5.065087

21 C 6.103766 7.394149 6.434280 6.989765 6.103766

22 C 4.761808 6.388764 5.623443 6.434280 5.793643

23 N 5.070507 5.124652 4.276774 5.070507 4.482102

24 H 7.145099 2.894897 4.303777 5.312442 6.492168

25 H 5.312442 4.631984 5.825726 7.145099 8.060933

26 H 2.193364 8.450329 8.358325 9.593484 9.401587

27 H 1.079696 7.637618 7.998623 9.401587 9.593484

28 H 9.401587 2.894897 2.253557 1.079696 2.193364

29 H 9.593484 4.631984 3.310913 2.193364 1.079696

30 H 8.060933 7.637618 6.403204 6.492168 5.312442

31 H 6.492168 8.450329 7.511166 8.060933 7.145099

32 Zn 4.332955 3.468166 3.097660 4.332955 4.332955

33 C 3.614082 6.903751 6.388764 7.394149 6.930345

34 C 4.209015 8.330068 7.792265 8.747595 8.193392

35 C 8.193392 1.426826 2.419938 2.885664 4.209015

36 C 4.982087 9.535226 8.983771 9.907092 9.297458

37 C 9.297458 2.632477 3.506235 3.621248 4.982087

38 C 2.885664 5.976030 6.750174 8.193392 8.747595

39 C 3.621248 6.994658 7.861962 9.297458 9.907092

40 C 8.747595 5.976030 4.583737 4.209015 2.885664

41 C 9.907092 6.994658 5.584925 4.982087 3.621248

42 H 10.939789 7.938753 6.527903 5.789850 4.445965

43 H 5.789850 10.600247 10.039528 10.939789 10.291900

44 H 4.445965 7.938753 8.865027 10.291900 10.939789

45 H 10.291900 3.698966 4.517752 4.445965 5.789850

16 17 18 19 20

16 C 0.000000

17 N 1.366814 0.000000

18 C 1.411895 2.469910 0.000000

19 C 2.516786 3.036143 1.411895 0.000000

20 C 3.852422 4.482102 2.533345 1.446863 0.000000

21 C 4.761808 5.070507 3.614082 2.254566 1.360953

22 C 4.356451 4.276774 3.566124 2.196738 2.254566

23 N 3.036143 2.920384 2.469910 1.366814 2.301574

24 H 6.403204 5.169224 7.637618 7.998623 9.401587

25 H 7.511166 6.146752 8.450329 8.358325 9.593484

26 H 7.998623 7.306330 7.637618 6.403204 6.492168

27 H 8.358325 7.306330 8.450329 7.511166 8.060933

28 H 3.310913 3.334815 4.631984 5.825726 7.145099

29 H 2.253557 3.334815 2.894897 4.303777 5.312442

30 H 4.303777 5.169224 2.894897 2.253557 1.079696

31 H 5.825726 6.146752 4.631984 3.310913 2.193364

32 Zn 3.097660 2.086288 3.468166 3.097660 4.332955

33 C 5.485664 5.124652 4.881689 3.566124 3.614082

34 C 6.750174 6.504800 5.976030 4.583737 4.209015

35 C 4.583737 3.717613 5.976030 6.750174 8.193392

36 C 7.861962 7.684192 6.994658 5.584925 4.982087

37 C 5.584925 4.849494 6.994658 7.861962 9.297458

38 C 7.792265 6.504800 8.330068 7.792265 8.747595

39 C 8.983771 7.684192 9.535226 8.983771 9.907092

40 C 2.419938 3.717613 1.426826 2.419938 2.885664

41 C 3.506235 4.849494 2.632477 3.506235 3.621248

42 H 4.517752 5.874945 3.698966 4.517752 4.445965

43 H 8.865027 8.732653 7.938753 6.527903 5.789850

44 H 10.039528 8.732653 10.600247 10.039528 10.939789

45 H 6.527903 5.874945 7.938753 8.865027 10.291900

21 22 23 24 25

21 C 0.000000

22 C 1.446863 0.000000

23 N 2.301574 1.366814 0.000000

24 H 9.593484 8.358325 7.306330 0.000000

25 H 9.401587 7.998623 7.306330 2.678345 0.000000

26 H 5.312442 4.303777 5.169224 9.129476 7.479350

27 H 7.145099 5.825726 6.146752 7.479350 5.341724

28 H 8.060933 7.511166 6.146752 5.341724 7.479350

29 H 6.492168 6.403204 5.169224 7.479350 9.129476

30 H 2.193364 3.310913 3.334815 10.232684 10.577398

31 H 1.079696 2.253557 3.334815 10.577398 10.232684

32 Zn 4.332955 3.097660 2.086288 5.305968 5.305968

33 C 2.533345 1.411895 2.469910 8.450329 7.637618

34 C 2.885664 2.419938 3.717613 9.813407 8.821903

35 C 8.747595 7.792265 6.504800 2.689647 5.070620

36 C 3.621248 3.506235 4.849494 10.977578 9.872509

37 C 9.907092 8.983771 7.684192 3.072226 5.699066

38 C 8.193392 6.750174 6.504800 5.070620 2.689647

39 C 9.297458 7.861962 7.684192 5.699066 3.072226

40 C 4.209015 4.583737 3.717613 8.821903 9.813407

41 C 4.982087 5.584925 4.849494 9.872509 10.977578

42 H 5.789850 6.527903 5.874945 10.827460 12.012708

43 H 4.445965 4.517752 5.874945 12.012708 10.827460

44 H 10.291900 8.865027 8.732653 6.393651 3.715849

45 H 10.939789 10.039528 8.732653 3.715849 6.393651

26 27 28 29 30

26 H 0.000000

27 H 2.678345 0.000000

28 H 10.577398 10.232684 0.000000

29 H 10.232684 10.577398 2.678345 0.000000

30 H 7.479350 9.129476 7.479350 5.341724 0.000000

31 H 5.341724 7.479350 9.129476 7.479350 2.678345

32 Zn 5.305968 5.305968 5.305968 5.305968 5.305968

33 C 2.894897 4.631984 8.450329 7.637618 4.631984

34 C 2.689647 5.070620 9.813407 8.821903 5.070620

35 C 9.813407 8.821903 2.689647 5.070620 8.821903

36 C 3.072226 5.699066 10.977578 9.872509 5.699066

37 C 10.977578 9.872509 3.072226 5.699066 9.872509

38 C 5.070620 2.689647 8.821903 9.813407 9.813407

39 C 5.699066 3.072226 9.872509 10.977578 10.977578

40 C 8.821903 9.813407 5.070620 2.689647 2.689647

41 C 9.872509 10.977578 5.699066 3.072226 3.072226

42 H 10.827460 12.012708 6.393651 3.715849 3.715849

43 H 3.715849 6.393651 12.012708 10.827460 6.393651

44 H 6.393651 3.715849 10.827460 12.012708 12.012708

45 H 12.012708 10.827460 3.715849 6.393651 10.827460

31 32 33 34 35

31 H 0.000000

32 Zn 5.305968 0.000000

33 C 2.894897 3.468166 0.000000

34 C 2.689647 4.892681 1.426826 0.000000

35 C 9.813407 4.892681 8.330068 9.756174 0.000000

36 C 3.072226 6.097526 2.632477 1.205666 10.961142

37 C 10.977578 6.097526 9.535226 10.961142 1.205666

38 C 8.821903 4.892681 5.976030 6.898657 6.898657

39 C 9.872509 6.097526 6.994658 7.797444 7.797444

40 C 5.070620 4.892681 5.976030 6.898657 6.898657

41 C 5.699066 6.097526 6.994658 7.797444 7.797444

42 H 6.393651 7.164743 7.938753 8.654005 8.654005

43 H 3.715849 7.164743 3.698966 2.272436 12.025791

44 H 10.827460 7.164743 7.938753 8.654005 8.654005

45 H 12.012708 7.164743 10.600247 12.025791 2.272436

36 37 38 39 40

36 C 0.000000

37 C 12.165938 0.000000

38 C 7.797444 7.797444 0.000000

39 C 8.602617 8.602617 1.205666 0.000000

40 C 7.797444 7.797444 9.756174 10.961142 0.000000

41 C 8.602617 8.602617 10.961142 12.165938 1.205666

42 H 9.385604 9.385604 12.025791 13.230272 2.272436

43 H 1.067245 13.230272 8.654005 9.385604 8.654005

44 H 9.385604 9.385604 2.272436 1.067245 12.025791

45 H 13.230272 1.067245 8.654005 9.385604 8.654005

41 42 43 44 45

41 C 0.000000

42 H 1.067245 0.000000

43 H 9.385604 10.107452 0.000000

44 H 13.230272 14.294096 10.107452 0.000000

45 H 9.385604 10.107452 14.294096 10.107452 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

RotChk: IX=3 Diff= 1.31D-16

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.680476 -4.262034 -0.067674

2 6 0 -1.098369 -2.878006 -0.010726

3 7 0 0.000000 -2.065023 0.017986

4 6 0 1.098369 -2.878006 -0.010726

5 6 0 0.680476 -4.262034 -0.067674

6 6 0 2.440845 -2.440845 -0.020653

7 6 0 2.878006 -1.098369 -0.010726

8 7 0 2.065023 0.000000 0.017986

9 6 0 2.878006 1.098369 -0.010726

10 6 0 4.262034 0.680476 -0.067674

11 6 0 4.262034 -0.680476 -0.067674

12 6 0 -2.440845 -2.440845 -0.020653

13 6 0 -2.878006 -1.098369 -0.010726

14 6 0 -4.262034 -0.680476 -0.067674

15 6 0 -4.262034 0.680476 -0.067674

16 6 0 -2.878006 1.098369 -0.010726

17 7 0 -2.065023 0.000000 0.017986

18 6 0 -2.440845 2.440845 -0.020653

19 6 0 -1.098369 2.878006 -0.010726

20 6 0 -0.680476 4.262034 -0.067674

21 6 0 0.680476 4.262034 -0.067674

22 6 0 1.098369 2.878006 -0.010726

23 7 0 0.000000 2.065023 0.017986

24 1 0 -1.339172 -5.116342 -0.112631

25 1 0 1.339172 -5.116342 -0.112631

26 1 0 5.116342 1.339172 -0.112631

27 1 0 5.116342 -1.339172 -0.112631

28 1 0 -5.116342 -1.339172 -0.112631

29 1 0 -5.116342 1.339172 -0.112631

30 1 0 -1.339172 5.116342 -0.112631

31 1 0 1.339172 5.116342 -0.112631

32 30 0 0.000000 0.000000 0.315102

33 6 0 2.440845 2.440845 -0.020653

34 6 0 3.449328 3.449328 -0.062521

35 6 0 -3.449328 -3.449328 -0.062521

36 6 0 4.301308 4.301308 -0.105988

37 6 0 -4.301308 -4.301308 -0.105988

38 6 0 3.449328 -3.449328 -0.062521

39 6 0 4.301308 -4.301308 -0.105988

40 6 0 -3.449328 3.449328 -0.062521

41 6 0 -4.301308 4.301308 -0.105988

42 1 0 -5.053726 5.053726 -0.188134

43 1 0 5.053726 5.053726 -0.188134

44 1 0 5.053726 -5.053726 -0.188134

45 1 0 -5.053726 -5.053726 -0.188134

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

Rotational constants (GHZ): 0.1470110 0.1470110 0.0736725

Leave Link 202 at Fri Jul 26 14:13:46 2019, MaxMem= 1342177280 cpu: 0.1

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 184 symmetry adapted cartesian basis functions of A1 symmetry.

There are 155 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3065.8831796193 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= 9 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= -0.1306400943 Hartrees.

Nuclear repulsion after empirical dispersion term = 3065.7525395250 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: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3842

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.77D-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) = 3.96%

GePol: Cavity surface area = 415.609 Ang\*\*2

GePol: Cavity volume = 419.607 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0084653982 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3065.7610049232 Hartrees.

Leave Link 301 at Fri Jul 26 14:13:46 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16227 LenP2D= 44892.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.37D-05 NBF= 172 148 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 172 148 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:13:47 2019, MaxMem= 1342177280 cpu: 6.7

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:13:47 2019, MaxMem= 1342177280 cpu: 0.8

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

Initial guess from the checkpoint file: "ZnTSPsim0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Occupied (E) (E) (B2) (A1) (E) (E) (B1) (A1) (B2) (E) (E)

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

(E) (E) (A1) (A2) (E) (E) (B1) (B1) (E) (E) (A1)

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

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

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(E) (E) (A2) (A1)

Virtual (A1) (A1) (B2) (A1) (B2) (A1) (A1) (B2) (A1) (B2)

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The electronic state of the initial guess is 1-A1.

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= -1359.45358205522

Leave Link 401 at Fri Jul 26 14:13:49 2019, MaxMem= 1342177280 cpu: 21.1

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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.

An orbital has undefined symmetry, so N\*\*3 symmetry is turned off.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 660000000 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= 0 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= 44282892.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.33D-15 for 3838.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.57D-15 for 3382 3167.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.33D-15 for 3838.

Iteration 1 A^-1\*A deviation from orthogonality is 1.02D-11 for 2337 2301.

E= -1359.05388430024

DIIS: error= 4.32D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.05388430024 IErMin= 1 ErrMin= 4.32D-03

ErrMax= 4.32D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.93D-03 BMatP= 4.93D-03

IDIUse=3 WtCom= 9.57D-01 WtEn= 4.32D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 3.215 Goal= None Shift= 0.000

GapD= 3.215 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=3.51D-04 MaxDP=1.86D-02 OVMax= 2.00D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.51D-04 CP: 1.00D+00

E= -1359.06095798557 Delta-E= -0.007073685328 Rises=F Damp=F

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

NSaved= 2 IEnMin= 2 EnMin= -1359.06095798557 IErMin= 2 ErrMin= 5.10D-04

ErrMax= 5.10D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.67D-05 BMatP= 4.93D-03

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

Coeff-Com: -0.285D-01 0.103D+01

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

Coeff: -0.283D-01 0.103D+01

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.81D-05 MaxDP=1.25D-03 DE=-7.07D-03 OVMax= 2.44D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.70D-05 CP: 1.00D+00 9.79D-01

E= -1359.06102295794 Delta-E= -0.000064972371 Rises=F Damp=F

DIIS: error= 7.47D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.06102295794 IErMin= 2 ErrMin= 5.10D-04

ErrMax= 7.47D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.29D-05 BMatP= 7.67D-05

IDIUse=3 WtCom= 9.93D-01 WtEn= 7.47D-03

Coeff-Com: -0.250D-01 0.521D+00 0.504D+00

Coeff-En: 0.000D+00 0.714D-01 0.929D+00

Coeff: -0.248D-01 0.517D+00 0.508D+00

Gap= 0.093 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.60D-05 MaxDP=6.96D-04 DE=-6.50D-05 OVMax= 2.06D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.19D-05 CP: 1.00D+00 9.82D-01 6.12D-01

E= -1359.06106593259 Delta-E= -0.000042974651 Rises=F Damp=F

DIIS: error= 2.10D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.06106593259 IErMin= 4 ErrMin= 2.10D-04

ErrMax= 2.10D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.23D-05 BMatP= 7.29D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.10D-03

Coeff-Com: -0.100D-01 0.138D+00 0.302D+00 0.571D+00

Coeff-En: 0.000D+00 0.000D+00 0.170D+00 0.830D+00

Coeff: -0.999D-02 0.137D+00 0.301D+00 0.571D+00

Gap= 0.093 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=5.17D-06 MaxDP=2.68D-04 DE=-4.30D-05 OVMax= 8.10D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.22D-06 CP: 1.00D+00 9.79D-01 7.05D-01 7.52D-01

E= -1359.06107565997 Delta-E= -0.000009727384 Rises=F Damp=F

DIIS: error= 9.56D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.06107565997 IErMin= 5 ErrMin= 9.56D-05

ErrMax= 9.56D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.92D-07 BMatP= 1.23D-05

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

Coeff-Com: -0.347D-02 0.348D-01 0.120D+00 0.299D+00 0.550D+00

Coeff: -0.347D-02 0.348D-01 0.120D+00 0.299D+00 0.550D+00

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=1.67D-06 MaxDP=4.72D-05 DE=-9.73D-06 OVMax= 1.59D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.04D-06 CP: 1.00D+00 9.78D-01 7.13D-01 8.07D-01 6.85D-01

E= -1359.06107622433 Delta-E= -0.000000564359 Rises=F Damp=F

DIIS: error= 3.14D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.06107622433 IErMin= 6 ErrMin= 3.14D-05

ErrMax= 3.14D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.75D-08 BMatP= 8.92D-07

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

Coeff-Com: 0.161D-03-0.937D-02-0.962D-04 0.326D-01 0.260D+00 0.717D+00

Coeff: 0.161D-03-0.937D-02-0.962D-04 0.326D-01 0.260D+00 0.717D+00

Gap= 0.093 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=5.59D-07 MaxDP=2.42D-05 DE=-5.64D-07 OVMax= 5.97D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.65D-07 CP: 1.00D+00 9.77D-01 7.16D-01 8.16D-01 7.73D-01

CP: 7.24D-01

E= -1359.06107626808 Delta-E= -0.000000043749 Rises=F Damp=F

DIIS: error= 9.45D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.06107626808 IErMin= 7 ErrMin= 9.45D-06

ErrMax= 9.45D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.17D-08 BMatP= 8.75D-08

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

Coeff-Com: 0.268D-03-0.783D-02-0.564D-02 0.726D-02 0.146D+00 0.477D+00

Coeff-Com: 0.384D+00

Coeff: 0.268D-03-0.783D-02-0.564D-02 0.726D-02 0.146D+00 0.477D+00

Coeff: 0.384D+00

Gap= 0.093 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.64D-07 MaxDP=9.68D-06 DE=-4.37D-08 OVMax= 2.99D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.06D-07 CP: 1.00D+00 9.77D-01 7.17D-01 8.15D-01 7.78D-01

CP: 7.26D-01 5.45D-01

E= -1359.06107628912 Delta-E= -0.000000021037 Rises=F Damp=F

DIIS: error= 1.35D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.06107628912 IErMin= 8 ErrMin= 1.35D-06

ErrMax= 1.35D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.36D-10 BMatP= 2.17D-08

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

Coeff-Com: 0.906D-04-0.231D-02-0.205D-02 0.198D-03 0.368D-01 0.136D+00

Coeff-Com: 0.161D+00 0.670D+00

Coeff: 0.906D-04-0.231D-02-0.205D-02 0.198D-03 0.368D-01 0.136D+00

Coeff: 0.161D+00 0.670D+00

Gap= 0.093 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=3.58D-08 MaxDP=1.39D-06 DE=-2.10D-08 OVMax= 3.93D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.04D-08 CP: 1.00D+00 9.77D-01 7.17D-01 8.15D-01 7.79D-01

CP: 7.34D-01 5.65D-01 8.69D-01

E= -1359.06107628898 Delta-E= 0.000000000140 Rises=F Damp=F

DIIS: error= 2.75D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 8 EnMin= -1359.06107628912 IErMin= 9 ErrMin= 2.75D-07

ErrMax= 2.75D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.28D-11 BMatP= 3.36D-10

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

Coeff-Com: 0.179D-04-0.357D-03-0.417D-03-0.584D-03 0.387D-02 0.206D-01

Coeff-Com: 0.391D-01 0.299D+00 0.639D+00

Coeff: 0.179D-04-0.357D-03-0.417D-03-0.584D-03 0.387D-02 0.206D-01

Coeff: 0.391D-01 0.299D+00 0.639D+00

Gap= 0.093 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.15D-08 MaxDP=4.79D-07 DE= 1.40D-10 OVMax= 1.43D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 8.58D-09 CP: 1.00D+00 9.77D-01 7.17D-01 8.16D-01 7.78D-01

CP: 7.36D-01 5.76D-01 8.91D-01 8.20D-01

E= -1359.06107628904 Delta-E= -0.000000000060 Rises=F Damp=F

DIIS: error= 7.66D-08 at cycle 10 NSaved= 10.

NSaved=10 IEnMin= 8 EnMin= -1359.06107628912 IErMin=10 ErrMin= 7.66D-08

ErrMax= 7.66D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.67D-12 BMatP= 3.28D-11

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

Coeff-Com: -0.329D-07 0.490D-04-0.366D-05-0.295D-03-0.159D-02-0.343D-02

Coeff-Com: 0.191D-02 0.688D-01 0.274D+00 0.661D+00

Coeff: -0.329D-07 0.490D-04-0.366D-05-0.295D-03-0.159D-02-0.343D-02

Coeff: 0.191D-02 0.688D-01 0.274D+00 0.661D+00

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=3.36D-09 MaxDP=1.02D-07 DE=-6.00D-11 OVMax= 4.11D-07

Error on total polarization charges = 0.06215

SCF Done: E(RB3LYP) = -1359.06107629 A.U. after 10 cycles

NFock= 10 Conv=0.34D-08 -V/T= 1.9681

KE= 1.403835427562D+03 PE=-9.373797333856D+03 EE= 3.545139825081D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.31

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:14:30 2019, MaxMem= 1342177280 cpu: 467.0

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16227 LenP2D= 44892.

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 = 255

Leave Link 701 at Fri Jul 26 14:14:34 2019, MaxMem= 1342177280 cpu: 43.5

(Enter /apps/gaussian/g09d01/g09/l702.exe)

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

Leave Link 702 at Fri Jul 26 14:14:34 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Fri Jul 26 14:14:38 2019, MaxMem= 1342177280 cpu: 43.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 0.00000000D+00 1.11555210D-12 4.80358093D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000229570 -0.000452106 0.000168134

2 6 0.000775671 0.000882577 -0.001223773

3 7 0.000000000 0.003945726 0.003548693

4 6 -0.000775671 0.000882577 -0.001223773

5 6 -0.000229570 -0.000452106 0.000168134

6 6 -0.000553408 0.000553408 0.001065062

7 6 -0.000882577 0.000775671 -0.001223773

8 7 -0.003945726 0.000000000 0.003548693

9 6 -0.000882577 -0.000775671 -0.001223773

10 6 0.000452106 -0.000229570 0.000168134

11 6 0.000452106 0.000229570 0.000168134

12 6 0.000553408 0.000553408 0.001065062

13 6 0.000882577 0.000775671 -0.001223773

14 6 -0.000452106 0.000229570 0.000168134

15 6 -0.000452106 -0.000229570 0.000168134

16 6 0.000882577 -0.000775671 -0.001223773

17 7 0.003945726 0.000000000 0.003548693

18 6 0.000553408 -0.000553408 0.001065062

19 6 0.000775671 -0.000882577 -0.001223773

20 6 0.000229570 0.000452106 0.000168134

21 6 -0.000229570 0.000452106 0.000168134

22 6 -0.000775671 -0.000882577 -0.001223773

23 7 0.000000000 -0.003945726 0.003548693

24 1 0.000167703 -0.000164982 0.000147734

25 1 -0.000167703 -0.000164982 0.000147734

26 1 0.000164982 -0.000167703 0.000147734

27 1 0.000164982 0.000167703 0.000147734

28 1 -0.000164982 0.000167703 0.000147734

29 1 -0.000164982 -0.000167703 0.000147734

30 1 0.000167703 0.000164982 0.000147734

31 1 -0.000167703 0.000164982 0.000147734

32 30 0.000000000 0.000000000 -0.009205105

33 6 -0.000553408 -0.000553408 0.001065062

34 6 0.000018546 0.000018546 -0.000116222

35 6 -0.000018546 -0.000018546 -0.000116222

36 6 -0.000081414 -0.000081414 -0.001418631

37 6 0.000081414 0.000081414 -0.001418631

38 6 0.000018546 -0.000018546 -0.000116222

39 6 -0.000081414 0.000081414 -0.001418631

40 6 -0.000018546 0.000018546 -0.000116222

41 6 0.000081414 -0.000081414 -0.001418631

42 1 0.000085953 -0.000085953 0.001038186

43 1 -0.000085953 -0.000085953 0.001038186

44 1 -0.000085953 0.000085953 0.001038186

45 1 0.000085953 0.000085953 0.001038186

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

Cartesian Forces: Max 0.009205105 RMS 0.001341160

Leave Link 716 at Fri Jul 26 14:14:38 2019, MaxMem= 1342177280 cpu: 1.7

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.003001845 RMS 0.000734194

Search for a local minimum.

Step number 3 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .73419D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3

DE= 1.38D-06 DEPred=-5.14D-04 R=-2.69D-03

Trust test=-2.69D-03 RLast= 2.13D-01 DXMaxT set to 7.50D-02

ITU= -1 -1 0

Eigenvalues --- 0.00533 0.00534 0.00534 0.00534 0.00534

Eigenvalues --- 0.00534 0.00534 0.00555 0.01188 0.01341

Eigenvalues --- 0.01341 0.01564 0.01662 0.01662 0.01662

Eigenvalues --- 0.01678 0.01806 0.01806 0.01815 0.01825

Eigenvalues --- 0.01830 0.01858 0.01859 0.01859 0.01868

Eigenvalues --- 0.01868 0.01868 0.01911 0.01919 0.01920

Eigenvalues --- 0.01920 0.01933 0.01954 0.01954 0.01970

Eigenvalues --- 0.01974 0.02171 0.02171 0.02178 0.02180

Eigenvalues --- 0.02458 0.02458 0.03324 0.04654 0.04654

Eigenvalues --- 0.04654 0.04654 0.04654 0.04654 0.04654

Eigenvalues --- 0.05201 0.08333 0.13855 0.15126 0.15126

Eigenvalues --- 0.15856 0.15998 0.15998 0.15998 0.15998

Eigenvalues --- 0.15999 0.15999 0.15999 0.22796 0.22864

Eigenvalues --- 0.22865 0.22865 0.23473 0.24431 0.24541

Eigenvalues --- 0.24592 0.24592 0.24668 0.24945 0.24945

Eigenvalues --- 0.24989 0.24997 0.24997 0.24997 0.24998

Eigenvalues --- 0.26184 0.35037 0.35037 0.35397 0.35476

Eigenvalues --- 0.35966 0.36034 0.36034 0.36034 0.36034

Eigenvalues --- 0.36034 0.36034 0.36034 0.36040 0.36779

Eigenvalues --- 0.36871 0.36871 0.37563 0.37563 0.37563

Eigenvalues --- 0.37566 0.38964 0.38964 0.39517 0.40347

Eigenvalues --- 0.41397 0.41397 0.41397 0.41422 0.41433

Eigenvalues --- 0.41433 0.41756 0.42448 0.43522 0.43790

Eigenvalues --- 0.43790 0.45814 0.47690 0.49042 0.49042

Eigenvalues --- 0.50109 0.51388 0.51892 0.51892 0.54457

Eigenvalues --- 1.01829 1.01831 1.01831 1.01831

En-DIIS/RFO-DIIS IScMMF= 0 using points: 3 2 1

RFO step: Lambda=-3.22160534D-04.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=F DC= -9.57D-05 SmlDif= 1.00D-05

RMS Error= 0.1942582749D-02 NUsed= 3 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.49532 0.70067 -0.19599

Iteration 1 RMS(Cart)= 0.01450514 RMS(Int)= 0.00069129

Iteration 2 RMS(Cart)= 0.00086006 RMS(Int)= 0.00002307

Iteration 3 RMS(Cart)= 0.00000143 RMS(Int)= 0.00002305

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002305

ITry= 1 IFail=0 DXMaxC= 9.59D-02 DCOld= 1.00D+10 DXMaxT= 7.50D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.09D-02 for atom 45.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73417 -0.00043 0.00048 -0.00148 -0.00101 2.73316

R2 2.57183 0.00103 0.00047 -0.00056 -0.00013 2.57170

R3 2.04033 -0.00004 -0.00004 0.00003 -0.00001 2.04032

R4 2.58290 0.00096 -0.00070 0.00227 0.00160 2.58450

R5 2.66810 0.00137 0.00145 -0.00276 -0.00085 2.66725

R6 2.58290 0.00096 -0.00070 0.00227 0.00160 2.58450

R7 3.94251 0.00300 0.01011 -0.02385 -0.01291 3.92960

R8 2.73417 -0.00043 0.00048 -0.00148 -0.00101 2.73316

R9 2.66810 0.00137 0.00145 -0.00276 -0.00085 2.66725

R10 2.04033 -0.00004 -0.00004 0.00003 -0.00001 2.04032

R11 2.66810 0.00137 0.00145 -0.00276 -0.00085 2.66725

R12 2.69631 0.00023 0.00017 -0.00008 -0.00103 2.69528

R13 2.58290 0.00096 -0.00070 0.00227 0.00160 2.58450

R14 2.73417 -0.00042 0.00048 -0.00147 -0.00101 2.73316

R15 2.58290 0.00096 -0.00070 0.00227 0.00160 2.58450

R16 3.94251 0.00300 0.01011 -0.02386 -0.01291 3.92960

R17 2.73417 -0.00043 0.00048 -0.00148 -0.00101 2.73316

R18 2.66810 0.00137 0.00145 -0.00276 -0.00085 2.66725

R19 2.57183 0.00103 0.00047 -0.00056 -0.00013 2.57170

R20 2.04033 -0.00004 -0.00004 0.00003 -0.00001 2.04032

R21 2.04033 -0.00003 -0.00004 0.00004 -0.00001 2.04032

R22 2.66810 0.00137 0.00145 -0.00276 -0.00085 2.66725

R23 2.69631 0.00023 0.00017 -0.00008 -0.00103 2.69528

R24 2.73417 -0.00042 0.00048 -0.00147 -0.00101 2.73316

R25 2.58290 0.00096 -0.00070 0.00227 0.00160 2.58450

R26 2.57183 0.00103 0.00047 -0.00056 -0.00013 2.57170

R27 2.04033 -0.00003 -0.00004 0.00004 -0.00001 2.04032

R28 2.73417 -0.00043 0.00048 -0.00148 -0.00101 2.73316

R29 2.04033 -0.00004 -0.00004 0.00003 -0.00001 2.04032

R30 2.58290 0.00096 -0.00070 0.00227 0.00160 2.58450

R31 2.66810 0.00137 0.00145 -0.00276 -0.00085 2.66725

R32 3.94251 0.00300 0.01011 -0.02386 -0.01291 3.92960

R33 2.66810 0.00137 0.00145 -0.00276 -0.00085 2.66725

R34 2.69631 0.00023 0.00017 -0.00008 -0.00103 2.69528

R35 2.73417 -0.00042 0.00048 -0.00147 -0.00101 2.73316

R36 2.58290 0.00096 -0.00070 0.00227 0.00160 2.58450

R37 2.57183 0.00103 0.00047 -0.00056 -0.00013 2.57170

R38 2.04033 -0.00003 -0.00004 0.00004 -0.00001 2.04032

R39 2.73417 -0.00042 0.00048 -0.00147 -0.00101 2.73316

R40 2.04033 -0.00003 -0.00004 0.00004 -0.00001 2.04032

R41 2.58290 0.00096 -0.00070 0.00227 0.00160 2.58450

R42 2.66810 0.00137 0.00145 -0.00276 -0.00085 2.66725

R43 3.94251 0.00300 0.01011 -0.02386 -0.01291 3.92960

R44 2.69631 0.00023 0.00017 -0.00008 -0.00103 2.69528

R45 2.27838 0.00026 0.00017 -0.00038 -0.00021 2.27817

R46 2.27838 0.00026 0.00017 -0.00038 -0.00021 2.27817

R47 2.01680 0.00004 0.00002 -0.00005 -0.00006 2.01674

R48 2.01680 0.00004 0.00002 -0.00005 -0.00006 2.01674

R49 2.27838 0.00026 0.00017 -0.00038 -0.00021 2.27817

R50 2.01680 0.00004 0.00002 -0.00005 -0.00006 2.01674

R51 2.27838 0.00026 0.00017 -0.00038 -0.00021 2.27817

R52 2.01680 0.00004 0.00002 -0.00005 -0.00006 2.01674

A1 1.86380 0.00040 0.00039 -0.00056 -0.00018 1.86362

A2 2.19237 -0.00045 0.00020 -0.00112 -0.00092 2.19145

A3 2.22695 0.00005 -0.00058 0.00169 0.00111 2.22806

A4 1.91526 -0.00085 -0.00165 0.00318 0.00156 1.91683

A5 2.17795 0.00052 0.00160 -0.00348 -0.00184 2.17611

A6 2.18961 0.00034 0.00019 0.00003 0.00012 2.18973

A7 1.86663 0.00088 0.00253 -0.00521 -0.00274 1.86389

A8 2.20400 -0.00042 -0.00205 0.00492 0.00281 2.20681

A9 2.20400 -0.00042 -0.00205 0.00492 0.00281 2.20681

A10 1.91526 -0.00085 -0.00165 0.00318 0.00156 1.91683

A11 2.18961 0.00034 0.00019 0.00003 0.00012 2.18973

A12 2.17795 0.00052 0.00160 -0.00348 -0.00184 2.17611

A13 1.86380 0.00040 0.00039 -0.00056 -0.00018 1.86362

A14 2.22695 0.00005 -0.00058 0.00169 0.00111 2.22806

A15 2.19237 -0.00045 0.00020 -0.00112 -0.00092 2.19145

A16 2.20032 0.00018 0.00197 -0.00478 -0.00263 2.19769

A17 2.04139 -0.00007 -0.00098 0.00240 0.00130 2.04269

A18 2.04139 -0.00010 -0.00098 0.00235 0.00130 2.04269

A19 2.18961 0.00034 0.00019 0.00004 0.00012 2.18973

A20 2.17795 0.00052 0.00160 -0.00349 -0.00184 2.17611

A21 1.91526 -0.00085 -0.00165 0.00318 0.00156 1.91683

A22 1.86663 0.00088 0.00253 -0.00521 -0.00274 1.86389

A23 2.20400 -0.00042 -0.00205 0.00492 0.00281 2.20681

A24 2.20400 -0.00042 -0.00205 0.00493 0.00281 2.20681

A25 1.91526 -0.00085 -0.00165 0.00318 0.00156 1.91683

A26 2.18961 0.00034 0.00019 0.00003 0.00012 2.18973

A27 2.17795 0.00052 0.00160 -0.00348 -0.00184 2.17611

A28 1.86380 0.00041 0.00039 -0.00056 -0.00018 1.86362

A29 2.19237 -0.00045 0.00020 -0.00112 -0.00092 2.19145

A30 2.22695 0.00004 -0.00058 0.00169 0.00111 2.22806

A31 1.86380 0.00040 0.00039 -0.00057 -0.00018 1.86362

A32 2.19237 -0.00044 0.00020 -0.00111 -0.00092 2.19145

A33 2.22695 0.00004 -0.00058 0.00168 0.00111 2.22806

A34 2.20032 0.00018 0.00197 -0.00478 -0.00263 2.19769

A35 2.04139 -0.00007 -0.00098 0.00240 0.00130 2.04269

A36 2.04139 -0.00010 -0.00098 0.00235 0.00130 2.04269

A37 2.17795 0.00052 0.00160 -0.00349 -0.00184 2.17611

A38 2.18961 0.00034 0.00019 0.00004 0.00012 2.18973

A39 1.91526 -0.00085 -0.00165 0.00318 0.00156 1.91683

A40 1.86380 0.00040 0.00039 -0.00057 -0.00018 1.86362

A41 2.19237 -0.00044 0.00020 -0.00111 -0.00092 2.19145

A42 2.22695 0.00004 -0.00058 0.00168 0.00111 2.22806

A43 1.86380 0.00041 0.00039 -0.00056 -0.00018 1.86362

A44 2.22695 0.00004 -0.00058 0.00169 0.00111 2.22806

A45 2.19237 -0.00045 0.00020 -0.00112 -0.00092 2.19145

A46 1.91526 -0.00085 -0.00165 0.00318 0.00156 1.91683

A47 2.17795 0.00052 0.00160 -0.00348 -0.00184 2.17611

A48 2.18961 0.00034 0.00019 0.00003 0.00012 2.18973

A49 1.86663 0.00088 0.00253 -0.00521 -0.00274 1.86389

A50 2.20400 -0.00042 -0.00205 0.00492 0.00281 2.20681

A51 2.20400 -0.00042 -0.00205 0.00493 0.00281 2.20681

A52 2.20032 0.00018 0.00197 -0.00478 -0.00263 2.19769

A53 2.04139 -0.00007 -0.00098 0.00240 0.00130 2.04269

A54 2.04139 -0.00010 -0.00098 0.00235 0.00130 2.04269

A55 2.17795 0.00052 0.00160 -0.00349 -0.00184 2.17611

A56 2.18961 0.00034 0.00019 0.00004 0.00012 2.18973

A57 1.91526 -0.00084 -0.00165 0.00318 0.00156 1.91683

A58 1.86380 0.00040 0.00039 -0.00056 -0.00018 1.86362

A59 2.19237 -0.00044 0.00020 -0.00111 -0.00092 2.19145

A60 2.22695 0.00004 -0.00058 0.00168 0.00111 2.22806

A61 1.86380 0.00040 0.00039 -0.00056 -0.00018 1.86362

A62 2.22695 0.00004 -0.00058 0.00168 0.00111 2.22806

A63 2.19237 -0.00044 0.00020 -0.00111 -0.00092 2.19145

A64 1.91526 -0.00084 -0.00165 0.00318 0.00156 1.91683

A65 2.17795 0.00052 0.00160 -0.00349 -0.00184 2.17611

A66 2.18961 0.00034 0.00019 0.00004 0.00012 2.18973

A67 1.86663 0.00088 0.00253 -0.00521 -0.00274 1.86389

A68 2.20400 -0.00042 -0.00205 0.00492 0.00281 2.20681

A69 2.20400 -0.00042 -0.00205 0.00492 0.00281 2.20681

A70 1.55051 0.00033 -0.00118 0.00399 0.00275 1.55327

A71 1.55051 0.00033 -0.00118 0.00399 0.00275 1.55327

A72 2.85579 0.00232 -0.00813 0.02832 0.02022 2.87602

A73 2.85579 0.00232 -0.00813 0.02832 0.02022 2.87602

A74 1.55051 0.00033 -0.00118 0.00399 0.00275 1.55327

A75 1.55051 0.00033 -0.00118 0.00399 0.00275 1.55327

A76 2.20032 0.00018 0.00197 -0.00478 -0.00263 2.19769

A77 2.04139 -0.00007 -0.00098 0.00240 0.00130 2.04269

A78 2.04139 -0.00010 -0.00098 0.00235 0.00130 2.04269

A79 3.14144 0.00007 0.00012 0.00037 0.00008 3.14153

A80 3.14144 0.00007 0.00012 0.00037 0.00008 3.14153

A81 3.14018 0.00010 0.00090 0.00555 0.00178 3.14195

A82 3.14018 0.00010 0.00090 0.00555 0.00178 3.14195

A83 3.14144 0.00007 0.00012 0.00037 0.00008 3.14153

A84 3.14018 0.00010 0.00090 0.00555 0.00178 3.14195

A85 3.14144 0.00007 0.00012 0.00037 0.00008 3.14153

A86 3.14018 0.00010 0.00090 0.00555 0.00178 3.14195

A87 3.13484 0.00125 0.00527 -0.00188 0.00343 3.13826

A88 3.14835 -0.00125 -0.00527 0.00188 -0.00343 3.14492

A89 3.09451 0.00183 0.03744 0.05574 0.09316 3.18766

A90 3.18868 -0.00183 -0.03744 -0.05574 -0.09316 3.09552

A91 3.13484 0.00125 0.00527 -0.00188 0.00343 3.13826

A92 3.09451 0.00183 0.03744 0.05574 0.09316 3.18766

A93 3.14835 -0.00125 -0.00527 0.00188 -0.00343 3.14492

A94 3.18868 -0.00183 -0.03744 -0.05574 -0.09316 3.09552

D1 0.00368 0.00006 0.00038 -0.00276 -0.00237 0.00132

D2 3.11754 0.00045 0.00506 -0.01289 -0.00782 3.10972

D3 -3.12675 -0.00018 0.00036 -0.00357 -0.00320 -3.12996

D4 -0.01290 0.00020 0.00504 -0.01370 -0.00866 -0.02155

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13014 -0.00025 -0.00003 -0.00080 -0.00084 -3.13099

D7 3.13014 0.00025 0.00003 0.00080 0.00084 3.13099

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 -0.00592 -0.00010 -0.00063 0.00446 0.00381 -0.00211

D10 -3.01390 -0.00043 0.01087 -0.03181 -0.02097 -3.03488

D11 -3.11955 -0.00050 -0.00538 0.01474 0.00935 -3.11020

D12 0.15566 -0.00082 0.00613 -0.02153 -0.01543 0.14023

D13 -3.10258 -0.00079 -0.00197 0.00344 0.00145 -3.10113

D14 0.02349 -0.00023 -0.00168 0.00175 0.00002 0.02351

D15 0.00696 -0.00036 0.00341 -0.00823 -0.00483 0.00213

D16 3.13303 0.00020 0.00370 -0.00993 -0.00626 3.12677

D17 0.00592 0.00010 0.00063 -0.00446 -0.00381 0.00211

D18 3.11955 0.00050 0.00538 -0.01474 -0.00935 3.11020

D19 3.01390 0.00043 -0.01087 0.03181 0.02097 3.03488

D20 -0.15566 0.00082 -0.00613 0.02153 0.01543 -0.14023

D21 -3.07950 -0.00088 -0.00272 0.00744 0.00473 -3.07477

D22 -0.22083 0.00137 -0.01059 0.03492 0.02439 -0.19644

D23 -1.65017 0.00024 -0.00665 0.02118 0.01456 -1.63561

D24 0.22083 -0.00137 0.01059 -0.03492 -0.02439 0.19644

D25 3.07950 0.00088 0.00272 -0.00744 -0.00473 3.07477

D26 1.65017 -0.00024 0.00665 -0.02118 -0.01456 1.63561

D27 -0.00368 -0.00006 -0.00038 0.00276 0.00237 -0.00132

D28 3.12675 0.00018 -0.00036 0.00357 0.00320 3.12996

D29 -3.11754 -0.00045 -0.00506 0.01289 0.00782 -3.10972

D30 0.01290 -0.00020 -0.00504 0.01370 0.00866 0.02155

D31 -0.00696 0.00036 -0.00341 0.00823 0.00483 -0.00213

D32 -3.13303 -0.00020 -0.00370 0.00993 0.00626 -3.12677

D33 3.10258 0.00079 0.00197 -0.00344 -0.00145 3.10113

D34 -0.02349 0.00023 0.00168 -0.00175 -0.00002 -0.02351

D35 0.00696 -0.00036 0.00341 -0.00823 -0.00483 0.00213

D36 -3.10258 -0.00079 -0.00197 0.00344 0.00145 -3.10113

D37 3.13303 0.00020 0.00370 -0.00992 -0.00626 3.12677

D38 0.02349 -0.00023 -0.00168 0.00175 0.00002 0.02351

D39 -3.11955 -0.00050 -0.00538 0.01474 0.00935 -3.11020

D40 0.15566 -0.00082 0.00613 -0.02153 -0.01543 0.14023

D41 -0.00592 -0.00010 -0.00063 0.00446 0.00381 -0.00211

D42 -3.01390 -0.00043 0.01087 -0.03181 -0.02097 -3.03488

D43 3.11754 0.00045 0.00506 -0.01289 -0.00782 3.10972

D44 -0.01290 0.00020 0.00504 -0.01370 -0.00866 -0.02155

D45 0.00368 0.00006 0.00038 -0.00276 -0.00237 0.00132

D46 -3.12675 -0.00018 0.00036 -0.00357 -0.00320 -3.12996

D47 0.00592 0.00010 0.00063 -0.00446 -0.00381 0.00211

D48 3.11955 0.00050 0.00538 -0.01474 -0.00935 3.11020

D49 3.01390 0.00043 -0.01087 0.03181 0.02097 3.03488

D50 -0.15566 0.00082 -0.00613 0.02153 0.01543 -0.14023

D51 -0.22083 0.00137 -0.01059 0.03492 0.02439 -0.19644

D52 -1.65017 0.00024 -0.00665 0.02118 0.01456 -1.63561

D53 -3.07950 -0.00088 -0.00272 0.00744 0.00473 -3.07477

D54 3.07950 0.00088 0.00272 -0.00744 -0.00473 3.07477

D55 1.65017 -0.00024 0.00665 -0.02118 -0.01456 1.63561

D56 0.22083 -0.00137 0.01059 -0.03492 -0.02439 0.19644

D57 -0.00368 -0.00006 -0.00038 0.00276 0.00237 -0.00132

D58 3.12675 0.00018 -0.00036 0.00357 0.00320 3.12996

D59 -3.11754 -0.00045 -0.00506 0.01289 0.00782 -3.10972

D60 0.01290 -0.00020 -0.00504 0.01370 0.00866 0.02155

D61 -0.00696 0.00036 -0.00341 0.00823 0.00483 -0.00213

D62 -3.13303 -0.00020 -0.00370 0.00993 0.00626 -3.12677

D63 3.10258 0.00079 0.00197 -0.00344 -0.00145 3.10113

D64 -0.02349 0.00023 0.00168 -0.00175 -0.00002 -0.02351

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13014 0.00025 0.00003 0.00081 0.00084 3.13099

D67 -3.13014 -0.00025 -0.00003 -0.00080 -0.00084 -3.13099

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.10258 0.00079 0.00197 -0.00344 -0.00145 3.10113

D70 -0.00696 0.00036 -0.00341 0.00823 0.00483 -0.00213

D71 -0.02349 0.00023 0.00168 -0.00175 -0.00002 -0.02351

D72 -3.13303 -0.00020 -0.00370 0.00992 0.00626 -3.12677

D73 -3.11754 -0.00045 -0.00506 0.01289 0.00782 -3.10972

D74 0.01290 -0.00020 -0.00504 0.01370 0.00866 0.02155

D75 -0.00368 -0.00006 -0.00038 0.00276 0.00237 -0.00132

D76 3.12675 0.00018 -0.00036 0.00357 0.00320 3.12996

D77 3.11955 0.00050 0.00538 -0.01474 -0.00935 3.11020

D78 -0.15566 0.00082 -0.00613 0.02153 0.01543 -0.14023

D79 0.00592 0.00010 0.00063 -0.00446 -0.00381 0.00211

D80 3.01390 0.00043 -0.01087 0.03181 0.02097 3.03488

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 3.13014 0.00025 0.00003 0.00080 0.00084 3.13099

D83 -3.13014 -0.00025 -0.00003 -0.00081 -0.00084 -3.13099

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 0.00368 0.00006 0.00038 -0.00276 -0.00237 0.00132

D86 3.11754 0.00045 0.00506 -0.01289 -0.00782 3.10972

D87 -3.12675 -0.00018 0.00036 -0.00357 -0.00320 -3.12996

D88 -0.01290 0.00020 0.00504 -0.01370 -0.00866 -0.02155

D89 -0.00592 -0.00010 -0.00063 0.00446 0.00381 -0.00211

D90 -3.01390 -0.00043 0.01087 -0.03181 -0.02097 -3.03488

D91 -3.11955 -0.00050 -0.00538 0.01474 0.00935 -3.11020

D92 0.15566 -0.00082 0.00613 -0.02153 -0.01543 0.14023

D93 -3.10258 -0.00079 -0.00197 0.00344 0.00145 -3.10113

D94 0.02349 -0.00023 -0.00168 0.00175 0.00002 0.02351

D95 0.00696 -0.00036 0.00341 -0.00823 -0.00483 0.00213

D96 3.13303 0.00020 0.00370 -0.00993 -0.00626 3.12677

D97 0.22083 -0.00137 0.01059 -0.03492 -0.02439 0.19644

D98 1.65017 -0.00024 0.00665 -0.02118 -0.01456 1.63561

D99 3.07950 0.00088 0.00272 -0.00744 -0.00473 3.07477

D100 -3.07950 -0.00088 -0.00272 0.00744 0.00473 -3.07477

D101 -1.65017 0.00024 -0.00665 0.02118 0.01456 -1.63561

D102 -0.22083 0.00137 -0.01059 0.03492 0.02439 -0.19644

D103 3.10258 0.00079 0.00197 -0.00344 -0.00145 3.10113

D104 -0.00696 0.00036 -0.00341 0.00823 0.00483 -0.00213

D105 -0.02349 0.00023 0.00168 -0.00175 -0.00002 -0.02351

D106 -3.13303 -0.00020 -0.00370 0.00992 0.00626 -3.12677

D107 -3.11754 -0.00045 -0.00506 0.01289 0.00782 -3.10972

D108 0.01290 -0.00020 -0.00504 0.01370 0.00866 0.02155

D109 -0.00368 -0.00006 -0.00038 0.00276 0.00237 -0.00132

D110 3.12675 0.00018 -0.00036 0.00357 0.00320 3.12996

D111 3.11955 0.00050 0.00538 -0.01474 -0.00935 3.11020

D112 -0.15566 0.00082 -0.00613 0.02153 0.01543 -0.14023

D113 0.00592 0.00010 0.00063 -0.00446 -0.00381 0.00211

D114 3.01390 0.00043 -0.01087 0.03181 0.02097 3.03488

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.13014 0.00025 0.00003 0.00081 0.00084 3.13099

D117 -3.13014 -0.00025 -0.00003 -0.00081 -0.00084 -3.13099

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 0.00368 0.00006 0.00038 -0.00276 -0.00237 0.00132

D120 3.11754 0.00045 0.00506 -0.01289 -0.00782 3.10972

D121 -3.12675 -0.00018 0.00036 -0.00357 -0.00320 -3.12996

D122 -0.01290 0.00020 0.00504 -0.01370 -0.00866 -0.02155

D123 -0.00592 -0.00010 -0.00063 0.00446 0.00381 -0.00211

D124 -3.01390 -0.00043 0.01087 -0.03181 -0.02097 -3.03488

D125 -3.11955 -0.00050 -0.00538 0.01474 0.00935 -3.11020

D126 0.15566 -0.00082 0.00613 -0.02153 -0.01543 0.14023

D127 -3.10258 -0.00079 -0.00197 0.00344 0.00145 -3.10113

D128 0.02349 -0.00023 -0.00168 0.00175 0.00002 0.02351

D129 0.00696 -0.00036 0.00341 -0.00823 -0.00483 0.00213

D130 3.13303 0.00020 0.00370 -0.00992 -0.00626 3.12677

D131 1.65017 -0.00024 0.00665 -0.02118 -0.01456 1.63561

D132 3.07950 0.00088 0.00272 -0.00744 -0.00473 3.07477

D133 0.22083 -0.00137 0.01059 -0.03492 -0.02439 0.19644

D134 -1.65017 0.00024 -0.00665 0.02118 0.01456 -1.63561

D135 -0.22083 0.00137 -0.01059 0.03492 0.02439 -0.19644

D136 -3.07950 -0.00088 -0.00272 0.00744 0.00473 -3.07477

Item Value Threshold Converged?

Maximum Force 0.003002 0.000450 NO

RMS Force 0.000734 0.000300 NO

Maximum Displacement 0.095847 0.001800 NO

RMS Displacement 0.014453 0.001200 NO

Predicted change in Energy=-5.270910D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:14:38 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/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 0.680443 4.259021 -0.044927

2 6 0 1.097932 2.875814 0.020651

3 7 0 0.000000 2.061150 0.057579

4 6 0 -1.097932 2.875814 0.020651

5 6 0 -0.680443 4.259021 -0.044927

6 6 0 -2.440460 2.440460 0.004260

7 6 0 -2.875814 1.097932 0.020651

8 7 0 -2.061150 0.000000 0.057579

9 6 0 -2.875814 -1.097932 0.020651

10 6 0 -4.259021 -0.680443 -0.044927

11 6 0 -4.259021 0.680443 -0.044927

12 6 0 2.440460 2.440460 0.004260

13 6 0 2.875814 1.097932 0.020651

14 6 0 4.259021 0.680443 -0.044927

15 6 0 4.259021 -0.680443 -0.044927

16 6 0 2.875814 -1.097932 0.020651

17 7 0 2.061150 0.000000 0.057579

18 6 0 2.440460 -2.440460 0.004260

19 6 0 1.097932 -2.875814 0.020651

20 6 0 0.680443 -4.259021 -0.044927

21 6 0 -0.680443 -4.259021 -0.044927

22 6 0 -1.097932 -2.875814 0.020651

23 7 0 0.000000 -2.061150 0.057579

24 1 0 1.340085 5.112341 -0.094459

25 1 0 -1.340085 5.112341 -0.094459

26 1 0 -5.112341 -1.340085 -0.094459

27 1 0 -5.112341 1.340085 -0.094459

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31 1 0 -1.340085 -5.112341 -0.094459

32 30 0 0.000000 0.000000 0.332895

33 6 0 -2.440460 -2.440460 0.004260

34 6 0 -3.448161 -3.448161 -0.053699

35 6 0 3.448161 3.448161 -0.053699

36 6 0 -4.299793 -4.299793 -0.106671

37 6 0 4.299793 4.299793 -0.106671

38 6 0 -3.448161 3.448161 -0.053699

39 6 0 -4.299793 4.299793 -0.106671

40 6 0 3.448161 -3.448161 -0.053699

41 6 0 4.299793 -4.299793 -0.106671

42 1 0 5.054423 -5.054423 -0.110844

43 1 0 -5.054423 -5.054423 -0.110844

44 1 0 -5.054423 5.054423 -0.110844

45 1 0 5.054423 5.054423 -0.110844

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.446326 0.000000

3 N 2.303074 1.367660 0.000000

4 C 2.253925 2.195863 1.367660 0.000000

5 C 1.360886 2.253925 2.303074 1.446326 0.000000

6 C 3.612425 3.565111 2.470337 1.411447 2.531253

7 C 4.758544 4.353334 3.033061 2.514305 3.849212

8 N 5.066172 4.272173 2.914906 3.033061 4.478405

9 C 6.430256 5.619724 4.272173 4.353334 5.789723

10 C 6.985456 6.430256 5.066172 4.758544 6.099551

11 C 6.099551 5.789723 4.478405 3.849212 5.060873

12 C 2.531253 1.411447 2.470337 3.565111 3.612425

13 C 3.849212 2.514305 3.033061 4.353334 4.758544

14 C 5.060873 3.849212 4.478405 5.789723 6.099551

15 C 6.099551 4.758544 5.066172 6.430256 6.985456

16 C 5.789723 4.353334 4.272173 5.619724 6.430256

17 N 4.478405 3.033061 2.914906 4.272173 5.066172

18 C 6.926985 5.483194 5.120857 6.386176 7.390906

19 C 7.147339 5.751627 5.057709 6.156544 7.353419

20 C 8.518041 7.147339 6.357520 7.353419 8.626067

21 C 8.626067 7.353419 6.357520 7.147339 8.518041

22 C 7.353419 6.156544 5.057709 5.751627 7.147339

23 N 6.357520 5.057709 4.122299 5.057709 6.357520

24 H 1.079693 2.252542 3.335973 3.310473 2.193888

25 H 2.193888 3.310473 3.335973 2.252542 1.079693

26 H 8.056599 7.506966 6.142275 5.822589 7.141020

27 H 6.486832 6.398375 5.165180 4.299674 5.307010

28 H 5.307010 4.299674 5.165180 6.398375 6.486832

29 H 7.141020 5.822589 6.142275 7.506966 8.056599

30 H 9.394679 7.992653 7.299172 8.352712 9.586835

31 H 9.586835 8.352712 7.299172 7.992653 9.394679

32 Zn 4.329551 3.094068 2.079456 3.094068 4.329551

33 C 7.390906 6.386176 5.120857 5.483194 6.926985

34 C 8.743346 7.788783 6.500362 6.746982 8.189078

35 C 2.884065 2.420060 3.718333 4.582583 4.207486

36 C 9.902518 8.980032 7.679635 7.858592 9.292836

37 C 3.620107 3.506544 4.850436 5.583849 4.980786

38 C 4.207486 4.582583 3.718333 2.420060 2.884065

39 C 4.980786 5.583849 4.850436 3.506544 3.620107

40 C 8.189078 6.746982 6.500362 7.788783 8.743346

41 C 9.292836 7.858592 7.679635 8.980032 9.902518

42 H 10.289620 8.863395 8.729658 10.037799 10.937699

43 H 10.937699 10.037799 8.729658 8.863395 10.289620

44 H 5.790138 6.528024 5.876669 4.518567 4.446202

45 H 4.446202 4.518567 5.876669 6.528024 5.790138

6 7 8 9 10

6 C 0.000000

7 C 1.411447 0.000000

8 N 2.470337 1.367660 0.000000

9 C 3.565111 2.195863 1.367660 0.000000

10 C 3.612425 2.253925 2.303074 1.446326 0.000000

11 C 2.531253 1.446326 2.303074 2.253925 1.360886

12 C 4.880920 5.483194 5.120857 6.386176 7.390906

13 C 5.483194 5.751627 5.057709 6.156544 7.353419

14 C 6.926985 7.147339 6.357520 7.353419 8.626067

15 C 7.390906 7.353419 6.357520 7.147339 8.518041

16 C 6.386176 6.156544 5.057709 5.751627 7.147339

17 N 5.120857 5.057709 4.122299 5.057709 6.357520

18 C 6.902663 6.386176 5.120857 5.483194 6.926985

19 C 6.386176 5.619724 4.272173 4.353334 5.789723

20 C 7.390906 6.430256 5.066172 4.758544 6.099551

21 C 6.926985 5.789723 4.478405 3.849212 5.060873

22 C 5.483194 4.353334 3.033061 2.514305 3.849212

23 N 5.120857 4.272173 2.914906 3.033061 4.478405

24 H 4.630466 5.822589 6.142275 7.506966 8.056599

25 H 2.891283 4.299674 5.165180 6.398375 6.486832

26 H 4.630466 3.310473 3.335973 2.252542 1.079693

27 H 2.891283 2.252542 3.335973 3.310473 2.193888

28 H 7.633176 7.992653 7.299172 8.352712 9.586835

29 H 8.446719 8.352712 7.299172 7.992653 9.394679

30 H 8.446719 7.506966 6.142275 5.822589 7.141020

31 H 7.633176 6.398375 5.165180 4.299674 5.307010

32 Zn 3.466942 3.094068 2.079456 3.094068 4.329551

33 C 4.880920 3.565111 2.470337 1.411447 2.531253

34 C 5.974502 4.582583 3.718333 2.420060 2.884065

35 C 5.974502 6.746982 6.500362 7.788783 8.743346

36 C 6.992885 5.583849 4.850436 3.506544 3.620107

37 C 6.992885 7.858592 7.679635 8.980032 9.902518

38 C 1.426283 2.420060 3.718333 4.582583 4.207486

39 C 2.631834 3.506544 4.850436 5.583849 4.980786

40 C 8.327969 7.788783 6.500362 6.746982 8.189078

41 C 9.532803 8.980032 7.679635 7.858592 9.292836

42 H 10.599990 10.037799 8.729658 8.863395 10.289620

43 H 7.938471 6.528024 5.876669 4.518567 4.446202

44 H 3.698494 4.518567 5.876669 6.528024 5.790138

45 H 7.938471 8.863395 8.729658 10.037799 10.937699

11 12 13 14 15

11 C 0.000000

12 C 6.926985 0.000000

13 C 7.147339 1.411447 0.000000

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17 N 6.357520 2.470337 1.367660 2.303074 2.303074

18 C 7.390906 4.880920 3.565111 3.612425 2.531253

19 C 6.430256 5.483194 4.353334 4.758544 3.849212

20 C 6.985456 6.926985 5.789723 6.099551 5.060873

21 C 6.099551 7.390906 6.430256 6.985456 6.099551

22 C 4.758544 6.386176 5.619724 6.430256 5.789723

23 N 5.066172 5.120857 4.272173 5.066172 4.478405

24 H 7.141020 2.891283 4.299674 5.307010 6.486832

25 H 5.307010 4.630466 5.822589 7.141020 8.056599

26 H 2.193888 8.446719 8.352712 9.586835 9.394679

27 H 1.079693 7.633176 7.992653 9.394679 9.586835

28 H 9.394679 2.891283 2.252542 1.079693 2.193888

29 H 9.586835 4.630466 3.310473 2.193888 1.079693

30 H 8.056599 7.633176 6.398375 6.486832 5.307010

31 H 6.486832 8.446719 7.506966 8.056599 7.141020

32 Zn 4.329551 3.466942 3.094068 4.329551 4.329551

33 C 3.612425 6.902663 6.386176 7.390906 6.926985

34 C 4.207486 8.327969 7.788783 8.743346 8.189078

35 C 8.189078 1.426283 2.420060 2.884065 4.207486

36 C 4.980786 9.532803 8.980032 9.902518 9.292836

37 C 9.292836 2.631834 3.506544 3.620107 4.980786

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39 C 3.620107 6.992885 7.858592 9.292836 9.902518

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41 C 9.902518 6.992885 5.583849 4.980786 3.620107

42 H 10.937699 7.938471 6.528024 5.790138 4.446202

43 H 5.790138 10.599990 10.037799 10.937699 10.289620

44 H 4.446202 7.938471 8.863395 10.289620 10.937699

45 H 10.289620 3.698494 4.518567 4.446202 5.790138

16 17 18 19 20

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17 N 1.367660 0.000000

18 C 1.411447 2.470337 0.000000

19 C 2.514305 3.033061 1.411447 0.000000

20 C 3.849212 4.478405 2.531253 1.446326 0.000000

21 C 4.758544 5.066172 3.612425 2.253925 1.360886

22 C 4.353334 4.272173 3.565111 2.195863 2.253925

23 N 3.033061 2.914906 2.470337 1.367660 2.303074

24 H 6.398375 5.165180 7.633176 7.992653 9.394679

25 H 7.506966 6.142275 8.446719 8.352712 9.586835

26 H 7.992653 7.299172 7.633176 6.398375 6.486832

27 H 8.352712 7.299172 8.446719 7.506966 8.056599

28 H 3.310473 3.335973 4.630466 5.822589 7.141020

29 H 2.252542 3.335973 2.891283 4.299674 5.307010

30 H 4.299674 5.165180 2.891283 2.252542 1.079693

31 H 5.822589 6.142275 4.630466 3.310473 2.193888

32 Zn 3.094068 2.079456 3.466942 3.094068 4.329551

33 C 5.483194 5.120857 4.880920 3.565111 3.612425

34 C 6.746982 6.500362 5.974502 4.582583 4.207486

35 C 4.582583 3.718333 5.974502 6.746982 8.189078

36 C 7.858592 7.679635 6.992885 5.583849 4.980786

37 C 5.583849 4.850436 6.992885 7.858592 9.292836

38 C 7.788783 6.500362 8.327969 7.788783 8.743346

39 C 8.980032 7.679635 9.532803 8.980032 9.902518

40 C 2.420060 3.718333 1.426283 2.420060 2.884065

41 C 3.506544 4.850436 2.631834 3.506544 3.620107

42 H 4.518567 5.876669 3.698494 4.518567 4.446202

43 H 8.863395 8.729658 7.938471 6.528024 5.790138

44 H 10.037799 8.729658 10.599990 10.037799 10.937699

45 H 6.528024 5.876669 7.938471 8.863395 10.289620

21 22 23 24 25

21 C 0.000000

22 C 1.446326 0.000000

23 N 2.303074 1.367660 0.000000

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26 H 5.307010 4.299674 5.165180 9.125109 7.474204

27 H 7.141020 5.822589 6.142275 7.474204 5.334776

28 H 8.056599 7.506966 6.142275 5.334776 7.474204

29 H 6.486832 6.398375 5.165180 7.474204 9.125109

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31 H 1.079693 2.252542 3.335973 10.570120 10.224682

32 Zn 4.329551 3.094068 2.079456 5.302310 5.302310

33 C 2.531253 1.411447 2.470337 8.446719 7.633176

34 C 2.884065 2.420060 3.718333 9.808729 8.816340

35 C 8.743346 7.788783 6.500362 2.686101 5.069365

36 C 3.620107 3.506544 4.850436 10.972541 9.866524

37 C 9.902518 8.980032 7.679635 3.069244 5.698124

38 C 8.189078 6.746982 6.500362 5.069365 2.686101

39 C 9.292836 7.858592 7.679635 5.698124 3.069244

40 C 4.207486 4.582583 3.718333 8.816340 9.808729

41 C 4.980786 5.583849 4.850436 9.866524 10.972541

42 H 5.790138 6.528024 5.876669 10.824032 12.010541

43 H 4.446202 4.518567 5.876669 12.010541 10.824032

44 H 10.289620 8.863395 8.729658 6.394791 3.714825

45 H 10.937699 10.037799 8.729658 3.714825 6.394791

26 27 28 29 30

26 H 0.000000

27 H 2.680170 0.000000

28 H 10.570120 10.224682 0.000000

29 H 10.224682 10.570120 2.680170 0.000000

30 H 7.474204 9.125109 7.474204 5.334776 0.000000

31 H 5.334776 7.474204 9.125109 7.474204 2.680170

32 Zn 5.302310 5.302310 5.302310 5.302310 5.302310

33 C 2.891283 4.630466 8.446719 7.633176 4.630466

34 C 2.686101 5.069365 9.808729 8.816340 5.069365

35 C 9.808729 8.816340 2.686101 5.069365 8.816340

36 C 3.069244 5.698124 10.972541 9.866524 5.698124

37 C 10.972541 9.866524 3.069244 5.698124 9.866524

38 C 5.069365 2.686101 8.816340 9.808729 9.808729

39 C 5.698124 3.069244 9.866524 10.972541 10.972541

40 C 8.816340 9.808729 5.069365 2.686101 2.686101

41 C 9.866524 10.972541 5.698124 3.069244 3.069244

42 H 10.824032 12.010541 6.394791 3.714825 3.714825

43 H 3.714825 6.394791 12.010541 10.824032 6.394791

44 H 6.394791 3.714825 10.824032 12.010541 12.010541

45 H 12.010541 10.824032 3.714825 6.394791 10.824032

31 32 33 34 35

31 H 0.000000

32 Zn 5.302310 0.000000

33 C 2.891283 3.466942 0.000000

34 C 2.686101 4.891736 1.426283 0.000000

35 C 9.808729 4.891736 8.327969 9.752872 0.000000

36 C 3.069244 6.096693 2.631834 1.205554 10.957391

37 C 10.972541 6.096693 9.532803 10.957391 1.205554

38 C 8.816340 4.891736 5.974502 6.896322 6.896322

39 C 9.866524 6.096693 6.992885 7.794799 7.794799

40 C 5.069365 4.891736 5.974502 6.896322 6.896322

41 C 5.698124 6.096693 6.992885 7.794799 7.794799

42 H 6.394791 7.161793 7.938471 8.653166 8.653166

43 H 3.714825 7.161793 3.698494 2.272316 12.024605

44 H 10.824032 7.161793 7.938471 8.653166 8.653166

45 H 12.010541 7.161793 10.599990 12.024605 2.272316

36 37 38 39 40

36 C 0.000000

37 C 12.161653 0.000000

38 C 7.794799 7.794799 0.000000

39 C 8.599587 8.599587 1.205554 0.000000

40 C 7.794799 7.794799 9.752872 10.957391 0.000000

41 C 8.599587 8.599587 10.957391 12.161653 1.205554

42 H 9.384607 9.384607 12.024605 13.228860 2.272316

43 H 1.067215 13.228860 8.653166 9.384607 8.653166

44 H 9.384607 9.384607 2.272316 1.067215 12.024605

45 H 13.228860 1.067215 8.653166 9.384607 8.653166

41 42 43 44 45

41 C 0.000000

42 H 1.067215 0.000000

43 H 9.384607 10.108846 0.000000

44 H 13.228860 14.296067 10.108846 0.000000

45 H 9.384607 10.108846 14.296067 10.108846 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

RotChk: IX=3 Diff= 3.63D-20

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 -0.680443 -4.259021 -0.067987

2 6 0 -1.097932 -2.875814 -0.002409

3 7 0 0.000000 -2.061150 0.034520

4 6 0 1.097932 -2.875814 -0.002409

5 6 0 0.680443 -4.259021 -0.067987

6 6 0 2.440460 -2.440460 -0.018799

7 6 0 2.875814 -1.097932 -0.002409

8 7 0 2.061150 0.000000 0.034520

9 6 0 2.875814 1.097932 -0.002409

10 6 0 4.259021 0.680443 -0.067987

11 6 0 4.259021 -0.680443 -0.067987

12 6 0 -2.440460 -2.440460 -0.018799

13 6 0 -2.875814 -1.097932 -0.002409

14 6 0 -4.259021 -0.680443 -0.067987

15 6 0 -4.259021 0.680443 -0.067987

16 6 0 -2.875814 1.097932 -0.002409

17 7 0 -2.061150 0.000000 0.034520

18 6 0 -2.440460 2.440460 -0.018799

19 6 0 -1.097932 2.875814 -0.002409

20 6 0 -0.680443 4.259021 -0.067987

21 6 0 0.680443 4.259021 -0.067987

22 6 0 1.097932 2.875814 -0.002409

23 7 0 0.000000 2.061150 0.034520

24 1 0 -1.340085 -5.112341 -0.117518

25 1 0 1.340085 -5.112341 -0.117518

26 1 0 5.112341 1.340085 -0.117518

27 1 0 5.112341 -1.340085 -0.117518

28 1 0 -5.112341 -1.340085 -0.117518

29 1 0 -5.112341 1.340085 -0.117518

30 1 0 -1.340085 5.112341 -0.117518

31 1 0 1.340085 5.112341 -0.117518

32 30 0 0.000000 0.000000 0.309835

33 6 0 2.440460 2.440460 -0.018799

34 6 0 3.448161 3.448161 -0.076758

35 6 0 -3.448161 -3.448161 -0.076758

36 6 0 4.299793 4.299793 -0.129730

37 6 0 -4.299793 -4.299793 -0.129730

38 6 0 3.448161 -3.448161 -0.076758

39 6 0 4.299793 -4.299793 -0.129730

40 6 0 -3.448161 3.448161 -0.076758

41 6 0 -4.299793 4.299793 -0.129730

42 1 0 -5.054423 5.054423 -0.133904

43 1 0 5.054423 5.054423 -0.133904

44 1 0 5.054423 -5.054423 -0.133904

45 1 0 -5.054423 -5.054423 -0.133904

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

Rotational constants (GHZ): 0.1471578 0.1471578 0.0737491

Leave Link 202 at Fri Jul 26 14:14:38 2019, MaxMem= 1342177280 cpu: 0.1

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 184 symmetry adapted cartesian basis functions of A1 symmetry.

There are 155 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3067.3757094727 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= 9 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= -0.1306991109 Hartrees.

Nuclear repulsion after empirical dispersion term = 3067.2450103618 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: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3818

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.45D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 180

GePol: Fraction of low-weight points (<1% of avg) = 4.71%

GePol: Cavity surface area = 416.323 Ang\*\*2

GePol: Cavity volume = 419.941 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0083909574 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3067.2534013191 Hartrees.

Leave Link 301 at Fri Jul 26 14:14:39 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16267 LenP2D= 44940.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.38D-05 NBF= 172 148 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 172 148 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:14:39 2019, MaxMem= 1342177280 cpu: 6.5

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:14:39 2019, MaxMem= 1342177280 cpu: 0.8

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

Initial guess from the checkpoint file: "ZnTSPsim0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Occupied (E) (E) (B2) (A1) (E) (E) (B1) (A1) (B2) (E) (E)

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

(E) (E) (A1) (A2) (E) (E) (B1) (B1) (E) (E) (A1)

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

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

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

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

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

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

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

(E) (E) (A2) (A1)

Virtual (A1) (A1) (B2) (A1) (B2) (A1) (A1) (B2) (A1) (B2)

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(E) (E) (E)

The electronic state of the initial guess is 1-A1.

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= -1359.45379658818

Leave Link 401 at Fri Jul 26 14:14:41 2019, MaxMem= 1342177280 cpu: 21.0

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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.

An orbital has undefined symmetry, so N\*\*3 symmetry is turned off.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 660000000 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= 0 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= 43731372.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.88D-15 for 309.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.10D-15 for 3033 2896.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.04D-14 for 307.

Iteration 1 A^-1\*A deviation from orthogonality is 5.87D-11 for 1387 1354.

E= -1359.05889747816

DIIS: error= 2.72D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.05889747816 IErMin= 1 ErrMin= 2.72D-03

ErrMax= 2.72D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.55D-03 BMatP= 1.55D-03

IDIUse=3 WtCom= 9.73D-01 WtEn= 2.72D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 3.225 Goal= None Shift= 0.000

GapD= 3.225 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=4.81D-04 MaxDP=2.66D-02 OVMax= 1.11D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.81D-04 CP: 9.99D-01

E= -1359.06127733168 Delta-E= -0.002379853522 Rises=F Damp=F

DIIS: error= 3.81D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.06127733168 IErMin= 2 ErrMin= 3.81D-04

ErrMax= 3.81D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.79D-05 BMatP= 1.55D-03

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.81D-03

Coeff-Com: 0.104D-02 0.999D+00

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

Coeff: 0.104D-02 0.999D+00

Gap= 0.093 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.65D-05 MaxDP=6.24D-04 DE=-2.38D-03 OVMax= 2.04D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.64D-05 CP: 9.99D-01 1.00D+00

E= -1359.06130584102 Delta-E= -0.000028509342 Rises=F Damp=F

DIIS: error= 5.24D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.06130584102 IErMin= 2 ErrMin= 3.81D-04

ErrMax= 5.24D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.92D-05 BMatP= 2.79D-05

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.24D-03

Coeff-Com: -0.149D-01 0.450D+00 0.565D+00

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

Coeff: -0.148D-01 0.448D+00 0.567D+00

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=7.88D-06 MaxDP=3.07D-04 DE=-2.85D-05 OVMax= 9.55D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.71D-06 CP: 9.99D-01 1.00D+00 7.52D-01

E= -1359.06131400812 Delta-E= -0.000008167099 Rises=F Damp=F

DIIS: error= 1.62D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.06131400812 IErMin= 4 ErrMin= 1.62D-04

ErrMax= 1.62D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.53D-06 BMatP= 1.92D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.62D-03

Coeff-Com: -0.971D-02 0.134D+00 0.341D+00 0.535D+00

Coeff-En: 0.000D+00 0.000D+00 0.231D+00 0.769D+00

Coeff: -0.969D-02 0.134D+00 0.341D+00 0.535D+00

Gap= 0.093 Goal= None Shift= 0.000

RMSDP=3.04D-06 MaxDP=1.51D-04 DE=-8.17D-06 OVMax= 4.58D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.82D-06 CP: 9.99D-01 1.00D+00 8.38D-01 7.20D-01

E= -1359.06131712870 Delta-E= -0.000003120577 Rises=F Damp=F

DIIS: error= 4.96D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.06131712870 IErMin= 5 ErrMin= 4.96D-05

ErrMax= 4.96D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.61D-07 BMatP= 4.53D-06

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

Coeff-Com: -0.465D-02 0.489D-01 0.158D+00 0.308D+00 0.490D+00

Coeff: -0.465D-02 0.489D-01 0.158D+00 0.308D+00 0.490D+00

Gap= 0.093 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=9.82D-07 MaxDP=3.20D-05 DE=-3.12D-06 OVMax= 1.02D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.77D-07 CP: 9.99D-01 1.00D+00 8.45D-01 7.74D-01 6.86D-01

E= -1359.06131738892 Delta-E= -0.000000260226 Rises=F Damp=F

DIIS: error= 1.51D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.06131738892 IErMin= 6 ErrMin= 1.51D-05

ErrMax= 1.51D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.36D-08 BMatP= 3.61D-07

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

Coeff-Com: -0.407D-05-0.655D-02-0.433D-02 0.185D-01 0.214D+00 0.779D+00

Coeff: -0.407D-05-0.655D-02-0.433D-02 0.185D-01 0.214D+00 0.779D+00

Gap= 0.093 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=3.49D-07 MaxDP=2.02D-05 DE=-2.60D-07 OVMax= 3.43D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.55D-07 CP: 9.99D-01 1.00D+00 8.49D-01 7.88D-01 7.83D-01

CP: 8.69D-01

E= -1359.06131740156 Delta-E= -0.000000012634 Rises=F Damp=F

DIIS: error= 4.61D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.06131740156 IErMin= 7 ErrMin= 4.61D-06

ErrMax= 4.61D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.11D-09 BMatP= 2.36D-08

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

Coeff-Com: 0.179D-03-0.614D-02-0.890D-02-0.270D-03 0.121D+00 0.514D+00

Coeff-Com: 0.380D+00

Coeff: 0.179D-03-0.614D-02-0.890D-02-0.270D-03 0.121D+00 0.514D+00

Coeff: 0.380D+00

Gap= 0.093 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=9.51D-08 MaxDP=4.85D-06 DE=-1.26D-08 OVMax= 1.47D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.59D-08 CP: 9.99D-01 1.00D+00 8.50D-01 7.87D-01 7.93D-01

CP: 8.59D-01 5.99D-01

E= -1359.06131740714 Delta-E= -0.000000005586 Rises=F Damp=F

DIIS: error= 5.61D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.06131740714 IErMin= 8 ErrMin= 5.61D-07

ErrMax= 5.61D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.13D-11 BMatP= 6.11D-09

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

Coeff-Com: 0.473D-04-0.111D-02-0.185D-02-0.166D-02 0.168D-01 0.873D-01

Coeff-Com: 0.129D+00 0.771D+00

Coeff: 0.473D-04-0.111D-02-0.185D-02-0.166D-02 0.168D-01 0.873D-01

Coeff: 0.129D+00 0.771D+00

Gap= 0.093 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.68D-08 MaxDP=5.59D-07 DE=-5.59D-09 OVMax= 1.62D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 9.51D-09 CP: 9.99D-01 1.00D+00 8.50D-01 7.88D-01 7.93D-01

CP: 8.71D-01 6.50D-01 9.31D-01

E= -1359.06131740729 Delta-E= -0.000000000145 Rises=F Damp=F

DIIS: error= 7.07D-08 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1359.06131740729 IErMin= 9 ErrMin= 7.07D-08

ErrMax= 7.07D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.35D-12 BMatP= 7.13D-11

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

Coeff-Com: 0.796D-05-0.114D-03-0.244D-03-0.565D-03 0.432D-03 0.684D-02

Coeff-Com: 0.227D-01 0.219D+00 0.752D+00

Coeff: 0.796D-05-0.114D-03-0.244D-03-0.565D-03 0.432D-03 0.684D-02

Coeff: 0.227D-01 0.219D+00 0.752D+00

Gap= 0.093 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=3.58D-09 MaxDP=1.29D-07 DE=-1.45D-10 OVMax= 5.99D-07

Error on total polarization charges = 0.06208

SCF Done: E(RB3LYP) = -1359.06131741 A.U. after 9 cycles

NFock= 9 Conv=0.36D-08 -V/T= 1.9681

KE= 1.403855121415D+03 PE=-9.376813743501D+03 EE= 3.546643903359D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.27

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:15:19 2019, MaxMem= 1342177280 cpu: 424.9

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16267 LenP2D= 44940.

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 Fri Jul 26 14:15:23 2019, MaxMem= 1342177280 cpu: 42.7

(Enter /apps/gaussian/g09d01/g09/l702.exe)

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

Leave Link 702 at Fri Jul 26 14:15:23 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Fri Jul 26 14:15:26 2019, MaxMem= 1342177280 cpu: 43.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-2.02504680D-13 4.19220214D-13 5.80904066D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000125988 -0.000372729 0.000233261

2 6 0.000699005 0.000644265 -0.001313813

3 7 0.000000000 0.006494122 0.003096490

4 6 -0.000699005 0.000644265 -0.001313813

5 6 -0.000125988 -0.000372729 0.000233261

6 6 -0.000106147 0.000106147 0.000476859

7 6 -0.000644265 0.000699005 -0.001313813

8 7 -0.006494122 0.000000000 0.003096490

9 6 -0.000644265 -0.000699005 -0.001313813

10 6 0.000372729 -0.000125988 0.000233261

11 6 0.000372729 0.000125988 0.000233261

12 6 0.000106147 0.000106147 0.000476859

13 6 0.000644265 0.000699005 -0.001313813

14 6 -0.000372729 0.000125988 0.000233261

15 6 -0.000372729 -0.000125988 0.000233261

16 6 0.000644265 -0.000699005 -0.001313813

17 7 0.006494122 0.000000000 0.003096490

18 6 0.000106147 -0.000106147 0.000476859

19 6 0.000699005 -0.000644265 -0.001313813

20 6 0.000125988 0.000372729 0.000233261

21 6 -0.000125988 0.000372729 0.000233261

22 6 -0.000699005 -0.000644265 -0.001313813

23 7 0.000000000 -0.006494122 0.003096490

24 1 0.000107949 -0.000135055 0.000103233

25 1 -0.000107949 -0.000135055 0.000103233

26 1 0.000135055 -0.000107949 0.000103233

27 1 0.000135055 0.000107949 0.000103233

28 1 -0.000135055 0.000107949 0.000103233

29 1 -0.000135055 -0.000107949 0.000103233

30 1 0.000107949 0.000135055 0.000103233

31 1 -0.000107949 0.000135055 0.000103233

32 30 0.000000000 0.000000000 -0.008640036

33 6 -0.000106147 -0.000106147 0.000476859

34 6 -0.000055114 -0.000055114 0.000254051

35 6 0.000055114 0.000055114 0.000254051

36 6 -0.000258645 -0.000258645 0.001181645

37 6 0.000258645 0.000258645 0.001181645

38 6 -0.000055114 0.000055114 0.000254051

39 6 -0.000258645 0.000258645 0.001181645

40 6 0.000055114 -0.000055114 0.000254051

41 6 0.000258645 -0.000258645 0.001181645

42 1 0.000075342 -0.000075342 -0.000894399

43 1 -0.000075342 -0.000075342 -0.000894399

44 1 -0.000075342 0.000075342 -0.000894399

45 1 0.000075342 0.000075342 -0.000894399

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

Cartesian Forces: Max 0.008640036 RMS 0.001528451

Leave Link 716 at Fri Jul 26 14:15:26 2019, MaxMem= 1342177280 cpu: 0.5

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.004547190 RMS 0.000882759

Search for a local minimum.

Step number 4 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .88276D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4

DE= -2.41D-04 DEPred=-5.27D-04 R= 4.57D-01

Trust test= 4.57D-01 RLast= 2.26D-01 DXMaxT set to 7.50D-02

ITU= 0 -1 -1 0

Eigenvalues --- 0.00534 0.00534 0.00534 0.00534 0.00534

Eigenvalues --- 0.00534 0.00534 0.00802 0.01179 0.01327

Eigenvalues --- 0.01327 0.01646 0.01646 0.01655 0.01677

Eigenvalues --- 0.01806 0.01806 0.01815 0.01825 0.01831

Eigenvalues --- 0.01849 0.01860 0.01860 0.01867 0.01868

Eigenvalues --- 0.01868 0.01868 0.01911 0.01916 0.01916

Eigenvalues --- 0.01919 0.01933 0.01951 0.01951 0.01970

Eigenvalues --- 0.02153 0.02153 0.02179 0.02181 0.02273

Eigenvalues --- 0.02273 0.02318 0.03320 0.04654 0.04654

Eigenvalues --- 0.04654 0.04654 0.04654 0.04654 0.04654

Eigenvalues --- 0.06477 0.07598 0.13869 0.15108 0.15108

Eigenvalues --- 0.15947 0.15998 0.15998 0.15998 0.15998

Eigenvalues --- 0.15999 0.15999 0.15999 0.22808 0.22863

Eigenvalues --- 0.22866 0.22866 0.24570 0.24647 0.24647

Eigenvalues --- 0.24662 0.24697 0.24770 0.24952 0.24952

Eigenvalues --- 0.24988 0.24997 0.24997 0.24997 0.24997

Eigenvalues --- 0.32303 0.35027 0.35027 0.35405 0.35472

Eigenvalues --- 0.36034 0.36034 0.36034 0.36034 0.36034

Eigenvalues --- 0.36034 0.36034 0.36038 0.36623 0.36781

Eigenvalues --- 0.36876 0.36876 0.37563 0.37563 0.37563

Eigenvalues --- 0.37569 0.38973 0.38973 0.39511 0.41215

Eigenvalues --- 0.41397 0.41397 0.41397 0.41455 0.41455

Eigenvalues --- 0.41770 0.42465 0.43174 0.43529 0.43797

Eigenvalues --- 0.43797 0.47103 0.47736 0.49046 0.49046

Eigenvalues --- 0.50104 0.51388 0.51894 0.51894 0.57332

Eigenvalues --- 1.01831 1.01831 1.01831 1.01970

En-DIIS/RFO-DIIS IScMMF= 0 using points: 4 3 2 1

RFO step: Lambda=-3.37007371D-04.

NNeg= 0 NP= 4 Switch= 2.50D-03 Rises=F DC= -9.57D-05 SmlDif= 1.00D-05

RMS Error= 0.1429926093D-02 NUsed= 4 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.62624 0.15949 -0.71159 0.92586

Iteration 1 RMS(Cart)= 0.01895482 RMS(Int)= 0.00020083

Iteration 2 RMS(Cart)= 0.00032695 RMS(Int)= 0.00014202

Iteration 3 RMS(Cart)= 0.00000003 RMS(Int)= 0.00014202

ITry= 1 IFail=0 DXMaxC= 7.74D-02 DCOld= 1.00D+10 DXMaxT= 7.50D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.14D-02 for atom 44.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73316 -0.00027 0.00103 -0.00007 0.00102 2.73418

R2 2.57170 0.00106 0.00209 0.00023 0.00254 2.57424

R3 2.04032 -0.00005 0.00001 -0.00021 -0.00021 2.04012

R4 2.58450 0.00058 -0.00153 0.00030 -0.00138 2.58312

R5 2.66725 0.00166 0.00545 0.00047 0.00657 2.67382

R6 2.58450 0.00058 -0.00153 0.00030 -0.00138 2.58312

R7 3.92960 0.00455 0.03043 0.00168 0.03273 3.96234

R8 2.73316 -0.00027 0.00103 -0.00007 0.00102 2.73418

R9 2.66725 0.00166 0.00545 0.00047 0.00657 2.67382

R10 2.04032 -0.00005 0.00001 -0.00021 -0.00021 2.04012

R11 2.66725 0.00166 0.00545 0.00047 0.00657 2.67382

R12 2.69528 0.00053 0.00071 0.00053 0.00006 2.69535

R13 2.58450 0.00058 -0.00153 0.00030 -0.00138 2.58312

R14 2.73316 -0.00026 0.00103 -0.00006 0.00102 2.73418

R15 2.58450 0.00058 -0.00153 0.00030 -0.00138 2.58312

R16 3.92960 0.00455 0.03043 0.00168 0.03273 3.96234

R17 2.73316 -0.00027 0.00103 -0.00007 0.00102 2.73418

R18 2.66725 0.00166 0.00545 0.00047 0.00657 2.67382

R19 2.57170 0.00106 0.00209 0.00024 0.00254 2.57424

R20 2.04032 -0.00005 0.00001 -0.00021 -0.00021 2.04012

R21 2.04032 -0.00005 0.00001 -0.00020 -0.00021 2.04012

R22 2.66725 0.00166 0.00545 0.00047 0.00657 2.67382

R23 2.69528 0.00053 0.00071 0.00053 0.00006 2.69535

R24 2.73316 -0.00026 0.00103 -0.00006 0.00102 2.73418

R25 2.58450 0.00058 -0.00153 0.00030 -0.00138 2.58312

R26 2.57170 0.00106 0.00209 0.00024 0.00254 2.57424

R27 2.04032 -0.00005 0.00001 -0.00020 -0.00021 2.04012

R28 2.73316 -0.00027 0.00103 -0.00007 0.00102 2.73418

R29 2.04032 -0.00005 0.00001 -0.00021 -0.00021 2.04012

R30 2.58450 0.00058 -0.00153 0.00030 -0.00138 2.58312

R31 2.66725 0.00166 0.00545 0.00047 0.00657 2.67382

R32 3.92960 0.00455 0.03043 0.00168 0.03273 3.96234

R33 2.66725 0.00166 0.00545 0.00047 0.00657 2.67382

R34 2.69528 0.00053 0.00071 0.00053 0.00006 2.69535

R35 2.73316 -0.00026 0.00103 -0.00006 0.00102 2.73418

R36 2.58450 0.00058 -0.00153 0.00030 -0.00138 2.58312

R37 2.57170 0.00106 0.00209 0.00024 0.00254 2.57424

R38 2.04032 -0.00005 0.00001 -0.00020 -0.00021 2.04012

R39 2.73316 -0.00026 0.00103 -0.00006 0.00102 2.73418

R40 2.04032 -0.00005 0.00001 -0.00020 -0.00021 2.04012

R41 2.58450 0.00058 -0.00153 0.00030 -0.00138 2.58312

R42 2.66725 0.00166 0.00545 0.00047 0.00657 2.67382

R43 3.92960 0.00455 0.03043 0.00168 0.03273 3.96234

R44 2.69528 0.00053 0.00071 0.00053 0.00006 2.69535

R45 2.27817 0.00047 0.00047 0.00013 0.00059 2.27876

R46 2.27817 0.00047 0.00047 0.00013 0.00059 2.27876

R47 2.01674 0.00011 0.00019 -0.00004 0.00012 2.01687

R48 2.01674 0.00011 0.00019 -0.00004 0.00012 2.01687

R49 2.27817 0.00047 0.00047 0.00013 0.00059 2.27876

R50 2.01674 0.00011 0.00019 -0.00004 0.00012 2.01687

R51 2.27817 0.00047 0.00047 0.00013 0.00059 2.27876

R52 2.01674 0.00011 0.00019 -0.00004 0.00012 2.01687

A1 1.86362 0.00041 0.00173 0.00022 0.00194 1.86556

A2 2.19145 -0.00038 -0.00039 -0.00013 -0.00051 2.19094

A3 2.22806 -0.00003 -0.00133 -0.00008 -0.00141 2.22665

A4 1.91683 -0.00110 -0.00638 -0.00049 -0.00699 1.90983

A5 2.17611 0.00076 0.00548 -0.00002 0.00600 2.18211

A6 2.18973 0.00036 0.00107 0.00037 0.00138 2.19111

A7 1.86389 0.00138 0.00930 0.00054 0.01010 1.87399

A8 2.20681 -0.00068 -0.00664 0.00009 -0.00625 2.20056

A9 2.20681 -0.00068 -0.00664 0.00009 -0.00625 2.20056

A10 1.91683 -0.00110 -0.00638 -0.00049 -0.00699 1.90983

A11 2.18973 0.00036 0.00107 0.00037 0.00138 2.19111

A12 2.17611 0.00076 0.00548 -0.00002 0.00600 2.18211

A13 1.86362 0.00041 0.00173 0.00022 0.00194 1.86556

A14 2.22806 -0.00003 -0.00133 -0.00008 -0.00141 2.22665

A15 2.19145 -0.00038 -0.00039 -0.00013 -0.00051 2.19094

A16 2.19769 0.00061 0.00675 -0.00002 0.00679 2.20448

A17 2.04269 -0.00029 -0.00334 -0.00002 -0.00339 2.03930

A18 2.04269 -0.00031 -0.00334 -0.00008 -0.00339 2.03930

A19 2.18973 0.00036 0.00107 0.00038 0.00138 2.19111

A20 2.17611 0.00075 0.00548 -0.00002 0.00600 2.18211

A21 1.91683 -0.00110 -0.00638 -0.00049 -0.00699 1.90983

A22 1.86389 0.00138 0.00930 0.00054 0.01010 1.87399

A23 2.20681 -0.00068 -0.00664 0.00009 -0.00625 2.20056

A24 2.20681 -0.00068 -0.00664 0.00009 -0.00625 2.20056

A25 1.91683 -0.00110 -0.00638 -0.00049 -0.00699 1.90983

A26 2.18973 0.00036 0.00107 0.00037 0.00138 2.19111

A27 2.17611 0.00076 0.00548 -0.00002 0.00600 2.18211

A28 1.86362 0.00041 0.00173 0.00022 0.00194 1.86556

A29 2.19145 -0.00038 -0.00039 -0.00013 -0.00051 2.19094

A30 2.22806 -0.00003 -0.00133 -0.00008 -0.00141 2.22665

A31 1.86362 0.00041 0.00173 0.00021 0.00194 1.86556

A32 2.19145 -0.00038 -0.00039 -0.00011 -0.00051 2.19094

A33 2.22806 -0.00003 -0.00133 -0.00009 -0.00141 2.22665

A34 2.19769 0.00061 0.00675 -0.00002 0.00679 2.20448

A35 2.04269 -0.00029 -0.00334 -0.00002 -0.00339 2.03930

A36 2.04269 -0.00031 -0.00334 -0.00008 -0.00339 2.03930

A37 2.17611 0.00075 0.00548 -0.00002 0.00600 2.18211

A38 2.18973 0.00036 0.00107 0.00038 0.00138 2.19111

A39 1.91683 -0.00110 -0.00638 -0.00049 -0.00699 1.90983

A40 1.86362 0.00041 0.00173 0.00021 0.00194 1.86556

A41 2.19145 -0.00038 -0.00039 -0.00011 -0.00051 2.19094

A42 2.22806 -0.00003 -0.00133 -0.00009 -0.00141 2.22665

A43 1.86362 0.00041 0.00173 0.00022 0.00194 1.86556

A44 2.22806 -0.00003 -0.00133 -0.00008 -0.00141 2.22665

A45 2.19145 -0.00038 -0.00039 -0.00013 -0.00051 2.19094

A46 1.91683 -0.00110 -0.00638 -0.00049 -0.00699 1.90983

A47 2.17611 0.00076 0.00548 -0.00002 0.00600 2.18211

A48 2.18973 0.00036 0.00107 0.00037 0.00138 2.19111

A49 1.86389 0.00138 0.00930 0.00054 0.01010 1.87399

A50 2.20681 -0.00068 -0.00664 0.00009 -0.00625 2.20056

A51 2.20681 -0.00068 -0.00664 0.00009 -0.00625 2.20056

A52 2.19769 0.00061 0.00675 -0.00002 0.00679 2.20448

A53 2.04269 -0.00029 -0.00334 -0.00002 -0.00339 2.03930

A54 2.04269 -0.00031 -0.00334 -0.00008 -0.00339 2.03930

A55 2.17611 0.00075 0.00548 -0.00002 0.00600 2.18211

A56 2.18973 0.00036 0.00107 0.00038 0.00138 2.19111

A57 1.91683 -0.00110 -0.00638 -0.00049 -0.00699 1.90983

A58 1.86362 0.00041 0.00173 0.00021 0.00194 1.86556

A59 2.19145 -0.00038 -0.00039 -0.00011 -0.00051 2.19094

A60 2.22806 -0.00003 -0.00133 -0.00009 -0.00141 2.22665

A61 1.86362 0.00041 0.00173 0.00021 0.00194 1.86556

A62 2.22806 -0.00003 -0.00133 -0.00009 -0.00141 2.22665

A63 2.19145 -0.00038 -0.00039 -0.00011 -0.00051 2.19094

A64 1.91683 -0.00110 -0.00638 -0.00049 -0.00699 1.90983

A65 2.17611 0.00075 0.00548 -0.00002 0.00600 2.18211

A66 2.18973 0.00036 0.00107 0.00038 0.00138 2.19111

A67 1.86389 0.00138 0.00930 0.00054 0.01010 1.87399

A68 2.20681 -0.00068 -0.00664 0.00009 -0.00625 2.20056

A69 2.20681 -0.00068 -0.00664 0.00009 -0.00625 2.20056

A70 1.55327 0.00033 -0.00083 0.00015 -0.00064 1.55263

A71 1.55327 0.00033 -0.00083 0.00015 -0.00064 1.55263

A72 2.87602 0.00248 -0.00623 0.00113 -0.00480 2.87122

A73 2.87602 0.00248 -0.00623 0.00113 -0.00480 2.87122

A74 1.55327 0.00033 -0.00083 0.00015 -0.00064 1.55263

A75 1.55327 0.00033 -0.00083 0.00015 -0.00064 1.55263

A76 2.19769 0.00061 0.00675 -0.00002 0.00679 2.20448

A77 2.04269 -0.00029 -0.00334 -0.00002 -0.00339 2.03930

A78 2.04269 -0.00031 -0.00334 -0.00008 -0.00339 2.03930

A79 3.14153 0.00001 0.00002 0.00047 0.00002 3.14155

A80 3.14153 0.00001 0.00002 0.00047 0.00002 3.14155

A81 3.14195 0.00000 -0.00063 0.00510 -0.00032 3.14163

A82 3.14195 0.00000 -0.00063 0.00510 -0.00032 3.14163

A83 3.14153 0.00001 0.00002 0.00047 0.00002 3.14155

A84 3.14195 0.00000 -0.00063 0.00510 -0.00032 3.14163

A85 3.14153 0.00001 0.00002 0.00047 0.00002 3.14155

A86 3.14195 0.00000 -0.00063 0.00510 -0.00032 3.14163

A87 3.13826 -0.00109 0.00229 -0.00136 0.00096 3.13923

A88 3.14492 0.00109 -0.00229 0.00136 -0.00096 3.14396

A89 3.18766 -0.00157 -0.04372 0.00013 -0.04349 3.14418

A90 3.09552 0.00157 0.04372 -0.00013 0.04349 3.13901

A91 3.13826 -0.00109 0.00229 -0.00136 0.00096 3.13923

A92 3.18766 -0.00157 -0.04372 0.00013 -0.04349 3.14418

A93 3.14492 0.00109 -0.00229 0.00136 -0.00096 3.14396

A94 3.09552 0.00157 0.04372 -0.00013 0.04349 3.13901

D1 0.00132 0.00011 -0.00175 0.00152 -0.00037 0.00095

D2 3.10972 0.00058 0.01872 -0.00268 0.01588 3.12560

D3 -3.12996 -0.00017 -0.00350 0.00085 -0.00270 -3.13265

D4 -0.02155 0.00030 0.01696 -0.00335 0.01355 -0.00800

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13099 -0.00029 -0.00180 -0.00069 -0.00240 -3.13339

D7 3.13099 0.00029 0.00180 0.00069 0.00240 3.13339

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 -0.00211 -0.00019 0.00282 -0.00244 0.00058 -0.00153

D10 -3.03488 -0.00037 0.03103 -0.00930 0.02177 -3.01311

D11 -3.11020 -0.00067 -0.01779 0.00181 -0.01588 -3.12608

D12 0.14023 -0.00085 0.01043 -0.00506 0.00531 0.14553

D13 -3.10113 -0.00082 -0.01630 0.00863 -0.00749 -3.10861

D14 0.02351 -0.00016 -0.00554 -0.00062 -0.00612 0.01739

D15 0.00213 -0.00031 0.00739 0.00377 0.01122 0.01334

D16 3.12677 0.00035 0.01815 -0.00548 0.01258 3.13935

D17 0.00211 0.00019 -0.00282 0.00244 -0.00058 0.00153

D18 3.11020 0.00067 0.01779 -0.00181 0.01588 3.12608

D19 3.03488 0.00037 -0.03103 0.00930 -0.02177 3.01311

D20 -0.14023 0.00085 -0.01043 0.00506 -0.00531 -0.14553

D21 -3.07477 -0.00104 -0.01297 0.00355 -0.00971 -3.08448

D22 -0.19644 0.00138 -0.01904 0.00465 -0.01439 -0.21083

D23 -1.63561 0.00017 -0.01600 0.00410 -0.01205 -1.64765

D24 0.19644 -0.00138 0.01904 -0.00465 0.01439 0.21083

D25 3.07477 0.00104 0.01297 -0.00355 0.00971 3.08448

D26 1.63561 -0.00017 0.01600 -0.00410 0.01205 1.64765

D27 -0.00132 -0.00011 0.00175 -0.00152 0.00037 -0.00095

D28 3.12996 0.00017 0.00350 -0.00085 0.00270 3.13265

D29 -3.10972 -0.00058 -0.01872 0.00268 -0.01588 -3.12560

D30 0.02155 -0.00030 -0.01696 0.00335 -0.01355 0.00800

D31 -0.00213 0.00031 -0.00739 -0.00377 -0.01122 -0.01334

D32 -3.12677 -0.00035 -0.01815 0.00548 -0.01258 -3.13935

D33 3.10113 0.00082 0.01630 -0.00863 0.00749 3.10861

D34 -0.02351 0.00016 0.00554 0.00062 0.00612 -0.01739

D35 0.00213 -0.00031 0.00739 0.00377 0.01122 0.01334

D36 -3.10113 -0.00082 -0.01630 0.00863 -0.00749 -3.10861

D37 3.12677 0.00035 0.01815 -0.00548 0.01258 3.13935

D38 0.02351 -0.00016 -0.00554 -0.00062 -0.00612 0.01739

D39 -3.11020 -0.00067 -0.01779 0.00181 -0.01588 -3.12608

D40 0.14023 -0.00085 0.01043 -0.00506 0.00531 0.14553

D41 -0.00211 -0.00019 0.00282 -0.00244 0.00058 -0.00153

D42 -3.03488 -0.00037 0.03103 -0.00930 0.02177 -3.01311

D43 3.10972 0.00058 0.01872 -0.00268 0.01588 3.12560

D44 -0.02155 0.00030 0.01696 -0.00335 0.01355 -0.00800

D45 0.00132 0.00011 -0.00175 0.00152 -0.00037 0.00095

D46 -3.12996 -0.00017 -0.00350 0.00084 -0.00270 -3.13265

D47 0.00211 0.00019 -0.00282 0.00244 -0.00058 0.00153

D48 3.11020 0.00067 0.01779 -0.00181 0.01588 3.12608

D49 3.03488 0.00037 -0.03103 0.00930 -0.02177 3.01311

D50 -0.14023 0.00085 -0.01043 0.00506 -0.00531 -0.14553

D51 -0.19644 0.00138 -0.01904 0.00465 -0.01439 -0.21083

D52 -1.63561 0.00017 -0.01600 0.00410 -0.01205 -1.64765

D53 -3.07477 -0.00104 -0.01297 0.00355 -0.00971 -3.08448

D54 3.07477 0.00104 0.01297 -0.00355 0.00971 3.08448

D55 1.63561 -0.00017 0.01600 -0.00411 0.01205 1.64765

D56 0.19644 -0.00138 0.01904 -0.00465 0.01439 0.21083

D57 -0.00132 -0.00011 0.00175 -0.00152 0.00037 -0.00095

D58 3.12996 0.00017 0.00350 -0.00084 0.00270 3.13265

D59 -3.10972 -0.00058 -0.01872 0.00268 -0.01588 -3.12560

D60 0.02155 -0.00030 -0.01696 0.00335 -0.01355 0.00800

D61 -0.00213 0.00031 -0.00739 -0.00377 -0.01122 -0.01334

D62 -3.12677 -0.00035 -0.01815 0.00548 -0.01258 -3.13935

D63 3.10113 0.00082 0.01630 -0.00863 0.00749 3.10861

D64 -0.02351 0.00016 0.00554 0.00062 0.00612 -0.01739

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13099 0.00029 0.00180 0.00069 0.00240 3.13339

D67 -3.13099 -0.00029 -0.00180 -0.00069 -0.00240 -3.13339

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.10113 0.00082 0.01630 -0.00863 0.00749 3.10861

D70 -0.00213 0.00031 -0.00739 -0.00377 -0.01122 -0.01334

D71 -0.02351 0.00016 0.00554 0.00062 0.00612 -0.01739

D72 -3.12677 -0.00035 -0.01815 0.00548 -0.01258 -3.13935

D73 -3.10972 -0.00058 -0.01872 0.00268 -0.01588 -3.12560

D74 0.02155 -0.00030 -0.01696 0.00335 -0.01355 0.00800

D75 -0.00132 -0.00011 0.00175 -0.00152 0.00037 -0.00095

D76 3.12996 0.00017 0.00350 -0.00084 0.00270 3.13265

D77 3.11020 0.00067 0.01779 -0.00181 0.01588 3.12608

D78 -0.14023 0.00085 -0.01043 0.00506 -0.00531 -0.14553

D79 0.00211 0.00019 -0.00282 0.00244 -0.00058 0.00153

D80 3.03488 0.00037 -0.03103 0.00930 -0.02177 3.01311

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 3.13099 0.00029 0.00180 0.00069 0.00240 3.13339

D83 -3.13099 -0.00029 -0.00180 -0.00069 -0.00240 -3.13339

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 0.00132 0.00011 -0.00175 0.00152 -0.00037 0.00095

D86 3.10972 0.00058 0.01872 -0.00268 0.01588 3.12560

D87 -3.12996 -0.00017 -0.00350 0.00084 -0.00270 -3.13265

D88 -0.02155 0.00030 0.01696 -0.00335 0.01355 -0.00800

D89 -0.00211 -0.00019 0.00282 -0.00244 0.00058 -0.00153

D90 -3.03488 -0.00037 0.03103 -0.00930 0.02177 -3.01311

D91 -3.11020 -0.00067 -0.01779 0.00181 -0.01588 -3.12608

D92 0.14023 -0.00085 0.01043 -0.00506 0.00531 0.14553

D93 -3.10113 -0.00082 -0.01630 0.00863 -0.00749 -3.10861

D94 0.02351 -0.00016 -0.00554 -0.00062 -0.00612 0.01739

D95 0.00213 -0.00031 0.00739 0.00377 0.01122 0.01334

D96 3.12677 0.00035 0.01815 -0.00548 0.01258 3.13935

D97 0.19644 -0.00138 0.01904 -0.00465 0.01439 0.21083

D98 1.63561 -0.00017 0.01600 -0.00410 0.01205 1.64765

D99 3.07477 0.00104 0.01297 -0.00355 0.00971 3.08448

D100 -3.07477 -0.00104 -0.01297 0.00355 -0.00971 -3.08448

D101 -1.63561 0.00017 -0.01600 0.00411 -0.01205 -1.64765

D102 -0.19644 0.00138 -0.01904 0.00465 -0.01439 -0.21083

D103 3.10113 0.00082 0.01630 -0.00863 0.00749 3.10861

D104 -0.00213 0.00031 -0.00739 -0.00377 -0.01122 -0.01334

D105 -0.02351 0.00016 0.00554 0.00062 0.00612 -0.01739

D106 -3.12677 -0.00035 -0.01815 0.00548 -0.01258 -3.13935

D107 -3.10972 -0.00058 -0.01872 0.00268 -0.01588 -3.12560

D108 0.02155 -0.00030 -0.01696 0.00335 -0.01355 0.00800

D109 -0.00132 -0.00011 0.00175 -0.00152 0.00037 -0.00095

D110 3.12996 0.00017 0.00350 -0.00084 0.00270 3.13265

D111 3.11020 0.00067 0.01779 -0.00181 0.01588 3.12608

D112 -0.14023 0.00085 -0.01043 0.00506 -0.00531 -0.14553

D113 0.00211 0.00019 -0.00282 0.00244 -0.00058 0.00153

D114 3.03488 0.00037 -0.03103 0.00930 -0.02177 3.01311

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.13099 0.00029 0.00180 0.00069 0.00240 3.13339

D117 -3.13099 -0.00029 -0.00180 -0.00069 -0.00240 -3.13339

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 0.00132 0.00011 -0.00175 0.00152 -0.00037 0.00095

D120 3.10972 0.00058 0.01872 -0.00268 0.01588 3.12560

D121 -3.12996 -0.00017 -0.00350 0.00084 -0.00270 -3.13265

D122 -0.02155 0.00030 0.01696 -0.00335 0.01355 -0.00800

D123 -0.00211 -0.00019 0.00282 -0.00244 0.00058 -0.00153

D124 -3.03488 -0.00037 0.03103 -0.00930 0.02177 -3.01311

D125 -3.11020 -0.00067 -0.01779 0.00181 -0.01588 -3.12608

D126 0.14023 -0.00085 0.01043 -0.00506 0.00531 0.14553

D127 -3.10113 -0.00082 -0.01630 0.00863 -0.00749 -3.10861

D128 0.02351 -0.00016 -0.00554 -0.00062 -0.00612 0.01739

D129 0.00213 -0.00031 0.00739 0.00377 0.01122 0.01334

D130 3.12677 0.00035 0.01815 -0.00548 0.01258 3.13935

D131 1.63561 -0.00017 0.01600 -0.00410 0.01205 1.64765

D132 3.07477 0.00104 0.01297 -0.00355 0.00971 3.08448

D133 0.19644 -0.00138 0.01904 -0.00465 0.01439 0.21083

D134 -1.63561 0.00017 -0.01600 0.00410 -0.01205 -1.64765

D135 -0.19644 0.00138 -0.01904 0.00465 -0.01439 -0.21083

D136 -3.07477 -0.00104 -0.01297 0.00355 -0.00971 -3.08448

Item Value Threshold Converged?

Maximum Force 0.004547 0.000450 NO

RMS Force 0.000883 0.000300 NO

Maximum Displacement 0.077395 0.001800 NO

RMS Displacement 0.018909 0.001200 NO

Predicted change in Energy=-1.201890D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:15:26 2019, MaxMem= 1342177280 cpu: 1.1

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.681115 4.270557 -0.046917

2 6 0 1.101449 2.886790 -0.003001

3 7 0 0.000000 2.077647 0.021454

4 6 0 -1.101449 2.886790 -0.003001

5 6 0 -0.681115 4.270557 -0.046917

6 6 0 -2.445931 2.445931 -0.007547

7 6 0 -2.886790 1.101449 -0.003001

8 7 0 -2.077647 0.000000 0.021454

9 6 0 -2.886790 -1.101449 -0.003001

10 6 0 -4.270557 -0.681115 -0.046917

11 6 0 -4.270557 0.681115 -0.046917

12 6 0 2.445931 2.445931 -0.007547

13 6 0 2.886790 1.101449 -0.003001

14 6 0 4.270557 0.681115 -0.046917

15 6 0 4.270557 -0.681115 -0.046917

16 6 0 2.886790 -1.101449 -0.003001

17 7 0 2.077647 0.000000 0.021454

18 6 0 2.445931 -2.445931 -0.007547

19 6 0 1.101449 -2.886790 -0.003001

20 6 0 0.681115 -4.270557 -0.046917

21 6 0 -0.681115 -4.270557 -0.046917

22 6 0 -1.101449 -2.886790 -0.003001

23 7 0 0.000000 -2.077647 0.021454

24 1 0 1.339486 5.125472 -0.081074

25 1 0 -1.339486 5.125472 -0.081074

26 1 0 -5.125472 -1.339486 -0.081074

27 1 0 -5.125472 1.339486 -0.081074

28 1 0 5.125472 1.339486 -0.081074

29 1 0 5.125472 -1.339486 -0.081074

30 1 0 1.339486 -5.125472 -0.081074

31 1 0 -1.339486 -5.125472 -0.081074

32 30 0 0.000000 0.000000 0.304052

33 6 0 -2.445931 -2.445931 -0.007547

34 6 0 -3.454266 -3.454266 -0.037532

35 6 0 3.454266 3.454266 -0.037532

36 6 0 -4.306710 -4.306710 -0.065715

37 6 0 4.306710 4.306710 -0.065715

38 6 0 -3.454266 3.454266 -0.037532

39 6 0 -4.306710 4.306710 -0.065715

40 6 0 3.454266 -3.454266 -0.037532

41 6 0 4.306710 -4.306710 -0.065715

42 1 0 5.061223 -5.061223 -0.088262

43 1 0 -5.061223 -5.061223 -0.088262

44 1 0 -5.061223 5.061223 -0.088262

45 1 0 5.061223 5.061223 -0.088262

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.446866 0.000000

3 N 2.297269 1.366931 0.000000

4 C 2.257050 2.202898 1.366931 0.000000

5 C 1.362230 2.257050 2.297269 1.446866 0.000000

6 C 3.620666 3.574672 2.473672 1.414924 2.538776

7 C 4.772328 4.369610 3.047477 2.524853 3.861369

8 N 5.084594 4.294275 2.938236 3.047477 4.493621

9 C 6.449055 5.640221 4.294275 4.369610 5.807355

10 C 7.002721 6.449055 5.084594 4.772328 6.115811

11 C 6.115811 5.807355 4.493621 3.861369 5.076237

12 C 2.538776 1.414924 2.473672 3.574672 3.620666

13 C 3.861369 2.524853 3.047477 4.369610 4.772328

14 C 5.076237 3.861369 4.493621 5.807355 6.115811

15 C 6.115811 4.772328 5.084594 6.449055 7.002721

16 C 5.807355 4.369610 4.294275 5.640221 6.449055

17 N 4.493621 3.047477 2.938236 4.294275 5.084594

18 C 6.944590 5.499597 5.142585 6.404829 7.408858

19 C 7.169813 5.773579 5.085215 6.179561 7.376115

20 C 8.541113 7.169813 6.385004 7.376115 8.649063

21 C 8.649063 7.376115 6.385004 7.169813 8.541113

22 C 7.376115 6.179561 5.085215 5.773579 7.169813

23 N 6.385004 5.085215 4.155293 5.085215 6.385004

24 H 1.079583 2.252655 3.330761 3.312998 2.194282

25 H 2.194282 3.312998 3.330761 2.252655 1.079583

26 H 8.074044 7.526091 6.160988 5.836117 7.157238

27 H 6.504520 6.416758 5.179368 4.311961 5.323969

28 H 5.323969 4.311961 5.179368 6.416758 6.504520

29 H 7.157238 5.836117 6.160988 7.526091 8.074044

30 H 9.419128 8.016177 7.327322 8.376192 9.610897

31 H 9.610897 8.376192 7.327322 8.016177 9.419128

32 Zn 4.338750 3.105000 2.096778 3.105000 4.338750

33 C 7.408858 6.404829 5.142585 5.499597 6.944590

34 C 8.762097 7.807990 6.522077 6.763573 8.207517

35 C 2.890810 2.420531 3.718939 4.591052 4.215186

36 C 9.922110 8.999920 7.701647 7.875536 9.312078

37 C 3.625824 3.506253 4.850163 5.591806 4.987992

38 C 4.215186 4.591052 3.718939 2.420531 2.890810

39 C 4.987992 5.591806 4.850163 3.506253 3.625824

40 C 8.207517 6.763573 6.522077 7.807990 8.762097

41 C 9.312078 7.875536 7.701647 8.999920 9.922110

42 H 10.308693 8.880201 8.751655 10.057668 10.957110

43 H 10.957110 10.057668 8.751655 8.880201 10.308693

44 H 5.796663 6.535591 5.876201 4.518322 4.451091

45 H 4.451091 4.518322 5.876201 6.535591 5.796663

6 7 8 9 10

6 C 0.000000

7 C 1.414924 0.000000

8 N 2.473672 1.366931 0.000000

9 C 3.574672 2.202898 1.366931 0.000000

10 C 3.620666 2.257050 2.297269 1.446866 0.000000

11 C 2.538776 1.446866 2.297269 2.257050 1.362230

12 C 4.891863 5.499597 5.142585 6.404829 7.408858

13 C 5.499597 5.773579 5.085215 6.179561 7.376115

14 C 6.944590 7.169813 6.385004 7.376115 8.649063

15 C 7.408858 7.376115 6.385004 7.169813 8.541113

16 C 6.404829 6.179561 5.085215 5.773579 7.169813

17 N 5.142585 5.085215 4.155293 5.085215 6.385004

18 C 6.918138 6.404829 5.142585 5.499597 6.944590

19 C 6.404829 5.640221 4.294275 4.369610 5.807355

20 C 7.408858 6.449055 5.084594 4.772328 6.115811

21 C 6.944590 5.807355 4.493621 3.861369 5.076237

22 C 5.499597 4.369610 3.047477 2.524853 3.861369

23 N 5.142585 4.294275 2.938236 3.047477 4.493621

24 H 4.638397 5.836117 6.160988 7.526091 8.074044

25 H 2.899925 4.311961 5.179368 6.416758 6.504520

26 H 4.638397 3.312998 3.330761 2.252655 1.079583

27 H 2.899925 2.252655 3.330761 3.312998 2.194282

28 H 7.652174 8.016177 7.327322 8.376192 9.610897

29 H 8.465278 8.376192 7.327322 8.016177 9.419128

30 H 8.465278 7.526091 6.160988 5.836117 7.157238

31 H 7.652174 6.416758 5.179368 4.311961 5.323969

32 Zn 3.473076 3.105000 2.096778 3.105000 4.338750

33 C 4.891863 3.574672 2.473672 1.414924 2.538776

34 C 5.985813 4.591052 3.718939 2.420531 2.890810

35 C 5.985813 6.763573 6.522077 7.807990 8.762097

36 C 7.004574 5.591806 4.850163 3.506253 3.625824

37 C 7.004574 7.875536 7.701647 8.999920 9.922110

38 C 1.426315 2.420531 3.718939 4.591052 4.215186

39 C 2.632182 3.506253 4.850163 5.591806 4.987992

40 C 8.344192 7.807990 6.522077 6.763573 8.207517

41 C 9.549854 8.999920 7.701647 7.875536 9.312078

42 H 10.617026 10.057668 8.751655 8.880201 10.308693

43 H 7.950071 6.535591 5.876201 4.518322 4.451091

44 H 3.699461 4.518322 5.876201 6.535591 5.796663

45 H 7.950071 8.880201 8.751655 10.057668 10.957110

11 12 13 14 15

11 C 0.000000

12 C 6.944590 0.000000

13 C 7.169813 1.414924 0.000000

14 C 8.541113 2.538776 1.446866 0.000000

15 C 8.649063 3.620666 2.257050 1.362230 0.000000

16 C 7.376115 3.574672 2.202898 2.257050 1.446866

17 N 6.385004 2.473672 1.366931 2.297269 2.297269

18 C 7.408858 4.891863 3.574672 3.620666 2.538776

19 C 6.449055 5.499597 4.369610 4.772328 3.861369

20 C 7.002721 6.944590 5.807355 6.115811 5.076237

21 C 6.115811 7.408858 6.449055 7.002721 6.115811

22 C 4.772328 6.404829 5.640221 6.449055 5.807355

23 N 5.084594 5.142585 4.294275 5.084594 4.493621

24 H 7.157238 2.899925 4.311961 5.323969 6.504520

25 H 5.323969 4.638397 5.836117 7.157238 8.074044

26 H 2.194282 8.465278 8.376192 9.610897 9.419128

27 H 1.079583 7.652174 8.016177 9.419128 9.610897

28 H 9.419128 2.899925 2.252655 1.079583 2.194282

29 H 9.610897 4.638397 3.312998 2.194282 1.079583

30 H 8.074044 7.652174 6.416758 6.504520 5.323969

31 H 6.504520 8.465278 7.526091 8.074044 7.157238

32 Zn 4.338750 3.473076 3.105000 4.338750 4.338750

33 C 3.620666 6.918138 6.404829 7.408858 6.944590

34 C 4.215186 8.344192 7.807990 8.762097 8.207517

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36 C 4.987992 9.549854 8.999920 9.922110 9.312078

37 C 9.312078 2.632182 3.506253 3.625824 4.987992

38 C 2.890810 5.985813 6.763573 8.207517 8.762097

39 C 3.625824 7.004574 7.875536 9.312078 9.922110

40 C 8.762097 5.985813 4.591052 4.215186 2.890810

41 C 9.922110 7.004574 5.591806 4.987992 3.625824

42 H 10.957110 7.950071 6.535591 5.796663 4.451091

43 H 5.796663 10.617026 10.057668 10.957110 10.308693

44 H 4.451091 7.950071 8.880201 10.308693 10.957110

45 H 10.308693 3.699461 4.518322 4.451091 5.796663

16 17 18 19 20

16 C 0.000000

17 N 1.366931 0.000000

18 C 1.414924 2.473672 0.000000

19 C 2.524853 3.047477 1.414924 0.000000

20 C 3.861369 4.493621 2.538776 1.446866 0.000000

21 C 4.772328 5.084594 3.620666 2.257050 1.362230

22 C 4.369610 4.294275 3.574672 2.202898 2.257050

23 N 3.047477 2.938236 2.473672 1.366931 2.297269

24 H 6.416758 5.179368 7.652174 8.016177 9.419128

25 H 7.526091 6.160988 8.465278 8.376192 9.610897

26 H 8.016177 7.327322 7.652174 6.416758 6.504520

27 H 8.376192 7.327322 8.465278 7.526091 8.074044

28 H 3.312998 3.330761 4.638397 5.836117 7.157238

29 H 2.252655 3.330761 2.899925 4.311961 5.323969

30 H 4.311961 5.179368 2.899925 2.252655 1.079583

31 H 5.836117 6.160988 4.638397 3.312998 2.194282

32 Zn 3.105000 2.096778 3.473076 3.105000 4.338750

33 C 5.499597 5.142585 4.891863 3.574672 3.620666

34 C 6.763573 6.522077 5.985813 4.591052 4.215186

35 C 4.591052 3.718939 5.985813 6.763573 8.207517

36 C 7.875536 7.701647 7.004574 5.591806 4.987992

37 C 5.591806 4.850163 7.004574 7.875536 9.312078

38 C 7.807990 6.522077 8.344192 7.807990 8.762097

39 C 8.999920 7.701647 9.549854 8.999920 9.922110

40 C 2.420531 3.718939 1.426315 2.420531 2.890810

41 C 3.506253 4.850163 2.632182 3.506253 3.625824

42 H 4.518322 5.876201 3.699461 4.518322 4.451091

43 H 8.880201 8.751655 7.950071 6.535591 5.796663

44 H 10.057668 8.751655 10.617026 10.057668 10.957110

45 H 6.535591 5.876201 7.950071 8.880201 10.308693

21 22 23 24 25

21 C 0.000000

22 C 1.446866 0.000000

23 N 2.297269 1.366931 0.000000

24 H 9.610897 8.376192 7.327322 0.000000

25 H 9.419128 8.016177 7.327322 2.678972 0.000000

26 H 5.323969 4.311961 5.179368 9.142831 7.491953

27 H 7.157238 5.836117 6.160988 7.491953 5.354192

28 H 8.074044 7.526091 6.160988 5.354192 7.491953

29 H 6.504520 6.416758 5.179368 7.491953 9.142831

30 H 2.194282 3.312998 3.330761 10.250943 10.595222

31 H 1.079583 2.252655 3.330761 10.595222 10.250943

32 Zn 4.338750 3.105000 2.096778 5.311592 5.311592

33 C 2.538776 1.414924 2.473672 8.465278 7.652174

34 C 2.890810 2.420531 3.718939 9.828217 8.836633

35 C 8.762097 7.807990 6.522077 2.695759 5.076897

36 C 3.625824 3.506253 4.850163 10.992990 9.887907

37 C 9.922110 8.999920 7.701647 3.078153 5.705273

38 C 8.207517 6.763573 6.522077 5.076897 2.695759

39 C 9.312078 7.875536 7.701647 5.705273 3.078153

40 C 4.215186 4.591052 3.718939 8.836633 9.828217

41 C 4.987992 5.591806 4.850163 9.887907 10.992990

42 H 5.796663 6.535591 5.876201 10.845281 12.030705

43 H 4.451091 4.518322 5.876201 12.030705 10.845281

44 H 10.308693 8.880201 8.751655 6.401035 3.722298

45 H 10.957110 10.057668 8.751655 3.722298 6.401035

26 27 28 29 30

26 H 0.000000

27 H 2.678972 0.000000

28 H 10.595222 10.250943 0.000000

29 H 10.250943 10.595222 2.678972 0.000000

30 H 7.491953 9.142831 7.491953 5.354192 0.000000

31 H 5.354192 7.491953 9.142831 7.491953 2.678972

32 Zn 5.311592 5.311592 5.311592 5.311592 5.311592

33 C 2.899925 4.638397 8.465278 7.652174 4.638397

34 C 2.695759 5.076897 9.828217 8.836633 5.076897

35 C 9.828217 8.836633 2.695759 5.076897 8.836633

36 C 3.078153 5.705273 10.992990 9.887907 5.705273

37 C 10.992990 9.887907 3.078153 5.705273 9.887907

38 C 5.076897 2.695759 8.836633 9.828217 9.828217

39 C 5.705273 3.078153 9.887907 10.992990 10.992990

40 C 8.836633 9.828217 5.076897 2.695759 2.695759

41 C 9.887907 10.992990 5.705273 3.078153 3.078153

42 H 10.845281 12.030705 6.401035 3.722298 3.722298

43 H 3.722298 6.401035 12.030705 10.845281 6.401035

44 H 6.401035 3.722298 10.845281 12.030705 12.030705

45 H 12.030705 10.845281 3.722298 6.401035 10.845281

31 32 33 34 35

31 H 0.000000

32 Zn 5.311592 0.000000

33 C 2.899925 3.473076 0.000000

34 C 2.695759 4.896997 1.426315 0.000000

35 C 9.828217 4.896997 8.344192 9.770139 0.000000

36 C 3.078153 6.101822 2.632182 1.205868 10.975714

37 C 10.992990 6.101822 9.549854 10.975714 1.205868

38 C 8.836633 4.896997 5.985813 6.908531 6.908531

39 C 9.887907 6.101822 7.004574 7.807702 7.807702

40 C 5.076897 4.896997 5.985813 6.908531 6.908531

41 C 5.705273 6.101822 7.004574 7.807702 7.807702

42 H 6.401035 7.168393 7.950071 8.665935 8.665935

43 H 3.722298 7.168393 3.699461 2.273146 12.042826

44 H 10.845281 7.168393 7.950071 8.665935 8.665935

45 H 12.030705 7.168393 10.617026 12.042826 2.273146

36 37 38 39 40

36 C 0.000000

37 C 12.181216 0.000000

38 C 7.807702 7.807702 0.000000

39 C 8.613421 8.613421 1.205868 0.000000

40 C 7.807702 7.807702 9.770139 10.975714 0.000000

41 C 8.613421 8.613421 10.975714 12.181216 1.205868

42 H 9.398296 9.398296 12.042826 13.248277 2.273146

43 H 1.067280 13.248277 8.665935 9.398296 8.665935

44 H 9.398296 9.398296 2.273146 1.067280 12.042826

45 H 13.248277 1.067280 8.665935 9.398296 8.665935

41 42 43 44 45

41 C 0.000000

42 H 1.067280 0.000000

43 H 9.398296 10.122445 0.000000

44 H 13.248277 14.315299 10.122445 0.000000

45 H 9.398296 10.122445 14.315299 10.122445 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

RotChk: IX=3 Diff= 3.53D-19

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681115 -4.270557 -0.062318

2 6 0 -1.101449 -2.886790 -0.018402

3 7 0 0.000000 -2.077647 0.006053

4 6 0 1.101449 -2.886790 -0.018402

5 6 0 0.681115 -4.270557 -0.062318

6 6 0 2.445931 -2.445931 -0.022948

7 6 0 2.886790 -1.101449 -0.018402

8 7 0 2.077647 0.000000 0.006053

9 6 0 2.886790 1.101449 -0.018402

10 6 0 4.270557 0.681115 -0.062318

11 6 0 4.270557 -0.681115 -0.062318

12 6 0 -2.445931 -2.445931 -0.022948

13 6 0 -2.886790 -1.101449 -0.018402

14 6 0 -4.270557 -0.681115 -0.062318

15 6 0 -4.270557 0.681115 -0.062318

16 6 0 -2.886790 1.101449 -0.018402

17 7 0 -2.077647 0.000000 0.006053

18 6 0 -2.445931 2.445931 -0.022948

19 6 0 -1.101449 2.886790 -0.018402

20 6 0 -0.681115 4.270557 -0.062318

21 6 0 0.681115 4.270557 -0.062318

22 6 0 1.101449 2.886790 -0.018402

23 7 0 0.000000 2.077647 0.006053

24 1 0 -1.339486 -5.125472 -0.096475

25 1 0 1.339486 -5.125472 -0.096475

26 1 0 5.125472 1.339486 -0.096475

27 1 0 5.125472 -1.339486 -0.096475

28 1 0 -5.125472 -1.339486 -0.096475

29 1 0 -5.125472 1.339486 -0.096475

30 1 0 -1.339486 5.125472 -0.096475

31 1 0 1.339486 5.125472 -0.096475

32 30 0 0.000000 0.000000 0.288651

33 6 0 2.445931 2.445931 -0.022948

34 6 0 3.454266 3.454266 -0.052933

35 6 0 -3.454266 -3.454266 -0.052933

36 6 0 4.306710 4.306710 -0.081117

37 6 0 -4.306710 -4.306710 -0.081117

38 6 0 3.454266 -3.454266 -0.052933

39 6 0 4.306710 -4.306710 -0.081117

40 6 0 -3.454266 3.454266 -0.052933

41 6 0 -4.306710 4.306710 -0.081117

42 1 0 -5.061223 5.061223 -0.103664

43 1 0 5.061223 5.061223 -0.103664

44 1 0 5.061223 -5.061223 -0.103664

45 1 0 -5.061223 -5.061223 -0.103664

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

Rotational constants (GHZ): 0.1464986 0.1464986 0.0733836

Leave Link 202 at Fri Jul 26 14:15:27 2019, MaxMem= 1342177280 cpu: 0.1

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 184 symmetry adapted cartesian basis functions of A1 symmetry.

There are 155 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3060.7524501237 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= 9 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= -0.1305121026 Hartrees.

Nuclear repulsion after empirical dispersion term = 3060.6219380211 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: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3890

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.13D-05

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 172

GePol: Fraction of low-weight points (<1% of avg) = 4.42%

GePol: Cavity surface area = 415.524 Ang\*\*2

GePol: Cavity volume = 419.874 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0084664208 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3060.6304044419 Hartrees.

Leave Link 301 at Fri Jul 26 14:15:27 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44832.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.38D-05 NBF= 172 148 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 172 148 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:15:27 2019, MaxMem= 1342177280 cpu: 6.5

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:15:27 2019, MaxMem= 1342177280 cpu: 0.8

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

Initial guess from the checkpoint file: "ZnTSPsim0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Occupied (E) (E) (B2) (A1) (E) (E) (B1) (A1) (B2) (E) (E)

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

(E) (E) (A1) (A2) (E) (E) (B1) (B1) (E) (E) (A1)

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

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

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(E) (E) (A2) (A1)

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(E) (E) (E) (E) (E) (E) (E) (E) (E) (E) (E) (E)

(E) (E) (E)

The electronic state of the initial guess is 1-A1.

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= -1359.45272755797

Leave Link 401 at Fri Jul 26 14:15:29 2019, MaxMem= 1342177280 cpu: 21.1

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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.

An orbital has undefined symmetry, so N\*\*3 symmetry is turned off.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 660000000 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= 0 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= 45396300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.77D-15 for 313.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.25D-15 for 2416 971.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.88D-15 for 318.

Iteration 1 A^-1\*A deviation from orthogonality is 1.89D-14 for 2135 2117.

E= -1359.05863816483

DIIS: error= 1.90D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.05863816483 IErMin= 1 ErrMin= 1.90D-03

ErrMax= 1.90D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.32D-03 BMatP= 2.32D-03

IDIUse=3 WtCom= 9.81D-01 WtEn= 1.90D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 3.207 Goal= None Shift= 0.000

GapD= 3.207 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=2.75D-04 MaxDP=1.24D-02 OVMax= 9.47D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.74D-04 CP: 9.97D-01

E= -1359.06174281677 Delta-E= -0.003104651938 Rises=F Damp=F

DIIS: error= 5.11D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.06174281677 IErMin= 2 ErrMin= 5.11D-04

ErrMax= 5.11D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.47D-05 BMatP= 2.32D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.11D-03

Coeff-Com: -0.221D-01 0.102D+01

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

Coeff: -0.220D-01 0.102D+01

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.61D-05 MaxDP=8.29D-04 DE=-3.10D-03 OVMax= 2.27D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.59D-05 CP: 9.98D-01 1.01D+00

E= -1359.06173296360 Delta-E= 0.000009853167 Rises=F Damp=F

DIIS: error= 7.54D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1359.06174281677 IErMin= 2 ErrMin= 5.11D-04

ErrMax= 7.54D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.86D-05 BMatP= 4.47D-05

IDIUse=3 WtCom= 2.67D-01 WtEn= 7.33D-01

Coeff-Com: -0.285D-01 0.619D+00 0.410D+00

Coeff-En: 0.000D+00 0.549D+00 0.451D+00

Coeff: -0.761D-02 0.567D+00 0.440D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.66D-05 MaxDP=7.20D-04 DE= 9.85D-06 OVMax= 2.12D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 7.83D-06 CP: 9.97D-01 1.02D+00 4.53D-01

E= -1359.06179621869 Delta-E= -0.000063255090 Rises=F Damp=F

DIIS: error= 1.54D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.06179621869 IErMin= 4 ErrMin= 1.54D-04

ErrMax= 1.54D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.06D-06 BMatP= 4.47D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.54D-03

Coeff-Com: -0.107D-01 0.165D+00 0.238D+00 0.608D+00

Coeff-En: 0.000D+00 0.000D+00 0.388D-01 0.961D+00

Coeff: -0.106D-01 0.165D+00 0.237D+00 0.608D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=3.69D-06 MaxDP=1.98D-04 DE=-6.33D-05 OVMax= 6.13D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.64D-06 CP: 9.97D-01 1.02D+00 5.29D-01 7.87D-01

E= -1359.06180111626 Delta-E= -0.000004897568 Rises=F Damp=F

DIIS: error= 8.18D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.06180111626 IErMin= 5 ErrMin= 8.18D-05

ErrMax= 8.18D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.37D-07 BMatP= 6.06D-06

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

Coeff-Com: -0.198D-02 0.735D-02 0.766D-01 0.347D+00 0.571D+00

Coeff: -0.198D-02 0.735D-02 0.766D-01 0.347D+00 0.571D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=1.28D-06 MaxDP=3.81D-05 DE=-4.90D-06 OVMax= 1.27D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 7.80D-07 CP: 9.98D-01 1.02D+00 5.32D-01 8.78D-01 7.32D-01

E= -1359.06180154320 Delta-E= -0.000000426940 Rises=F Damp=F

DIIS: error= 1.20D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.06180154320 IErMin= 6 ErrMin= 1.20D-05

ErrMax= 1.20D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.78D-08 BMatP= 6.37D-07

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

Coeff-Com: 0.180D-03-0.128D-01 0.779D-02 0.745D-01 0.203D+00 0.727D+00

Coeff: 0.180D-03-0.128D-01 0.779D-02 0.745D-01 0.203D+00 0.727D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=3.08D-07 MaxDP=6.97D-06 DE=-4.27D-07 OVMax= 2.06D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.75D-07 CP: 9.98D-01 1.02D+00 5.36D-01 8.79D-01 7.62D-01

CP: 7.31D-01

E= -1359.06180155282 Delta-E= -0.000000009621 Rises=F Damp=F

DIIS: error= 4.65D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.06180155282 IErMin= 7 ErrMin= 4.65D-06

ErrMax= 4.65D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.76D-09 BMatP= 1.78D-08

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

Coeff-Com: 0.221D-03-0.841D-02 0.761D-03 0.270D-01 0.940D-01 0.455D+00

Coeff-Com: 0.431D+00

Coeff: 0.221D-03-0.841D-02 0.761D-03 0.270D-01 0.940D-01 0.455D+00

Coeff: 0.431D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=9.34D-08 MaxDP=5.69D-06 DE=-9.62D-09 OVMax= 1.59D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.90D-08 CP: 9.98D-01 1.02D+00 5.37D-01 8.80D-01 7.64D-01

CP: 7.21D-01 6.56D-01

E= -1359.06180155749 Delta-E= -0.000000004668 Rises=F Damp=F

DIIS: error= 1.12D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.06180155749 IErMin= 8 ErrMin= 1.12D-06

ErrMax= 1.12D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.52D-10 BMatP= 5.76D-09

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

Coeff-Com: 0.996D-04-0.316D-02-0.298D-03 0.653D-02 0.279D-01 0.172D+00

Coeff-Com: 0.241D+00 0.556D+00

Coeff: 0.996D-04-0.316D-02-0.298D-03 0.653D-02 0.279D-01 0.172D+00

Coeff: 0.241D+00 0.556D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=2.84D-08 MaxDP=1.50D-06 DE=-4.67D-09 OVMax= 4.19D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.36D-08 CP: 9.98D-01 1.02D+00 5.37D-01 8.80D-01 7.65D-01

CP: 7.21D-01 6.47D-01 7.88D-01

E= -1359.06180155800 Delta-E= -0.000000000512 Rises=F Damp=F

DIIS: error= 2.60D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1359.06180155800 IErMin= 9 ErrMin= 2.60D-07

ErrMax= 2.60D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.63D-11 BMatP= 3.52D-10

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

Coeff-Com: 0.121D-04-0.105D-03-0.252D-03-0.152D-02-0.282D-02 0.829D-02

Coeff-Com: 0.455D-01 0.283D+00 0.668D+00

Coeff: 0.121D-04-0.105D-03-0.252D-03-0.152D-02-0.282D-02 0.829D-02

Coeff: 0.455D-01 0.283D+00 0.668D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=1.11D-08 MaxDP=5.43D-07 DE=-5.12D-10 OVMax= 1.34D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 7.62D-09 CP: 9.98D-01 1.02D+00 5.37D-01 8.80D-01 7.63D-01

CP: 7.26D-01 6.65D-01 8.09D-01 7.96D-01

E= -1359.06180155797 Delta-E= 0.000000000032 Rises=F Damp=F

DIIS: error= 9.32D-08 at cycle 10 NSaved= 10.

NSaved=10 IEnMin= 9 EnMin= -1359.06180155800 IErMin=10 ErrMin= 9.32D-08

ErrMax= 9.32D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.85D-12 BMatP= 3.63D-11

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

Coeff-Com: 0.135D-05 0.852D-04-0.997D-04-0.942D-03-0.228D-02-0.392D-02

Coeff-Com: 0.960D-02 0.105D+00 0.294D+00 0.599D+00

Coeff: 0.135D-05 0.852D-04-0.997D-04-0.942D-03-0.228D-02-0.392D-02

Coeff: 0.960D-02 0.105D+00 0.294D+00 0.599D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.69D-09 MaxDP=1.41D-07 DE= 3.18D-11 OVMax= 3.33D-07

Error on total polarization charges = 0.06220

SCF Done: E(RB3LYP) = -1359.06180156 A.U. after 10 cycles

NFock= 10 Conv=0.27D-08 -V/T= 1.9682

KE= 1.403735714491D+03 PE=-9.363419476404D+03 EE= 3.539991555913D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.31

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:16:10 2019, MaxMem= 1342177280 cpu: 460.6

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44832.

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 = 260

Leave Link 701 at Fri Jul 26 14:16:14 2019, MaxMem= 1342177280 cpu: 43.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

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

Leave Link 702 at Fri Jul 26 14:16:14 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Fri Jul 26 14:16:17 2019, MaxMem= 1342177280 cpu: 43.0

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-1.56319402D-13-8.73967565D-13 5.89065833D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000170936 -0.000099116 0.000005701

2 6 0.000047647 0.000043516 -0.000334839

3 7 0.000000000 -0.000308254 0.003237973

4 6 -0.000047647 0.000043516 -0.000334839

5 6 0.000170936 -0.000099116 0.000005701

6 6 0.000581911 -0.000581911 -0.000040714

7 6 -0.000043516 0.000047647 -0.000334839

8 7 0.000308254 0.000000000 0.003237973

9 6 -0.000043516 -0.000047647 -0.000334839

10 6 0.000099116 0.000170936 0.000005701

11 6 0.000099116 -0.000170936 0.000005701

12 6 -0.000581911 -0.000581911 -0.000040714

13 6 0.000043516 0.000047647 -0.000334839

14 6 -0.000099116 -0.000170936 0.000005701

15 6 -0.000099116 0.000170936 0.000005701

16 6 0.000043516 -0.000047647 -0.000334839

17 7 -0.000308254 0.000000000 0.003237973

18 6 -0.000581911 0.000581911 -0.000040714

19 6 0.000047647 -0.000043516 -0.000334839

20 6 -0.000170936 0.000099116 0.000005701

21 6 0.000170936 0.000099116 0.000005701

22 6 -0.000047647 -0.000043516 -0.000334839

23 7 0.000000000 0.000308254 0.003237973

24 1 0.000095322 0.000052720 0.000032215

25 1 -0.000095322 0.000052720 0.000032215

26 1 -0.000052720 -0.000095322 0.000032215

27 1 -0.000052720 0.000095322 0.000032215

28 1 0.000052720 0.000095322 0.000032215

29 1 0.000052720 -0.000095322 0.000032215

30 1 0.000095322 -0.000052720 0.000032215

31 1 -0.000095322 -0.000052720 0.000032215

32 30 0.000000000 0.000000000 -0.010554774

33 6 0.000581911 0.000581911 -0.000040714

34 6 -0.000361085 -0.000361085 0.000051316

35 6 0.000361085 0.000361085 0.000051316

36 6 0.000106043 0.000106043 -0.000003244

37 6 -0.000106043 -0.000106043 -0.000003244

38 6 -0.000361085 0.000361085 0.000051316

39 6 0.000106043 -0.000106043 -0.000003244

40 6 0.000361085 -0.000361085 0.000051316

41 6 -0.000106043 0.000106043 -0.000003244

42 1 0.000030742 -0.000030742 -0.000012791

43 1 -0.000030742 -0.000030742 -0.000012791

44 1 -0.000030742 0.000030742 -0.000012791

45 1 0.000030742 0.000030742 -0.000012791

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

Cartesian Forces: Max 0.010554774 RMS 0.001085032

Leave Link 716 at Fri Jul 26 14:16:18 2019, MaxMem= 1342177280 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002127429 RMS 0.000400904

Search for a local minimum.

Step number 5 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .40090D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

DE= -4.84D-04 DEPred=-1.20D-04 R= 4.03D+00

TightC=F SS= 1.41D+00 RLast= 1.74D-01 DXNew= 1.2613D-01 5.2187D-01

Trust test= 4.03D+00 RLast= 1.74D-01 DXMaxT set to 1.26D-01

ITU= 1 0 -1 -1 0

Eigenvalues --- 0.00227 0.00534 0.00534 0.00534 0.00534

Eigenvalues --- 0.00534 0.00534 0.00534 0.01187 0.01339

Eigenvalues --- 0.01339 0.01527 0.01655 0.01655 0.01662

Eigenvalues --- 0.01678 0.01805 0.01805 0.01826 0.01828

Eigenvalues --- 0.01831 0.01856 0.01859 0.01859 0.01868

Eigenvalues --- 0.01868 0.01868 0.01909 0.01919 0.01919

Eigenvalues --- 0.01920 0.01930 0.01933 0.01952 0.01952

Eigenvalues --- 0.02146 0.02162 0.02162 0.02178 0.02181

Eigenvalues --- 0.02317 0.02317 0.03322 0.03584 0.04654

Eigenvalues --- 0.04654 0.04654 0.04654 0.04654 0.04654

Eigenvalues --- 0.04654 0.05715 0.13838 0.14328 0.15096

Eigenvalues --- 0.15096 0.15999 0.15999 0.15999 0.15999

Eigenvalues --- 0.15999 0.15999 0.15999 0.16491 0.22801

Eigenvalues --- 0.22864 0.22866 0.22866 0.24468 0.24566

Eigenvalues --- 0.24616 0.24616 0.24679 0.24950 0.24950

Eigenvalues --- 0.24993 0.24997 0.24997 0.24998 0.24998

Eigenvalues --- 0.26050 0.35051 0.35051 0.35424 0.35493

Eigenvalues --- 0.35697 0.36034 0.36034 0.36034 0.36034

Eigenvalues --- 0.36034 0.36034 0.36034 0.36063 0.36772

Eigenvalues --- 0.36861 0.36861 0.37563 0.37563 0.37563

Eigenvalues --- 0.37565 0.38963 0.38963 0.39534 0.39851

Eigenvalues --- 0.41397 0.41397 0.41397 0.41451 0.41451

Eigenvalues --- 0.41737 0.41758 0.42464 0.43513 0.43779

Eigenvalues --- 0.43779 0.46561 0.47751 0.49061 0.49061

Eigenvalues --- 0.50126 0.51393 0.51895 0.51895 0.59938

Eigenvalues --- 1.01810 1.01831 1.01831 1.01831

En-DIIS/RFO-DIIS IScMMF= 0 using points: 5 4 3 2 1

RFO step: Lambda=-4.86966187D-04.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= -9.57D-05 SmlDif= 1.00D-05

RMS Error= 0.5340981900D-02 NUsed= 5 EDIIS=T

EnCoef did 1 forward-backward iterations

Rare condition: small coef for last iteration: -0.204D+01

DidBck=T Rises=F En-DIIS coefs: 0.58340 0.29349 0.00000 0.00000 0.12311

Iteration 1 RMS(Cart)= 0.09778700 RMS(Int)= 0.02657663

New curvilinear step failed, DQL= 8.78D+00 SP=-2.10D-01.

ITry= 1 IFail=1 DXMaxC= 5.66D-01 DCOld= 1.00D+10 DXMaxT= 1.26D-01 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.08880215 RMS(Int)= 0.01843800

New curvilinear step failed, DQL= 8.82D+00 SP=-2.13D-01.

ITry= 2 IFail=1 DXMaxC= 5.10D-01 DCOld= 1.00D+10 DXMaxT= 1.26D-01 DXLimC= 3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.08006824 RMS(Int)= 0.01114547

Iteration 2 RMS(Cart)= 0.01036946 RMS(Int)= 0.00354914

Iteration 3 RMS(Cart)= 0.00027795 RMS(Int)= 0.00354188

Iteration 4 RMS(Cart)= 0.00000179 RMS(Int)= 0.00354130

Iteration 5 RMS(Cart)= 0.00000022 RMS(Int)= 0.00354130

ITry= 3 IFail=0 DXMaxC= 4.39D-01 DCOld= 1.00D+10 DXMaxT= 1.26D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.77D-02 for atom 44.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73418 -0.00005 -0.00011 -0.00630 -0.00644 2.72774

R2 2.57424 -0.00010 -0.00062 0.00884 0.00206 2.57630

R3 2.04012 0.00010 0.00008 -0.00124 -0.00091 2.03920

R4 2.58312 -0.00016 0.00010 0.00919 0.00996 2.59309

R5 2.67382 -0.00018 -0.00151 0.02012 0.00769 2.68151

R6 2.58312 -0.00016 0.00010 0.00919 0.00996 2.59309

R7 3.96234 -0.00082 -0.00597 -0.03620 -0.02673 3.93560

R8 2.73418 -0.00005 -0.00011 -0.00630 -0.00644 2.72774

R9 2.67382 -0.00018 -0.00151 0.02012 0.00769 2.68151

R10 2.04012 0.00010 0.00008 -0.00124 -0.00091 2.03920

R11 2.67382 -0.00018 -0.00151 0.02012 0.00769 2.68151

R12 2.69535 0.00040 0.00018 -0.01108 -0.00676 2.68859

R13 2.58312 -0.00016 0.00010 0.00919 0.00996 2.59309

R14 2.73418 -0.00005 -0.00011 -0.00632 -0.00644 2.72774

R15 2.58312 -0.00016 0.00010 0.00919 0.00996 2.59309

R16 3.96234 -0.00082 -0.00597 -0.03619 -0.02673 3.93560

R17 2.73418 -0.00005 -0.00011 -0.00630 -0.00644 2.72774

R18 2.67382 -0.00018 -0.00151 0.02011 0.00769 2.68151

R19 2.57424 -0.00010 -0.00062 0.00884 0.00206 2.57630

R20 2.04012 0.00010 0.00008 -0.00124 -0.00091 2.03920

R21 2.04012 0.00010 0.00008 -0.00127 -0.00091 2.03920

R22 2.67382 -0.00018 -0.00151 0.02012 0.00769 2.68151

R23 2.69535 0.00040 0.00018 -0.01108 -0.00676 2.68859

R24 2.73418 -0.00005 -0.00011 -0.00632 -0.00644 2.72774

R25 2.58312 -0.00016 0.00010 0.00919 0.00996 2.59309

R26 2.57424 -0.00010 -0.00062 0.00884 0.00206 2.57630

R27 2.04012 0.00010 0.00008 -0.00127 -0.00091 2.03920

R28 2.73418 -0.00005 -0.00011 -0.00630 -0.00644 2.72774

R29 2.04012 0.00010 0.00008 -0.00124 -0.00091 2.03920

R30 2.58312 -0.00016 0.00010 0.00919 0.00996 2.59309

R31 2.67382 -0.00018 -0.00151 0.02011 0.00769 2.68151

R32 3.96234 -0.00082 -0.00597 -0.03619 -0.02673 3.93560

R33 2.67382 -0.00018 -0.00151 0.02012 0.00769 2.68151

R34 2.69535 0.00040 0.00018 -0.01108 -0.00676 2.68859

R35 2.73418 -0.00005 -0.00011 -0.00632 -0.00644 2.72774

R36 2.58312 -0.00016 0.00010 0.00919 0.00996 2.59309

R37 2.57424 -0.00010 -0.00062 0.00883 0.00206 2.57630

R38 2.04012 0.00010 0.00008 -0.00127 -0.00091 2.03920

R39 2.73418 -0.00005 -0.00011 -0.00632 -0.00644 2.72774

R40 2.04012 0.00010 0.00008 -0.00127 -0.00091 2.03920

R41 2.58312 -0.00016 0.00010 0.00919 0.00996 2.59309

R42 2.67382 -0.00018 -0.00151 0.02012 0.00769 2.68151

R43 3.96234 -0.00082 -0.00597 -0.03619 -0.02673 3.93560

R44 2.69535 0.00040 0.00018 -0.01108 -0.00676 2.68859

R45 2.27876 -0.00011 -0.00013 0.00060 0.00035 2.27911

R46 2.27876 -0.00011 -0.00013 0.00060 0.00035 2.27911

R47 2.01687 0.00004 -0.00001 -0.00003 -0.00010 2.01677

R48 2.01687 0.00004 -0.00001 -0.00003 -0.00010 2.01677

R49 2.27876 -0.00011 -0.00013 0.00060 0.00035 2.27911

R50 2.01687 0.00004 -0.00001 -0.00003 -0.00010 2.01677

R51 2.27876 -0.00011 -0.00013 0.00060 0.00035 2.27911

R52 2.01687 0.00004 -0.00001 -0.00003 -0.00010 2.01677

A1 1.86556 -0.00004 -0.00044 0.00555 0.00289 1.86845

A2 2.19094 -0.00003 0.00024 -0.01141 -0.00844 2.18250

A3 2.22665 0.00006 0.00019 0.00607 0.00550 2.23215

A4 1.90983 0.00006 0.00146 -0.01189 -0.00208 1.90775

A5 2.18211 0.00006 -0.00119 0.00575 -0.00069 2.18142

A6 2.19111 -0.00012 -0.00037 0.00576 0.00222 2.19333

A7 1.87399 -0.00005 -0.00203 0.01270 -0.00172 1.87227

A8 2.20056 0.00004 0.00096 0.01130 0.00267 2.20322

A9 2.20056 0.00004 0.00096 0.01130 0.00267 2.20322

A10 1.90983 0.00006 0.00146 -0.01189 -0.00208 1.90775

A11 2.19111 -0.00012 -0.00037 0.00576 0.00222 2.19333

A12 2.18211 0.00006 -0.00119 0.00575 -0.00069 2.18142

A13 1.86556 -0.00004 -0.00044 0.00555 0.00289 1.86845

A14 2.22665 0.00006 0.00019 0.00607 0.00550 2.23215

A15 2.19094 -0.00003 0.00024 -0.01141 -0.00844 2.18250

A16 2.20448 0.00017 -0.00119 0.00270 -0.00390 2.20059

A17 2.03930 -0.00008 0.00060 -0.00174 0.00137 2.04067

A18 2.03930 -0.00008 0.00060 -0.00161 0.00137 2.04067

A19 2.19111 -0.00012 -0.00037 0.00575 0.00222 2.19333

A20 2.18211 0.00006 -0.00119 0.00576 -0.00069 2.18142

A21 1.90983 0.00006 0.00146 -0.01189 -0.00208 1.90775

A22 1.87399 -0.00005 -0.00203 0.01270 -0.00172 1.87227

A23 2.20056 0.00004 0.00096 0.01130 0.00267 2.20322

A24 2.20056 0.00004 0.00096 0.01129 0.00267 2.20322

A25 1.90983 0.00006 0.00146 -0.01189 -0.00208 1.90775

A26 2.19111 -0.00012 -0.00037 0.00576 0.00222 2.19333

A27 2.18211 0.00006 -0.00119 0.00575 -0.00069 2.18142

A28 1.86556 -0.00004 -0.00044 0.00555 0.00289 1.86845

A29 2.19094 -0.00003 0.00024 -0.01141 -0.00844 2.18250

A30 2.22665 0.00006 0.00019 0.00607 0.00550 2.23215

A31 1.86556 -0.00004 -0.00044 0.00556 0.00289 1.86845

A32 2.19094 -0.00003 0.00024 -0.01144 -0.00844 2.18250

A33 2.22665 0.00006 0.00019 0.00608 0.00550 2.23215

A34 2.20448 0.00017 -0.00119 0.00270 -0.00390 2.20059

A35 2.03930 -0.00008 0.00060 -0.00174 0.00137 2.04067

A36 2.03930 -0.00008 0.00060 -0.00161 0.00137 2.04067

A37 2.18211 0.00006 -0.00119 0.00576 -0.00069 2.18142

A38 2.19111 -0.00012 -0.00037 0.00575 0.00222 2.19333

A39 1.90983 0.00006 0.00146 -0.01189 -0.00208 1.90775

A40 1.86556 -0.00004 -0.00044 0.00556 0.00289 1.86845

A41 2.19094 -0.00003 0.00024 -0.01144 -0.00844 2.18250

A42 2.22665 0.00006 0.00019 0.00608 0.00550 2.23215

A43 1.86556 -0.00004 -0.00044 0.00555 0.00289 1.86845

A44 2.22665 0.00006 0.00019 0.00607 0.00550 2.23215

A45 2.19094 -0.00003 0.00024 -0.01141 -0.00844 2.18250

A46 1.90983 0.00006 0.00146 -0.01189 -0.00208 1.90775

A47 2.18211 0.00006 -0.00119 0.00575 -0.00069 2.18142

A48 2.19111 -0.00012 -0.00037 0.00576 0.00222 2.19333

A49 1.87399 -0.00005 -0.00203 0.01270 -0.00172 1.87227

A50 2.20056 0.00004 0.00096 0.01130 0.00267 2.20322

A51 2.20056 0.00004 0.00096 0.01129 0.00267 2.20322

A52 2.20448 0.00017 -0.00119 0.00270 -0.00390 2.20059

A53 2.03930 -0.00008 0.00060 -0.00174 0.00137 2.04067

A54 2.03930 -0.00008 0.00060 -0.00161 0.00137 2.04067

A55 2.18211 0.00006 -0.00119 0.00576 -0.00069 2.18142

A56 2.19111 -0.00012 -0.00037 0.00575 0.00222 2.19333

A57 1.90983 0.00006 0.00146 -0.01189 -0.00208 1.90775

A58 1.86556 -0.00004 -0.00044 0.00556 0.00289 1.86845

A59 2.19094 -0.00003 0.00024 -0.01144 -0.00844 2.18250

A60 2.22665 0.00006 0.00019 0.00609 0.00550 2.23215

A61 1.86556 -0.00004 -0.00044 0.00556 0.00289 1.86845

A62 2.22665 0.00006 0.00019 0.00609 0.00550 2.23215

A63 2.19094 -0.00003 0.00024 -0.01144 -0.00844 2.18250

A64 1.90983 0.00006 0.00146 -0.01189 -0.00208 1.90775

A65 2.18211 0.00006 -0.00119 0.00576 -0.00069 2.18142

A66 2.19111 -0.00012 -0.00037 0.00575 0.00222 2.19333

A67 1.87399 -0.00005 -0.00203 0.01270 -0.00172 1.87227

A68 2.20056 0.00004 0.00096 0.01130 0.00267 2.20322

A69 2.20056 0.00004 0.00096 0.01130 0.00267 2.20322

A70 1.55263 0.00028 -0.00024 0.04559 0.01817 1.57080

A71 1.55263 0.00028 -0.00024 0.04559 0.01817 1.57080

A72 2.87122 0.00213 -0.00166 0.34136 0.26907 3.14029

A73 2.87122 0.00213 -0.00166 0.34136 0.26907 3.14029

A74 1.55263 0.00028 -0.00024 0.04560 0.01817 1.57080

A75 1.55263 0.00028 -0.00024 0.04560 0.01817 1.57080

A76 2.20448 0.00017 -0.00119 0.00270 -0.00390 2.20059

A77 2.03930 -0.00008 0.00060 -0.00174 0.00137 2.04067

A78 2.03930 -0.00008 0.00060 -0.00161 0.00137 2.04067

A79 3.14155 0.00000 0.00001 -0.00170 -0.00016 3.14139

A80 3.14155 0.00000 0.00001 -0.00170 -0.00016 3.14139

A81 3.14163 0.00000 0.00008 -0.00829 -0.00005 3.14159

A82 3.14163 0.00000 0.00008 -0.00829 -0.00005 3.14159

A83 3.14155 0.00000 0.00001 -0.00170 -0.00016 3.14139

A84 3.14163 0.00000 0.00008 -0.00829 -0.00005 3.14159

A85 3.14155 0.00000 0.00001 -0.00170 -0.00016 3.14139

A86 3.14163 0.00000 0.00008 -0.00829 -0.00005 3.14159

A87 3.13923 -0.00007 0.00069 -0.04005 -0.03144 3.10778

A88 3.14396 0.00007 -0.00069 0.04005 0.03144 3.17540

A89 3.14418 -0.00002 0.01158 0.02416 0.03100 3.17517

A90 3.13901 0.00002 -0.01158 -0.02416 -0.03100 3.10801

A91 3.13923 -0.00007 0.00069 -0.04005 -0.03144 3.10778

A92 3.14418 -0.00002 0.01158 0.02416 0.03100 3.17517

A93 3.14396 0.00007 -0.00069 0.04005 0.03144 3.17540

A94 3.13901 0.00002 -0.01158 -0.02416 -0.03100 3.10801

D1 0.00095 0.00013 0.00006 -0.01171 -0.00931 -0.00836

D2 3.12560 0.00029 -0.00211 -0.03526 -0.03031 3.09529

D3 -3.13265 -0.00003 0.00078 -0.03826 -0.02975 3.12078

D4 -0.00800 0.00013 -0.00139 -0.06181 -0.05076 -0.05876

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13339 -0.00016 0.00074 -0.02716 -0.02112 3.12867

D7 3.13339 0.00016 -0.00074 0.02716 0.02112 -3.12867

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 -0.00153 -0.00021 -0.00010 0.01891 0.01501 0.01348

D10 -3.01311 -0.00054 -0.00069 -0.26441 -0.21170 3.05838

D11 -3.12608 -0.00037 0.00212 0.04261 0.03623 -3.08985

D12 0.14553 -0.00070 0.00153 -0.24070 -0.19048 -0.04494

D13 -3.10861 -0.00062 -0.00007 0.02580 0.02082 -3.08780

D14 0.01739 -0.00008 0.00132 -0.02612 -0.01950 -0.00211

D15 0.01334 -0.00043 -0.00255 -0.00166 -0.00364 0.00971

D16 3.13935 0.00010 -0.00116 -0.05358 -0.04395 3.09539

D17 0.00153 0.00021 0.00010 -0.01891 -0.01501 -0.01348

D18 3.12608 0.00037 -0.00212 -0.04261 -0.03623 3.08985

D19 3.01311 0.00054 0.00069 0.26441 0.21170 -3.05838

D20 -0.14553 0.00070 -0.00153 0.24070 0.19048 0.04494

D21 -3.08448 -0.00085 0.00110 0.00141 0.00081 -3.08367

D22 -0.21083 0.00122 -0.00051 0.33363 0.26745 0.05662

D23 -1.64765 0.00019 0.00029 0.16752 0.13413 -1.51353

D24 0.21083 -0.00122 0.00051 -0.33363 -0.26745 -0.05662

D25 3.08448 0.00085 -0.00110 -0.00141 -0.00081 3.08367

D26 1.64765 -0.00019 -0.00029 -0.16752 -0.13413 1.51353

D27 -0.00095 -0.00013 -0.00006 0.01171 0.00931 0.00836

D28 3.13265 0.00003 -0.00078 0.03826 0.02975 -3.12078

D29 -3.12560 -0.00029 0.00211 0.03526 0.03031 -3.09529

D30 0.00800 -0.00013 0.00139 0.06181 0.05076 0.05876

D31 -0.01334 0.00043 0.00255 0.00166 0.00364 -0.00971

D32 -3.13935 -0.00010 0.00116 0.05358 0.04395 -3.09539

D33 3.10861 0.00062 0.00007 -0.02580 -0.02082 3.08780

D34 -0.01739 0.00008 -0.00132 0.02612 0.01950 0.00211

D35 0.01334 -0.00043 -0.00255 -0.00166 -0.00364 0.00971

D36 -3.10861 -0.00062 -0.00007 0.02580 0.02082 -3.08780

D37 3.13935 0.00010 -0.00116 -0.05358 -0.04395 3.09539

D38 0.01739 -0.00008 0.00132 -0.02612 -0.01950 -0.00211

D39 -3.12608 -0.00037 0.00212 0.04261 0.03623 -3.08985

D40 0.14553 -0.00070 0.00153 -0.24070 -0.19048 -0.04494

D41 -0.00153 -0.00021 -0.00010 0.01890 0.01501 0.01348

D42 -3.01311 -0.00054 -0.00069 -0.26441 -0.21170 3.05838

D43 3.12560 0.00029 -0.00211 -0.03526 -0.03031 3.09529

D44 -0.00800 0.00013 -0.00139 -0.06181 -0.05076 -0.05876

D45 0.00095 0.00013 0.00006 -0.01171 -0.00931 -0.00836

D46 -3.13265 -0.00003 0.00078 -0.03825 -0.02975 3.12078

D47 0.00153 0.00021 0.00010 -0.01891 -0.01501 -0.01348

D48 3.12608 0.00037 -0.00212 -0.04261 -0.03623 3.08985

D49 3.01311 0.00054 0.00069 0.26441 0.21170 -3.05838

D50 -0.14553 0.00070 -0.00153 0.24070 0.19048 0.04494

D51 -0.21083 0.00122 -0.00051 0.33363 0.26745 0.05662

D52 -1.64765 0.00019 0.00029 0.16753 0.13413 -1.51353

D53 -3.08448 -0.00085 0.00110 0.00141 0.00081 -3.08367

D54 3.08448 0.00085 -0.00110 -0.00142 -0.00081 3.08367

D55 1.64765 -0.00019 -0.00029 -0.16751 -0.13413 1.51353

D56 0.21083 -0.00122 0.00051 -0.33363 -0.26745 -0.05662

D57 -0.00095 -0.00013 -0.00006 0.01171 0.00931 0.00836

D58 3.13265 0.00003 -0.00078 0.03826 0.02975 -3.12078

D59 -3.12560 -0.00029 0.00211 0.03526 0.03031 -3.09529

D60 0.00800 -0.00013 0.00139 0.06181 0.05076 0.05876

D61 -0.01334 0.00043 0.00255 0.00166 0.00364 -0.00971

D62 -3.13935 -0.00010 0.00116 0.05358 0.04395 -3.09539

D63 3.10861 0.00062 0.00007 -0.02580 -0.02082 3.08780

D64 -0.01739 0.00008 -0.00132 0.02612 0.01950 0.00211

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13339 0.00016 -0.00074 0.02715 0.02112 -3.12867

D67 -3.13339 -0.00016 0.00074 -0.02716 -0.02112 3.12867

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.10861 0.00062 0.00007 -0.02580 -0.02082 3.08780

D70 -0.01334 0.00043 0.00255 0.00166 0.00364 -0.00971

D71 -0.01739 0.00008 -0.00132 0.02612 0.01950 0.00211

D72 -3.13935 -0.00010 0.00116 0.05358 0.04395 -3.09539

D73 -3.12560 -0.00029 0.00211 0.03526 0.03031 -3.09529

D74 0.00800 -0.00013 0.00139 0.06181 0.05076 0.05876

D75 -0.00095 -0.00013 -0.00006 0.01171 0.00931 0.00836

D76 3.13265 0.00003 -0.00078 0.03825 0.02975 -3.12078

D77 3.12608 0.00037 -0.00212 -0.04261 -0.03623 3.08985

D78 -0.14553 0.00070 -0.00153 0.24070 0.19048 0.04494

D79 0.00153 0.00021 0.00010 -0.01890 -0.01501 -0.01348

D80 3.01311 0.00054 0.00069 0.26441 0.21170 -3.05838

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 3.13339 0.00016 -0.00074 0.02716 0.02112 -3.12867

D83 -3.13339 -0.00016 0.00074 -0.02715 -0.02112 3.12867

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 0.00095 0.00013 0.00006 -0.01171 -0.00931 -0.00836

D86 3.12560 0.00029 -0.00211 -0.03526 -0.03031 3.09529

D87 -3.13265 -0.00003 0.00078 -0.03826 -0.02975 3.12078

D88 -0.00800 0.00013 -0.00139 -0.06181 -0.05076 -0.05876

D89 -0.00153 -0.00021 -0.00010 0.01891 0.01501 0.01348

D90 -3.01311 -0.00054 -0.00069 -0.26441 -0.21170 3.05838

D91 -3.12608 -0.00037 0.00212 0.04261 0.03623 -3.08985

D92 0.14553 -0.00070 0.00153 -0.24070 -0.19048 -0.04494

D93 -3.10861 -0.00062 -0.00007 0.02580 0.02082 -3.08780

D94 0.01739 -0.00008 0.00132 -0.02612 -0.01950 -0.00211

D95 0.01334 -0.00043 -0.00255 -0.00166 -0.00364 0.00971

D96 3.13935 0.00010 -0.00116 -0.05358 -0.04395 3.09539

D97 0.21083 -0.00122 0.00051 -0.33363 -0.26745 -0.05662

D98 1.64765 -0.00019 -0.00029 -0.16753 -0.13413 1.51353

D99 3.08448 0.00085 -0.00110 -0.00141 -0.00081 3.08367

D100 -3.08448 -0.00085 0.00110 0.00142 0.00081 -3.08367

D101 -1.64765 0.00019 0.00029 0.16751 0.13413 -1.51353

D102 -0.21083 0.00122 -0.00051 0.33363 0.26745 0.05662

D103 3.10861 0.00062 0.00007 -0.02580 -0.02082 3.08780

D104 -0.01334 0.00043 0.00255 0.00166 0.00364 -0.00971

D105 -0.01739 0.00008 -0.00132 0.02612 0.01950 0.00211

D106 -3.13935 -0.00010 0.00116 0.05358 0.04395 -3.09539

D107 -3.12560 -0.00029 0.00211 0.03527 0.03031 -3.09529

D108 0.00800 -0.00013 0.00139 0.06181 0.05076 0.05876

D109 -0.00095 -0.00013 -0.00006 0.01171 0.00931 0.00836

D110 3.13265 0.00003 -0.00078 0.03825 0.02975 -3.12078

D111 3.12608 0.00037 -0.00212 -0.04261 -0.03623 3.08985

D112 -0.14553 0.00070 -0.00153 0.24070 0.19048 0.04494

D113 0.00153 0.00021 0.00010 -0.01890 -0.01501 -0.01348

D114 3.01311 0.00054 0.00069 0.26441 0.21170 -3.05838

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.13339 0.00016 -0.00074 0.02715 0.02112 -3.12867

D117 -3.13339 -0.00016 0.00074 -0.02715 -0.02112 3.12867

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 0.00095 0.00013 0.00006 -0.01171 -0.00931 -0.00836

D120 3.12560 0.00029 -0.00211 -0.03527 -0.03031 3.09529

D121 -3.13265 -0.00003 0.00078 -0.03825 -0.02975 3.12078

D122 -0.00800 0.00013 -0.00139 -0.06181 -0.05076 -0.05876

D123 -0.00153 -0.00021 -0.00010 0.01890 0.01501 0.01348

D124 -3.01311 -0.00054 -0.00069 -0.26441 -0.21170 3.05838

D125 -3.12608 -0.00037 0.00212 0.04261 0.03623 -3.08985

D126 0.14553 -0.00070 0.00153 -0.24070 -0.19048 -0.04494

D127 -3.10861 -0.00062 -0.00007 0.02580 0.02082 -3.08780

D128 0.01739 -0.00008 0.00132 -0.02612 -0.01950 -0.00211

D129 0.01334 -0.00043 -0.00255 -0.00166 -0.00364 0.00971

D130 3.13935 0.00010 -0.00116 -0.05358 -0.04395 3.09539

D131 1.64765 -0.00019 -0.00029 -0.16753 -0.13413 1.51353

D132 3.08448 0.00085 -0.00110 -0.00142 -0.00081 3.08367

D133 0.21083 -0.00122 0.00051 -0.33363 -0.26745 -0.05662

D134 -1.64765 0.00019 0.00029 0.16753 0.13413 -1.51353

D135 -0.21083 0.00122 -0.00051 0.33363 0.26745 0.05662

D136 -3.08448 -0.00085 0.00110 0.00142 0.00081 -3.08367

Item Value Threshold Converged?

Maximum Force 0.002127 0.000450 NO

RMS Force 0.000401 0.000300 NO

Maximum Displacement 0.438565 0.001800 NO

RMS Displacement 0.078373 0.001200 NO

Predicted change in Energy=-3.208916D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:16:18 2019, MaxMem= 1342177280 cpu: 1.3

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.681660 4.270748 -0.011835

2 6 0 1.104997 2.893703 0.078208

3 7 0 0.000000 2.082630 0.142090

4 6 0 -1.104997 2.893703 0.078208

5 6 0 -0.681660 4.270748 -0.011835

6 6 0 -2.453869 2.453869 0.053039

7 6 0 -2.893703 1.104997 0.078208

8 7 0 -2.082630 0.000000 0.142090

9 6 0 -2.893703 -1.104997 0.078208

10 6 0 -4.270748 -0.681660 -0.011835

11 6 0 -4.270748 0.681660 -0.011835

12 6 0 2.453869 2.453869 0.053039

13 6 0 2.893703 1.104997 0.078208

14 6 0 4.270748 0.681660 -0.011835

15 6 0 4.270748 -0.681660 -0.011835

16 6 0 2.893703 -1.104997 0.078208

17 7 0 2.082630 0.000000 0.142090

18 6 0 2.453869 -2.453869 0.053039

19 6 0 1.104997 -2.893703 0.078208

20 6 0 0.681660 -4.270748 -0.011835

21 6 0 -0.681660 -4.270748 -0.011835

22 6 0 -1.104997 -2.893703 0.078208

23 7 0 0.000000 -2.082630 0.142090

24 1 0 1.344432 5.121162 -0.056418

25 1 0 -1.344432 5.121162 -0.056418

26 1 0 -5.121162 -1.344432 -0.056418

27 1 0 -5.121162 1.344432 -0.056418

28 1 0 5.121162 1.344432 -0.056418

29 1 0 5.121162 -1.344432 -0.056418

30 1 0 1.344432 -5.121162 -0.056418

31 1 0 -1.344432 -5.121162 -0.056418

32 30 0 0.000000 0.000000 0.143448

33 6 0 -2.453869 -2.453869 0.053039

34 6 0 -3.455918 -3.455918 -0.073389

35 6 0 3.455918 3.455918 -0.073389

36 6 0 -4.302331 -4.302331 -0.220829

37 6 0 4.302331 4.302331 -0.220829

38 6 0 -3.455918 3.455918 -0.073389

39 6 0 -4.302331 4.302331 -0.220829

40 6 0 3.455918 -3.455918 -0.073389

41 6 0 4.302331 -4.302331 -0.220829

42 1 0 5.053686 -5.053686 -0.320341

43 1 0 -5.053686 -5.053686 -0.320341

44 1 0 -5.053686 5.053686 -0.320341

45 1 0 5.053686 5.053686 -0.320341

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.443460 0.000000

3 N 2.297001 1.372202 0.000000

4 C 2.257544 2.209995 1.372202 0.000000

5 C 1.363320 2.257544 2.297001 1.443460 0.000000

6 C 3.624472 3.586031 2.483390 1.418994 2.538894

7 C 4.776328 4.380533 3.055055 2.529612 3.863058

8 N 5.089625 4.305644 2.945284 3.055055 4.497299

9 C 6.456777 5.655016 4.305644 4.380533 5.813767

10 C 7.003763 6.456777 5.089625 4.776328 6.116200

11 C 6.116200 5.813767 4.497299 3.863058 5.075737

12 C 2.538894 1.418994 2.483390 3.586031 3.624472

13 C 3.863058 2.529612 3.055055 4.380533 4.776328

14 C 5.075737 3.863058 4.497299 5.813767 6.116200

15 C 6.116200 4.776328 5.089625 6.456777 7.003763

16 C 5.813767 4.380533 4.305644 5.655016 6.456777

17 N 4.497299 3.055055 2.945284 4.305644 5.089625

18 C 6.954525 5.515126 5.158414 6.423605 7.419989

19 C 7.177512 5.787406 5.097940 6.195010 7.384417

20 C 8.541496 7.177512 6.391695 7.384417 8.649613

21 C 8.649613 7.384417 6.391695 7.177512 8.541496

22 C 7.384417 6.195010 5.097940 5.787406 7.177512

23 N 6.391695 5.097940 4.165260 5.097940 6.391695

24 H 1.079100 2.244332 3.328600 3.313518 2.197780

25 H 2.197780 3.313518 3.328600 2.244332 1.079100

26 H 8.074960 7.532926 6.165262 5.840333 7.158311

27 H 6.499081 6.417431 5.177899 4.306732 5.317376

28 H 5.317376 4.306732 5.177899 6.417431 6.499081

29 H 7.158311 5.840333 6.165262 7.532926 8.074960

30 H 9.415372 8.019570 7.330861 8.381878 9.608070

31 H 9.608070 8.381878 7.330861 8.019570 9.415372

32 Zn 4.327593 3.098192 2.082630 3.098192 4.327593

33 C 7.419989 6.423605 5.158414 5.515126 6.954525

34 C 8.764971 7.819375 6.531870 6.772555 8.209852

35 C 2.892101 2.421961 3.725013 4.597936 4.217498

36 C 9.918746 9.006194 7.707755 7.880055 9.308631

37 C 3.626835 3.506650 4.854774 5.595789 4.988470

38 C 4.217498 4.597936 3.725013 2.421961 2.892101

39 C 4.988470 5.595789 4.854774 3.506650 3.626835

40 C 8.209852 6.772555 6.531870 7.819375 8.764971

41 C 9.308631 7.880055 7.707755 9.006194 9.918746

42 H 10.303148 8.883241 8.756745 10.062267 10.951458

43 H 10.951458 10.062267 8.756745 8.883241 10.303148

44 H 5.796754 6.538635 5.880541 4.518463 4.452278

45 H 4.452278 4.518463 5.880541 6.538635 5.796754

6 7 8 9 10

6 C 0.000000

7 C 1.418994 0.000000

8 N 2.483390 1.372202 0.000000

9 C 3.586031 2.209995 1.372202 0.000000

10 C 3.624472 2.257544 2.297001 1.443460 0.000000

11 C 2.538894 1.443460 2.297001 2.257544 1.363320

12 C 4.907739 5.515126 5.158414 6.423605 7.419989

13 C 5.515126 5.787406 5.097940 6.195010 7.384417

14 C 6.954525 7.177512 6.391695 7.384417 8.649613

15 C 7.419989 7.384417 6.391695 7.177512 8.541496

16 C 6.423605 6.195010 5.097940 5.787406 7.177512

17 N 5.158414 5.097940 4.165260 5.097940 6.391695

18 C 6.940591 6.423605 5.158414 5.515126 6.954525

19 C 6.423605 5.655016 4.305644 4.380533 5.813767

20 C 7.419989 6.456777 5.089625 4.776328 6.116200

21 C 6.954525 5.813767 4.497299 3.863058 5.075737

22 C 5.515126 4.380533 3.055055 2.529612 3.863058

23 N 5.158414 4.305644 2.945284 3.055055 4.497299

24 H 4.642577 5.840333 6.165262 7.532926 8.074960

25 H 2.890896 4.306732 5.177899 6.417431 6.499081

26 H 4.642577 3.313518 3.328600 2.244332 1.079100

27 H 2.890896 2.244332 3.328600 3.313518 2.197780

28 H 7.656627 8.019570 7.330861 8.381878 9.608070

29 H 8.474678 8.381878 7.330861 8.019570 9.415372

30 H 8.474678 7.532926 6.165262 5.840333 7.158311

31 H 7.656627 6.417431 5.177899 4.306732 5.317376

32 Zn 3.471473 3.098192 2.082630 3.098192 4.327593

33 C 4.907739 3.586031 2.483390 1.418994 2.538894

34 C 5.995471 4.597936 3.725013 2.421961 2.892101

35 C 5.995471 6.772555 6.531870 7.819375 8.764971

36 C 7.009854 5.595789 4.854774 3.506650 3.626835

37 C 7.009854 7.880055 7.707755 9.006194 9.918746

38 C 1.422740 2.421961 3.725013 4.597936 4.217498

39 C 2.628426 3.506650 4.854774 5.595789 4.988470

40 C 8.358658 7.819375 6.531870 6.772555 8.209852

41 C 9.558634 9.006194 7.707755 7.880055 9.308631

42 H 10.623850 10.062267 8.756745 8.883241 10.303148

43 H 7.953732 6.538635 5.880541 4.518463 4.452278

44 H 3.695606 4.518463 5.880541 6.538635 5.796754

45 H 7.953732 8.883241 8.756745 10.062267 10.951458

11 12 13 14 15

11 C 0.000000

12 C 6.954525 0.000000

13 C 7.177512 1.418994 0.000000

14 C 8.541496 2.538894 1.443460 0.000000

15 C 8.649613 3.624472 2.257544 1.363320 0.000000

16 C 7.384417 3.586031 2.209995 2.257544 1.443460

17 N 6.391695 2.483390 1.372202 2.297001 2.297001

18 C 7.419989 4.907739 3.586031 3.624472 2.538894

19 C 6.456777 5.515126 4.380533 4.776328 3.863058

20 C 7.003763 6.954525 5.813767 6.116200 5.075737

21 C 6.116200 7.419989 6.456777 7.003763 6.116200

22 C 4.776328 6.423605 5.655016 6.456777 5.813767

23 N 5.089625 5.158414 4.305644 5.089625 4.497299

24 H 7.158311 2.890896 4.306732 5.317376 6.499081

25 H 5.317376 4.642577 5.840333 7.158311 8.074960

26 H 2.197780 8.474678 8.381878 9.608070 9.415372

27 H 1.079100 7.656627 8.019570 9.415372 9.608070

28 H 9.415372 2.890896 2.244332 1.079100 2.197780

29 H 9.608070 4.642577 3.313518 2.197780 1.079100

30 H 8.074960 7.656627 6.417431 6.499081 5.317376

31 H 6.499081 8.474678 7.532926 8.074960 7.158311

32 Zn 4.327593 3.471473 3.098192 4.327593 4.327593

33 C 3.624472 6.940591 6.423605 7.419989 6.954525

34 C 4.217498 8.358658 7.819375 8.764971 8.209852

35 C 8.209852 1.422740 2.421961 2.892101 4.217498

36 C 4.988470 9.558634 9.006194 9.918746 9.308631

37 C 9.308631 2.628426 3.506650 3.626835 4.988470

38 C 2.892101 5.995471 6.772555 8.209852 8.764971

39 C 3.626835 7.009854 7.880055 9.308631 9.918746

40 C 8.764971 5.995471 4.597936 4.217498 2.892101

41 C 9.918746 7.009854 5.595789 4.988470 3.626835

42 H 10.951458 7.953732 6.538635 5.796754 4.452278

43 H 5.796754 10.623850 10.062267 10.951458 10.303148

44 H 4.452278 7.953732 8.883241 10.303148 10.951458

45 H 10.303148 3.695606 4.518463 4.452278 5.796754

16 17 18 19 20

16 C 0.000000

17 N 1.372202 0.000000

18 C 1.418994 2.483390 0.000000

19 C 2.529612 3.055055 1.418994 0.000000

20 C 3.863058 4.497299 2.538894 1.443460 0.000000

21 C 4.776328 5.089625 3.624472 2.257544 1.363320

22 C 4.380533 4.305644 3.586031 2.209995 2.257544

23 N 3.055055 2.945284 2.483390 1.372202 2.297001

24 H 6.417431 5.177899 7.656627 8.019570 9.415372

25 H 7.532926 6.165262 8.474678 8.381878 9.608070

26 H 8.019570 7.330861 7.656627 6.417431 6.499081

27 H 8.381878 7.330861 8.474678 7.532926 8.074960

28 H 3.313518 3.328600 4.642577 5.840333 7.158311

29 H 2.244332 3.328600 2.890896 4.306732 5.317376

30 H 4.306732 5.177899 2.890896 2.244332 1.079100

31 H 5.840333 6.165262 4.642577 3.313518 2.197780

32 Zn 3.098192 2.082630 3.471473 3.098192 4.327593

33 C 5.515126 5.158414 4.907739 3.586031 3.624472

34 C 6.772555 6.531870 5.995471 4.597936 4.217498

35 C 4.597936 3.725013 5.995471 6.772555 8.209852

36 C 7.880055 7.707755 7.009854 5.595789 4.988470

37 C 5.595789 4.854774 7.009854 7.880055 9.308631

38 C 7.819375 6.531870 8.358658 7.819375 8.764971

39 C 9.006194 7.707755 9.558634 9.006194 9.918746

40 C 2.421961 3.725013 1.422740 2.421961 2.892101

41 C 3.506650 4.854774 2.628426 3.506650 3.626835

42 H 4.518463 5.880541 3.695606 4.518463 4.452278

43 H 8.883241 8.756745 7.953732 6.538635 5.796754

44 H 10.062267 8.756745 10.623850 10.062267 10.951458

45 H 6.538635 5.880541 7.953732 8.883241 10.303148

21 22 23 24 25

21 C 0.000000

22 C 1.443460 0.000000

23 N 2.297001 1.372202 0.000000

24 H 9.608070 8.381878 7.330861 0.000000

25 H 9.415372 8.019570 7.330861 2.688864 0.000000

26 H 5.317376 4.306732 5.177899 9.143730 7.487829

27 H 7.158311 5.840333 6.165262 7.487829 5.341103

28 H 8.074960 7.532926 6.165262 5.341103 7.487829

29 H 6.499081 6.417431 5.177899 7.487829 9.143730

30 H 2.197780 3.313518 3.328600 10.242324 10.589390

31 H 1.079100 2.244332 3.328600 10.589390 10.242324

32 Zn 4.327593 3.098192 2.082630 5.298466 5.298466

33 C 2.538894 1.418994 2.483390 8.474678 7.656627

34 C 2.892101 2.421961 3.725013 9.829036 8.833174

35 C 8.764971 7.819375 6.531870 2.689182 5.081012

36 C 3.626835 3.506650 4.854774 10.987046 9.878178

37 C 9.918746 9.006194 7.707755 3.073545 5.708191

38 C 8.209852 6.772555 6.531870 5.081012 2.689182

39 C 9.308631 7.880055 7.707755 5.708191 3.073545

40 C 4.217498 4.597936 3.725013 8.833174 9.829036

41 C 4.988470 5.595789 4.854774 9.878178 10.987046

42 H 5.796754 6.538635 5.880541 10.833086 12.022192

43 H 4.452278 4.518463 5.880541 12.022192 10.833086

44 H 10.303148 8.883241 8.756745 6.403914 3.719244

45 H 10.951458 10.062267 8.756745 3.719244 6.403914

26 27 28 29 30

26 H 0.000000

27 H 2.688864 0.000000

28 H 10.589390 10.242324 0.000000

29 H 10.242324 10.589390 2.688864 0.000000

30 H 7.487829 9.143730 7.487829 5.341103 0.000000

31 H 5.341103 7.487829 9.143730 7.487829 2.688864

32 Zn 5.298466 5.298466 5.298466 5.298466 5.298466

33 C 2.890896 4.642577 8.474678 7.656627 4.642577

34 C 2.689182 5.081012 9.829036 8.833174 5.081012

35 C 9.829036 8.833174 2.689182 5.081012 8.833174

36 C 3.073545 5.708191 10.987046 9.878178 5.708191

37 C 10.987046 9.878178 3.073545 5.708191 9.878178

38 C 5.081012 2.689182 8.833174 9.829036 9.829036

39 C 5.708191 3.073545 9.878178 10.987046 10.987046

40 C 8.833174 9.829036 5.081012 2.689182 2.689182

41 C 9.878178 10.987046 5.708191 3.073545 3.073545

42 H 10.833086 12.022192 6.403914 3.719244 3.719244

43 H 3.719244 6.403914 12.022192 10.833086 6.403914

44 H 6.403914 3.719244 10.833086 12.022192 12.022192

45 H 12.022192 10.833086 3.719244 6.403914 10.833086

31 32 33 34 35

31 H 0.000000

32 Zn 5.298466 0.000000

33 C 2.890896 3.471473 0.000000

34 C 2.689182 4.892214 1.422740 0.000000

35 C 9.829036 4.892214 8.358658 9.774813 0.000000

36 C 3.073545 6.095309 2.628426 1.206054 10.972812

37 C 10.987046 6.095309 9.558634 10.972812 1.206054

38 C 8.833174 4.892214 5.995471 6.911837 6.911837

39 C 9.878178 6.095309 7.009854 7.805676 7.805676

40 C 5.081012 4.892214 5.995471 6.911837 6.911837

41 C 5.708191 6.095309 7.009854 7.805676 7.805676

42 H 6.403914 7.162024 7.953732 8.661825 8.661825

43 H 3.719244 7.162024 3.695606 2.273039 12.036931

44 H 10.833086 7.162024 7.953732 8.661825 8.661825

45 H 12.022192 7.162024 10.623850 12.036931 2.273039

36 37 38 39 40

36 C 0.000000

37 C 12.168829 0.000000

38 C 7.805676 7.805676 0.000000

39 C 8.604661 8.604661 1.206054 0.000000

40 C 7.805676 7.805676 9.774813 10.972812 0.000000

41 C 8.604661 8.604661 10.972812 12.168829 1.206054

42 H 9.386665 9.386665 12.036931 13.231780 2.273039

43 H 1.067226 13.231780 8.661825 9.386665 8.661825

44 H 9.386665 9.386665 2.273039 1.067226 12.036931

45 H 13.231780 1.067226 8.661825 9.386665 8.661825

41 42 43 44 45

41 C 0.000000

42 H 1.067226 0.000000

43 H 9.386665 10.107372 0.000000

44 H 13.231780 14.293983 10.107372 0.000000

45 H 9.386665 10.107372 14.293983 10.107372 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

RotChk: IX=3 Diff= 3.92D-19

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681660 -4.270748 -0.028419

2 6 0 -1.104997 -2.893703 0.061624

3 7 0 0.000000 -2.082630 0.125507

4 6 0 1.104997 -2.893703 0.061624

5 6 0 0.681660 -4.270748 -0.028419

6 6 0 2.453869 -2.453869 0.036455

7 6 0 2.893703 -1.104997 0.061624

8 7 0 2.082630 0.000000 0.125507

9 6 0 2.893703 1.104997 0.061624

10 6 0 4.270748 0.681660 -0.028419

11 6 0 4.270748 -0.681660 -0.028419

12 6 0 -2.453869 -2.453869 0.036455

13 6 0 -2.893703 -1.104997 0.061624

14 6 0 -4.270748 -0.681660 -0.028419

15 6 0 -4.270748 0.681660 -0.028419

16 6 0 -2.893703 1.104997 0.061624

17 7 0 -2.082630 0.000000 0.125507

18 6 0 -2.453869 2.453869 0.036455

19 6 0 -1.104997 2.893703 0.061624

20 6 0 -0.681660 4.270748 -0.028419

21 6 0 0.681660 4.270748 -0.028419

22 6 0 1.104997 2.893703 0.061624

23 7 0 0.000000 2.082630 0.125507

24 1 0 -1.344432 -5.121162 -0.073002

25 1 0 1.344432 -5.121162 -0.073002

26 1 0 5.121162 1.344432 -0.073002

27 1 0 5.121162 -1.344432 -0.073002

28 1 0 -5.121162 -1.344432 -0.073002

29 1 0 -5.121162 1.344432 -0.073002

30 1 0 -1.344432 5.121162 -0.073002

31 1 0 1.344432 5.121162 -0.073002

32 30 0 0.000000 0.000000 0.126865

33 6 0 2.453869 2.453869 0.036455

34 6 0 3.455918 3.455918 -0.089972

35 6 0 -3.455918 -3.455918 -0.089972

36 6 0 4.302331 4.302331 -0.237413

37 6 0 -4.302331 -4.302331 -0.237413

38 6 0 3.455918 -3.455918 -0.089972

39 6 0 4.302331 -4.302331 -0.237413

40 6 0 -3.455918 3.455918 -0.089972

41 6 0 -4.302331 4.302331 -0.237413

42 1 0 -5.053686 5.053686 -0.336924

43 1 0 5.053686 5.053686 -0.336924

44 1 0 5.053686 -5.053686 -0.336924

45 1 0 -5.053686 -5.053686 -0.336924

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

Rotational constants (GHZ): 0.1463778 0.1463778 0.0733163

Leave Link 202 at Fri Jul 26 14:16:18 2019, MaxMem= 1342177280 cpu: 0.1

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 184 symmetry adapted cartesian basis functions of A1 symmetry.

There are 155 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3059.0858917776 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= 9 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= -0.1306116627 Hartrees.

Nuclear repulsion after empirical dispersion term = 3058.9552801148 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: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3770

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.37D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 164

GePol: Fraction of low-weight points (<1% of avg) = 4.35%

GePol: Cavity surface area = 420.994 Ang\*\*2

GePol: Cavity volume = 422.768 Ang\*\*3

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

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

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PCM non-electrostatic energy = 0.0082902222 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3058.9635703370 Hartrees.

Leave Link 301 at Fri Jul 26 14:16:18 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16219 LenP2D= 44804.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.53D-05 NBF= 172 148 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 172 148 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:16:18 2019, MaxMem= 1342177280 cpu: 6.6

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:16:19 2019, MaxMem= 1342177280 cpu: 0.8

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

Initial guess from the checkpoint file: "ZnTSPsim0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Occupied (E) (E) (B2) (A1) (E) (E) (B1) (A1) (B2) (E) (E)

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

(E) (E) (A1) (A2) (E) (E) (B1) (B1) (E) (E) (A1)

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

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

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

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

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

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

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

(E) (E) (A2) (A1)

Virtual (A1) (A1) (B2) (A1) (B2) (A1) (A1) (B2) (A1) (B2)

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(E) (E) (E)

The electronic state of the initial guess is 1-A1.

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= -1359.45045751893

Leave Link 401 at Fri Jul 26 14:16:20 2019, MaxMem= 1342177280 cpu: 21.1

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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.

An orbital has undefined symmetry, so N\*\*3 symmetry is turned off.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 660000000 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= 0 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= 42638700.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.88D-15 for 1247.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.49D-15 for 3752 536.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.55D-15 for 3769.

Iteration 1 A^-1\*A deviation from orthogonality is 3.11D-12 for 2474 2446.

E= -1359.02106825546

DIIS: error= 9.25D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.02106825546 IErMin= 1 ErrMin= 9.25D-03

ErrMax= 9.25D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.32D-02 BMatP= 3.32D-02

IDIUse=3 WtCom= 9.07D-01 WtEn= 9.25D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 3.232 Goal= None Shift= 0.000

GapD= 3.232 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=6.40D-04 MaxDP=2.70D-02 OVMax= 4.09D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.38D-04 CP: 9.95D-01

E= -1359.06118816273 Delta-E= -0.040119907262 Rises=F Damp=F

DIIS: error= 3.55D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.06118816273 IErMin= 2 ErrMin= 3.55D-03

ErrMax= 3.55D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.92D-04 BMatP= 3.32D-02

IDIUse=3 WtCom= 9.64D-01 WtEn= 3.55D-02

Coeff-Com: -0.209D-01 0.102D+01

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

Coeff: -0.202D-01 0.102D+01

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=7.40D-05 MaxDP=2.32D-03 DE=-4.01D-02 OVMax= 5.15D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 6.77D-05 CP: 9.94D-01 1.04D+00

E= -1359.06145345095 Delta-E= -0.000265288220 Rises=F Damp=F

DIIS: error= 4.74D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.06145345095 IErMin= 2 ErrMin= 3.55D-03

ErrMax= 4.74D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.06D-04 BMatP= 5.92D-04

IDIUse=3 WtCom= 1.27D-01 WtEn= 8.73D-01

Coeff-Com: -0.269D-01 0.565D+00 0.462D+00

Coeff-En: 0.000D+00 0.206D+00 0.794D+00

Coeff: -0.341D-02 0.251D+00 0.752D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=5.62D-05 MaxDP=2.39D-03 DE=-2.65D-04 OVMax= 4.38D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.23D-05 CP: 9.95D-01 1.05D+00 3.28D-01

E= -1359.06155696642 Delta-E= -0.000103515471 Rises=F Damp=F

DIIS: error= 3.60D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.06155696642 IErMin= 2 ErrMin= 3.55D-03

ErrMax= 3.60D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.86D-04 BMatP= 5.92D-04

IDIUse=3 WtCom= 9.64D-01 WtEn= 3.60D-02

Coeff-Com: -0.560D-02 0.696D-01 0.438D+00 0.498D+00

Coeff-En: 0.000D+00 0.000D+00 0.404D+00 0.596D+00

Coeff: -0.540D-02 0.671D-01 0.437D+00 0.501D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=2.62D-05 MaxDP=1.06D-03 DE=-1.04D-04 OVMax= 1.90D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 5.70D-06 CP: 9.94D-01 1.05D+00 6.31D-01 5.30D-01

E= -1359.06173767837 Delta-E= -0.000180711953 Rises=F Damp=F

DIIS: error= 1.81D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.06173767837 IErMin= 5 ErrMin= 1.81D-04

ErrMax= 1.81D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.49D-06 BMatP= 4.86D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.81D-03

Coeff-Com: -0.125D-02-0.575D-02 0.246D+00 0.331D+00 0.430D+00

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

Coeff: -0.125D-02-0.574D-02 0.246D+00 0.331D+00 0.431D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 305122 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=3.24D-06 MaxDP=2.12D-04 DE=-1.81D-04 OVMax= 6.44D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.26D-06 CP: 9.94D-01 1.05D+00 6.34D-01 5.56D-01 6.22D-01

E= -1359.06174479835 Delta-E= -0.000007119982 Rises=F Damp=F

DIIS: error= 3.85D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.06174479835 IErMin= 6 ErrMin= 3.85D-05

ErrMax= 3.85D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.13D-07 BMatP= 7.49D-06

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

Coeff-Com: 0.308D-03-0.144D-01 0.500D-01 0.835D-01 0.228D+00 0.653D+00

Coeff: 0.308D-03-0.144D-01 0.500D-01 0.835D-01 0.228D+00 0.653D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=9.71D-07 MaxDP=3.36D-05 DE=-7.12D-06 OVMax= 1.08D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.51D-07 CP: 9.94D-01 1.05D+00 6.36D-01 5.71D-01 6.64D-01

CP: 7.54D-01

E= -1359.06174517444 Delta-E= -0.000000376092 Rises=F Damp=F

DIIS: error= 5.94D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.06174517444 IErMin= 7 ErrMin= 5.94D-06

ErrMax= 5.94D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.27D-08 BMatP= 4.13D-07

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

Coeff-Com: 0.163D-03-0.619D-02 0.144D-01 0.262D-01 0.890D-01 0.295D+00

Coeff-Com: 0.581D+00

Coeff: 0.163D-03-0.619D-02 0.144D-01 0.262D-01 0.890D-01 0.295D+00

Coeff: 0.581D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.11D-07 MaxDP=8.02D-06 DE=-3.76D-07 OVMax= 2.82D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.73D-07 CP: 9.94D-01 1.05D+00 6.36D-01 5.71D-01 6.69D-01

CP: 7.59D-01 7.93D-01

E= -1359.06174518481 Delta-E= -0.000000010363 Rises=F Damp=F

DIIS: error= 2.83D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.06174518481 IErMin= 8 ErrMin= 2.83D-06

ErrMax= 2.83D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.31D-09 BMatP= 1.27D-08

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

Coeff-Com: 0.551D-04-0.174D-02 0.189D-02 0.432D-02 0.212D-01 0.834D-01

Coeff-Com: 0.324D+00 0.566D+00

Coeff: 0.551D-04-0.174D-02 0.189D-02 0.432D-02 0.212D-01 0.834D-01

Coeff: 0.324D+00 0.566D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=7.59D-08 MaxDP=3.28D-06 DE=-1.04D-08 OVMax= 1.14D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.94D-08 CP: 9.94D-01 1.05D+00 6.36D-01 5.70D-01 6.72D-01

CP: 7.69D-01 8.22D-01 7.42D-01

E= -1359.06174518689 Delta-E= -0.000000002086 Rises=F Damp=F

DIIS: error= 6.95D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1359.06174518689 IErMin= 9 ErrMin= 6.95D-07

ErrMax= 6.95D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.79D-10 BMatP= 2.31D-09

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

Coeff-Com: 0.953D-05-0.176D-03-0.650D-03-0.772D-03 0.917D-03 0.107D-01

Coeff-Com: 0.100D+00 0.279D+00 0.610D+00

Coeff: 0.953D-05-0.176D-03-0.650D-03-0.772D-03 0.917D-03 0.107D-01

Coeff: 0.100D+00 0.279D+00 0.610D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.51D-08 MaxDP=9.33D-07 DE=-2.09D-09 OVMax= 4.33D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.09D-08 CP: 9.94D-01 1.05D+00 6.36D-01 5.71D-01 6.71D-01

CP: 7.69D-01 8.32D-01 7.89D-01 8.68D-01

E= -1359.06174518724 Delta-E= -0.000000000348 Rises=F Damp=F

DIIS: error= 3.16D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1359.06174518724 IErMin=10 ErrMin= 3.16D-07

ErrMax= 3.16D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.61D-11 BMatP= 1.79D-10

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

Coeff-Com: -0.301D-06 0.921D-04-0.577D-03-0.915D-03-0.184D-02-0.320D-02

Coeff-Com: 0.216D-01 0.997D-01 0.371D+00 0.514D+00

Coeff: -0.301D-06 0.921D-04-0.577D-03-0.915D-03-0.184D-02-0.320D-02

Coeff: 0.216D-01 0.997D-01 0.371D+00 0.514D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=9.81D-09 MaxDP=3.19D-07 DE=-3.48D-10 OVMax= 1.77D-06

Error on total polarization charges = 0.06214

SCF Done: E(RB3LYP) = -1359.06174519 A.U. after 10 cycles

NFock= 10 Conv=0.98D-08 -V/T= 1.9682

KE= 1.403644734219D+03 PE=-9.359984199559D+03 EE= 3.538314149815D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.20

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:17:00 2019, MaxMem= 1342177280 cpu: 451.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16219 LenP2D= 44804.

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 Fri Jul 26 14:17:04 2019, MaxMem= 1342177280 cpu: 41.9

(Enter /apps/gaussian/g09d01/g09/l702.exe)

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

Leave Link 702 at Fri Jul 26 14:17:04 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Fri Jul 26 14:17:08 2019, MaxMem= 1342177280 cpu: 43.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-1.77635684D-14-6.82121026D-13-2.59144761D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000458790 0.001221325 0.001294745

2 6 -0.001402542 -0.003978012 -0.000242780

3 7 0.000000000 0.009550398 -0.001450470

4 6 0.001402542 -0.003978012 -0.000242780

5 6 0.000458790 0.001221325 0.001294745

6 6 0.004802143 -0.004802143 -0.000124045

7 6 0.003978012 -0.001402542 -0.000242780

8 7 -0.009550398 0.000000000 -0.001450470

9 6 0.003978012 0.001402542 -0.000242780

10 6 -0.001221325 0.000458790 0.001294745

11 6 -0.001221325 -0.000458790 0.001294745

12 6 -0.004802143 -0.004802143 -0.000124045

13 6 -0.003978012 -0.001402542 -0.000242780

14 6 0.001221325 -0.000458790 0.001294745

15 6 0.001221325 0.000458790 0.001294745

16 6 -0.003978012 0.001402542 -0.000242780

17 7 0.009550398 0.000000000 -0.001450470

18 6 -0.004802143 0.004802143 -0.000124045

19 6 -0.001402542 0.003978012 -0.000242780

20 6 -0.000458790 -0.001221325 0.001294745

21 6 0.000458790 -0.001221325 0.001294745

22 6 0.001402542 0.003978012 -0.000242780

23 7 0.000000000 -0.009550398 -0.001450470

24 1 -0.000234946 0.000802627 -0.000575252

25 1 0.000234946 0.000802627 -0.000575252

26 1 -0.000802627 0.000234946 -0.000575252

27 1 -0.000802627 -0.000234946 -0.000575252

28 1 0.000802627 -0.000234946 -0.000575252

29 1 0.000802627 0.000234946 -0.000575252

30 1 -0.000234946 -0.000802627 -0.000575252

31 1 0.000234946 -0.000802627 -0.000575252

32 30 0.000000000 0.000000000 0.001309196

33 6 0.004802143 0.004802143 -0.000124045

34 6 -0.001644130 -0.001644130 -0.000919629

35 6 0.001644130 0.001644130 -0.000919629

36 6 0.000091102 0.000091102 0.001536266

37 6 -0.000091102 -0.000091102 0.001536266

38 6 -0.001644130 0.001644130 -0.000919629

39 6 0.000091102 -0.000091102 0.001536266

40 6 0.001644130 -0.001644130 -0.000919629

41 6 -0.000091102 0.000091102 0.001536266

42 1 0.000016483 -0.000016483 -0.000322847

43 1 -0.000016483 -0.000016483 -0.000322847

44 1 -0.000016483 0.000016483 -0.000322847

45 1 0.000016483 0.000016483 -0.000322847

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

Cartesian Forces: Max 0.009550398 RMS 0.002392157

Leave Link 716 at Fri Jul 26 14:17:08 2019, MaxMem= 1342177280 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.004558763 RMS 0.001190956

Search for a local minimum.

Step number 6 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .11910D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 2 3 4 6

5

DE= 5.64D-05 DEPred=-3.21D-03 R=-1.76D-02

Trust test=-1.76D-02 RLast= 1.26D+00 DXMaxT set to 6.31D-02

ITU= -1 1 0 -1 -1 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.55703.

Iteration 1 RMS(Cart)= 0.04389646 RMS(Int)= 0.00156194

Iteration 2 RMS(Cart)= 0.00276936 RMS(Int)= 0.00086780

Iteration 3 RMS(Cart)= 0.00000220 RMS(Int)= 0.00086780

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00086780

ITry= 1 IFail=0 DXMaxC= 2.44D-01 DCOld= 1.00D+10 DXMaxT= 6.31D-02 DXLimC= 3.00D+00 Rises=T

ClnCor: largest displacement from symmetrization is 2.09D-04 for atom 37.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.72774 0.00186 0.00359 0.00000 0.00390 2.73164

R2 2.57630 -0.00077 -0.00115 0.00000 -0.00007 2.57623

R3 2.03920 0.00051 0.00051 0.00000 0.00051 2.03971

R4 2.59309 -0.00456 -0.00555 0.00000 -0.00617 2.58692

R5 2.68151 -0.00132 -0.00428 0.00000 -0.00280 2.67871

R6 2.59309 -0.00456 -0.00555 0.00000 -0.00617 2.58692

R7 3.93560 0.00286 0.01489 0.00000 0.01259 3.94819

R8 2.72774 0.00186 0.00359 0.00000 0.00390 2.73164

R9 2.68151 -0.00132 -0.00428 0.00000 -0.00280 2.67871

R10 2.03920 0.00051 0.00051 0.00000 0.00051 2.03971

R11 2.68151 -0.00132 -0.00428 0.00000 -0.00280 2.67871

R12 2.68859 0.00219 0.00376 0.00000 0.00373 2.69232

R13 2.59309 -0.00456 -0.00555 0.00000 -0.00617 2.58692

R14 2.72774 0.00186 0.00359 0.00000 0.00390 2.73164

R15 2.59309 -0.00456 -0.00555 0.00000 -0.00617 2.58692

R16 3.93560 0.00286 0.01489 0.00000 0.01259 3.94819

R17 2.72774 0.00186 0.00359 0.00000 0.00390 2.73164

R18 2.68151 -0.00132 -0.00428 0.00000 -0.00280 2.67871

R19 2.57630 -0.00077 -0.00115 0.00000 -0.00007 2.57623

R20 2.03920 0.00051 0.00051 0.00000 0.00051 2.03971

R21 2.03920 0.00051 0.00051 0.00000 0.00051 2.03971

R22 2.68151 -0.00132 -0.00428 0.00000 -0.00280 2.67871

R23 2.68859 0.00219 0.00376 0.00000 0.00373 2.69232

R24 2.72774 0.00186 0.00359 0.00000 0.00390 2.73164

R25 2.59309 -0.00456 -0.00555 0.00000 -0.00617 2.58692

R26 2.57630 -0.00077 -0.00115 0.00000 -0.00007 2.57623

R27 2.03920 0.00051 0.00051 0.00000 0.00051 2.03971

R28 2.72774 0.00186 0.00359 0.00000 0.00390 2.73164

R29 2.03920 0.00051 0.00051 0.00000 0.00051 2.03971

R30 2.59309 -0.00456 -0.00555 0.00000 -0.00617 2.58692

R31 2.68151 -0.00132 -0.00428 0.00000 -0.00280 2.67871

R32 3.93560 0.00286 0.01489 0.00000 0.01259 3.94819

R33 2.68151 -0.00132 -0.00428 0.00000 -0.00280 2.67871

R34 2.68859 0.00219 0.00376 0.00000 0.00373 2.69232

R35 2.72774 0.00186 0.00359 0.00000 0.00390 2.73164

R36 2.59309 -0.00456 -0.00555 0.00000 -0.00617 2.58692

R37 2.57630 -0.00077 -0.00115 0.00000 -0.00007 2.57623

R38 2.03920 0.00051 0.00051 0.00000 0.00051 2.03971

R39 2.72774 0.00186 0.00359 0.00000 0.00390 2.73164

R40 2.03920 0.00051 0.00051 0.00000 0.00051 2.03971

R41 2.59309 -0.00456 -0.00555 0.00000 -0.00617 2.58692

R42 2.68151 -0.00132 -0.00428 0.00000 -0.00280 2.67871

R43 3.93560 0.00286 0.01489 0.00000 0.01259 3.94819

R44 2.68859 0.00219 0.00376 0.00000 0.00373 2.69232

R45 2.27911 -0.00025 -0.00020 0.00000 -0.00020 2.27892

R46 2.27911 -0.00025 -0.00020 0.00000 -0.00020 2.27892

R47 2.01677 0.00005 0.00006 0.00000 0.00006 2.01682

R48 2.01677 0.00005 0.00006 0.00000 0.00006 2.01682

R49 2.27911 -0.00025 -0.00020 0.00000 -0.00020 2.27892

R50 2.01677 0.00005 0.00006 0.00000 0.00006 2.01682

R51 2.27911 -0.00025 -0.00020 0.00000 -0.00020 2.27892

R52 2.01677 0.00005 0.00006 0.00000 0.00006 2.01682

A1 1.86845 -0.00095 -0.00161 0.00000 -0.00134 1.86711

A2 2.18250 0.00119 0.00470 0.00000 0.00459 2.18709

A3 2.23215 -0.00024 -0.00306 0.00000 -0.00317 2.22898

A4 1.90775 0.00006 0.00116 0.00000 -0.00030 1.90745

A5 2.18142 0.00048 0.00038 0.00000 0.00136 2.18278

A6 2.19333 -0.00052 -0.00124 0.00000 -0.00070 2.19262

A7 1.87227 0.00178 0.00096 0.00000 0.00336 1.87563

A8 2.20322 -0.00086 -0.00148 0.00000 0.00035 2.20357

A9 2.20322 -0.00086 -0.00148 0.00000 0.00035 2.20357

A10 1.90775 0.00006 0.00116 0.00000 -0.00030 1.90745

A11 2.19333 -0.00052 -0.00124 0.00000 -0.00070 2.19262

A12 2.18142 0.00048 0.00038 0.00000 0.00136 2.18278

A13 1.86845 -0.00095 -0.00161 0.00000 -0.00134 1.86711

A14 2.23215 -0.00024 -0.00306 0.00000 -0.00317 2.22898

A15 2.18250 0.00119 0.00470 0.00000 0.00459 2.18709

A16 2.20059 0.00277 0.00217 0.00000 0.00327 2.20385

A17 2.04067 -0.00135 -0.00076 0.00000 -0.00123 2.03944

A18 2.04067 -0.00136 -0.00076 0.00000 -0.00123 2.03944

A19 2.19333 -0.00052 -0.00124 0.00000 -0.00070 2.19262

A20 2.18142 0.00048 0.00038 0.00000 0.00136 2.18278

A21 1.90775 0.00006 0.00116 0.00000 -0.00030 1.90745

A22 1.87227 0.00178 0.00096 0.00000 0.00336 1.87563

A23 2.20322 -0.00086 -0.00148 0.00000 0.00035 2.20357

A24 2.20322 -0.00086 -0.00148 0.00000 0.00035 2.20357

A25 1.90775 0.00006 0.00116 0.00000 -0.00030 1.90745

A26 2.19333 -0.00052 -0.00124 0.00000 -0.00070 2.19262

A27 2.18142 0.00048 0.00038 0.00000 0.00136 2.18278

A28 1.86845 -0.00095 -0.00161 0.00000 -0.00134 1.86711

A29 2.18250 0.00119 0.00470 0.00000 0.00459 2.18709

A30 2.23215 -0.00024 -0.00306 0.00000 -0.00317 2.22898

A31 1.86845 -0.00095 -0.00161 0.00000 -0.00134 1.86711

A32 2.18250 0.00119 0.00470 0.00000 0.00459 2.18709

A33 2.23215 -0.00024 -0.00306 0.00000 -0.00317 2.22898

A34 2.20059 0.00277 0.00217 0.00000 0.00327 2.20385

A35 2.04067 -0.00135 -0.00076 0.00000 -0.00123 2.03944

A36 2.04067 -0.00136 -0.00076 0.00000 -0.00123 2.03944

A37 2.18142 0.00048 0.00038 0.00000 0.00136 2.18278

A38 2.19333 -0.00052 -0.00124 0.00000 -0.00070 2.19262

A39 1.90775 0.00006 0.00116 0.00000 -0.00030 1.90745

A40 1.86845 -0.00095 -0.00161 0.00000 -0.00134 1.86711

A41 2.18250 0.00119 0.00470 0.00000 0.00459 2.18709

A42 2.23215 -0.00024 -0.00306 0.00000 -0.00317 2.22898

A43 1.86845 -0.00095 -0.00161 0.00000 -0.00134 1.86711

A44 2.23215 -0.00024 -0.00306 0.00000 -0.00317 2.22898

A45 2.18250 0.00119 0.00470 0.00000 0.00459 2.18709

A46 1.90775 0.00006 0.00116 0.00000 -0.00030 1.90745

A47 2.18142 0.00048 0.00038 0.00000 0.00136 2.18278

A48 2.19333 -0.00052 -0.00124 0.00000 -0.00070 2.19262

A49 1.87227 0.00178 0.00096 0.00000 0.00336 1.87563

A50 2.20322 -0.00086 -0.00148 0.00000 0.00035 2.20357

A51 2.20322 -0.00086 -0.00148 0.00000 0.00035 2.20357

A52 2.20059 0.00277 0.00217 0.00000 0.00327 2.20385

A53 2.04067 -0.00135 -0.00076 0.00000 -0.00123 2.03944

A54 2.04067 -0.00136 -0.00076 0.00000 -0.00123 2.03944

A55 2.18142 0.00048 0.00038 0.00000 0.00136 2.18278

A56 2.19333 -0.00052 -0.00124 0.00000 -0.00070 2.19262

A57 1.90775 0.00006 0.00116 0.00000 -0.00030 1.90745

A58 1.86845 -0.00095 -0.00161 0.00000 -0.00134 1.86711

A59 2.18250 0.00119 0.00470 0.00000 0.00459 2.18709

A60 2.23215 -0.00024 -0.00306 0.00000 -0.00317 2.22898

A61 1.86845 -0.00095 -0.00161 0.00000 -0.00134 1.86711

A62 2.23215 -0.00024 -0.00306 0.00000 -0.00317 2.22898

A63 2.18250 0.00119 0.00470 0.00000 0.00459 2.18709

A64 1.90775 0.00006 0.00116 0.00000 -0.00030 1.90745

A65 2.18142 0.00048 0.00038 0.00000 0.00136 2.18278

A66 2.19333 -0.00052 -0.00124 0.00000 -0.00070 2.19262

A67 1.87227 0.00178 0.00096 0.00000 0.00336 1.87563

A68 2.20322 -0.00086 -0.00148 0.00000 0.00035 2.20357

A69 2.20322 -0.00086 -0.00148 0.00000 0.00035 2.20357

A70 1.57080 0.00000 -0.01012 0.00000 -0.00569 1.56511

A71 1.57080 0.00000 -0.01012 0.00000 -0.00569 1.56511

A72 3.14029 0.00068 -0.14988 0.00000 -0.14972 2.99057

A73 3.14029 0.00068 -0.14988 0.00000 -0.14972 2.99057

A74 1.57080 0.00000 -0.01012 0.00000 -0.00569 1.56511

A75 1.57080 0.00000 -0.01012 0.00000 -0.00569 1.56511

A76 2.20059 0.00277 0.00217 0.00000 0.00327 2.20385

A77 2.04067 -0.00135 -0.00076 0.00000 -0.00123 2.03944

A78 2.04067 -0.00136 -0.00076 0.00000 -0.00123 2.03944

A79 3.14139 0.00003 0.00009 0.00000 -0.00001 3.14138

A80 3.14139 0.00003 0.00009 0.00000 -0.00001 3.14138

A81 3.14159 0.00001 0.00003 0.00000 0.00015 3.14174

A82 3.14159 0.00001 0.00003 0.00000 0.00015 3.14174

A83 3.14139 0.00003 0.00009 0.00000 -0.00001 3.14138

A84 3.14159 0.00001 0.00003 0.00000 0.00015 3.14174

A85 3.14139 0.00003 0.00009 0.00000 -0.00001 3.14138

A86 3.14159 0.00001 0.00003 0.00000 0.00015 3.14174

A87 3.10778 0.00206 0.01752 0.00000 0.01752 3.12530

A88 3.17540 -0.00206 -0.01752 0.00000 -0.01752 3.15788

A89 3.17517 -0.00056 -0.01727 0.00000 -0.01727 3.15790

A90 3.10801 0.00056 0.01727 0.00000 0.01727 3.12528

A91 3.10778 0.00206 0.01752 0.00000 0.01752 3.12530

A92 3.17517 -0.00056 -0.01727 0.00000 -0.01727 3.15790

A93 3.17540 -0.00206 -0.01752 0.00000 -0.01752 3.15788

A94 3.10801 0.00056 0.01727 0.00000 0.01727 3.12528

D1 -0.00836 -0.00005 0.00518 0.00000 0.00516 -0.00319

D2 3.09529 0.00043 0.01689 0.00000 0.01685 3.11214

D3 3.12078 0.00011 0.01657 0.00000 0.01655 3.13733

D4 -0.05876 0.00058 0.02827 0.00000 0.02824 -0.03052

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 3.12867 0.00018 0.01177 0.00000 0.01182 3.14049

D7 -3.12867 -0.00018 -0.01177 0.00000 -0.01182 -3.14049

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.01348 0.00010 -0.00836 0.00000 -0.00831 0.00516

D10 3.05838 0.00061 0.11792 0.00000 0.11791 -3.10689

D11 -3.08985 -0.00041 -0.02018 0.00000 -0.02014 -3.10999

D12 -0.04494 0.00011 0.10610 0.00000 0.10609 0.06114

D13 -3.08780 -0.00073 -0.01160 0.00000 -0.01155 -3.09935

D14 -0.00211 0.00049 0.01086 0.00000 0.01088 0.00877

D15 0.00971 -0.00016 0.00203 0.00000 0.00204 0.01175

D16 3.09539 0.00105 0.02448 0.00000 0.02447 3.11986

D17 -0.01348 -0.00010 0.00836 0.00000 0.00831 -0.00516

D18 3.08985 0.00041 0.02018 0.00000 0.02014 3.10999

D19 -3.05838 -0.00061 -0.11792 0.00000 -0.11791 3.10689

D20 0.04494 -0.00011 -0.10610 0.00000 -0.10609 -0.06114

D21 -3.08367 -0.00071 -0.00045 0.00000 -0.00010 -3.08377

D22 0.05662 -0.00003 -0.14898 0.00000 -0.14939 -0.09277

D23 -1.51353 -0.00037 -0.07471 0.00000 -0.07474 -1.58827

D24 -0.05662 0.00003 0.14898 0.00000 0.14939 0.09277

D25 3.08367 0.00071 0.00045 0.00000 0.00010 3.08377

D26 1.51353 0.00037 0.07471 0.00000 0.07474 1.58827

D27 0.00836 0.00005 -0.00518 0.00000 -0.00516 0.00319

D28 -3.12078 -0.00011 -0.01657 0.00000 -0.01655 -3.13733

D29 -3.09529 -0.00043 -0.01689 0.00000 -0.01685 -3.11214

D30 0.05876 -0.00058 -0.02827 0.00000 -0.02824 0.03052

D31 -0.00971 0.00016 -0.00203 0.00000 -0.00204 -0.01175

D32 -3.09539 -0.00105 -0.02448 0.00000 -0.02447 -3.11986

D33 3.08780 0.00073 0.01160 0.00000 0.01155 3.09935

D34 0.00211 -0.00049 -0.01086 0.00000 -0.01088 -0.00877

D35 0.00971 -0.00016 0.00203 0.00000 0.00204 0.01175

D36 -3.08780 -0.00073 -0.01160 0.00000 -0.01155 -3.09935

D37 3.09539 0.00106 0.02448 0.00000 0.02447 3.11986

D38 -0.00211 0.00049 0.01086 0.00000 0.01088 0.00877

D39 -3.08985 -0.00041 -0.02018 0.00000 -0.02014 -3.10999

D40 -0.04494 0.00011 0.10610 0.00000 0.10609 0.06114

D41 0.01348 0.00010 -0.00836 0.00000 -0.00831 0.00516

D42 3.05838 0.00061 0.11792 0.00000 0.11791 -3.10689

D43 3.09529 0.00043 0.01689 0.00000 0.01685 3.11214

D44 -0.05876 0.00058 0.02827 0.00000 0.02824 -0.03052

D45 -0.00836 -0.00005 0.00518 0.00000 0.00516 -0.00319

D46 3.12078 0.00011 0.01657 0.00000 0.01655 3.13733

D47 -0.01348 -0.00010 0.00836 0.00000 0.00831 -0.00516

D48 3.08985 0.00041 0.02018 0.00000 0.02014 3.10999

D49 -3.05838 -0.00061 -0.11792 0.00000 -0.11791 3.10689

D50 0.04494 -0.00011 -0.10610 0.00000 -0.10609 -0.06114

D51 0.05662 -0.00003 -0.14898 0.00000 -0.14939 -0.09277

D52 -1.51353 -0.00037 -0.07471 0.00000 -0.07474 -1.58827

D53 -3.08367 -0.00071 -0.00045 0.00000 -0.00010 -3.08377

D54 3.08367 0.00071 0.00045 0.00000 0.00010 3.08377

D55 1.51353 0.00037 0.07471 0.00000 0.07474 1.58827

D56 -0.05662 0.00003 0.14898 0.00000 0.14939 0.09277

D57 0.00836 0.00005 -0.00518 0.00000 -0.00516 0.00319

D58 -3.12078 -0.00011 -0.01657 0.00000 -0.01655 -3.13733

D59 -3.09529 -0.00043 -0.01689 0.00000 -0.01685 -3.11214

D60 0.05876 -0.00058 -0.02827 0.00000 -0.02824 0.03052

D61 -0.00971 0.00016 -0.00203 0.00000 -0.00204 -0.01175

D62 -3.09539 -0.00105 -0.02448 0.00000 -0.02447 -3.11986

D63 3.08780 0.00073 0.01160 0.00000 0.01155 3.09935

D64 0.00211 -0.00049 -0.01086 0.00000 -0.01088 -0.00877

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 -3.12867 -0.00018 -0.01177 0.00000 -0.01182 -3.14049

D67 3.12867 0.00018 0.01177 0.00000 0.01182 3.14049

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.08780 0.00073 0.01160 0.00000 0.01155 3.09935

D70 -0.00971 0.00016 -0.00203 0.00000 -0.00204 -0.01175

D71 0.00211 -0.00049 -0.01086 0.00000 -0.01088 -0.00877

D72 -3.09539 -0.00106 -0.02448 0.00000 -0.02447 -3.11986

D73 -3.09529 -0.00043 -0.01689 0.00000 -0.01685 -3.11214

D74 0.05876 -0.00058 -0.02827 0.00000 -0.02824 0.03052

D75 0.00836 0.00005 -0.00518 0.00000 -0.00516 0.00319

D76 -3.12078 -0.00011 -0.01657 0.00000 -0.01655 -3.13733

D77 3.08985 0.00041 0.02018 0.00000 0.02014 3.10999

D78 0.04494 -0.00011 -0.10610 0.00000 -0.10609 -0.06114

D79 -0.01348 -0.00010 0.00836 0.00000 0.00831 -0.00516

D80 -3.05838 -0.00061 -0.11792 0.00000 -0.11791 3.10689

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 -3.12867 -0.00018 -0.01177 0.00000 -0.01182 -3.14049

D83 3.12867 0.00018 0.01177 0.00000 0.01182 3.14049

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 -0.00836 -0.00005 0.00518 0.00000 0.00516 -0.00319

D86 3.09529 0.00043 0.01689 0.00000 0.01685 3.11214

D87 3.12078 0.00011 0.01657 0.00000 0.01655 3.13733

D88 -0.05876 0.00058 0.02827 0.00000 0.02824 -0.03052

D89 0.01348 0.00010 -0.00836 0.00000 -0.00831 0.00516

D90 3.05838 0.00061 0.11792 0.00000 0.11791 -3.10689

D91 -3.08985 -0.00041 -0.02018 0.00000 -0.02014 -3.10999

D92 -0.04494 0.00011 0.10610 0.00000 0.10609 0.06114

D93 -3.08780 -0.00073 -0.01160 0.00000 -0.01155 -3.09935

D94 -0.00211 0.00049 0.01086 0.00000 0.01088 0.00877

D95 0.00971 -0.00016 0.00203 0.00000 0.00204 0.01175

D96 3.09539 0.00105 0.02448 0.00000 0.02447 3.11986

D97 -0.05662 0.00003 0.14898 0.00000 0.14939 0.09277

D98 1.51353 0.00037 0.07471 0.00000 0.07474 1.58827

D99 3.08367 0.00071 0.00045 0.00000 0.00010 3.08377

D100 -3.08367 -0.00071 -0.00045 0.00000 -0.00010 -3.08377

D101 -1.51353 -0.00037 -0.07471 0.00000 -0.07474 -1.58827

D102 0.05662 -0.00003 -0.14898 0.00000 -0.14939 -0.09277

D103 3.08780 0.00073 0.01160 0.00000 0.01155 3.09935

D104 -0.00971 0.00016 -0.00203 0.00000 -0.00204 -0.01175

D105 0.00211 -0.00049 -0.01086 0.00000 -0.01088 -0.00877

D106 -3.09539 -0.00106 -0.02448 0.00000 -0.02447 -3.11986

D107 -3.09529 -0.00043 -0.01689 0.00000 -0.01685 -3.11214

D108 0.05876 -0.00058 -0.02827 0.00000 -0.02824 0.03052

D109 0.00836 0.00005 -0.00518 0.00000 -0.00516 0.00319

D110 -3.12078 -0.00011 -0.01657 0.00000 -0.01655 -3.13733

D111 3.08985 0.00041 0.02018 0.00000 0.02014 3.10999

D112 0.04494 -0.00011 -0.10610 0.00000 -0.10609 -0.06114

D113 -0.01348 -0.00010 0.00836 0.00000 0.00831 -0.00516

D114 -3.05838 -0.00061 -0.11792 0.00000 -0.11791 3.10689

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 -3.12867 -0.00018 -0.01177 0.00000 -0.01182 -3.14049

D117 3.12867 0.00018 0.01177 0.00000 0.01182 3.14049

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 -0.00836 -0.00005 0.00518 0.00000 0.00516 -0.00319

D120 3.09529 0.00043 0.01689 0.00000 0.01685 3.11214

D121 3.12078 0.00011 0.01657 0.00000 0.01655 3.13733

D122 -0.05876 0.00058 0.02827 0.00000 0.02824 -0.03052

D123 0.01348 0.00010 -0.00836 0.00000 -0.00831 0.00516

D124 3.05838 0.00061 0.11792 0.00000 0.11791 -3.10689

D125 -3.08985 -0.00041 -0.02018 0.00000 -0.02014 -3.10999

D126 -0.04494 0.00011 0.10610 0.00000 0.10609 0.06114

D127 -3.08780 -0.00073 -0.01160 0.00000 -0.01155 -3.09935

D128 -0.00211 0.00049 0.01086 0.00000 0.01088 0.00877

D129 0.00971 -0.00016 0.00203 0.00000 0.00204 0.01175

D130 3.09539 0.00106 0.02448 0.00000 0.02447 3.11986

D131 1.51353 0.00037 0.07471 0.00000 0.07474 1.58827

D132 3.08367 0.00071 0.00045 0.00000 0.00010 3.08377

D133 -0.05662 0.00003 0.14898 0.00000 0.14939 0.09277

D134 -1.51353 -0.00037 -0.07471 0.00000 -0.07474 -1.58827

D135 0.05662 -0.00003 -0.14898 0.00000 -0.14939 -0.09277

D136 -3.08367 -0.00071 -0.00045 0.00000 -0.00010 -3.08377

Item Value Threshold Converged?

Maximum Force 0.004559 0.000450 NO

RMS Force 0.001191 0.000300 NO

Maximum Displacement 0.244036 0.001800 NO

RMS Displacement 0.043668 0.001200 NO

Predicted change in Energy=-5.865051D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:17:08 2019, MaxMem= 1342177280 cpu: 1.0

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.681641 4.273079 -0.031351

2 6 0 1.103732 2.892054 0.033052

3 7 0 0.000000 2.083340 0.074896

4 6 0 -1.103732 2.892054 0.033052

5 6 0 -0.681641 4.273079 -0.031351

6 6 0 -2.450724 2.450724 0.019427

7 6 0 -2.892054 1.103732 0.033052

8 7 0 -2.083340 0.000000 0.074896

9 6 0 -2.892054 -1.103732 0.033052

10 6 0 -4.273079 -0.681641 -0.031351

11 6 0 -4.273079 0.681641 -0.031351

12 6 0 2.450724 2.450724 0.019427

13 6 0 2.892054 1.103732 0.033052

14 6 0 4.273079 0.681641 -0.031351

15 6 0 4.273079 -0.681641 -0.031351

16 6 0 2.892054 -1.103732 0.033052

17 7 0 2.083340 0.000000 0.074896

18 6 0 2.450724 -2.450724 0.019427

19 6 0 1.103732 -2.892054 0.033052

20 6 0 0.681641 -4.273079 -0.031351

21 6 0 -0.681641 -4.273079 -0.031351

22 6 0 -1.103732 -2.892054 0.033052

23 7 0 0.000000 -2.083340 0.074896

24 1 0 1.341871 5.126089 -0.070191

25 1 0 -1.341871 5.126089 -0.070191

26 1 0 -5.126089 -1.341871 -0.070191

27 1 0 -5.126089 1.341871 -0.070191

28 1 0 5.126089 1.341871 -0.070191

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31 1 0 -1.341871 -5.126089 -0.070191

32 30 0 0.000000 0.000000 0.232513

33 6 0 -2.450724 -2.450724 0.019427

34 6 0 -3.456831 -3.456831 -0.053399

35 6 0 3.456831 3.456831 -0.053399

36 6 0 -4.307635 -4.307635 -0.134522

37 6 0 4.307635 4.307635 -0.134522

38 6 0 -3.456831 3.456831 -0.053399

39 6 0 -4.307635 4.307635 -0.134522

40 6 0 3.456831 -3.456831 -0.053399

41 6 0 4.307635 -4.307635 -0.134522

42 1 0 5.061234 -5.061234 -0.191202

43 1 0 -5.061234 -5.061234 -0.191202

44 1 0 -5.061234 5.061234 -0.191202

45 1 0 5.061234 5.061234 -0.191202

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.445523 0.000000

3 N 2.295840 1.368939 0.000000

4 C 2.258082 2.207464 1.368939 0.000000

5 C 1.363283 2.258082 2.295840 1.445523 0.000000

6 C 3.624261 3.581775 2.478728 1.417513 2.540317

7 C 4.777050 4.377717 3.053745 2.529069 3.864561

8 N 5.090738 4.303854 2.946287 3.053745 4.498361

9 C 6.456434 5.650895 4.303854 4.377717 5.813791

10 C 7.007033 6.456434 5.090738 4.777050 6.119451

11 C 6.119451 5.813791 4.498361 3.864561 5.079060

12 C 2.540317 1.417513 2.478728 3.581775 3.624261

13 C 3.864561 2.529069 3.053745 4.377717 4.777050

14 C 5.079060 3.864561 4.498361 5.813791 6.119451

15 C 6.119451 4.777050 5.090738 6.456434 7.007033

16 C 5.813791 4.377717 4.303854 5.650895 6.456434

17 N 4.498361 3.053745 2.946287 4.303854 5.090738

18 C 6.952823 5.509977 5.154304 6.417135 7.417803

19 C 7.177844 5.784108 5.096520 6.191026 7.384500

20 C 8.546158 7.177844 6.393746 7.384500 8.654210

21 C 8.654210 7.384500 6.393746 7.177844 8.546158

22 C 7.384500 6.191026 5.096520 5.784108 7.177844

23 N 6.393746 5.096520 4.166680 5.096520 6.393746

24 H 1.079369 2.249062 3.328662 3.313992 2.196301

25 H 2.196301 3.313992 3.328662 2.249062 1.079369

26 H 8.078298 7.533091 6.166839 5.840902 7.161165

27 H 6.505630 6.420623 5.181468 4.311969 5.324153

28 H 5.324153 4.311969 5.181468 6.420623 6.505630

29 H 7.161165 5.840902 6.166839 7.533091 8.078298

30 H 9.422408 8.022343 7.334680 8.383451 9.614597

31 H 9.614597 8.383451 7.334680 8.022343 9.422408

32 Zn 4.335143 3.101933 2.089294 3.101933 4.335143

33 C 7.417803 6.417135 5.154304 5.509977 6.952823

34 C 8.768064 7.817579 6.531434 6.771476 8.213018

35 C 2.892823 2.421470 3.721910 4.596214 4.218258

36 C 9.926337 9.008135 7.710002 7.882170 9.315961

37 C 3.627626 3.506700 4.852532 5.595967 4.990463

38 C 4.218258 4.596214 3.721910 2.421470 2.892823

39 C 4.990463 5.595967 4.852532 3.506700 3.627626

40 C 8.213018 6.771476 6.531434 7.817579 8.768064

41 C 9.315961 7.882170 7.710002 9.008135 9.926337

42 H 10.311924 8.886332 8.759671 10.065381 10.960637

43 H 10.960637 10.065381 8.759671 8.886332 10.311924

44 H 5.798910 6.539300 5.878329 4.518567 4.452816

45 H 4.452816 4.518567 5.878329 6.539300 5.798910

6 7 8 9 10

6 C 0.000000

7 C 1.417513 0.000000

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12 C 4.901447 5.509977 5.154304 6.417135 7.417803

13 C 5.509977 5.784108 5.096520 6.191026 7.384500

14 C 6.952823 7.177844 6.393746 7.384500 8.654210

15 C 7.417803 7.384500 6.393746 7.177844 8.546158

16 C 6.417135 6.191026 5.096520 5.784108 7.177844

17 N 5.154304 5.096520 4.166680 5.096520 6.393746

18 C 6.931693 6.417135 5.154304 5.509977 6.952823

19 C 6.417135 5.650895 4.303854 4.377717 5.813791

20 C 7.417803 6.456434 5.090738 4.777050 6.119451

21 C 6.952823 5.813791 4.498361 3.864561 5.079060

22 C 5.509977 4.377717 3.053745 2.529069 3.864561

23 N 5.154304 4.303854 2.946287 3.053745 4.498361

24 H 4.642131 5.840902 6.166839 7.533091 8.078298

25 H 2.897441 4.311969 5.181468 6.420623 6.505630

26 H 4.642131 3.313992 3.328662 2.249062 1.079369

27 H 2.897441 2.249062 3.328662 3.313992 2.196301

28 H 7.658046 8.022343 7.334680 8.383451 9.614597

29 H 8.473482 8.383451 7.334680 8.022343 9.422408

30 H 8.473482 7.533091 6.166839 5.840902 7.161165

31 H 7.658046 6.420623 5.181468 4.311969 5.324153

32 Zn 3.472391 3.101933 2.089294 3.101933 4.335143

33 C 4.901447 3.581775 2.478728 1.417513 2.540317

34 C 5.993059 4.596214 3.721910 2.421470 2.892823

35 C 5.993059 6.771476 6.531434 7.817579 8.768064

36 C 7.010509 5.595967 4.852532 3.506700 3.627626

37 C 7.010509 7.882170 7.710002 9.008135 9.926337

38 C 1.424713 2.421470 3.721910 4.596214 4.218258

39 C 2.630578 3.506700 4.852532 5.595967 4.990463

40 C 8.354861 7.817579 6.531434 6.771476 8.213018

41 C 9.559002 9.008135 7.710002 7.882170 9.315961

42 H 10.625600 10.065381 8.759671 8.886332 10.311924

43 H 7.955416 6.539300 5.878329 4.518567 4.452816

44 H 3.697823 4.518567 5.878329 6.539300 5.798910

45 H 7.955416 8.886332 8.759671 10.065381 10.960637

11 12 13 14 15

11 C 0.000000

12 C 6.952823 0.000000

13 C 7.177844 1.417513 0.000000

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15 C 8.654210 3.624261 2.258082 1.363283 0.000000

16 C 7.384500 3.581775 2.207464 2.258082 1.445523

17 N 6.393746 2.478728 1.368939 2.295840 2.295840

18 C 7.417803 4.901447 3.581775 3.624261 2.540317

19 C 6.456434 5.509977 4.377717 4.777050 3.864561

20 C 7.007033 6.952823 5.813791 6.119451 5.079060

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23 N 5.090738 5.154304 4.303854 5.090738 4.498361

24 H 7.161165 2.897441 4.311969 5.324153 6.505630

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26 H 2.196301 8.473482 8.383451 9.614597 9.422408

27 H 1.079369 7.658046 8.022343 9.422408 9.614597

28 H 9.422408 2.897441 2.249062 1.079369 2.196301

29 H 9.614597 4.642131 3.313992 2.196301 1.079369

30 H 8.078298 7.658046 6.420623 6.505630 5.324153

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32 Zn 4.335143 3.472391 3.101933 4.335143 4.335143

33 C 3.624261 6.931693 6.417135 7.417803 6.952823

34 C 4.218258 8.354861 7.817579 8.768064 8.213018

35 C 8.213018 1.424713 2.421470 2.892823 4.218258

36 C 4.990463 9.559002 9.008135 9.926337 9.315961

37 C 9.315961 2.630578 3.506700 3.627626 4.990463

38 C 2.892823 5.993059 6.771476 8.213018 8.768064

39 C 3.627626 7.010509 7.882170 9.315961 9.926337

40 C 8.768064 5.993059 4.596214 4.218258 2.892823

41 C 9.926337 7.010509 5.595967 4.990463 3.627626

42 H 10.960637 7.955416 6.539300 5.798910 4.452816

43 H 5.798910 10.625600 10.065381 10.960637 10.311924

44 H 4.452816 7.955416 8.886332 10.311924 10.960637

45 H 10.311924 3.697823 4.518567 4.452816 5.798910

16 17 18 19 20

16 C 0.000000

17 N 1.368939 0.000000

18 C 1.417513 2.478728 0.000000

19 C 2.529069 3.053745 1.417513 0.000000

20 C 3.864561 4.498361 2.540317 1.445523 0.000000

21 C 4.777050 5.090738 3.624261 2.258082 1.363283

22 C 4.377717 4.303854 3.581775 2.207464 2.258082

23 N 3.053745 2.946287 2.478728 1.368939 2.295840

24 H 6.420623 5.181468 7.658046 8.022343 9.422408

25 H 7.533091 6.166839 8.473482 8.383451 9.614597

26 H 8.022343 7.334680 7.658046 6.420623 6.505630

27 H 8.383451 7.334680 8.473482 7.533091 8.078298

28 H 3.313992 3.328662 4.642131 5.840902 7.161165

29 H 2.249062 3.328662 2.897441 4.311969 5.324153

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32 Zn 3.101933 2.089294 3.472391 3.101933 4.335143

33 C 5.509977 5.154304 4.901447 3.581775 3.624261

34 C 6.771476 6.531434 5.993059 4.596214 4.218258

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36 C 7.882170 7.710002 7.010509 5.595967 4.990463

37 C 5.595967 4.852532 7.010509 7.882170 9.315961

38 C 7.817579 6.531434 8.354861 7.817579 8.768064

39 C 9.008135 7.710002 9.559002 9.008135 9.926337

40 C 2.421470 3.721910 1.424713 2.421470 2.892823

41 C 3.506700 4.852532 2.630578 3.506700 3.627626

42 H 4.518567 5.878329 3.697823 4.518567 4.452816

43 H 8.886332 8.759671 7.955416 6.539300 5.798910

44 H 10.065381 8.759671 10.625600 10.065381 10.960637

45 H 6.539300 5.878329 7.955416 8.886332 10.311924

21 22 23 24 25

21 C 0.000000

22 C 1.445523 0.000000

23 N 2.295840 1.368939 0.000000

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25 H 9.422408 8.022343 7.334680 2.683742 0.000000

26 H 5.324153 4.311969 5.181468 9.147077 7.493651

27 H 7.161165 5.840902 6.166839 7.493651 5.351692

28 H 8.078298 7.533091 6.166839 5.351692 7.493651

29 H 6.505630 6.420623 5.181468 7.493651 9.147077

30 H 2.196301 3.313992 3.328662 10.252178 10.597623

31 H 1.079369 2.249062 3.328662 10.597623 10.252178

32 Zn 4.335143 3.101933 2.089294 5.307451 5.307451

33 C 2.540317 1.417513 2.478728 8.473482 7.658046

34 C 2.892823 2.421470 3.721910 9.833328 8.839675

35 C 8.768064 7.817579 6.531434 2.694394 5.080772

36 C 3.627626 3.506700 4.852532 10.996190 9.889138

37 C 9.926337 9.008135 7.710002 3.077298 5.708846

38 C 8.213018 6.771476 6.531434 5.080772 2.694394

39 C 9.315961 7.882170 7.710002 5.708846 3.077298

40 C 4.218258 4.596214 3.721910 8.839675 9.833328

41 C 4.990463 5.595967 4.852532 9.889138 10.996190

42 H 5.798910 6.539300 5.878329 10.845730 12.033119

43 H 4.452816 4.518567 5.878329 12.033119 10.845730

44 H 10.311924 8.886332 8.759671 6.404577 3.721896

45 H 10.960637 10.065381 8.759671 3.721896 6.404577

26 27 28 29 30

26 H 0.000000

27 H 2.683742 0.000000

28 H 10.597623 10.252178 0.000000

29 H 10.252178 10.597623 2.683742 0.000000

30 H 7.493651 9.147077 7.493651 5.351692 0.000000

31 H 5.351692 7.493651 9.147077 7.493651 2.683742

32 Zn 5.307451 5.307451 5.307451 5.307451 5.307451

33 C 2.897441 4.642131 8.473482 7.658046 4.642131

34 C 2.694394 5.080772 9.833328 8.839675 5.080772

35 C 9.833328 8.839675 2.694394 5.080772 8.839675

36 C 3.077298 5.708846 10.996190 9.889138 5.708846

37 C 10.996190 9.889138 3.077298 5.708846 9.889138

38 C 5.080772 2.694394 8.839675 9.833328 9.833328

39 C 5.708846 3.077298 9.889138 10.996190 10.996190

40 C 8.839675 9.833328 5.080772 2.694394 2.694394

41 C 9.889138 10.996190 5.708846 3.077298 3.077298

42 H 10.845730 12.033119 6.404577 3.721896 3.721896

43 H 3.721896 6.404577 12.033119 10.845730 6.404577

44 H 6.404577 3.721896 10.845730 12.033119 12.033119

45 H 12.033119 10.845730 3.721896 6.404577 10.845730

31 32 33 34 35

31 H 0.000000

32 Zn 5.307451 0.000000

33 C 2.897441 3.472391 0.000000

34 C 2.694394 4.897050 1.424713 0.000000

35 C 9.833328 4.897050 8.354861 9.777394 0.000000

36 C 3.077298 6.102963 2.630578 1.205951 10.980913

37 C 10.996190 6.102963 9.559002 10.980913 1.205951

38 C 8.839675 4.897050 5.993059 6.913662 6.913662

39 C 9.889138 6.102963 7.010509 7.811362 7.811362

40 C 5.080772 4.897050 5.993059 6.913662 6.913662

41 C 5.708846 6.102963 7.010509 7.811362 7.811362

42 H 6.404577 7.170196 7.955416 8.668940 8.668940

43 H 3.721896 7.170196 3.697823 2.273150 12.047151

44 H 10.845730 7.170196 7.955416 8.668940 8.668940

45 H 12.033119 7.170196 10.625600 12.047151 2.273150

36 37 38 39 40

36 C 0.000000

37 C 12.183832 0.000000

38 C 7.811362 7.811362 0.000000

39 C 8.615270 8.615270 1.205951 0.000000

40 C 7.811362 7.811362 9.777394 10.980913 0.000000

41 C 8.615270 8.615270 10.980913 12.183832 1.205951

42 H 9.399300 9.399300 12.047151 13.249703 2.273150

43 H 1.067256 13.249703 8.668940 9.399300 8.668940

44 H 9.399300 9.399300 2.273150 1.067256 12.047151

45 H 13.249703 1.067256 8.668940 9.399300 8.668940

41 42 43 44 45

41 C 0.000000

42 H 1.067256 0.000000

43 H 9.399300 10.122468 0.000000

44 H 13.249703 14.315332 10.122468 0.000000

45 H 9.399300 10.122468 14.315332 10.122468 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(C6H2),2SGD(N2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

Omega: Change in point group or standard orientation.

Old FWG=C04V [C4(Zn1),2SGV(N2),2SGD(C6H2),X(C16H8)]

New FWG=C04V [C4(Zn1),2SGV(C6H2),2SGD(N2),X(C16H8)]

RotChk: IX=3 Diff= 1.08D+00

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -3.503516 -2.539530 -0.047250

2 6 0 -2.825448 -1.264535 0.017153

3 7 0 -1.473144 -1.473144 0.058997

4 6 0 -1.264535 -2.825448 0.017153

5 6 0 -2.539530 -3.503516 -0.047250

6 6 0 0.000000 -3.465847 0.003528

7 6 0 1.264535 -2.825448 0.017153

8 7 0 1.473144 -1.473144 0.058997

9 6 0 2.825448 -1.264535 0.017153

10 6 0 3.503516 -2.539530 -0.047250

11 6 0 2.539530 -3.503516 -0.047250

12 6 0 -3.465847 0.000000 0.003528

13 6 0 -2.825448 1.264535 0.017153

14 6 0 -3.503516 2.539530 -0.047250

15 6 0 -2.539530 3.503516 -0.047250

16 6 0 -1.264535 2.825448 0.017153

17 7 0 -1.473144 1.473144 0.058997

18 6 0 0.000000 3.465847 0.003528

19 6 0 1.264535 2.825448 0.017153

20 6 0 2.539530 3.503516 -0.047250

21 6 0 3.503516 2.539530 -0.047250

22 6 0 2.825448 1.264535 0.017153

23 7 0 1.473144 1.473144 0.058997

24 1 0 -4.573538 -2.675846 -0.086090

25 1 0 -2.675846 -4.573538 -0.086090

26 1 0 4.573538 -2.675846 -0.086090

27 1 0 2.675846 -4.573538 -0.086090

28 1 0 -4.573538 2.675846 -0.086090

29 1 0 -2.675846 4.573538 -0.086090

30 1 0 2.675846 4.573538 -0.086090

31 1 0 4.573538 2.675846 -0.086090

32 30 0 0.000000 0.000000 0.216614

33 6 0 3.465847 0.000000 0.003528

34 6 0 4.888697 0.000000 -0.069297

35 6 0 -4.888697 0.000000 -0.069297

36 6 0 6.091916 0.000000 -0.150420

37 6 0 -6.091916 0.000000 -0.150420

38 6 0 0.000000 -4.888697 -0.069297

39 6 0 0.000000 -6.091916 -0.150420

40 6 0 0.000000 4.888697 -0.069297

41 6 0 0.000000 6.091916 -0.150420

42 1 0 0.000000 7.157666 -0.207101

43 1 0 7.157666 0.000000 -0.207101

44 1 0 0.000000 -7.157666 -0.207101

45 1 0 -7.157666 0.000000 -0.207101

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

Rotational constants (GHZ): 0.1463075 0.1463075 0.0732593

Leave Link 202 at Fri Jul 26 14:17:08 2019, MaxMem= 1342177280 cpu: 0.1

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 205 symmetry adapted cartesian basis functions of A1 symmetry.

There are 134 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 191 symmetry adapted basis functions of A1 symmetry.

There are 129 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3058.8292454383 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= 9 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= -0.1305207357 Hartrees.

Nuclear repulsion after empirical dispersion term = 3058.6987247025 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: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3910

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.49D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 232

GePol: Fraction of low-weight points (<1% of avg) = 5.93%

GePol: Cavity surface area = 416.041 Ang\*\*2

GePol: Cavity volume = 421.150 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0083302219 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3058.7070549244 Hartrees.

Leave Link 301 at Fri Jul 26 14:17:08 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16211 LenP2D= 44788.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 5.12D-05 NBF= 191 129 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 191 129 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:17:09 2019, MaxMem= 1342177280 cpu: 6.6

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:17:09 2019, MaxMem= 1342177280 cpu: 0.8

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

Lowest energy guess from the checkpoint file: "ZnTSPsim0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.923880 0.000000 0.000000 0.382683 Ang= 45.00 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.923880 0.000000 0.000000 0.382683 Ang= 45.00 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 4.43D-01

Max alpha theta= 3.003 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Occupied (B2) (E) (E) (A1) (A1) (A1) (B2) (E) (E) (B1)

(A1) (B2) (E) (E) (A1) (E) (E) (B2) (E) (E) (B2)

(A2) (E) (E) (E) (E) (A2) (B1) (A1) (E) (E) (E)

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

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

(B1) (A2) (E) (E) (B1) (E) (E) (A1) (E) (E) (E)

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

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

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

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

(B2) (B1) (E) (E)

Virtual (B2) (E) (E) (A1) (A1) (A1) (B2) (E) (E) (B1)

(A1) (B2) (E) (E) (A1) (E) (E) (B2) (E) (E) (B2)

(A2) (E) (E) (E) (E) (A2) (B1) (A1) (E) (E) (E)

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The electronic state of the initial guess is 1-A1.

Leave Link 401 at Fri Jul 26 14:17:10 2019, MaxMem= 1342177280 cpu: 16.8

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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.

An orbital has undefined symmetry, so N\*\*3 symmetry is turned off.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 660000000 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= 0 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= 45864300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.66D-15 for 3906.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.56D-15 for 3906 846.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.66D-15 for 3906.

Iteration 1 A^-1\*A deviation from orthogonality is 5.21D-14 for 939 918.

E= -1359.06211047953

DIIS: error= 8.60D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.06211047953 IErMin= 1 ErrMin= 8.60D-04

ErrMax= 8.60D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.99D-05 BMatP= 4.99D-05

IDIUse=3 WtCom= 9.91D-01 WtEn= 8.60D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 10.463 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=6.95D-05 MaxDP=1.99D-03 OVMax= 2.55D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.92D-05 CP: 1.00D+00

E= -1359.06214963893 Delta-E= -0.000039159401 Rises=F Damp=F

DIIS: error= 1.07D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.06214963893 IErMin= 1 ErrMin= 8.60D-04

ErrMax= 1.07D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.21D-05 BMatP= 4.99D-05

IDIUse=3 WtCom= 9.89D-01 WtEn= 1.07D-02

Coeff-Com: 0.472D+00 0.528D+00

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

Coeff: 0.467D+00 0.533D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.01D-05 MaxDP=3.40D-04 DE=-3.92D-05 OVMax= 7.42D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 9.59D-06 CP: 1.00D+00 9.57D-01

E= -1359.06216676251 Delta-E= -0.000017123584 Rises=F Damp=F

DIIS: error= 2.87D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.06216676251 IErMin= 3 ErrMin= 2.87D-04

ErrMax= 2.87D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.94D-06 BMatP= 4.21D-05

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.87D-03

Coeff-Com: 0.512D-02 0.202D+00 0.793D+00

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

Coeff: 0.511D-02 0.201D+00 0.794D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.68D-06 MaxDP=1.20D-04 DE=-1.71D-05 OVMax= 2.66D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.91D-06 CP: 1.00D+00 9.75D-01 8.59D-01

E= -1359.06216770039 Delta-E= -0.000000937875 Rises=F Damp=F

DIIS: error= 3.26D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.06216770039 IErMin= 4 ErrMin= 3.26D-05

ErrMax= 3.26D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.48D-07 BMatP= 2.94D-06

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

Coeff-Com: -0.827D-02 0.106D+00 0.471D+00 0.431D+00

Coeff: -0.827D-02 0.106D+00 0.471D+00 0.431D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=1.09D-06 MaxDP=6.15D-05 DE=-9.38D-07 OVMax= 1.61D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.02D-06 CP: 1.00D+00 9.73D-01 8.55D-01 8.19D-01

E= -1359.06216814605 Delta-E= -0.000000445659 Rises=F Damp=F

DIIS: error= 8.16D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.06216814605 IErMin= 5 ErrMin= 8.16D-06

ErrMax= 8.16D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.33D-08 BMatP= 5.48D-07

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

Coeff-Com: -0.437D-02 0.259D-01 0.121D+00 0.214D+00 0.643D+00

Coeff: -0.437D-02 0.259D-01 0.121D+00 0.214D+00 0.643D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=3.84D-07 MaxDP=1.05D-05 DE=-4.46D-07 OVMax= 3.49D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.06D-07 CP: 1.00D+00 9.75D-01 8.53D-01 7.65D-01 7.30D-01

E= -1359.06216816572 Delta-E= -0.000000019676 Rises=F Damp=F

DIIS: error= 4.42D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.06216816572 IErMin= 6 ErrMin= 4.42D-06

ErrMax= 4.42D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.79D-09 BMatP= 2.33D-08

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

Coeff-Com: -0.844D-03 0.178D-02 0.734D-02 0.593D-01 0.304D+00 0.629D+00

Coeff: -0.844D-03 0.178D-02 0.734D-02 0.593D-01 0.304D+00 0.629D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=8.21D-08 MaxDP=3.45D-06 DE=-1.97D-08 OVMax= 8.52D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.75D-08 CP: 1.00D+00 9.75D-01 8.55D-01 7.80D-01 7.18D-01

CP: 7.83D-01

E= -1359.06216816716 Delta-E= -0.000000001435 Rises=F Damp=F

DIIS: error= 6.10D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.06216816716 IErMin= 7 ErrMin= 6.10D-07

ErrMax= 6.10D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.19D-10 BMatP= 1.79D-09

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

Coeff-Com: -0.793D-04-0.893D-03-0.499D-02 0.868D-02 0.833D-01 0.262D+00

Coeff-Com: 0.652D+00

Coeff: -0.793D-04-0.893D-03-0.499D-02 0.868D-02 0.833D-01 0.262D+00

Coeff: 0.652D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.63D-08 MaxDP=1.00D-06 DE=-1.44D-09 OVMax= 3.24D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.55D-08 CP: 1.00D+00 9.75D-01 8.55D-01 7.84D-01 7.33D-01

CP: 7.94D-01 8.14D-01

E= -1359.06216816682 Delta-E= 0.000000000333 Rises=F Damp=F

DIIS: error= 6.71D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 7 EnMin= -1359.06216816716 IErMin= 7 ErrMin= 6.10D-07

ErrMax= 6.71D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.69D-11 BMatP= 1.19D-10

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

Coeff-Com: 0.701D-05-0.746D-03-0.388D-02 0.653D-03 0.305D-01 0.121D+00

Coeff-Com: 0.441D+00 0.412D+00

Coeff: 0.701D-05-0.746D-03-0.388D-02 0.653D-03 0.305D-01 0.121D+00

Coeff: 0.441D+00 0.412D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=9.03D-09 MaxDP=5.50D-07 DE= 3.33D-10 OVMax= 1.59D-06

Error on total polarization charges = 0.06219

SCF Done: E(RB3LYP) = -1359.06216817 A.U. after 8 cycles

NFock= 8 Conv=0.90D-08 -V/T= 1.9682

KE= 1.403670770256D+03 PE=-9.359518099389D+03 EE= 3.538078106041D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.23

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:17:45 2019, MaxMem= 1342177280 cpu: 392.0

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16211 LenP2D= 44788.

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 = 250

Leave Link 701 at Fri Jul 26 14:17:49 2019, MaxMem= 1342177280 cpu: 43.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

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

Leave Link 702 at Fri Jul 26 14:17:49 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Fri Jul 26 14:17:53 2019, MaxMem= 1342177280 cpu: 42.8

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-4.44089210D-14 1.25233157D-13 2.18207423D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000549125 0.000525581 0.000671851

2 6 -0.000505219 -0.001832542 -0.000426370

3 7 0.000000000 0.004648958 0.000350594

4 6 0.000505219 -0.001832542 -0.000426370

5 6 0.000549125 0.000525581 0.000671851

6 6 0.002545253 -0.002545253 -0.000152492

7 6 0.001832542 -0.000505219 -0.000426370

8 7 -0.004648958 0.000000000 0.000350594

9 6 0.001832542 0.000505219 -0.000426370

10 6 -0.000525581 0.000549125 0.000671851

11 6 -0.000525581 -0.000549125 0.000671851

12 6 -0.002545253 -0.002545253 -0.000152492

13 6 -0.001832542 -0.000505219 -0.000426370

14 6 0.000525581 -0.000549125 0.000671851

15 6 0.000525581 0.000549125 0.000671851

16 6 -0.001832542 0.000505219 -0.000426370

17 7 0.004648958 0.000000000 0.000350594

18 6 -0.002545253 0.002545253 -0.000152492

19 6 -0.000505219 0.001832542 -0.000426370

20 6 -0.000549125 -0.000525581 0.000671851

21 6 0.000549125 -0.000525581 0.000671851

22 6 0.000505219 0.001832542 -0.000426370

23 7 0.000000000 -0.004648958 0.000350594

24 1 -0.000198004 0.000374896 -0.000207981

25 1 0.000198004 0.000374896 -0.000207981

26 1 -0.000374896 0.000198004 -0.000207981

27 1 -0.000374896 -0.000198004 -0.000207981

28 1 0.000374896 -0.000198004 -0.000207981

29 1 0.000374896 0.000198004 -0.000207981

30 1 -0.000198004 -0.000374896 -0.000207981

31 1 0.000198004 -0.000374896 -0.000207981

32 30 0.000000000 0.000000000 -0.001766452

33 6 0.002545253 0.002545253 -0.000152492

34 6 -0.000828369 -0.000828369 -0.000436615

35 6 0.000828369 0.000828369 -0.000436615

36 6 -0.000058792 -0.000058792 0.000759221

37 6 0.000058792 0.000058792 0.000759221

38 6 -0.000828369 0.000828369 -0.000436615

39 6 -0.000058792 0.000058792 0.000759221

40 6 0.000828369 -0.000828369 -0.000436615

41 6 0.000058792 -0.000058792 0.000759221

42 1 -0.000017094 0.000017094 -0.000154096

43 1 0.000017094 0.000017094 -0.000154096

44 1 0.000017094 -0.000017094 -0.000154096

45 1 -0.000017094 -0.000017094 -0.000154096

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

Cartesian Forces: Max 0.004648958 RMS 0.001189599

Leave Link 716 at Fri Jul 26 14:17:53 2019, MaxMem= 1342177280 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002194059 RMS 0.000608671

Search for a local minimum.

Step number 7 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .60867D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 4 5 7

ITU= 0 -1 1 0 -1 -1 0

Use linear search instead of GDIIS.

Linear search step of 0.097 exceeds DXMaxT= 0.063 but not scaled.

Quartic linear search produced a step of -0.51636.

Iteration 1 RMS(Cart)= 0.01793687 RMS(Int)= 0.00028269

Iteration 2 RMS(Cart)= 0.00047093 RMS(Int)= 0.00017409

Iteration 3 RMS(Cart)= 0.00000007 RMS(Int)= 0.00017409

ITry= 1 IFail=0 DXMaxC= 1.00D-01 DCOld= 1.00D+10 DXMaxT= 6.31D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 4.14D-05 for atom 39.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73164 0.00085 0.00131 0.00000 0.00137 2.73302

R2 2.57623 -0.00070 -0.00103 0.00000 -0.00081 2.57542

R3 2.03971 0.00018 0.00021 0.00000 0.00021 2.03992

R4 2.58692 -0.00219 -0.00196 0.00000 -0.00208 2.58484

R5 2.67871 -0.00068 -0.00253 0.00000 -0.00223 2.67648

R6 2.58692 -0.00219 -0.00196 0.00000 -0.00208 2.58484

R7 3.94819 0.00131 0.00730 0.00000 0.00684 3.95503

R8 2.73164 0.00085 0.00131 0.00000 0.00137 2.73302

R9 2.67871 -0.00068 -0.00253 0.00000 -0.00223 2.67648

R10 2.03971 0.00018 0.00021 0.00000 0.00021 2.03992

R11 2.67871 -0.00068 -0.00253 0.00000 -0.00223 2.67648

R12 2.69232 0.00122 0.00156 0.00000 0.00156 2.69387

R13 2.58692 -0.00219 -0.00196 0.00000 -0.00208 2.58484

R14 2.73164 0.00085 0.00131 0.00000 0.00137 2.73302

R15 2.58692 -0.00219 -0.00196 0.00000 -0.00208 2.58484

R16 3.94819 0.00131 0.00730 0.00000 0.00684 3.95503

R17 2.73164 0.00085 0.00131 0.00000 0.00137 2.73302

R18 2.67871 -0.00068 -0.00253 0.00000 -0.00223 2.67648

R19 2.57623 -0.00070 -0.00103 0.00000 -0.00081 2.57542

R20 2.03971 0.00018 0.00021 0.00000 0.00021 2.03992

R21 2.03971 0.00018 0.00021 0.00000 0.00021 2.03992

R22 2.67871 -0.00068 -0.00253 0.00000 -0.00223 2.67648

R23 2.69232 0.00122 0.00156 0.00000 0.00156 2.69387

R24 2.73164 0.00085 0.00131 0.00000 0.00137 2.73302

R25 2.58692 -0.00219 -0.00196 0.00000 -0.00208 2.58484

R26 2.57623 -0.00070 -0.00103 0.00000 -0.00081 2.57542

R27 2.03971 0.00018 0.00021 0.00000 0.00021 2.03992

R28 2.73164 0.00085 0.00131 0.00000 0.00137 2.73302

R29 2.03971 0.00018 0.00021 0.00000 0.00021 2.03992

R30 2.58692 -0.00219 -0.00196 0.00000 -0.00208 2.58484

R31 2.67871 -0.00068 -0.00253 0.00000 -0.00223 2.67648

R32 3.94819 0.00131 0.00730 0.00000 0.00684 3.95503

R33 2.67871 -0.00068 -0.00253 0.00000 -0.00223 2.67648

R34 2.69232 0.00122 0.00156 0.00000 0.00156 2.69387

R35 2.73164 0.00085 0.00131 0.00000 0.00137 2.73302

R36 2.58692 -0.00219 -0.00196 0.00000 -0.00208 2.58484

R37 2.57623 -0.00070 -0.00103 0.00000 -0.00081 2.57542

R38 2.03971 0.00018 0.00021 0.00000 0.00021 2.03992

R39 2.73164 0.00085 0.00131 0.00000 0.00137 2.73302

R40 2.03971 0.00018 0.00021 0.00000 0.00021 2.03992

R41 2.58692 -0.00219 -0.00196 0.00000 -0.00208 2.58484

R42 2.67871 -0.00068 -0.00253 0.00000 -0.00223 2.67648

R43 3.94819 0.00131 0.00730 0.00000 0.00684 3.95503

R44 2.69232 0.00122 0.00156 0.00000 0.00156 2.69387

R45 2.27892 0.00002 -0.00008 0.00000 -0.00008 2.27884

R46 2.27892 0.00002 -0.00008 0.00000 -0.00008 2.27884

R47 2.01682 -0.00002 0.00002 0.00000 0.00002 2.01684

R48 2.01682 -0.00002 0.00002 0.00000 0.00002 2.01684

R49 2.27892 0.00002 -0.00008 0.00000 -0.00008 2.27884

R50 2.01682 -0.00002 0.00002 0.00000 0.00002 2.01684

R51 2.27892 0.00002 -0.00008 0.00000 -0.00008 2.27884

R52 2.01682 -0.00002 0.00002 0.00000 0.00002 2.01684

A1 1.86711 -0.00037 -0.00080 0.00000 -0.00075 1.86636

A2 2.18709 0.00059 0.00199 0.00000 0.00197 2.18906

A3 2.22898 -0.00021 -0.00120 0.00000 -0.00122 2.22776

A4 1.90745 -0.00008 0.00123 0.00000 0.00094 1.90839

A5 2.18278 0.00034 -0.00035 0.00000 -0.00015 2.18263

A6 2.19262 -0.00026 -0.00078 0.00000 -0.00068 2.19195

A7 1.87563 0.00090 -0.00085 0.00000 -0.00036 1.87527

A8 2.20357 -0.00045 -0.00155 0.00000 -0.00119 2.20238

A9 2.20357 -0.00045 -0.00155 0.00000 -0.00119 2.20238

A10 1.90745 -0.00008 0.00123 0.00000 0.00094 1.90839

A11 2.19262 -0.00026 -0.00078 0.00000 -0.00068 2.19195

A12 2.18278 0.00034 -0.00035 0.00000 -0.00015 2.18263

A13 1.86711 -0.00037 -0.00080 0.00000 -0.00075 1.86636

A14 2.22898 -0.00021 -0.00120 0.00000 -0.00122 2.22776

A15 2.18709 0.00059 0.00199 0.00000 0.00197 2.18906

A16 2.20385 0.00139 0.00033 0.00000 0.00055 2.20440

A17 2.03944 -0.00068 -0.00007 0.00000 -0.00017 2.03927

A18 2.03944 -0.00069 -0.00007 0.00000 -0.00017 2.03927

A19 2.19262 -0.00026 -0.00078 0.00000 -0.00068 2.19195

A20 2.18278 0.00034 -0.00035 0.00000 -0.00015 2.18263

A21 1.90745 -0.00008 0.00123 0.00000 0.00094 1.90839

A22 1.87563 0.00090 -0.00085 0.00000 -0.00036 1.87527

A23 2.20357 -0.00045 -0.00155 0.00000 -0.00119 2.20238

A24 2.20357 -0.00045 -0.00155 0.00000 -0.00119 2.20238

A25 1.90745 -0.00008 0.00123 0.00000 0.00094 1.90839

A26 2.19262 -0.00026 -0.00078 0.00000 -0.00068 2.19195

A27 2.18278 0.00034 -0.00035 0.00000 -0.00015 2.18263

A28 1.86711 -0.00037 -0.00080 0.00000 -0.00075 1.86636

A29 2.18709 0.00059 0.00199 0.00000 0.00197 2.18906

A30 2.22898 -0.00021 -0.00120 0.00000 -0.00122 2.22776

A31 1.86711 -0.00037 -0.00080 0.00000 -0.00075 1.86636

A32 2.18709 0.00059 0.00199 0.00000 0.00197 2.18906

A33 2.22898 -0.00021 -0.00120 0.00000 -0.00122 2.22776

A34 2.20385 0.00139 0.00033 0.00000 0.00055 2.20440

A35 2.03944 -0.00068 -0.00007 0.00000 -0.00017 2.03927

A36 2.03944 -0.00069 -0.00007 0.00000 -0.00017 2.03927

A37 2.18278 0.00034 -0.00035 0.00000 -0.00015 2.18263

A38 2.19262 -0.00026 -0.00078 0.00000 -0.00068 2.19195

A39 1.90745 -0.00008 0.00123 0.00000 0.00094 1.90839

A40 1.86711 -0.00037 -0.00080 0.00000 -0.00075 1.86636

A41 2.18709 0.00059 0.00199 0.00000 0.00197 2.18906

A42 2.22898 -0.00021 -0.00120 0.00000 -0.00122 2.22776

A43 1.86711 -0.00037 -0.00080 0.00000 -0.00075 1.86636

A44 2.22898 -0.00021 -0.00120 0.00000 -0.00122 2.22776

A45 2.18709 0.00059 0.00199 0.00000 0.00197 2.18906

A46 1.90745 -0.00008 0.00123 0.00000 0.00094 1.90839

A47 2.18278 0.00034 -0.00035 0.00000 -0.00015 2.18263

A48 2.19262 -0.00026 -0.00078 0.00000 -0.00068 2.19195

A49 1.87563 0.00090 -0.00085 0.00000 -0.00036 1.87527

A50 2.20357 -0.00045 -0.00155 0.00000 -0.00119 2.20238

A51 2.20357 -0.00045 -0.00155 0.00000 -0.00119 2.20238

A52 2.20385 0.00139 0.00033 0.00000 0.00055 2.20440

A53 2.03944 -0.00068 -0.00007 0.00000 -0.00017 2.03927

A54 2.03944 -0.00069 -0.00007 0.00000 -0.00017 2.03927

A55 2.18278 0.00034 -0.00035 0.00000 -0.00015 2.18263

A56 2.19262 -0.00026 -0.00078 0.00000 -0.00068 2.19195

A57 1.90745 -0.00008 0.00123 0.00000 0.00094 1.90839

A58 1.86711 -0.00037 -0.00080 0.00000 -0.00075 1.86636

A59 2.18709 0.00059 0.00199 0.00000 0.00197 2.18906

A60 2.22898 -0.00021 -0.00120 0.00000 -0.00122 2.22776

A61 1.86711 -0.00037 -0.00080 0.00000 -0.00075 1.86636

A62 2.22898 -0.00021 -0.00120 0.00000 -0.00122 2.22776

A63 2.18709 0.00059 0.00199 0.00000 0.00197 2.18906

A64 1.90745 -0.00008 0.00123 0.00000 0.00094 1.90839

A65 2.18278 0.00034 -0.00035 0.00000 -0.00015 2.18263

A66 2.19262 -0.00026 -0.00078 0.00000 -0.00068 2.19195

A67 1.87563 0.00090 -0.00085 0.00000 -0.00036 1.87527

A68 2.20357 -0.00045 -0.00155 0.00000 -0.00119 2.20238

A69 2.20357 -0.00045 -0.00155 0.00000 -0.00119 2.20238

A70 1.56511 0.00007 -0.00644 0.00000 -0.00557 1.55954

A71 1.56511 0.00007 -0.00644 0.00000 -0.00557 1.55954

A72 2.99057 0.00091 -0.06163 0.00000 -0.06157 2.92900

A73 2.99057 0.00091 -0.06163 0.00000 -0.06157 2.92900

A74 1.56511 0.00007 -0.00644 0.00000 -0.00557 1.55954

A75 1.56511 0.00007 -0.00644 0.00000 -0.00557 1.55954

A76 2.20385 0.00139 0.00033 0.00000 0.00055 2.20440

A77 2.03944 -0.00068 -0.00007 0.00000 -0.00017 2.03927

A78 2.03944 -0.00069 -0.00007 0.00000 -0.00017 2.03927

A79 3.14138 0.00002 0.00009 0.00000 0.00007 3.14145

A80 3.14138 0.00002 0.00009 0.00000 0.00007 3.14145

A81 3.14174 0.00000 -0.00005 0.00000 -0.00003 3.14171

A82 3.14174 0.00000 -0.00005 0.00000 -0.00003 3.14171

A83 3.14138 0.00002 0.00009 0.00000 0.00007 3.14145

A84 3.14174 0.00000 -0.00005 0.00000 -0.00003 3.14171

A85 3.14138 0.00002 0.00009 0.00000 0.00007 3.14145

A86 3.14174 0.00000 -0.00005 0.00000 -0.00003 3.14171

A87 3.12530 0.00106 0.00719 0.00000 0.00719 3.13249

A88 3.15788 -0.00106 -0.00719 0.00000 -0.00719 3.15069

A89 3.15790 -0.00027 -0.00709 0.00000 -0.00709 3.15082

A90 3.12528 0.00027 0.00709 0.00000 0.00709 3.13237

A91 3.12530 0.00106 0.00719 0.00000 0.00719 3.13249

A92 3.15790 -0.00027 -0.00709 0.00000 -0.00709 3.15082

A93 3.15788 -0.00106 -0.00719 0.00000 -0.00719 3.15069

A94 3.12528 0.00027 0.00709 0.00000 0.00709 3.13237

D1 -0.00319 -0.00002 0.00214 0.00000 0.00214 -0.00106

D2 3.11214 0.00032 0.00695 0.00000 0.00695 3.11908

D3 3.13733 -0.00001 0.00682 0.00000 0.00681 -3.13904

D4 -0.03052 0.00033 0.01163 0.00000 0.01162 -0.01890

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 3.14049 0.00000 0.00480 0.00000 0.00481 -3.13788

D7 -3.14049 0.00000 -0.00480 0.00000 -0.00481 3.13788

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00516 0.00003 -0.00346 0.00000 -0.00345 0.00171

D10 -3.10689 0.00020 0.04843 0.00000 0.04843 -3.05846

D11 -3.10999 -0.00032 -0.00831 0.00000 -0.00830 -3.11829

D12 0.06114 -0.00015 0.04358 0.00000 0.04358 0.10472

D13 -3.09935 -0.00061 -0.00478 0.00000 -0.00478 -3.10413

D14 0.00877 0.00018 0.00445 0.00000 0.00445 0.01322

D15 0.01175 -0.00021 0.00082 0.00000 0.00083 0.01258

D16 3.11986 0.00058 0.01006 0.00000 0.01006 3.12992

D17 -0.00516 -0.00003 0.00346 0.00000 0.00345 -0.00171

D18 3.10999 0.00032 0.00831 0.00000 0.00830 3.11829

D19 3.10689 -0.00020 -0.04843 0.00000 -0.04843 3.05846

D20 -0.06114 0.00015 -0.04358 0.00000 -0.04358 -0.10472

D21 -3.08377 -0.00054 -0.00037 0.00000 -0.00027 -3.08403

D22 -0.09277 0.00036 -0.06096 0.00000 -0.06108 -0.15384

D23 -1.58827 -0.00009 -0.03067 0.00000 -0.03067 -1.61894

D24 0.09277 -0.00036 0.06096 0.00000 0.06108 0.15384

D25 3.08377 0.00054 0.00037 0.00000 0.00027 3.08403

D26 1.58827 0.00009 0.03067 0.00000 0.03067 1.61894

D27 0.00319 0.00002 -0.00214 0.00000 -0.00214 0.00106

D28 -3.13733 0.00001 -0.00682 0.00000 -0.00681 3.13904

D29 -3.11214 -0.00032 -0.00695 0.00000 -0.00695 -3.11908

D30 0.03052 -0.00033 -0.01163 0.00000 -0.01162 0.01890

D31 -0.01175 0.00021 -0.00082 0.00000 -0.00083 -0.01258

D32 -3.11986 -0.00058 -0.01006 0.00000 -0.01006 -3.12992

D33 3.09935 0.00061 0.00478 0.00000 0.00478 3.10413

D34 -0.00877 -0.00018 -0.00445 0.00000 -0.00445 -0.01322

D35 0.01175 -0.00021 0.00082 0.00000 0.00083 0.01258

D36 -3.09935 -0.00061 -0.00478 0.00000 -0.00478 -3.10413

D37 3.11986 0.00058 0.01006 0.00000 0.01006 3.12992

D38 0.00877 0.00018 0.00445 0.00000 0.00445 0.01322

D39 -3.10999 -0.00032 -0.00831 0.00000 -0.00830 -3.11829

D40 0.06114 -0.00015 0.04358 0.00000 0.04358 0.10472

D41 0.00516 0.00003 -0.00346 0.00000 -0.00345 0.00171

D42 -3.10689 0.00020 0.04843 0.00000 0.04843 -3.05846

D43 3.11214 0.00032 0.00695 0.00000 0.00695 3.11908

D44 -0.03052 0.00033 0.01163 0.00000 0.01162 -0.01890

D45 -0.00319 -0.00002 0.00214 0.00000 0.00214 -0.00106

D46 3.13733 -0.00001 0.00682 0.00000 0.00681 -3.13904

D47 -0.00516 -0.00003 0.00346 0.00000 0.00345 -0.00171

D48 3.10999 0.00032 0.00831 0.00000 0.00830 3.11829

D49 3.10689 -0.00020 -0.04843 0.00000 -0.04843 3.05846

D50 -0.06114 0.00015 -0.04358 0.00000 -0.04358 -0.10472

D51 -0.09277 0.00036 -0.06096 0.00000 -0.06108 -0.15384

D52 -1.58827 -0.00009 -0.03067 0.00000 -0.03067 -1.61894

D53 -3.08377 -0.00054 -0.00037 0.00000 -0.00027 -3.08403

D54 3.08377 0.00054 0.00037 0.00000 0.00027 3.08403

D55 1.58827 0.00009 0.03067 0.00000 0.03067 1.61894

D56 0.09277 -0.00036 0.06096 0.00000 0.06108 0.15384

D57 0.00319 0.00002 -0.00214 0.00000 -0.00214 0.00106

D58 -3.13733 0.00001 -0.00682 0.00000 -0.00681 3.13904

D59 -3.11214 -0.00032 -0.00695 0.00000 -0.00695 -3.11908

D60 0.03052 -0.00033 -0.01163 0.00000 -0.01162 0.01890

D61 -0.01175 0.00021 -0.00082 0.00000 -0.00083 -0.01258

D62 -3.11986 -0.00058 -0.01006 0.00000 -0.01006 -3.12992

D63 3.09935 0.00061 0.00478 0.00000 0.00478 3.10413

D64 -0.00877 -0.00018 -0.00445 0.00000 -0.00445 -0.01322

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 -3.14049 0.00000 -0.00480 0.00000 -0.00481 3.13788

D67 3.14049 0.00000 0.00480 0.00000 0.00481 -3.13788

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.09935 0.00061 0.00478 0.00000 0.00478 3.10413

D70 -0.01175 0.00021 -0.00082 0.00000 -0.00083 -0.01258

D71 -0.00877 -0.00018 -0.00445 0.00000 -0.00445 -0.01322

D72 -3.11986 -0.00058 -0.01006 0.00000 -0.01006 -3.12992

D73 -3.11214 -0.00032 -0.00695 0.00000 -0.00695 -3.11908

D74 0.03052 -0.00033 -0.01163 0.00000 -0.01162 0.01890

D75 0.00319 0.00002 -0.00214 0.00000 -0.00214 0.00106

D76 -3.13733 0.00001 -0.00682 0.00000 -0.00681 3.13904

D77 3.10999 0.00032 0.00831 0.00000 0.00830 3.11829

D78 -0.06114 0.00015 -0.04358 0.00000 -0.04358 -0.10472

D79 -0.00516 -0.00003 0.00346 0.00000 0.00345 -0.00171

D80 3.10689 -0.00020 -0.04843 0.00000 -0.04843 3.05846

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 -3.14049 0.00000 -0.00480 0.00000 -0.00481 3.13788

D83 3.14049 0.00000 0.00480 0.00000 0.00481 -3.13788

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 -0.00319 -0.00002 0.00214 0.00000 0.00214 -0.00106

D86 3.11214 0.00032 0.00695 0.00000 0.00695 3.11908

D87 3.13733 -0.00001 0.00682 0.00000 0.00681 -3.13904

D88 -0.03052 0.00033 0.01163 0.00000 0.01162 -0.01890

D89 0.00516 0.00003 -0.00346 0.00000 -0.00345 0.00171

D90 -3.10689 0.00020 0.04843 0.00000 0.04843 -3.05846

D91 -3.10999 -0.00032 -0.00831 0.00000 -0.00830 -3.11829

D92 0.06114 -0.00015 0.04358 0.00000 0.04358 0.10472

D93 -3.09935 -0.00061 -0.00478 0.00000 -0.00478 -3.10413

D94 0.00877 0.00018 0.00445 0.00000 0.00445 0.01322

D95 0.01175 -0.00021 0.00082 0.00000 0.00083 0.01258

D96 3.11986 0.00058 0.01006 0.00000 0.01006 3.12992

D97 0.09277 -0.00036 0.06096 0.00000 0.06108 0.15384

D98 1.58827 0.00009 0.03067 0.00000 0.03067 1.61894

D99 3.08377 0.00054 0.00037 0.00000 0.00027 3.08403

D100 -3.08377 -0.00054 -0.00037 0.00000 -0.00027 -3.08403

D101 -1.58827 -0.00009 -0.03067 0.00000 -0.03067 -1.61894

D102 -0.09277 0.00036 -0.06096 0.00000 -0.06108 -0.15384

D103 3.09935 0.00061 0.00478 0.00000 0.00478 3.10413

D104 -0.01175 0.00021 -0.00082 0.00000 -0.00083 -0.01258

D105 -0.00877 -0.00018 -0.00445 0.00000 -0.00445 -0.01322

D106 -3.11986 -0.00058 -0.01006 0.00000 -0.01006 -3.12992

D107 -3.11214 -0.00032 -0.00695 0.00000 -0.00695 -3.11908

D108 0.03052 -0.00033 -0.01163 0.00000 -0.01162 0.01890

D109 0.00319 0.00002 -0.00214 0.00000 -0.00214 0.00106

D110 -3.13733 0.00001 -0.00682 0.00000 -0.00681 3.13904

D111 3.10999 0.00032 0.00831 0.00000 0.00830 3.11829

D112 -0.06114 0.00015 -0.04358 0.00000 -0.04358 -0.10472

D113 -0.00516 -0.00003 0.00346 0.00000 0.00345 -0.00171

D114 3.10689 -0.00020 -0.04843 0.00000 -0.04843 3.05846

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 -3.14049 0.00000 -0.00480 0.00000 -0.00481 3.13788

D117 3.14049 0.00000 0.00480 0.00000 0.00481 -3.13788

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 -0.00319 -0.00002 0.00214 0.00000 0.00214 -0.00106

D120 3.11214 0.00032 0.00695 0.00000 0.00695 3.11908

D121 3.13733 -0.00001 0.00682 0.00000 0.00681 -3.13904

D122 -0.03052 0.00033 0.01163 0.00000 0.01162 -0.01890

D123 0.00516 0.00003 -0.00346 0.00000 -0.00345 0.00171

D124 -3.10689 0.00020 0.04843 0.00000 0.04843 -3.05846

D125 -3.10999 -0.00032 -0.00831 0.00000 -0.00830 -3.11829

D126 0.06114 -0.00015 0.04358 0.00000 0.04358 0.10472

D127 -3.09935 -0.00061 -0.00478 0.00000 -0.00478 -3.10413

D128 0.00877 0.00018 0.00445 0.00000 0.00445 0.01322

D129 0.01175 -0.00021 0.00082 0.00000 0.00083 0.01258

D130 3.11986 0.00058 0.01006 0.00000 0.01006 3.12992

D131 1.58827 0.00009 0.03067 0.00000 0.03067 1.61894

D132 3.08377 0.00054 0.00037 0.00000 0.00027 3.08403

D133 0.09277 -0.00036 0.06096 0.00000 0.06108 0.15384

D134 -1.58827 -0.00009 -0.03067 0.00000 -0.03067 -1.61894

D135 -0.09277 0.00036 -0.06096 0.00000 -0.06108 -0.15384

D136 -3.08377 -0.00054 -0.00037 0.00000 -0.00027 -3.08403

Item Value Threshold Converged?

Maximum Force 0.002194 0.000450 NO

RMS Force 0.000609 0.000300 NO

Maximum Displacement 0.100396 0.001800 NO

RMS Displacement 0.017954 0.001200 NO

Predicted change in Energy=-2.838567D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:17:53 2019, MaxMem= 1342177280 cpu: 1.0

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.681427 4.272266 -0.039389

2 6 0 1.102696 2.889778 0.014450

3 7 0 0.000000 2.081100 0.047309

4 6 0 -1.102696 2.889778 0.014450

5 6 0 -0.681427 4.272266 -0.039389

6 6 0 -2.448505 2.448505 0.005521

7 6 0 -2.889778 1.102696 0.014450

8 7 0 -2.081100 0.000000 0.047309

9 6 0 -2.889778 -1.102696 0.014450

10 6 0 -4.272266 -0.681427 -0.039389

11 6 0 -4.272266 0.681427 -0.039389

12 6 0 2.448505 2.448505 0.005521

13 6 0 2.889778 1.102696 0.014450

14 6 0 4.272266 0.681427 -0.039389

15 6 0 4.272266 -0.681427 -0.039389

16 6 0 2.889778 -1.102696 0.014450

17 7 0 2.081100 0.000000 0.047309

18 6 0 2.448505 -2.448505 0.005521

19 6 0 1.102696 -2.889778 0.014450

20 6 0 0.681427 -4.272266 -0.039389

21 6 0 -0.681427 -4.272266 -0.039389

22 6 0 -1.102696 -2.889778 0.014450

23 7 0 0.000000 -2.081100 0.047309

24 1 0 1.340678 5.126277 -0.075826

25 1 0 -1.340678 5.126277 -0.075826

26 1 0 -5.126277 -1.340678 -0.075826

27 1 0 -5.126277 1.340678 -0.075826

28 1 0 5.126277 1.340678 -0.075826

29 1 0 5.126277 -1.340678 -0.075826

30 1 0 1.340678 -5.126277 -0.075826

31 1 0 -1.340678 -5.126277 -0.075826

32 30 0 0.000000 0.000000 0.269364

33 6 0 -2.448505 -2.448505 0.005521

34 6 0 -3.455873 -3.455873 -0.045207

35 6 0 3.455873 3.455873 -0.045207

36 6 0 -4.307730 -4.307730 -0.099012

37 6 0 4.307730 4.307730 -0.099012

38 6 0 -3.455873 3.455873 -0.045207

39 6 0 -4.307730 4.307730 -0.099012

40 6 0 3.455873 -3.455873 -0.045207

41 6 0 4.307730 -4.307730 -0.099012

42 1 0 5.061897 -5.061897 -0.138075

43 1 0 -5.061897 -5.061897 -0.138075

44 1 0 -5.061897 5.061897 -0.138075

45 1 0 5.061897 5.061897 -0.138075

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.446250 0.000000

3 N 2.296316 1.367837 0.000000

4 C 2.257712 2.205391 1.367837 0.000000

5 C 1.362853 2.257712 2.296316 1.446250 0.000000

6 C 3.622788 3.578523 2.476269 1.416335 2.539820

7 C 4.775204 4.374187 3.051094 2.527316 3.863404

8 N 5.088352 4.299820 2.943120 3.051094 4.496539

9 C 6.453419 5.646211 4.299820 4.374187 5.811190

10 C 7.005579 6.453419 5.088352 4.775204 6.118267

11 C 6.118267 5.811190 4.496539 3.863404 5.078214

12 C 2.539820 1.416335 2.476269 3.578523 3.622788

13 C 3.863404 2.527316 3.051094 4.374187 4.775204

14 C 5.078214 3.863404 4.496539 5.811190 6.118267

15 C 6.118267 4.775204 5.088352 6.453419 7.005579

16 C 5.811190 4.374187 4.299820 5.646211 6.453419

17 N 4.496539 3.051094 2.943120 4.299820 5.088352

18 C 6.949341 5.505320 5.149199 6.411581 7.413990

19 C 7.174625 5.779556 5.091822 6.186035 7.381116

20 C 8.544532 7.174625 6.390393 7.381116 8.652537

21 C 8.652537 7.381116 6.390393 7.174625 8.544532

22 C 7.381116 6.186035 5.091822 5.779556 7.174625

23 N 6.390393 5.091822 4.162201 5.091822 6.390393

24 H 1.079480 2.250936 3.329517 3.313632 2.195352

25 H 2.195352 3.313632 3.329517 2.250936 1.079480

26 H 8.076874 7.530273 6.164613 5.839017 7.159830

27 H 6.505764 6.419343 5.180937 4.312432 5.324681

28 H 5.324681 4.312432 5.180937 6.419343 6.505764

29 H 7.159830 5.839017 6.164613 7.530273 8.076874

30 H 9.421707 8.020096 7.332044 8.380655 9.613680

31 H 9.613680 8.380655 7.332044 8.020096 9.421707

32 Zn 4.337272 3.103504 2.092913 3.103504 4.337272

33 C 7.413990 6.411581 5.149199 5.505320 6.949341

34 C 8.765924 7.813540 6.527610 6.768182 8.211073

35 C 2.892073 2.421047 3.720433 4.593971 4.217082

36 C 9.925299 9.004982 7.706821 7.879672 9.315039

37 C 3.626967 3.506523 4.851373 5.594297 4.989638

38 C 4.217082 4.593971 3.720433 2.421047 2.892073

39 C 4.989638 5.594297 4.851373 3.506523 3.626967

40 C 8.211073 6.768182 6.527610 7.813540 8.765924

41 C 9.315039 7.879672 7.706821 9.004982 9.925299

42 H 10.311394 8.884125 8.756687 10.062534 10.960022

43 H 10.960022 10.062534 8.756687 8.884125 10.311394

44 H 5.798191 6.537856 5.877271 4.518477 4.452165

45 H 4.452165 4.518477 5.877271 6.537856 5.798191

6 7 8 9 10

6 C 0.000000

7 C 1.416335 0.000000

8 N 2.476269 1.367837 0.000000

9 C 3.578523 2.205391 1.367837 0.000000

10 C 3.622788 2.257712 2.296316 1.446250 0.000000

11 C 2.539820 1.446250 2.296316 2.257712 1.362853

12 C 4.897010 5.505320 5.149199 6.411581 7.413990

13 C 5.505320 5.779556 5.091822 6.186035 7.381116

14 C 6.949341 7.174625 6.390393 7.381116 8.652537

15 C 7.413990 7.381116 6.390393 7.174625 8.544532

16 C 6.411581 6.186035 5.091822 5.779556 7.174625

17 N 5.149199 5.091822 4.162201 5.091822 6.390393

18 C 6.925418 6.411581 5.149199 5.505320 6.949341

19 C 6.411581 5.646211 4.299820 4.374187 5.811190

20 C 7.413990 6.453419 5.088352 4.775204 6.118267

21 C 6.949341 5.811190 4.496539 3.863404 5.078214

22 C 5.505320 4.374187 3.051094 2.527316 3.863404

23 N 5.149199 4.299820 2.943120 3.051094 4.496539

24 H 4.640581 5.839017 6.164613 7.530273 8.076874

25 H 2.899028 4.312432 5.180937 6.419343 6.505764

26 H 4.640581 3.313632 3.329517 2.250936 1.079480

27 H 2.899028 2.250936 3.329517 3.313632 2.195352

28 H 7.655797 8.020096 7.332044 8.380655 9.613680

29 H 8.470056 8.380655 7.332044 8.020096 9.421707

30 H 8.470056 7.530273 6.164613 5.839017 7.159830

31 H 7.655797 6.419343 5.180937 4.312432 5.324681

32 Zn 3.472746 3.103504 2.092913 3.103504 4.337272

33 C 4.897010 3.578523 2.476269 1.416335 2.539820

34 C 5.989912 4.593971 3.720433 2.421047 2.892073

35 C 5.989912 6.768182 6.527610 7.813540 8.765924

36 C 7.008163 5.594297 4.851373 3.506523 3.626967

37 C 7.008163 7.879672 7.706821 9.004982 9.925299

38 C 1.425537 2.421047 3.720433 4.593971 4.217082

39 C 2.631418 3.506523 4.851373 5.594297 4.989638

40 C 8.350206 7.813540 6.527610 6.768182 8.211073

41 C 9.555330 9.004982 7.706821 7.879672 9.315039

42 H 10.622282 10.062534 8.756687 8.884125 10.311394

43 H 7.953400 6.537856 5.877271 4.518477 4.452165

44 H 3.698683 4.518477 5.877271 6.537856 5.798191

45 H 7.953400 8.884125 8.756687 10.062534 10.960022

11 12 13 14 15

11 C 0.000000

12 C 6.949341 0.000000

13 C 7.174625 1.416335 0.000000

14 C 8.544532 2.539820 1.446250 0.000000

15 C 8.652537 3.622788 2.257712 1.362853 0.000000

16 C 7.381116 3.578523 2.205391 2.257712 1.446250

17 N 6.390393 2.476269 1.367837 2.296316 2.296316

18 C 7.413990 4.897010 3.578523 3.622788 2.539820

19 C 6.453419 5.505320 4.374187 4.775204 3.863404

20 C 7.005579 6.949341 5.811190 6.118267 5.078214

21 C 6.118267 7.413990 6.453419 7.005579 6.118267

22 C 4.775204 6.411581 5.646211 6.453419 5.811190

23 N 5.088352 5.149199 4.299820 5.088352 4.496539

24 H 7.159830 2.899028 4.312432 5.324681 6.505764

25 H 5.324681 4.640581 5.839017 7.159830 8.076874

26 H 2.195352 8.470056 8.380655 9.613680 9.421707

27 H 1.079480 7.655797 8.020096 9.421707 9.613680

28 H 9.421707 2.899028 2.250936 1.079480 2.195352

29 H 9.613680 4.640581 3.313632 2.195352 1.079480

30 H 8.076874 7.655797 6.419343 6.505764 5.324681

31 H 6.505764 8.470056 7.530273 8.076874 7.159830

32 Zn 4.337272 3.472746 3.103504 4.337272 4.337272

33 C 3.622788 6.925418 6.411581 7.413990 6.949341

34 C 4.217082 8.350206 7.813540 8.765924 8.211073

35 C 8.211073 1.425537 2.421047 2.892073 4.217082

36 C 4.989638 9.555330 9.004982 9.925299 9.315039

37 C 9.315039 2.631418 3.506523 3.626967 4.989638

38 C 2.892073 5.989912 6.768182 8.211073 8.765924

39 C 3.626967 7.008163 7.879672 9.315039 9.925299

40 C 8.765924 5.989912 4.593971 4.217082 2.892073

41 C 9.925299 7.008163 5.594297 4.989638 3.626967

42 H 10.960022 7.953400 6.537856 5.798191 4.452165

43 H 5.798191 10.622282 10.062534 10.960022 10.311394

44 H 4.452165 7.953400 8.884125 10.311394 10.960022

45 H 10.311394 3.698683 4.518477 4.452165 5.798191

16 17 18 19 20

16 C 0.000000

17 N 1.367837 0.000000

18 C 1.416335 2.476269 0.000000

19 C 2.527316 3.051094 1.416335 0.000000

20 C 3.863404 4.496539 2.539820 1.446250 0.000000

21 C 4.775204 5.088352 3.622788 2.257712 1.362853

22 C 4.374187 4.299820 3.578523 2.205391 2.257712

23 N 3.051094 2.943120 2.476269 1.367837 2.296316

24 H 6.419343 5.180937 7.655797 8.020096 9.421707

25 H 7.530273 6.164613 8.470056 8.380655 9.613680

26 H 8.020096 7.332044 7.655797 6.419343 6.505764

27 H 8.380655 7.332044 8.470056 7.530273 8.076874

28 H 3.313632 3.329517 4.640581 5.839017 7.159830

29 H 2.250936 3.329517 2.899028 4.312432 5.324681

30 H 4.312432 5.180937 2.899028 2.250936 1.079480

31 H 5.839017 6.164613 4.640581 3.313632 2.195352

32 Zn 3.103504 2.092913 3.472746 3.103504 4.337272

33 C 5.505320 5.149199 4.897010 3.578523 3.622788

34 C 6.768182 6.527610 5.989912 4.593971 4.217082

35 C 4.593971 3.720433 5.989912 6.768182 8.211073

36 C 7.879672 7.706821 7.008163 5.594297 4.989638

37 C 5.594297 4.851373 7.008163 7.879672 9.315039

38 C 7.813540 6.527610 8.350206 7.813540 8.765924

39 C 9.004982 7.706821 9.555330 9.004982 9.925299

40 C 2.421047 3.720433 1.425537 2.421047 2.892073

41 C 3.506523 4.851373 2.631418 3.506523 3.626967

42 H 4.518477 5.877271 3.698683 4.518477 4.452165

43 H 8.884125 8.756687 7.953400 6.537856 5.798191

44 H 10.062534 8.756687 10.622282 10.062534 10.960022

45 H 6.537856 5.877271 7.953400 8.884125 10.311394

21 22 23 24 25

21 C 0.000000

22 C 1.446250 0.000000

23 N 2.296316 1.367837 0.000000

24 H 9.613680 8.380655 7.332044 0.000000

25 H 9.421707 8.020096 7.332044 2.681356 0.000000

26 H 5.324681 4.312432 5.180937 9.145656 7.493482

27 H 7.159830 5.839017 6.164613 7.493482 5.353646

28 H 8.076874 7.530273 6.164613 5.353646 7.493482

29 H 6.505764 6.419343 5.180937 7.493482 9.145656

30 H 2.195352 3.313632 3.329517 10.252555 10.597384

31 H 1.079480 2.250936 3.329517 10.597384 10.252555

32 Zn 4.337272 3.103504 2.092913 5.309924 5.309924

33 C 2.539820 1.416335 2.476269 8.470056 7.655797

34 C 2.892073 2.421047 3.720433 9.831640 8.839021

35 C 8.765924 7.813540 6.527610 2.695410 5.079182

36 C 3.626967 3.506523 4.851373 10.995705 9.889612

37 C 9.925299 9.004982 7.706821 3.077979 5.707457

38 C 8.211073 6.768182 6.527610 5.079182 2.695410

39 C 9.315039 7.879672 7.706821 5.707457 3.077979

40 C 4.217082 4.593971 3.720433 8.839021 9.831640

41 C 4.989638 5.594297 4.851373 9.889612 10.995705

42 H 5.798191 6.537856 5.877271 10.846669 12.033110

43 H 4.452165 4.518477 5.877271 12.033110 10.846669

44 H 10.311394 8.884125 8.756687 6.403201 3.722296

45 H 10.960022 10.062534 8.756687 3.722296 6.403201

26 27 28 29 30

26 H 0.000000

27 H 2.681356 0.000000

28 H 10.597384 10.252555 0.000000

29 H 10.252555 10.597384 2.681356 0.000000

30 H 7.493482 9.145656 7.493482 5.353646 0.000000

31 H 5.353646 7.493482 9.145656 7.493482 2.681356

32 Zn 5.309924 5.309924 5.309924 5.309924 5.309924

33 C 2.899028 4.640581 8.470056 7.655797 4.640581

34 C 2.695410 5.079182 9.831640 8.839021 5.079182

35 C 9.831640 8.839021 2.695410 5.079182 8.839021

36 C 3.077979 5.707457 10.995705 9.889612 5.707457

37 C 10.995705 9.889612 3.077979 5.707457 9.889612

38 C 5.079182 2.695410 8.839021 9.831640 9.831640

39 C 5.707457 3.077979 9.889612 10.995705 10.995705

40 C 8.839021 9.831640 5.079182 2.695410 2.695410

41 C 9.889612 10.995705 5.707457 3.077979 3.077979

42 H 10.846669 12.033110 6.403201 3.722296 3.722296

43 H 3.722296 6.403201 12.033110 10.846669 6.403201

44 H 6.403201 3.722296 10.846669 12.033110 12.033110

45 H 12.033110 10.846669 3.722296 6.403201 10.846669

31 32 33 34 35

31 H 0.000000

32 Zn 5.309924 0.000000

33 C 2.899028 3.472746 0.000000

34 C 2.695410 4.897456 1.425537 0.000000

35 C 9.831640 4.897456 8.350206 9.774685 0.000000

36 C 3.077979 6.103177 2.631418 1.205908 10.979524

37 C 10.995705 6.103177 9.555330 10.979524 1.205908

38 C 8.839021 4.897456 5.989912 6.911746 6.911746

39 C 9.889612 6.103177 7.008163 7.810383 7.810383

40 C 5.079182 4.897456 5.989912 6.911746 6.911746

41 C 5.707457 6.103177 7.008163 7.810383 7.810383

42 H 6.403201 7.170188 7.953400 8.668353 8.668353

43 H 3.722296 7.170188 3.698683 2.273158 12.046303

44 H 10.846669 7.170188 7.953400 8.668353 8.668353

45 H 12.033110 7.170188 10.622282 12.046303 2.273158

36 37 38 39 40

36 C 0.000000

37 C 12.184099 0.000000

38 C 7.810383 7.810383 0.000000

39 C 8.615459 8.615459 1.205908 0.000000

40 C 7.810383 7.810383 9.774685 10.979524 0.000000

41 C 8.615459 8.615459 10.979524 12.184099 1.205908

42 H 9.400010 9.400010 12.046303 13.250710 2.273158

43 H 1.067268 13.250710 8.668353 9.400010 8.668353

44 H 9.400010 9.400010 2.273158 1.067268 12.046303

45 H 13.250710 1.067268 8.668353 9.400010 8.668353

41 42 43 44 45

41 C 0.000000

42 H 1.067268 0.000000

43 H 9.400010 10.123793 0.000000

44 H 13.250710 14.317206 10.123793 0.000000

45 H 9.400010 10.123793 14.317206 10.123793 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

Omega: Change in point group or standard orientation.

Old FWG=C04V [C4(Zn1),2SGV(C6H2),2SGD(N2),X(C16H8)]

New FWG=C04V [C4(Zn1),2SGV(N2),2SGD(C6H2),X(C16H8)]

RotChk: IX=3 Diff= 1.08D+00

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681427 -4.272266 -0.055023

2 6 0 -1.102696 -2.889778 -0.001184

3 7 0 0.000000 -2.081100 0.031675

4 6 0 1.102696 -2.889778 -0.001184

5 6 0 0.681427 -4.272266 -0.055023

6 6 0 2.448505 -2.448505 -0.010113

7 6 0 2.889778 -1.102696 -0.001184

8 7 0 2.081100 0.000000 0.031675

9 6 0 2.889778 1.102696 -0.001184

10 6 0 4.272266 0.681427 -0.055023

11 6 0 4.272266 -0.681427 -0.055023

12 6 0 -2.448505 -2.448505 -0.010113

13 6 0 -2.889778 -1.102696 -0.001184

14 6 0 -4.272266 -0.681427 -0.055023

15 6 0 -4.272266 0.681427 -0.055023

16 6 0 -2.889778 1.102696 -0.001184

17 7 0 -2.081100 0.000000 0.031675

18 6 0 -2.448505 2.448505 -0.010113

19 6 0 -1.102696 2.889778 -0.001184

20 6 0 -0.681427 4.272266 -0.055023

21 6 0 0.681427 4.272266 -0.055023

22 6 0 1.102696 2.889778 -0.001184

23 7 0 0.000000 2.081100 0.031675

24 1 0 -1.340678 -5.126277 -0.091460

25 1 0 1.340678 -5.126277 -0.091460

26 1 0 5.126277 1.340678 -0.091460

27 1 0 5.126277 -1.340678 -0.091460

28 1 0 -5.126277 -1.340678 -0.091460

29 1 0 -5.126277 1.340678 -0.091460

30 1 0 -1.340678 5.126277 -0.091460

31 1 0 1.340678 5.126277 -0.091460

32 30 0 0.000000 0.000000 0.253730

33 6 0 2.448505 2.448505 -0.010113

34 6 0 3.455873 3.455873 -0.060841

35 6 0 -3.455873 -3.455873 -0.060841

36 6 0 4.307730 4.307730 -0.114645

37 6 0 -4.307730 -4.307730 -0.114645

38 6 0 3.455873 -3.455873 -0.060841

39 6 0 4.307730 -4.307730 -0.114645

40 6 0 -3.455873 3.455873 -0.060841

41 6 0 -4.307730 4.307730 -0.114645

42 1 0 -5.061897 5.061897 -0.153709

43 1 0 5.061897 5.061897 -0.153709

44 1 0 5.061897 -5.061897 -0.153709

45 1 0 -5.061897 -5.061897 -0.153709

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

Rotational constants (GHZ): 0.1463786 0.1463786 0.0733045

Leave Link 202 at Fri Jul 26 14:17:53 2019, MaxMem= 1342177280 cpu: 0.1

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 184 symmetry adapted cartesian basis functions of A1 symmetry.

There are 155 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3059.5838261618 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= 9 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= -0.1305095028 Hartrees.

Nuclear repulsion after empirical dispersion term = 3059.4533166590 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: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3850

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.26D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 168

GePol: Fraction of low-weight points (<1% of avg) = 4.36%

GePol: Cavity surface area = 416.835 Ang\*\*2

GePol: Cavity volume = 420.500 Ang\*\*3

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

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

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PCM non-electrostatic energy = 0.0084076316 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3059.4617242906 Hartrees.

Leave Link 301 at Fri Jul 26 14:17:53 2019, MaxMem= 1342177280 cpu: 1.0

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44800.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.41D-05 NBF= 172 148 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 172 148 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:17:54 2019, MaxMem= 1342177280 cpu: 6.5

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:17:54 2019, MaxMem= 1342177280 cpu: 0.8

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

Lowest energy guess from the checkpoint file: "ZnTSPsim0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.923880 0.000000 0.000000 -0.382683 Ang= -45.00 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 4.84D-01

Max alpha theta= 1.331 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Occupied (B1) (E) (E) (A1) (A1) (A1) (B1) (E) (E) (A1)

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

(A2) (E) (E) (A2) (E) (E) (B2) (A1) (E) (E) (E)

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

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

(B2) (E) (E) (A2) (B2) (E) (E) (A1) (E) (E) (E)

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

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

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

(A2) (B2) (E) (E)

Virtual (B1) (E) (E) (A1) (A1) (A1) (B1) (E) (E) (A1)

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The electronic state of the initial guess is 1-A1.

Leave Link 401 at Fri Jul 26 14:17:55 2019, MaxMem= 1342177280 cpu: 16.7

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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.

An orbital has undefined symmetry, so N\*\*3 symmetry is turned off.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 660000000 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= 0 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= 44467500.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.10D-15 for 3849.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.01D-15 for 2252 1939.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.99D-15 for 3849.

Iteration 1 A^-1\*A deviation from orthogonality is 1.71D-13 for 916 864.

E= -1359.06272248912

DIIS: error= 1.24D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.06272248912 IErMin= 1 ErrMin= 1.24D-04

ErrMax= 1.24D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.51D-06 BMatP= 2.51D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.24D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 10.472 Goal= None Shift= 0.000

RMSDP=1.58D-05 MaxDP=8.46D-04 OVMax= 6.12D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.58D-05 CP: 1.00D+00

E= -1359.06272498700 Delta-E= -0.000002497879 Rises=F Damp=F

DIIS: error= 2.23D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.06272498700 IErMin= 1 ErrMin= 1.24D-04

ErrMax= 2.23D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.96D-06 BMatP= 2.51D-06

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.23D-03

Coeff-Com: 0.459D+00 0.541D+00

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

Coeff: 0.458D+00 0.542D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=3.59D-06 MaxDP=1.05D-04 DE=-2.50D-06 OVMax= 1.54D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.27D-06 CP: 1.00D+00 9.07D-01

E= -1359.06272594066 Delta-E= -0.000000953662 Rises=F Damp=F

DIIS: error= 6.53D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.06272594066 IErMin= 3 ErrMin= 6.53D-05

ErrMax= 6.53D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.15D-07 BMatP= 1.96D-06

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

Coeff-Com: 0.379D-01 0.245D+00 0.717D+00

Coeff: 0.379D-01 0.245D+00 0.717D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 305122 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=6.85D-07 MaxDP=2.83D-05 DE=-9.54D-07 OVMax= 8.84D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.49D-07 CP: 1.00D+00 9.17D-01 1.04D+00

E= -1359.06272601586 Delta-E= -0.000000075202 Rises=F Damp=F

DIIS: error= 9.58D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.06272601586 IErMin= 4 ErrMin= 9.58D-06

ErrMax= 9.58D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.72D-08 BMatP= 2.15D-07

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

Coeff-Com: 0.462D-02 0.125D+00 0.380D+00 0.491D+00

Coeff: 0.462D-02 0.125D+00 0.380D+00 0.491D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.64D-07 MaxDP=1.47D-05 DE=-7.52D-08 OVMax= 4.53D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.49D-07 CP: 1.00D+00 9.19D-01 1.05D+00 8.89D-01

E= -1359.06272603433 Delta-E= -0.000000018469 Rises=F Damp=F

DIIS: error= 3.99D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.06272603433 IErMin= 5 ErrMin= 3.99D-06

ErrMax= 3.99D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.34D-09 BMatP= 2.72D-08

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

Coeff-Com: -0.285D-02 0.353D-01 0.792D-01 0.289D+00 0.600D+00

Coeff: -0.285D-02 0.353D-01 0.792D-01 0.289D+00 0.600D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.44D-07 MaxDP=3.97D-06 DE=-1.85D-08 OVMax= 1.52D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 7.12D-08 CP: 1.00D+00 9.22D-01 1.03D+00 8.94D-01 7.15D-01

E= -1359.06272603849 Delta-E= -0.000000004162 Rises=F Damp=F

DIIS: error= 1.23D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.06272603849 IErMin= 6 ErrMin= 1.23D-06

ErrMax= 1.23D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.17D-10 BMatP= 4.34D-09

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

Coeff-Com: -0.121D-02 0.987D-02 0.115D-01 0.104D+00 0.302D+00 0.574D+00

Coeff: -0.121D-02 0.987D-02 0.115D-01 0.104D+00 0.302D+00 0.574D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.58D-08 MaxDP=1.37D-06 DE=-4.16D-09 OVMax= 3.08D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.11D-08 CP: 1.00D+00 9.22D-01 1.02D+00 8.94D-01 7.03D-01

CP: 8.18D-01

E= -1359.06272603825 Delta-E= 0.000000000244 Rises=F Damp=F

DIIS: error= 3.43D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 6 EnMin= -1359.06272603849 IErMin= 7 ErrMin= 3.43D-07

ErrMax= 3.43D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.03D-11 BMatP= 2.17D-10

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

Coeff-Com: -0.467D-03 0.183D-02-0.224D-02 0.284D-01 0.121D+00 0.354D+00

Coeff-Com: 0.497D+00

Coeff: -0.467D-03 0.183D-02-0.224D-02 0.284D-01 0.121D+00 0.354D+00

Coeff: 0.497D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.01D-08 MaxDP=4.45D-07 DE= 2.44D-10 OVMax= 1.28D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.86D-09 CP: 1.00D+00 9.22D-01 1.03D+00 8.96D-01 7.15D-01

CP: 8.01D-01 7.83D-01

E= -1359.06272603874 Delta-E= -0.000000000491 Rises=F Damp=F

DIIS: error= 1.72D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.06272603874 IErMin= 8 ErrMin= 1.72D-07

ErrMax= 1.72D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.23D-12 BMatP= 4.03D-11

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

Coeff-Com: -0.103D-03-0.516D-03-0.255D-02-0.318D-03 0.248D-01 0.115D+00

Coeff-Com: 0.274D+00 0.589D+00

Coeff: -0.103D-03-0.516D-03-0.255D-02-0.318D-03 0.248D-01 0.115D+00

Coeff: 0.274D+00 0.589D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=3.95D-09 MaxDP=2.18D-07 DE=-4.91D-10 OVMax= 4.61D-07

Error on total polarization charges = 0.06215

SCF Done: E(RB3LYP) = -1359.06272604 A.U. after 8 cycles

NFock= 8 Conv=0.40D-08 -V/T= 1.9682

KE= 1.403700510366D+03 PE=-9.361028125022D+03 EE= 3.538803164327D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.28

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:18:30 2019, MaxMem= 1342177280 cpu: 387.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44800.

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 = 250

Leave Link 701 at Fri Jul 26 14:18:34 2019, MaxMem= 1342177280 cpu: 42.7

(Enter /apps/gaussian/g09d01/g09/l702.exe)

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

Leave Link 702 at Fri Jul 26 14:18:34 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Fri Jul 26 14:18:37 2019, MaxMem= 1342177280 cpu: 43.4

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-2.30926389D-14 4.33431069D-13 4.07259995D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000478350 0.000204669 0.000283340

2 6 -0.000282706 -0.000805977 -0.000321054

3 7 0.000000000 0.000132353 0.001687706

4 6 0.000282706 -0.000805977 -0.000321054

5 6 0.000478350 0.000204669 0.000283340

6 6 0.001644567 -0.001644567 -0.000093833

7 6 0.000805977 -0.000282706 -0.000321054

8 7 -0.000132353 0.000000000 0.001687706

9 6 0.000805977 0.000282706 -0.000321054

10 6 -0.000204669 0.000478350 0.000283340

11 6 -0.000204669 -0.000478350 0.000283340

12 6 -0.001644567 -0.001644567 -0.000093833

13 6 -0.000805977 -0.000282706 -0.000321054

14 6 0.000204669 -0.000478350 0.000283340

15 6 0.000204669 0.000478350 0.000283340

16 6 -0.000805977 0.000282706 -0.000321054

17 7 0.000132353 0.000000000 0.001687706

18 6 -0.001644567 0.001644567 -0.000093833

19 6 -0.000282706 0.000805977 -0.000321054

20 6 -0.000478350 -0.000204669 0.000283340

21 6 0.000478350 -0.000204669 0.000283340

22 6 0.000282706 0.000805977 -0.000321054

23 7 0.000000000 -0.000132353 0.001687706

24 1 -0.000001205 0.000230311 -0.000090453

25 1 0.000001205 0.000230311 -0.000090453

26 1 -0.000230311 0.000001205 -0.000090453

27 1 -0.000230311 -0.000001205 -0.000090453

28 1 0.000230311 -0.000001205 -0.000090453

29 1 0.000230311 0.000001205 -0.000090453

30 1 -0.000001205 -0.000230311 -0.000090453

31 1 0.000001205 -0.000230311 -0.000090453

32 30 0.000000000 0.000000000 -0.005653188

33 6 0.001644567 0.001644567 -0.000093833

34 6 -0.000628220 -0.000628220 -0.000106619

35 6 0.000628220 0.000628220 -0.000106619

36 6 0.000118215 0.000118215 0.000244054

37 6 -0.000118215 -0.000118215 0.000244054

38 6 -0.000628220 0.000628220 -0.000106619

39 6 0.000118215 -0.000118215 0.000244054

40 6 0.000628220 -0.000628220 -0.000106619

41 6 -0.000118215 0.000118215 0.000244054

42 1 0.000028450 -0.000028450 -0.000061678

43 1 -0.000028450 -0.000028450 -0.000061678

44 1 -0.000028450 0.000028450 -0.000061678

45 1 0.000028450 0.000028450 -0.000061678

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

Cartesian Forces: Max 0.005653188 RMS 0.000763166

Leave Link 716 at Fri Jul 26 14:18:37 2019, MaxMem= 1342177280 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001221641 RMS 0.000402882

Search for a local minimum.

Step number 8 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .40288D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

7 8

ITU= 0 0 -1 1 0 -1 -1 0

Eigenvalues --- 0.00338 0.00485 0.00534 0.00534 0.00534

Eigenvalues --- 0.00534 0.00534 0.00534 0.00536 0.01172

Eigenvalues --- 0.01297 0.01297 0.01541 0.01541 0.01599

Eigenvalues --- 0.01650 0.01675 0.01800 0.01800 0.01813

Eigenvalues --- 0.01813 0.01826 0.01832 0.01860 0.01860

Eigenvalues --- 0.01869 0.01869 0.01869 0.01870 0.01909

Eigenvalues --- 0.01921 0.01932 0.01932 0.01934 0.01936

Eigenvalues --- 0.01970 0.01970 0.02160 0.02179 0.02181

Eigenvalues --- 0.02189 0.02189 0.02746 0.03314 0.04654

Eigenvalues --- 0.04654 0.04654 0.04654 0.04654 0.04654

Eigenvalues --- 0.04654 0.06004 0.13447 0.13845 0.15038

Eigenvalues --- 0.15038 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16474 0.22823

Eigenvalues --- 0.22865 0.22869 0.22869 0.24734 0.24734

Eigenvalues --- 0.24740 0.24750 0.24794 0.24966 0.24966

Eigenvalues --- 0.24993 0.24994 0.24994 0.24994 0.24994

Eigenvalues --- 0.26541 0.34768 0.35044 0.35044 0.35458

Eigenvalues --- 0.35500 0.36030 0.36034 0.36034 0.36034

Eigenvalues --- 0.36034 0.36034 0.36034 0.36034 0.36771

Eigenvalues --- 0.36864 0.36864 0.37561 0.37563 0.37563

Eigenvalues --- 0.37563 0.38975 0.38975 0.39536 0.39963

Eigenvalues --- 0.41397 0.41397 0.41397 0.41500 0.41500

Eigenvalues --- 0.41602 0.41785 0.42504 0.43516 0.43781

Eigenvalues --- 0.43781 0.47378 0.47869 0.49080 0.49080

Eigenvalues --- 0.50129 0.51397 0.51900 0.51900 0.76501

Eigenvalues --- 1.01673 1.01831 1.01831 1.01831

En-DIIS/RFO-DIIS IScMMF= 0 using points: 8 7

RFO step: Lambda=-1.64376646D-04.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 5.58D-04 SmlDif= 1.00D-05

RMS Error= 0.2325968670D-02 NUsed= 2 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.12117 0.87883

Iteration 1 RMS(Cart)= 0.03710689 RMS(Int)= 0.00124539

Iteration 2 RMS(Cart)= 0.00250381 RMS(Int)= 0.00058262

Iteration 3 RMS(Cart)= 0.00000037 RMS(Int)= 0.00058262

ITry= 1 IFail=0 DXMaxC= 3.39D-01 DCOld= 1.00D+10 DXMaxT= 6.31D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 8.06D-03 for atom 44.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73302 0.00036 -0.00121 -0.00200 -0.00338 2.72964

R2 2.57542 -0.00065 0.00071 0.00233 0.00245 2.57787

R3 2.03992 0.00018 -0.00018 0.00088 0.00070 2.04062

R4 2.58484 -0.00116 0.00183 0.00289 0.00501 2.58984

R5 2.67648 -0.00085 0.00196 0.00140 0.00258 2.67907

R6 2.58484 -0.00116 0.00183 0.00289 0.00501 2.58984

R7 3.95503 -0.00108 -0.00601 -0.00762 -0.01129 3.94374

R8 2.73302 0.00036 -0.00121 -0.00200 -0.00338 2.72964

R9 2.67648 -0.00085 0.00196 0.00140 0.00258 2.67907

R10 2.03992 0.00018 -0.00018 0.00088 0.00070 2.04062

R11 2.67648 -0.00085 0.00196 0.00140 0.00258 2.67907

R12 2.69387 0.00076 -0.00137 0.00161 -0.00055 2.69333

R13 2.58484 -0.00116 0.00183 0.00289 0.00501 2.58984

R14 2.73302 0.00036 -0.00121 -0.00198 -0.00338 2.72964

R15 2.58484 -0.00116 0.00183 0.00289 0.00501 2.58984

R16 3.95503 -0.00108 -0.00601 -0.00762 -0.01129 3.94374

R17 2.73302 0.00036 -0.00121 -0.00199 -0.00338 2.72964

R18 2.67648 -0.00085 0.00196 0.00140 0.00258 2.67907

R19 2.57542 -0.00065 0.00071 0.00233 0.00245 2.57787

R20 2.03992 0.00018 -0.00018 0.00088 0.00070 2.04062

R21 2.03992 0.00018 -0.00018 0.00090 0.00070 2.04062

R22 2.67648 -0.00085 0.00196 0.00140 0.00258 2.67907

R23 2.69387 0.00076 -0.00137 0.00161 -0.00055 2.69333

R24 2.73302 0.00036 -0.00121 -0.00198 -0.00338 2.72964

R25 2.58484 -0.00116 0.00183 0.00289 0.00501 2.58984

R26 2.57542 -0.00065 0.00071 0.00233 0.00245 2.57787

R27 2.03992 0.00018 -0.00018 0.00090 0.00070 2.04062

R28 2.73302 0.00036 -0.00121 -0.00199 -0.00338 2.72964

R29 2.03992 0.00018 -0.00018 0.00088 0.00070 2.04062

R30 2.58484 -0.00116 0.00183 0.00289 0.00501 2.58984

R31 2.67648 -0.00085 0.00196 0.00140 0.00258 2.67907

R32 3.95503 -0.00108 -0.00601 -0.00762 -0.01129 3.94374

R33 2.67648 -0.00085 0.00196 0.00140 0.00258 2.67907

R34 2.69387 0.00076 -0.00137 0.00161 -0.00055 2.69333

R35 2.73302 0.00036 -0.00121 -0.00198 -0.00338 2.72964

R36 2.58484 -0.00116 0.00183 0.00289 0.00501 2.58984

R37 2.57542 -0.00065 0.00071 0.00233 0.00245 2.57787

R38 2.03992 0.00018 -0.00018 0.00090 0.00070 2.04062

R39 2.73302 0.00036 -0.00121 -0.00198 -0.00338 2.72964

R40 2.03992 0.00018 -0.00018 0.00090 0.00070 2.04062

R41 2.58484 -0.00116 0.00183 0.00289 0.00501 2.58984

R42 2.67648 -0.00085 0.00196 0.00140 0.00258 2.67907

R43 3.95503 -0.00108 -0.00601 -0.00763 -0.01129 3.94374

R44 2.69387 0.00076 -0.00137 0.00161 -0.00055 2.69333

R45 2.27884 -0.00013 0.00007 -0.00063 -0.00056 2.27828

R46 2.27884 -0.00013 0.00007 -0.00063 -0.00056 2.27828

R47 2.01684 0.00004 -0.00002 0.00039 0.00035 2.01720

R48 2.01684 0.00004 -0.00002 0.00039 0.00035 2.01720

R49 2.27884 -0.00013 0.00007 -0.00063 -0.00056 2.27828

R50 2.01684 0.00004 -0.00002 0.00039 0.00035 2.01720

R51 2.27884 -0.00013 0.00007 -0.00063 -0.00056 2.27828

R52 2.01684 0.00004 -0.00002 0.00039 0.00035 2.01720

A1 1.86636 -0.00027 0.00066 0.00179 0.00224 1.86860

A2 2.18906 0.00028 -0.00173 -0.00414 -0.00577 2.18328

A3 2.22776 -0.00001 0.00108 0.00237 0.00353 2.23129

A4 1.90839 0.00026 -0.00082 -0.00373 -0.00401 1.90438

A5 2.18263 0.00004 0.00013 0.00284 0.00234 2.18497

A6 2.19195 -0.00030 0.00059 0.00160 0.00185 2.19380

A7 1.87527 0.00001 0.00032 0.00383 0.00267 1.87794

A8 2.20238 0.00000 0.00105 -0.00084 0.00023 2.20261

A9 2.20238 0.00000 0.00105 -0.00084 0.00023 2.20261

A10 1.90839 0.00026 -0.00082 -0.00373 -0.00401 1.90438

A11 2.19195 -0.00030 0.00059 0.00160 0.00185 2.19380

A12 2.18263 0.00004 0.00013 0.00284 0.00234 2.18497

A13 1.86636 -0.00027 0.00066 0.00179 0.00224 1.86860

A14 2.22776 -0.00001 0.00108 0.00237 0.00353 2.23129

A15 2.18906 0.00028 -0.00173 -0.00414 -0.00577 2.18328

A16 2.20440 0.00060 -0.00048 0.00030 -0.00124 2.20316

A17 2.03927 -0.00029 0.00015 0.00055 0.00049 2.03977

A18 2.03927 -0.00029 0.00015 0.00047 0.00049 2.03977

A19 2.19195 -0.00030 0.00059 0.00160 0.00185 2.19380

A20 2.18263 0.00004 0.00013 0.00283 0.00234 2.18497

A21 1.90839 0.00026 -0.00082 -0.00373 -0.00401 1.90438

A22 1.87527 0.00001 0.00032 0.00382 0.00267 1.87794

A23 2.20238 0.00000 0.00105 -0.00085 0.00023 2.20261

A24 2.20238 0.00000 0.00105 -0.00084 0.00023 2.20261

A25 1.90839 0.00026 -0.00082 -0.00373 -0.00401 1.90438

A26 2.19195 -0.00030 0.00059 0.00159 0.00185 2.19380

A27 2.18263 0.00004 0.00013 0.00284 0.00234 2.18497

A28 1.86636 -0.00027 0.00066 0.00179 0.00224 1.86860

A29 2.18906 0.00028 -0.00173 -0.00414 -0.00577 2.18328

A30 2.22776 -0.00001 0.00108 0.00236 0.00353 2.23129

A31 1.86636 -0.00027 0.00066 0.00178 0.00224 1.86860

A32 2.18906 0.00028 -0.00173 -0.00412 -0.00577 2.18328

A33 2.22776 -0.00001 0.00108 0.00235 0.00353 2.23129

A34 2.20440 0.00060 -0.00048 0.00030 -0.00124 2.20316

A35 2.03927 -0.00029 0.00015 0.00055 0.00049 2.03977

A36 2.03927 -0.00029 0.00015 0.00047 0.00049 2.03977

A37 2.18263 0.00004 0.00013 0.00283 0.00234 2.18497

A38 2.19195 -0.00030 0.00059 0.00160 0.00185 2.19380

A39 1.90839 0.00026 -0.00082 -0.00373 -0.00401 1.90438

A40 1.86636 -0.00027 0.00066 0.00178 0.00224 1.86860

A41 2.18906 0.00028 -0.00173 -0.00412 -0.00577 2.18328

A42 2.22776 -0.00001 0.00108 0.00235 0.00353 2.23129

A43 1.86636 -0.00027 0.00066 0.00179 0.00224 1.86860

A44 2.22776 -0.00001 0.00108 0.00236 0.00353 2.23129

A45 2.18906 0.00028 -0.00173 -0.00414 -0.00577 2.18328

A46 1.90839 0.00026 -0.00082 -0.00373 -0.00401 1.90438

A47 2.18263 0.00004 0.00013 0.00284 0.00234 2.18497

A48 2.19195 -0.00030 0.00059 0.00159 0.00185 2.19380

A49 1.87527 0.00001 0.00032 0.00382 0.00267 1.87794

A50 2.20238 0.00000 0.00105 -0.00085 0.00023 2.20261

A51 2.20238 0.00000 0.00105 -0.00084 0.00023 2.20261

A52 2.20440 0.00060 -0.00048 0.00029 -0.00124 2.20316

A53 2.03927 -0.00029 0.00015 0.00055 0.00049 2.03977

A54 2.03927 -0.00029 0.00015 0.00047 0.00049 2.03977

A55 2.18263 0.00004 0.00013 0.00283 0.00234 2.18497

A56 2.19195 -0.00030 0.00059 0.00160 0.00185 2.19380

A57 1.90839 0.00026 -0.00082 -0.00373 -0.00401 1.90438

A58 1.86636 -0.00027 0.00066 0.00178 0.00224 1.86860

A59 2.18906 0.00028 -0.00173 -0.00412 -0.00577 2.18328

A60 2.22776 -0.00001 0.00108 0.00235 0.00353 2.23129

A61 1.86636 -0.00027 0.00066 0.00178 0.00224 1.86860

A62 2.22776 -0.00001 0.00108 0.00235 0.00353 2.23129

A63 2.18906 0.00028 -0.00173 -0.00412 -0.00577 2.18328

A64 1.90839 0.00026 -0.00082 -0.00373 -0.00401 1.90438

A65 2.18263 0.00004 0.00013 0.00283 0.00234 2.18497

A66 2.19195 -0.00030 0.00059 0.00160 0.00185 2.19380

A67 1.87527 0.00001 0.00032 0.00382 0.00267 1.87794

A68 2.20238 0.00000 0.00105 -0.00084 0.00023 2.20261

A69 2.20238 0.00000 0.00105 -0.00084 0.00023 2.20261

A70 1.55954 0.00013 0.00489 0.00811 0.00958 1.56912

A71 1.55954 0.00013 0.00489 0.00811 0.00958 1.56912

A72 2.92900 0.00122 0.05411 0.07682 0.13073 3.05972

A73 2.92900 0.00122 0.05411 0.07682 0.13073 3.05972

A74 1.55954 0.00013 0.00489 0.00810 0.00958 1.56912

A75 1.55954 0.00013 0.00489 0.00810 0.00958 1.56912

A76 2.20440 0.00060 -0.00048 0.00029 -0.00124 2.20316

A77 2.03927 -0.00029 0.00015 0.00055 0.00049 2.03977

A78 2.03927 -0.00029 0.00015 0.00047 0.00049 2.03977

A79 3.14145 0.00001 -0.00006 0.00037 0.00030 3.14175

A80 3.14145 0.00001 -0.00006 0.00037 0.00030 3.14175

A81 3.14171 0.00000 0.00003 0.00324 -0.00072 3.14099

A82 3.14171 0.00000 0.00003 0.00324 -0.00072 3.14099

A83 3.14145 0.00001 -0.00006 0.00037 0.00030 3.14175

A84 3.14171 0.00000 0.00003 0.00324 -0.00072 3.14099

A85 3.14145 0.00001 -0.00006 0.00037 0.00030 3.14175

A86 3.14171 0.00000 0.00003 0.00324 -0.00072 3.14099

A87 3.13249 0.00028 -0.00632 0.00138 -0.00493 3.12756

A88 3.15069 -0.00028 0.00632 -0.00138 0.00493 3.15562

A89 3.15082 -0.00011 0.00623 -0.09358 -0.08721 3.06360

A90 3.13237 0.00011 -0.00623 0.09358 0.08721 3.21958

A91 3.13249 0.00028 -0.00632 0.00138 -0.00493 3.12756

A92 3.15082 -0.00011 0.00623 -0.09358 -0.08721 3.06360

A93 3.15069 -0.00028 0.00632 -0.00138 0.00493 3.15562

A94 3.13237 0.00011 -0.00623 0.09358 0.08721 3.21958

D1 -0.00106 0.00004 -0.00188 -0.02100 -0.02288 -0.02394

D2 3.11908 0.00022 -0.00610 0.01326 0.00711 3.12619

D3 -3.13904 0.00000 -0.00599 -0.02506 -0.03102 3.11313

D4 -0.01890 0.00018 -0.01021 0.00919 -0.00103 -0.01993

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13788 -0.00004 -0.00423 -0.00416 -0.00841 3.13690

D7 3.13788 0.00004 0.00423 0.00416 0.00841 -3.13690

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00171 -0.00007 0.00304 0.03395 0.03704 0.03875

D10 -3.05846 -0.00017 -0.04256 0.00652 -0.03604 -3.09450

D11 -3.11829 -0.00025 0.00730 -0.00055 0.00686 -3.11143

D12 0.10472 -0.00035 -0.03830 -0.02798 -0.06622 0.03850

D13 -3.10413 -0.00048 0.00420 -0.06404 -0.05982 3.11924

D14 0.01322 0.00002 -0.00392 0.00334 -0.00062 0.01260

D15 0.01258 -0.00027 -0.00073 -0.02435 -0.02500 -0.01243

D16 3.12992 0.00023 -0.00884 0.04303 0.03420 -3.11906

D17 -0.00171 0.00007 -0.00304 -0.03395 -0.03704 -0.03875

D18 3.11829 0.00025 -0.00730 0.00055 -0.00686 3.11143

D19 3.05846 0.00017 0.04256 -0.00652 0.03604 3.09450

D20 -0.10472 0.00035 0.03830 0.02798 0.06622 -0.03850

D21 -3.08403 -0.00054 0.00023 -0.02145 -0.02158 -3.10562

D22 -0.15384 0.00066 0.05368 0.05408 0.10802 -0.04583

D23 -1.61894 0.00006 0.02695 0.01632 0.04322 -1.57572

D24 0.15384 -0.00066 -0.05368 -0.05408 -0.10802 0.04583

D25 3.08403 0.00054 -0.00023 0.02145 0.02158 3.10562

D26 1.61894 -0.00006 -0.02695 -0.01632 -0.04322 1.57572

D27 0.00106 -0.00004 0.00188 0.02100 0.02288 0.02394

D28 3.13904 0.00000 0.00599 0.02506 0.03102 -3.11313

D29 -3.11908 -0.00022 0.00610 -0.01326 -0.00711 -3.12619

D30 0.01890 -0.00018 0.01021 -0.00919 0.00103 0.01993

D31 -0.01258 0.00027 0.00073 0.02435 0.02500 0.01243

D32 -3.12992 -0.00023 0.00884 -0.04303 -0.03420 3.11906

D33 3.10413 0.00048 -0.00420 0.06404 0.05982 -3.11924

D34 -0.01322 -0.00002 0.00392 -0.00334 0.00062 -0.01260

D35 0.01258 -0.00027 -0.00073 -0.02435 -0.02500 -0.01243

D36 -3.10413 -0.00048 0.00420 -0.06404 -0.05982 3.11924

D37 3.12992 0.00023 -0.00884 0.04303 0.03420 -3.11906

D38 0.01322 0.00002 -0.00392 0.00334 -0.00062 0.01260

D39 -3.11829 -0.00025 0.00730 -0.00055 0.00686 -3.11143

D40 0.10472 -0.00035 -0.03830 -0.02798 -0.06622 0.03850

D41 0.00171 -0.00007 0.00304 0.03395 0.03704 0.03875

D42 -3.05846 -0.00017 -0.04256 0.00652 -0.03604 -3.09450

D43 3.11908 0.00022 -0.00610 0.01326 0.00711 3.12619

D44 -0.01890 0.00018 -0.01021 0.00919 -0.00103 -0.01993

D45 -0.00106 0.00004 -0.00188 -0.02100 -0.02288 -0.02394

D46 -3.13904 0.00000 -0.00599 -0.02506 -0.03102 3.11313

D47 -0.00171 0.00007 -0.00304 -0.03395 -0.03704 -0.03875

D48 3.11829 0.00025 -0.00730 0.00055 -0.00686 3.11143

D49 3.05846 0.00017 0.04256 -0.00652 0.03604 3.09450

D50 -0.10472 0.00035 0.03830 0.02798 0.06622 -0.03850

D51 -0.15384 0.00066 0.05368 0.05409 0.10802 -0.04583

D52 -1.61894 0.00006 0.02695 0.01631 0.04322 -1.57572

D53 -3.08403 -0.00054 0.00023 -0.02145 -0.02158 -3.10562

D54 3.08403 0.00054 -0.00023 0.02145 0.02158 3.10562

D55 1.61894 -0.00006 -0.02695 -0.01633 -0.04322 1.57572

D56 0.15384 -0.00066 -0.05368 -0.05408 -0.10802 0.04583

D57 0.00106 -0.00004 0.00188 0.02100 0.02288 0.02394

D58 3.13904 0.00000 0.00599 0.02506 0.03102 -3.11313

D59 -3.11908 -0.00022 0.00610 -0.01326 -0.00711 -3.12619

D60 0.01890 -0.00018 0.01021 -0.00919 0.00103 0.01993

D61 -0.01258 0.00027 0.00073 0.02435 0.02500 0.01243

D62 -3.12992 -0.00023 0.00884 -0.04303 -0.03420 3.11906

D63 3.10413 0.00048 -0.00420 0.06404 0.05982 -3.11924

D64 -0.01322 -0.00002 0.00392 -0.00334 0.00062 -0.01260

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13788 0.00004 0.00423 0.00417 0.00841 -3.13690

D67 -3.13788 -0.00004 -0.00423 -0.00416 -0.00841 3.13690

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.10413 0.00048 -0.00420 0.06404 0.05982 -3.11924

D70 -0.01258 0.00027 0.00073 0.02435 0.02500 0.01243

D71 -0.01322 -0.00002 0.00392 -0.00334 0.00062 -0.01260

D72 -3.12992 -0.00023 0.00884 -0.04303 -0.03420 3.11906

D73 -3.11908 -0.00022 0.00610 -0.01326 -0.00711 -3.12619

D74 0.01890 -0.00018 0.01021 -0.00919 0.00103 0.01993

D75 0.00106 -0.00004 0.00188 0.02100 0.02288 0.02394

D76 3.13904 0.00000 0.00599 0.02506 0.03102 -3.11313

D77 3.11829 0.00025 -0.00730 0.00055 -0.00686 3.11143

D78 -0.10472 0.00035 0.03830 0.02798 0.06622 -0.03850

D79 -0.00171 0.00007 -0.00304 -0.03395 -0.03704 -0.03875

D80 3.05846 0.00017 0.04256 -0.00652 0.03604 3.09450

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 3.13788 0.00004 0.00423 0.00416 0.00841 -3.13690

D83 -3.13788 -0.00004 -0.00423 -0.00417 -0.00841 3.13690

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 -0.00106 0.00004 -0.00188 -0.02100 -0.02288 -0.02394

D86 3.11908 0.00022 -0.00610 0.01326 0.00711 3.12619

D87 -3.13904 0.00000 -0.00599 -0.02506 -0.03102 3.11313

D88 -0.01890 0.00018 -0.01021 0.00919 -0.00103 -0.01993

D89 0.00171 -0.00007 0.00304 0.03395 0.03704 0.03875

D90 -3.05846 -0.00017 -0.04256 0.00652 -0.03604 -3.09450

D91 -3.11829 -0.00025 0.00730 -0.00055 0.00686 -3.11143

D92 0.10472 -0.00035 -0.03830 -0.02798 -0.06622 0.03850

D93 -3.10413 -0.00048 0.00420 -0.06404 -0.05982 3.11924

D94 0.01322 0.00002 -0.00392 0.00334 -0.00062 0.01260

D95 0.01258 -0.00027 -0.00073 -0.02435 -0.02500 -0.01243

D96 3.12992 0.00023 -0.00884 0.04303 0.03420 -3.11906

D97 0.15384 -0.00066 -0.05368 -0.05409 -0.10802 0.04583

D98 1.61894 -0.00006 -0.02695 -0.01631 -0.04322 1.57572

D99 3.08403 0.00054 -0.00023 0.02145 0.02158 3.10562

D100 -3.08403 -0.00054 0.00023 -0.02145 -0.02158 -3.10562

D101 -1.61894 0.00006 0.02695 0.01633 0.04322 -1.57572

D102 -0.15384 0.00066 0.05368 0.05408 0.10802 -0.04583

D103 3.10413 0.00048 -0.00420 0.06404 0.05982 -3.11924

D104 -0.01258 0.00027 0.00073 0.02435 0.02500 0.01243

D105 -0.01322 -0.00002 0.00392 -0.00334 0.00062 -0.01260

D106 -3.12992 -0.00023 0.00884 -0.04303 -0.03420 3.11906

D107 -3.11908 -0.00022 0.00610 -0.01326 -0.00711 -3.12619

D108 0.01890 -0.00018 0.01021 -0.00919 0.00103 0.01993

D109 0.00106 -0.00004 0.00188 0.02100 0.02288 0.02394

D110 3.13904 0.00000 0.00599 0.02506 0.03102 -3.11313

D111 3.11829 0.00025 -0.00730 0.00055 -0.00686 3.11143

D112 -0.10472 0.00035 0.03830 0.02798 0.06622 -0.03850

D113 -0.00171 0.00007 -0.00304 -0.03395 -0.03704 -0.03875

D114 3.05846 0.00017 0.04256 -0.00653 0.03604 3.09450

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.13788 0.00004 0.00423 0.00417 0.00841 -3.13690

D117 -3.13788 -0.00004 -0.00423 -0.00417 -0.00841 3.13690

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 -0.00106 0.00004 -0.00188 -0.02100 -0.02288 -0.02394

D120 3.11908 0.00022 -0.00610 0.01326 0.00711 3.12619

D121 -3.13904 0.00000 -0.00599 -0.02506 -0.03102 3.11313

D122 -0.01890 0.00018 -0.01021 0.00919 -0.00103 -0.01993

D123 0.00171 -0.00007 0.00304 0.03395 0.03704 0.03875

D124 -3.05846 -0.00017 -0.04256 0.00653 -0.03604 -3.09450

D125 -3.11829 -0.00025 0.00730 -0.00055 0.00686 -3.11143

D126 0.10472 -0.00035 -0.03830 -0.02798 -0.06622 0.03850

D127 -3.10413 -0.00048 0.00420 -0.06404 -0.05982 3.11924

D128 0.01322 0.00002 -0.00392 0.00334 -0.00062 0.01260

D129 0.01258 -0.00027 -0.00073 -0.02435 -0.02500 -0.01243

D130 3.12992 0.00023 -0.00884 0.04303 0.03420 -3.11906

D131 1.61894 -0.00006 -0.02695 -0.01632 -0.04322 1.57572

D132 3.08403 0.00054 -0.00023 0.02145 0.02158 3.10562

D133 0.15384 -0.00066 -0.05368 -0.05408 -0.10802 0.04583

D134 -1.61894 0.00006 0.02695 0.01632 0.04322 -1.57572

D135 -0.15384 0.00066 0.05368 0.05408 0.10802 -0.04583

D136 -3.08403 -0.00054 0.00023 -0.02145 -0.02158 -3.10562

Item Value Threshold Converged?

Maximum Force 0.001222 0.000450 NO

RMS Force 0.000403 0.000300 NO

Maximum Displacement 0.339309 0.001800 NO

RMS Displacement 0.036771 0.001200 NO

Predicted change in Energy=-7.704968D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:18:38 2019, MaxMem= 1342177280 cpu: 1.4

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.682075 4.275026 -0.017630

2 6 0 1.105913 2.894156 -0.023280

3 7 0 0.000000 2.085190 0.004403

4 6 0 -1.105913 2.894156 -0.023280

5 6 0 -0.682075 4.275026 -0.017630

6 6 0 -2.453125 2.453125 -0.042929

7 6 0 -2.894156 1.105913 -0.023280

8 7 0 -2.085190 0.000000 0.004403

9 6 0 -2.894156 -1.105913 -0.023280

10 6 0 -4.275026 -0.682075 -0.017630

11 6 0 -4.275026 0.682075 -0.017630

12 6 0 2.453125 2.453125 -0.042929

13 6 0 2.894156 1.105913 -0.023280

14 6 0 4.275026 0.682075 -0.017630

15 6 0 4.275026 -0.682075 -0.017630

16 6 0 2.894156 -1.105913 -0.023280

17 7 0 2.085190 0.000000 0.004403

18 6 0 2.453125 -2.453125 -0.042929

19 6 0 1.105913 -2.894156 -0.023280

20 6 0 0.682075 -4.275026 -0.017630

21 6 0 -0.682075 -4.275026 -0.017630

22 6 0 -1.105913 -2.894156 -0.023280

23 7 0 0.000000 -2.085190 0.004403

24 1 0 1.344570 5.127740 -0.010140

25 1 0 -1.344570 5.127740 -0.010140

26 1 0 -5.127740 -1.344570 -0.010140

27 1 0 -5.127740 1.344570 -0.010140

28 1 0 5.127740 1.344570 -0.010140

29 1 0 5.127740 -1.344570 -0.010140

30 1 0 1.344570 -5.127740 -0.010140

31 1 0 -1.344570 -5.127740 -0.010140

32 30 0 0.000000 0.000000 0.089809

33 6 0 -2.453125 -2.453125 -0.042929

34 6 0 -3.460928 -3.460928 -0.042180

35 6 0 3.460928 3.460928 -0.042180

36 6 0 -4.313348 -4.313348 -0.058343

37 6 0 4.313348 4.313348 -0.058343

38 6 0 -3.460928 3.460928 -0.042180

39 6 0 -4.313348 4.313348 -0.058343

40 6 0 3.460928 -3.460928 -0.042180

41 6 0 4.313348 -4.313348 -0.058343

42 1 0 5.065667 -5.065667 -0.144906

43 1 0 -5.065667 -5.065667 -0.144906

44 1 0 -5.065667 5.065667 -0.144906

45 1 0 5.065667 5.065667 -0.144906

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.444463 0.000000

3 N 2.293707 1.370487 0.000000

4 C 2.259145 2.211825 1.370487 0.000000

5 C 1.364151 2.259145 2.293707 1.444463 0.000000

6 C 3.626216 3.586314 2.481016 1.417701 2.540980

7 C 4.778362 4.381593 3.055469 2.528957 3.864791

8 N 5.092553 4.308137 2.948904 3.055469 4.499452

9 C 6.460957 5.656951 4.308137 4.381593 5.817889

10 C 7.010400 6.460957 5.092553 4.778362 6.122267

11 C 6.122267 5.817889 4.499452 3.864791 5.081200

12 C 2.540980 1.417701 2.481016 3.586314 3.626216

13 C 3.864791 2.528957 3.055469 4.381593 4.778362

14 C 5.081200 3.864791 4.499452 5.817889 6.122267

15 C 6.122267 4.778362 5.092553 6.460957 7.010400

16 C 5.817889 4.381593 4.308137 5.656951 6.460957

17 N 4.499452 3.055469 2.948904 4.308137 5.092553

18 C 6.957390 5.514416 5.159106 6.423438 7.422812

19 C 7.181702 5.788311 5.100754 6.196509 7.388782

20 C 8.550052 7.181702 6.396723 7.388782 8.658193

21 C 8.658193 7.388782 6.396723 7.181702 8.550052

22 C 7.388782 6.196509 5.100754 5.788311 7.181702

23 N 6.396723 5.100754 4.170381 5.100754 6.396723

24 H 1.079850 2.246337 3.326438 3.315711 2.198743

25 H 2.198743 3.315711 3.326438 2.246337 1.079850

26 H 8.082937 7.538262 6.169051 5.843121 7.165463

27 H 6.507041 6.423380 5.180970 4.310044 5.324619

28 H 5.324619 4.310044 5.180970 6.423380 6.507041

29 H 7.165463 5.843121 6.169051 7.538262 8.082937

30 H 9.426079 8.025456 7.337196 8.387839 9.618698

31 H 9.618698 8.387839 7.337196 8.025456 9.426079

32 Zn 4.330429 3.100318 2.086939 3.100318 4.330429

33 C 7.422812 6.423438 5.159106 5.514416 6.957390

34 C 8.775538 7.825821 6.537554 6.777429 8.219952

35 C 2.895752 2.422330 3.724627 4.601915 4.222302

36 C 9.935596 9.017633 7.716877 7.889041 9.324589

37 C 3.631703 3.507559 4.855264 5.602117 4.995736

38 C 4.222302 4.601915 3.724627 2.422330 2.895752

39 C 4.995736 5.602117 4.855264 3.507559 3.631703

40 C 8.219952 6.777429 6.537554 7.825821 8.775538

41 C 9.324589 7.889041 7.716877 9.017633 9.935596

42 H 10.318944 8.891187 8.764589 10.072832 10.968194

43 H 10.968194 10.072832 8.764589 8.891187 10.318944

44 H 5.803262 6.543596 5.879329 4.517732 4.456140

45 H 4.456140 4.517732 5.879329 6.543596 5.803262

6 7 8 9 10

6 C 0.000000

7 C 1.417701 0.000000

8 N 2.481016 1.370487 0.000000

9 C 3.586314 2.211825 1.370487 0.000000

10 C 3.626216 2.259145 2.293707 1.444463 0.000000

11 C 2.540980 1.444463 2.293707 2.259145 1.364151

12 C 4.906251 5.514416 5.159106 6.423438 7.422812

13 C 5.514416 5.788311 5.100754 6.196509 7.388782

14 C 6.957390 7.181702 6.396723 7.388782 8.658193

15 C 7.422812 7.388782 6.396723 7.181702 8.550052

16 C 6.423438 6.196509 5.100754 5.788311 7.181702

17 N 5.159106 5.100754 4.170381 5.100754 6.396723

18 C 6.938486 6.423438 5.159106 5.514416 6.957390

19 C 6.423438 5.656951 4.308137 4.381593 5.817889

20 C 7.422812 6.460957 5.092553 4.778362 6.122267

21 C 6.957390 5.817889 4.499452 3.864791 5.081200

22 C 5.514416 4.381593 3.055469 2.528957 3.864791

23 N 5.159106 4.308137 2.948904 3.055469 4.499452

24 H 4.645119 5.843121 6.169051 7.538262 8.082937

25 H 2.895433 4.310044 5.180970 6.423380 6.507041

26 H 4.645119 3.315711 3.326438 2.246337 1.079850

27 H 2.895433 2.246337 3.326438 3.315711 2.198743

28 H 7.661559 8.025456 7.337196 8.387839 9.618698

29 H 8.478979 8.387839 7.337196 8.025456 9.426079

30 H 8.478979 7.538262 6.169051 5.843121 7.165463

31 H 7.661559 6.423380 5.180970 4.310044 5.324619

32 Zn 3.471782 3.100318 2.086939 3.100318 4.330429

33 C 4.906251 3.586314 2.481016 1.417701 2.540980

34 C 5.999307 4.601915 3.724627 2.422330 2.895752

35 C 5.999307 6.777429 6.537554 7.825821 8.775538

36 C 7.017537 5.602117 4.855264 3.507559 3.631703

37 C 7.017537 7.889041 7.716877 9.017633 9.935596

38 C 1.425248 2.422330 3.724627 4.601915 4.222302

39 C 2.630797 3.507559 4.855264 5.602117 4.995736

40 C 8.363734 7.825821 6.537554 6.777429 8.219952

41 C 9.569250 9.017633 7.716877 7.889041 9.324589

42 H 10.633666 10.072832 8.764589 8.891187 10.318944

43 H 7.960402 6.543596 5.879329 4.517732 4.456140

44 H 3.696098 4.517732 5.879329 6.543596 5.803262

45 H 7.960402 8.891187 8.764589 10.072832 10.968194

11 12 13 14 15

11 C 0.000000

12 C 6.957390 0.000000

13 C 7.181702 1.417701 0.000000

14 C 8.550052 2.540980 1.444463 0.000000

15 C 8.658193 3.626216 2.259145 1.364151 0.000000

16 C 7.388782 3.586314 2.211825 2.259145 1.444463

17 N 6.396723 2.481016 1.370487 2.293707 2.293707

18 C 7.422812 4.906251 3.586314 3.626216 2.540980

19 C 6.460957 5.514416 4.381593 4.778362 3.864791

20 C 7.010400 6.957390 5.817889 6.122267 5.081200

21 C 6.122267 7.422812 6.460957 7.010400 6.122267

22 C 4.778362 6.423438 5.656951 6.460957 5.817889

23 N 5.092553 5.159106 4.308137 5.092553 4.499452

24 H 7.165463 2.895433 4.310044 5.324619 6.507041

25 H 5.324619 4.645119 5.843121 7.165463 8.082937

26 H 2.198743 8.478979 8.387839 9.618698 9.426079

27 H 1.079850 7.661559 8.025456 9.426079 9.618698

28 H 9.426079 2.895433 2.246337 1.079850 2.198743

29 H 9.618698 4.645119 3.315711 2.198743 1.079850

30 H 8.082937 7.661559 6.423380 6.507041 5.324619

31 H 6.507041 8.478979 7.538262 8.082937 7.165463

32 Zn 4.330429 3.471782 3.100318 4.330429 4.330429

33 C 3.626216 6.938486 6.423438 7.422812 6.957390

34 C 4.222302 8.363734 7.825821 8.775538 8.219952

35 C 8.219952 1.425248 2.422330 2.895752 4.222302

36 C 4.995736 9.569250 9.017633 9.935596 9.324589

37 C 9.324589 2.630797 3.507559 3.631703 4.995736

38 C 2.895752 5.999307 6.777429 8.219952 8.775538

39 C 3.631703 7.017537 7.889041 9.324589 9.935596

40 C 8.775538 5.999307 4.601915 4.222302 2.895752

41 C 9.935596 7.017537 5.602117 4.995736 3.631703

42 H 10.968194 7.960402 6.543596 5.803262 4.456140

43 H 5.803262 10.633666 10.072832 10.968194 10.318944

44 H 4.456140 7.960402 8.891187 10.318944 10.968194

45 H 10.318944 3.696098 4.517732 4.456140 5.803262

16 17 18 19 20

16 C 0.000000

17 N 1.370487 0.000000

18 C 1.417701 2.481016 0.000000

19 C 2.528957 3.055469 1.417701 0.000000

20 C 3.864791 4.499452 2.540980 1.444463 0.000000

21 C 4.778362 5.092553 3.626216 2.259145 1.364151

22 C 4.381593 4.308137 3.586314 2.211825 2.259145

23 N 3.055469 2.948904 2.481016 1.370487 2.293707

24 H 6.423380 5.180970 7.661559 8.025456 9.426079

25 H 7.538262 6.169051 8.478979 8.387839 9.618698

26 H 8.025456 7.337196 7.661559 6.423380 6.507041

27 H 8.387839 7.337196 8.478979 7.538262 8.082937

28 H 3.315711 3.326438 4.645119 5.843121 7.165463

29 H 2.246337 3.326438 2.895433 4.310044 5.324619

30 H 4.310044 5.180970 2.895433 2.246337 1.079850

31 H 5.843121 6.169051 4.645119 3.315711 2.198743

32 Zn 3.100318 2.086939 3.471782 3.100318 4.330429

33 C 5.514416 5.159106 4.906251 3.586314 3.626216

34 C 6.777429 6.537554 5.999307 4.601915 4.222302

35 C 4.601915 3.724627 5.999307 6.777429 8.219952

36 C 7.889041 7.716877 7.017537 5.602117 4.995736

37 C 5.602117 4.855264 7.017537 7.889041 9.324589

38 C 7.825821 6.537554 8.363734 7.825821 8.775538

39 C 9.017633 7.716877 9.569250 9.017633 9.935596

40 C 2.422330 3.724627 1.425248 2.422330 2.895752

41 C 3.507559 4.855264 2.630797 3.507559 3.631703

42 H 4.517732 5.879329 3.696098 4.517732 4.456140

43 H 8.891187 8.764589 7.960402 6.543596 5.803262

44 H 10.072832 8.764589 10.633666 10.072832 10.968194

45 H 6.543596 5.879329 7.960402 8.891187 10.318944

21 22 23 24 25

21 C 0.000000

22 C 1.444463 0.000000

23 N 2.293707 1.370487 0.000000

24 H 9.618698 8.387839 7.337196 0.000000

25 H 9.426079 8.025456 7.337196 2.689140 0.000000

26 H 5.324619 4.310044 5.180970 9.153229 7.496877

27 H 7.165463 5.843121 6.169051 7.496877 5.350210

28 H 8.082937 7.538262 6.169051 5.350210 7.496877

29 H 6.507041 6.423380 5.180970 7.496877 9.153229

30 H 2.198743 3.315711 3.326438 10.255480 10.602186

31 H 1.079850 2.246337 3.326438 10.602186 10.255480

32 Zn 4.330429 3.100318 2.086939 5.302035 5.302035

33 C 2.540980 1.417701 2.481016 8.478979 7.661559

34 C 2.895752 2.422330 3.724627 9.841700 8.845632

35 C 8.775538 7.825821 6.537554 2.694116 5.086462

36 C 3.631703 3.507559 4.855264 11.006747 9.896974

37 C 9.935596 9.017633 7.716877 3.078830 5.716432

38 C 8.219952 6.777429 6.537554 5.086462 2.694116

39 C 9.324589 7.889041 7.716877 5.716432 3.078830

40 C 4.222302 4.601915 3.724627 8.845632 9.841700

41 C 4.995736 5.602117 4.855264 9.896974 11.006747

42 H 5.803262 6.543596 5.879329 10.852201 12.042211

43 H 4.456140 4.517732 5.879329 12.042211 10.852201

44 H 10.318944 8.891187 8.764589 6.411954 3.724053

45 H 10.968194 10.072832 8.764589 3.724053 6.411954

26 27 28 29 30

26 H 0.000000

27 H 2.689140 0.000000

28 H 10.602186 10.255480 0.000000

29 H 10.255480 10.602186 2.689140 0.000000

30 H 7.496877 9.153229 7.496877 5.350210 0.000000

31 H 5.350210 7.496877 9.153229 7.496877 2.689140

32 Zn 5.302035 5.302035 5.302035 5.302035 5.302035

33 C 2.895433 4.645119 8.478979 7.661559 4.645119

34 C 2.694116 5.086462 9.841700 8.845632 5.086462

35 C 9.841700 8.845632 2.694116 5.086462 8.845632

36 C 3.078830 5.716432 11.006747 9.896974 5.716432

37 C 11.006747 9.896974 3.078830 5.716432 9.896974

38 C 5.086462 2.694116 8.845632 9.841700 9.841700

39 C 5.716432 3.078830 9.896974 11.006747 11.006747

40 C 8.845632 9.841700 5.086462 2.694116 2.694116

41 C 9.896974 11.006747 5.716432 3.078830 3.078830

42 H 10.852201 12.042211 6.411954 3.724053 3.724053

43 H 3.724053 6.411954 12.042211 10.852201 6.411954

44 H 6.411954 3.724053 10.852201 12.042211 12.042211

45 H 12.042211 10.852201 3.724053 6.411954 10.852201

31 32 33 34 35

31 H 0.000000

32 Zn 5.302035 0.000000

33 C 2.895433 3.471782 0.000000

34 C 2.694116 4.896270 1.425248 0.000000

35 C 9.841700 4.896270 8.363734 9.788982 0.000000

36 C 3.078830 6.101793 2.630797 1.205612 10.994497

37 C 11.006747 6.101793 9.569250 10.994497 1.205612

38 C 8.845632 4.896270 5.999307 6.921855 6.921855

39 C 9.896974 6.101793 7.017537 7.820885 7.820885

40 C 5.086462 4.896270 5.999307 6.921855 6.921855

41 C 5.716432 6.101793 7.017537 7.820885 7.820885

42 H 6.411954 7.167778 7.960402 8.676897 8.676897

43 H 3.724053 7.167778 3.696098 2.271767 12.058863

44 H 10.852201 7.167778 7.960402 8.676897 8.676897

45 H 12.042211 7.167778 10.633666 12.058863 2.271767

36 37 38 39 40

36 C 0.000000

37 C 12.199989 0.000000

38 C 7.820885 7.820885 0.000000

39 C 8.626695 8.626695 1.205612 0.000000

40 C 7.820885 7.820885 9.788982 10.994497 0.000000

41 C 8.626695 8.626695 10.994497 12.199989 1.205612

42 H 9.409537 9.409537 12.058863 13.264211 2.271767

43 H 1.067455 13.264211 8.676897 9.409537 8.676897

44 H 9.409537 9.409537 2.271767 1.067455 12.058863

45 H 13.264211 1.067455 8.676897 9.409537 8.676897

41 42 43 44 45

41 C 0.000000

42 H 1.067455 0.000000

43 H 9.409537 10.131333 0.000000

44 H 13.264211 14.327869 10.131333 0.000000

45 H 9.409537 10.131333 14.327869 10.131333 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

RotChk: IX=3 Diff= 3.91D-19

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.682075 -4.275026 -0.003976

2 6 0 -1.105913 -2.894156 -0.009626

3 7 0 0.000000 -2.085190 0.018057

4 6 0 1.105913 -2.894156 -0.009626

5 6 0 0.682075 -4.275026 -0.003976

6 6 0 2.453125 -2.453125 -0.029275

7 6 0 2.894156 -1.105913 -0.009626

8 7 0 2.085190 0.000000 0.018057

9 6 0 2.894156 1.105913 -0.009626

10 6 0 4.275026 0.682075 -0.003976

11 6 0 4.275026 -0.682075 -0.003976

12 6 0 -2.453125 -2.453125 -0.029275

13 6 0 -2.894156 -1.105913 -0.009626

14 6 0 -4.275026 -0.682075 -0.003976

15 6 0 -4.275026 0.682075 -0.003976

16 6 0 -2.894156 1.105913 -0.009626

17 7 0 -2.085190 0.000000 0.018057

18 6 0 -2.453125 2.453125 -0.029275

19 6 0 -1.105913 2.894156 -0.009626

20 6 0 -0.682075 4.275026 -0.003976

21 6 0 0.682075 4.275026 -0.003976

22 6 0 1.105913 2.894156 -0.009626

23 7 0 0.000000 2.085190 0.018057

24 1 0 -1.344570 -5.127740 0.003515

25 1 0 1.344570 -5.127740 0.003515

26 1 0 5.127740 1.344570 0.003515

27 1 0 5.127740 -1.344570 0.003515

28 1 0 -5.127740 -1.344570 0.003515

29 1 0 -5.127740 1.344570 0.003515

30 1 0 -1.344570 5.127740 0.003515

31 1 0 1.344570 5.127740 0.003515

32 30 0 0.000000 0.000000 0.103463

33 6 0 2.453125 2.453125 -0.029275

34 6 0 3.460928 3.460928 -0.028525

35 6 0 -3.460928 -3.460928 -0.028525

36 6 0 4.313348 4.313348 -0.044688

37 6 0 -4.313348 -4.313348 -0.044688

38 6 0 3.460928 -3.460928 -0.028525

39 6 0 4.313348 -4.313348 -0.044688

40 6 0 -3.460928 3.460928 -0.028525

41 6 0 -4.313348 4.313348 -0.044688

42 1 0 -5.065667 5.065667 -0.131251

43 1 0 5.065667 5.065667 -0.131251

44 1 0 5.065667 -5.065667 -0.131251

45 1 0 -5.065667 -5.065667 -0.131251

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

Rotational constants (GHZ): 0.1462056 0.1462056 0.0731230

Leave Link 202 at Fri Jul 26 14:18:38 2019, MaxMem= 1342177280 cpu: 0.1

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 184 symmetry adapted cartesian basis functions of A1 symmetry.

There are 155 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3057.5821107338 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= 9 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= -0.1305525960 Hartrees.

Nuclear repulsion after empirical dispersion term = 3057.4515581378 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: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3870

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.15D-04

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 124

GePol: Fraction of low-weight points (<1% of avg) = 3.20%

GePol: Cavity surface area = 415.391 Ang\*\*2

GePol: Cavity volume = 420.085 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0084864122 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3057.4600445500 Hartrees.

Leave Link 301 at Fri Jul 26 14:18:38 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16211 LenP2D= 44788.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.52D-05 NBF= 172 148 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 172 148 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:18:38 2019, MaxMem= 1342177280 cpu: 6.5

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:18:39 2019, MaxMem= 1342177280 cpu: 0.8

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

Initial guess from the checkpoint file: "ZnTSPsim0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Occupied (E) (E) (B2) (A1) (E) (E) (B1) (A1) (B2) (E) (E)

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

(E) (E) (A1) (A2) (E) (E) (B1) (B1) (E) (E) (A1)

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

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

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

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

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

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

(E) (E) (A2) (A1)

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(E) (E) (E)

The electronic state of the initial guess is 1-A1.

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= -1359.45037519773

Leave Link 401 at Fri Jul 26 14:18:40 2019, MaxMem= 1342177280 cpu: 21.0

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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.

An orbital has undefined symmetry, so N\*\*3 symmetry is turned off.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 660000000 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= 0 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= 44930700.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.55D-15 for 3866.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.66D-15 for 2247 667.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.44D-15 for 3866.

Iteration 1 A^-1\*A deviation from orthogonality is 2.35D-14 for 2294 2250.

E= -1359.04899599300

DIIS: error= 3.94D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.04899599300 IErMin= 1 ErrMin= 3.94D-03

ErrMax= 3.94D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.93D-03 BMatP= 7.93D-03

IDIUse=3 WtCom= 9.61D-01 WtEn= 3.94D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 3.231 Goal= None Shift= 0.000

GapD= 3.231 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=5.41D-04 MaxDP=2.03D-02 OVMax= 2.12D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.40D-04 CP: 9.98D-01

E= -1359.06113843658 Delta-E= -0.012142443578 Rises=F Damp=F

DIIS: error= 1.28D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.06113843658 IErMin= 2 ErrMin= 1.28D-03

ErrMax= 1.28D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.30D-04 BMatP= 7.93D-03

IDIUse=3 WtCom= 9.87D-01 WtEn= 1.28D-02

Coeff-Com: -0.283D-01 0.103D+01

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

Coeff: -0.279D-01 0.103D+01

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=4.61D-05 MaxDP=8.56D-04 DE=-1.21D-02 OVMax= 3.26D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.96D-05 CP: 9.97D-01 1.04D+00

E= -1359.06128623290 Delta-E= -0.000147796326 Rises=F Damp=F

DIIS: error= 1.71D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.06128623290 IErMin= 2 ErrMin= 1.28D-03

ErrMax= 1.71D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-04 BMatP= 1.30D-04

IDIUse=3 WtCom= 9.83D-01 WtEn= 1.71D-02

Coeff-Com: -0.261D-01 0.503D+00 0.523D+00

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

Coeff: -0.256D-01 0.494D+00 0.531D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=1.50D-05 MaxDP=5.76D-04 DE=-1.48D-04 OVMax= 1.09D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.20D-05 CP: 9.97D-01 1.04D+00 7.79D-01

E= -1359.06132667032 Delta-E= -0.000040437417 Rises=F Damp=F

DIIS: error= 3.65D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.06132667032 IErMin= 4 ErrMin= 3.65D-04

ErrMax= 3.65D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.14D-06 BMatP= 1.10D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.65D-03

Coeff-Com: -0.667D-02 0.795D-01 0.214D+00 0.713D+00

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

Coeff: -0.665D-02 0.793D-01 0.213D+00 0.714D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=4.47D-06 MaxDP=1.58D-04 DE=-4.04D-05 OVMax= 3.34D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.07D-06 CP: 9.97D-01 1.04D+00 7.97D-01 8.60D-01

E= -1359.06132929396 Delta-E= -0.000002623637 Rises=F Damp=F

DIIS: error= 4.25D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.06132929396 IErMin= 5 ErrMin= 4.25D-05

ErrMax= 4.25D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.12D-07 BMatP= 6.14D-06

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

Coeff-Com: -0.160D-02 0.628D-02 0.694D-01 0.349D+00 0.577D+00

Coeff: -0.160D-02 0.628D-02 0.694D-01 0.349D+00 0.577D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.58D-06 MaxDP=7.00D-05 DE=-2.62D-06 OVMax= 2.10D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.47D-06 CP: 9.97D-01 1.04D+00 8.02D-01 8.82D-01 8.88D-01

E= -1359.06132975362 Delta-E= -0.000000459661 Rises=F Damp=F

DIIS: error= 2.76D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.06132975362 IErMin= 6 ErrMin= 2.76D-05

ErrMax= 2.76D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.56D-07 BMatP= 7.12D-07

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

Coeff-Com: 0.404D-03-0.139D-01-0.159D-02 0.756D-01 0.401D+00 0.539D+00

Coeff: 0.404D-03-0.139D-01-0.159D-02 0.756D-01 0.401D+00 0.539D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=7.15D-07 MaxDP=3.07D-05 DE=-4.60D-07 OVMax= 8.59D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.78D-07 CP: 9.97D-01 1.04D+00 8.09D-01 8.99D-01 8.79D-01

CP: 6.17D-01

E= -1359.06132999412 Delta-E= -0.000000240507 Rises=F Damp=F

DIIS: error= 3.78D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.06132999412 IErMin= 7 ErrMin= 3.78D-06

ErrMax= 3.78D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.99D-09 BMatP= 2.56D-07

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

Coeff-Com: 0.248D-03-0.738D-02-0.230D-02 0.308D-01 0.197D+00 0.279D+00

Coeff-Com: 0.502D+00

Coeff: 0.248D-03-0.738D-02-0.230D-02 0.308D-01 0.197D+00 0.279D+00

Coeff: 0.502D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=1.14D-07 MaxDP=6.05D-06 DE=-2.41D-07 OVMax= 1.33D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 9.59D-08 CP: 9.97D-01 1.04D+00 8.10D-01 9.00D-01 8.80D-01

CP: 5.97D-01 8.46D-01

E= -1359.06132999752 Delta-E= -0.000000003395 Rises=F Damp=F

DIIS: error= 1.53D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.06132999752 IErMin= 8 ErrMin= 1.53D-06

ErrMax= 1.53D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.57D-10 BMatP= 4.99D-09

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

Coeff-Com: 0.721D-04-0.173D-02-0.871D-03 0.413D-02 0.400D-01 0.602D-01

Coeff-Com: 0.295D+00 0.603D+00

Coeff: 0.721D-04-0.173D-02-0.871D-03 0.413D-02 0.400D-01 0.602D-01

Coeff: 0.295D+00 0.603D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=4.64D-08 MaxDP=1.74D-06 DE=-3.40D-09 OVMax= 6.85D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.57D-08 CP: 9.97D-01 1.04D+00 8.10D-01 9.00D-01 8.81D-01

CP: 6.04D-01 8.89D-01 7.55D-01

E= -1359.06132999839 Delta-E= -0.000000000870 Rises=F Damp=F

DIIS: error= 4.98D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1359.06132999839 IErMin= 9 ErrMin= 4.98D-07

ErrMax= 4.98D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.29D-10 BMatP= 8.57D-10

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

Coeff-Com: 0.524D-05 0.916D-04-0.158D-03-0.217D-02-0.603D-02-0.640D-02

Coeff-Com: 0.921D-01 0.351D+00 0.572D+00

Coeff: 0.524D-05 0.916D-04-0.158D-03-0.217D-02-0.603D-02-0.640D-02

Coeff: 0.921D-01 0.351D+00 0.572D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.83D-08 MaxDP=8.05D-07 DE=-8.70D-10 OVMax= 2.11D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.06D-08 CP: 9.97D-01 1.04D+00 8.10D-01 9.00D-01 8.81D-01

CP: 6.04D-01 8.98D-01 7.97D-01 6.21D-01

E= -1359.06132999856 Delta-E= -0.000000000171 Rises=F Damp=F

DIIS: error= 9.16D-08 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1359.06132999856 IErMin=10 ErrMin= 9.16D-08

ErrMax= 9.16D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.04D-12 BMatP= 1.29D-10

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

Coeff-Com: -0.191D-05 0.116D-03-0.992D-05-0.911D-03-0.417D-02-0.522D-02

Coeff-Com: 0.166D-01 0.870D-01 0.195D+00 0.711D+00

Coeff: -0.191D-05 0.116D-03-0.992D-05-0.911D-03-0.417D-02-0.522D-02

Coeff: 0.166D-01 0.870D-01 0.195D+00 0.711D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=3.51D-09 MaxDP=1.31D-07 DE=-1.71D-10 OVMax= 2.49D-07

Error on total polarization charges = 0.06213

SCF Done: E(RB3LYP) = -1359.06133000 A.U. after 10 cycles

NFock= 10 Conv=0.35D-08 -V/T= 1.9682

KE= 1.403638407624D+03 PE=-9.356961062506D+03 EE= 3.536801280334D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.33

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:19:21 2019, MaxMem= 1342177280 cpu: 456.5

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16211 LenP2D= 44788.

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 = 255

Leave Link 701 at Fri Jul 26 14:19:25 2019, MaxMem= 1342177280 cpu: 43.0

(Enter /apps/gaussian/g09d01/g09/l702.exe)

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

Leave Link 702 at Fri Jul 26 14:19:25 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Fri Jul 26 14:19:28 2019, MaxMem= 1342177280 cpu: 42.9

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.77635684D-14 2.13162821D-14 5.99171368D-02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000712598 0.001434224 -0.000766102

2 6 -0.002603027 -0.002435550 0.002463924

3 7 0.000000000 0.003600212 -0.004312091

4 6 0.002603027 -0.002435550 0.002463924

5 6 0.000712598 0.001434224 -0.000766102

6 6 0.002693363 -0.002693363 0.004837592

7 6 0.002435550 -0.002603027 0.002463924

8 7 -0.003600212 0.000000000 -0.004312091

9 6 0.002435550 0.002603027 0.002463924

10 6 -0.001434224 0.000712598 -0.000766102

11 6 -0.001434224 -0.000712598 -0.000766102

12 6 -0.002693363 -0.002693363 0.004837592

13 6 -0.002435550 -0.002603027 0.002463924

14 6 0.001434224 -0.000712598 -0.000766102

15 6 0.001434224 0.000712598 -0.000766102

16 6 -0.002435550 0.002603027 0.002463924

17 7 0.003600212 0.000000000 -0.004312091

18 6 -0.002693363 0.002693363 0.004837592

19 6 -0.002603027 0.002435550 0.002463924

20 6 -0.000712598 -0.001434224 -0.000766102

21 6 0.000712598 -0.001434224 -0.000766102

22 6 0.002603027 0.002435550 0.002463924

23 7 0.000000000 -0.003600212 -0.004312091

24 1 -0.000567320 0.000426288 -0.000447815

25 1 0.000567320 0.000426288 -0.000447815

26 1 -0.000426288 0.000567320 -0.000447815

27 1 -0.000426288 -0.000567320 -0.000447815

28 1 0.000426288 -0.000567320 -0.000447815

29 1 0.000426288 0.000567320 -0.000447815

30 1 -0.000567320 -0.000426288 -0.000447815

31 1 0.000567320 -0.000426288 -0.000447815

32 30 0.000000000 0.000000000 -0.003373631

33 6 0.002693363 0.002693363 0.004837592

34 6 -0.000014397 -0.000014397 -0.001721848

35 6 0.000014397 0.000014397 -0.001721848

36 6 -0.000393843 -0.000393843 -0.002243003

37 6 0.000393843 0.000393843 -0.002243003

38 6 -0.000014397 0.000014397 -0.001721848

39 6 -0.000393843 0.000393843 -0.002243003

40 6 0.000014397 -0.000014397 -0.001721848

41 6 0.000393843 -0.000393843 -0.002243003

42 1 0.000050845 -0.000050845 0.001782742

43 1 -0.000050845 -0.000050845 0.001782742

44 1 -0.000050845 0.000050845 0.001782742

45 1 0.000050845 0.000050845 0.001782742

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

Cartesian Forces: Max 0.004837592 RMS 0.001955583

Leave Link 716 at Fri Jul 26 14:19:28 2019, MaxMem= 1342177280 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.003653814 RMS 0.001079421

Search for a local minimum.

Step number 9 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .10794D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 2 3 4 5

7 9 8

DE= 1.40D-03 DEPred=-7.70D-04 R=-1.81D+00

Trust test=-1.81D+00 RLast= 5.40D-01 DXMaxT set to 5.00D-02

ITU= -1 0 0 -1 1 0 -1 -1 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.83789.

Iteration 1 RMS(Cart)= 0.03063503 RMS(Int)= 0.00077669

Iteration 2 RMS(Cart)= 0.00175279 RMS(Int)= 0.00009936

Iteration 3 RMS(Cart)= 0.00000042 RMS(Int)= 0.00009936

ITry= 1 IFail=0 DXMaxC= 2.84D-01 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=T

ClnCor: largest displacement from symmetrization is 1.83D-04 for atom 44.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.72964 0.00161 0.00283 0.00000 0.00286 2.73250

R2 2.57787 -0.00178 -0.00205 0.00000 -0.00195 2.57592

R3 2.04062 -0.00004 -0.00059 0.00000 -0.00059 2.04003

R4 2.58984 -0.00365 -0.00420 0.00000 -0.00425 2.58559

R5 2.67907 -0.00075 -0.00216 0.00000 -0.00196 2.67710

R6 2.58984 -0.00365 -0.00420 0.00000 -0.00425 2.58559

R7 3.94374 0.00021 0.00946 0.00000 0.00918 3.95292

R8 2.72964 0.00161 0.00283 0.00000 0.00286 2.73250

R9 2.67907 -0.00075 -0.00216 0.00000 -0.00196 2.67710

R10 2.04062 -0.00004 -0.00059 0.00000 -0.00059 2.04003

R11 2.67907 -0.00075 -0.00216 0.00000 -0.00196 2.67710

R12 2.69333 0.00067 0.00046 0.00000 0.00044 2.69376

R13 2.58984 -0.00365 -0.00420 0.00000 -0.00425 2.58559

R14 2.72964 0.00162 0.00283 0.00000 0.00286 2.73250

R15 2.58984 -0.00365 -0.00420 0.00000 -0.00425 2.58559

R16 3.94374 0.00021 0.00946 0.00000 0.00918 3.95292

R17 2.72964 0.00161 0.00283 0.00000 0.00286 2.73250

R18 2.67907 -0.00075 -0.00216 0.00000 -0.00196 2.67710

R19 2.57787 -0.00178 -0.00205 0.00000 -0.00195 2.57592

R20 2.04062 -0.00004 -0.00059 0.00000 -0.00059 2.04003

R21 2.04062 -0.00001 -0.00059 0.00000 -0.00059 2.04003

R22 2.67907 -0.00075 -0.00216 0.00000 -0.00196 2.67710

R23 2.69333 0.00067 0.00046 0.00000 0.00044 2.69376

R24 2.72964 0.00162 0.00283 0.00000 0.00286 2.73250

R25 2.58984 -0.00365 -0.00420 0.00000 -0.00425 2.58559

R26 2.57787 -0.00178 -0.00205 0.00000 -0.00195 2.57592

R27 2.04062 -0.00001 -0.00059 0.00000 -0.00059 2.04003

R28 2.72964 0.00161 0.00283 0.00000 0.00286 2.73250

R29 2.04062 -0.00004 -0.00059 0.00000 -0.00059 2.04003

R30 2.58984 -0.00365 -0.00420 0.00000 -0.00425 2.58559

R31 2.67907 -0.00075 -0.00216 0.00000 -0.00196 2.67710

R32 3.94374 0.00021 0.00946 0.00000 0.00918 3.95292

R33 2.67907 -0.00075 -0.00216 0.00000 -0.00196 2.67710

R34 2.69333 0.00067 0.00046 0.00000 0.00044 2.69376

R35 2.72964 0.00163 0.00283 0.00000 0.00286 2.73250

R36 2.58984 -0.00365 -0.00420 0.00000 -0.00425 2.58559

R37 2.57787 -0.00178 -0.00205 0.00000 -0.00195 2.57592

R38 2.04062 -0.00001 -0.00059 0.00000 -0.00059 2.04003

R39 2.72964 0.00163 0.00283 0.00000 0.00286 2.73250

R40 2.04062 -0.00001 -0.00059 0.00000 -0.00059 2.04003

R41 2.58984 -0.00365 -0.00420 0.00000 -0.00425 2.58559

R42 2.67907 -0.00075 -0.00216 0.00000 -0.00196 2.67710

R43 3.94374 0.00020 0.00946 0.00000 0.00918 3.95292

R44 2.69333 0.00067 0.00046 0.00000 0.00044 2.69376

R45 2.27828 0.00066 0.00047 0.00000 0.00047 2.27875

R46 2.27828 0.00066 0.00047 0.00000 0.00047 2.27875

R47 2.01720 -0.00007 -0.00030 0.00000 -0.00030 2.01690

R48 2.01720 -0.00007 -0.00030 0.00000 -0.00030 2.01690

R49 2.27828 0.00066 0.00047 0.00000 0.00047 2.27875

R50 2.01720 -0.00007 -0.00030 0.00000 -0.00030 2.01690

R51 2.27828 0.00066 0.00047 0.00000 0.00047 2.27875

R52 2.01720 -0.00007 -0.00030 0.00000 -0.00030 2.01690

A1 1.86860 -0.00090 -0.00187 0.00000 -0.00184 1.86676

A2 2.18328 0.00117 0.00484 0.00000 0.00482 2.18811

A3 2.23129 -0.00026 -0.00296 0.00000 -0.00298 2.22831

A4 1.90438 0.00082 0.00336 0.00000 0.00325 1.90763

A5 2.18497 0.00005 -0.00196 0.00000 -0.00184 2.18313

A6 2.19380 -0.00087 -0.00155 0.00000 -0.00151 2.19230

A7 1.87794 0.00022 -0.00224 0.00000 -0.00197 1.87596

A8 2.20261 -0.00011 -0.00019 0.00000 -0.00015 2.20246

A9 2.20261 -0.00011 -0.00019 0.00000 -0.00015 2.20246

A10 1.90438 0.00082 0.00336 0.00000 0.00325 1.90763

A11 2.19380 -0.00087 -0.00155 0.00000 -0.00151 2.19230

A12 2.18497 0.00005 -0.00196 0.00000 -0.00184 2.18313

A13 1.86860 -0.00090 -0.00187 0.00000 -0.00184 1.86676

A14 2.23129 -0.00026 -0.00296 0.00000 -0.00298 2.22831

A15 2.18328 0.00117 0.00484 0.00000 0.00482 2.18811

A16 2.20316 0.00193 0.00104 0.00000 0.00123 2.20439

A17 2.03977 -0.00090 -0.00041 0.00000 -0.00041 2.03935

A18 2.03977 -0.00099 -0.00041 0.00000 -0.00041 2.03935

A19 2.19380 -0.00086 -0.00155 0.00000 -0.00151 2.19230

A20 2.18497 0.00004 -0.00196 0.00000 -0.00184 2.18313

A21 1.90438 0.00083 0.00336 0.00000 0.00325 1.90763

A22 1.87794 0.00022 -0.00224 0.00000 -0.00197 1.87596

A23 2.20261 -0.00011 -0.00019 0.00000 -0.00015 2.20246

A24 2.20261 -0.00011 -0.00019 0.00000 -0.00015 2.20246

A25 1.90438 0.00083 0.00336 0.00000 0.00325 1.90763

A26 2.19380 -0.00087 -0.00155 0.00000 -0.00151 2.19230

A27 2.18497 0.00005 -0.00196 0.00000 -0.00184 2.18313

A28 1.86860 -0.00090 -0.00187 0.00000 -0.00184 1.86676

A29 2.18328 0.00116 0.00484 0.00000 0.00482 2.18811

A30 2.23129 -0.00027 -0.00296 0.00000 -0.00298 2.22831

A31 1.86860 -0.00091 -0.00187 0.00000 -0.00184 1.86676

A32 2.18328 0.00118 0.00484 0.00000 0.00482 2.18811

A33 2.23129 -0.00027 -0.00296 0.00000 -0.00298 2.22831

A34 2.20316 0.00193 0.00104 0.00000 0.00123 2.20439

A35 2.03977 -0.00090 -0.00041 0.00000 -0.00041 2.03935

A36 2.03977 -0.00099 -0.00041 0.00000 -0.00041 2.03935

A37 2.18497 0.00004 -0.00196 0.00000 -0.00184 2.18313

A38 2.19380 -0.00086 -0.00155 0.00000 -0.00151 2.19230

A39 1.90438 0.00083 0.00336 0.00000 0.00325 1.90763

A40 1.86860 -0.00091 -0.00187 0.00000 -0.00184 1.86676

A41 2.18328 0.00118 0.00484 0.00000 0.00482 2.18811

A42 2.23129 -0.00027 -0.00296 0.00000 -0.00298 2.22831

A43 1.86860 -0.00090 -0.00187 0.00000 -0.00184 1.86676

A44 2.23129 -0.00027 -0.00296 0.00000 -0.00298 2.22831

A45 2.18328 0.00116 0.00484 0.00000 0.00482 2.18811

A46 1.90438 0.00083 0.00336 0.00000 0.00325 1.90763

A47 2.18497 0.00005 -0.00196 0.00000 -0.00184 2.18313

A48 2.19380 -0.00087 -0.00155 0.00000 -0.00151 2.19230

A49 1.87794 0.00022 -0.00224 0.00000 -0.00197 1.87596

A50 2.20261 -0.00011 -0.00019 0.00000 -0.00015 2.20246

A51 2.20261 -0.00011 -0.00019 0.00000 -0.00015 2.20246

A52 2.20316 0.00193 0.00104 0.00000 0.00123 2.20439

A53 2.03977 -0.00090 -0.00041 0.00000 -0.00041 2.03935

A54 2.03977 -0.00099 -0.00041 0.00000 -0.00041 2.03935

A55 2.18497 0.00004 -0.00196 0.00000 -0.00184 2.18313

A56 2.19380 -0.00086 -0.00155 0.00000 -0.00151 2.19230

A57 1.90438 0.00083 0.00336 0.00000 0.00325 1.90763

A58 1.86860 -0.00091 -0.00187 0.00000 -0.00184 1.86676

A59 2.18328 0.00118 0.00484 0.00000 0.00482 2.18811

A60 2.23129 -0.00027 -0.00296 0.00000 -0.00298 2.22831

A61 1.86860 -0.00091 -0.00187 0.00000 -0.00184 1.86676

A62 2.23129 -0.00027 -0.00296 0.00000 -0.00298 2.22831

A63 2.18328 0.00118 0.00484 0.00000 0.00482 2.18811

A64 1.90438 0.00083 0.00336 0.00000 0.00325 1.90763

A65 2.18497 0.00004 -0.00196 0.00000 -0.00184 2.18313

A66 2.19380 -0.00086 -0.00155 0.00000 -0.00151 2.19230

A67 1.87794 0.00022 -0.00224 0.00000 -0.00197 1.87596

A68 2.20261 -0.00011 -0.00019 0.00000 -0.00015 2.20246

A69 2.20261 -0.00011 -0.00019 0.00000 -0.00015 2.20246

A70 1.56912 0.00003 -0.00803 0.00000 -0.00746 1.56167

A71 1.56912 0.00003 -0.00803 0.00000 -0.00746 1.56167

A72 3.05972 0.00081 -0.10953 0.00000 -0.10952 2.95020

A73 3.05972 0.00081 -0.10953 0.00000 -0.10952 2.95020

A74 1.56912 0.00003 -0.00803 0.00000 -0.00746 1.56167

A75 1.56912 0.00003 -0.00803 0.00000 -0.00746 1.56167

A76 2.20316 0.00193 0.00104 0.00000 0.00123 2.20439

A77 2.03977 -0.00090 -0.00041 0.00000 -0.00041 2.03935

A78 2.03977 -0.00099 -0.00041 0.00000 -0.00041 2.03935

A79 3.14175 0.00009 -0.00025 0.00000 -0.00027 3.14148

A80 3.14175 0.00009 -0.00025 0.00000 -0.00027 3.14148

A81 3.14099 0.00010 0.00060 0.00000 0.00055 3.14153

A82 3.14099 0.00010 0.00060 0.00000 0.00055 3.14153

A83 3.14175 0.00009 -0.00025 0.00000 -0.00027 3.14148

A84 3.14099 0.00010 0.00060 0.00000 0.00055 3.14153

A85 3.14175 0.00009 -0.00025 0.00000 -0.00027 3.14148

A86 3.14099 0.00010 0.00060 0.00000 0.00055 3.14153

A87 3.12756 0.00255 0.00413 0.00000 0.00413 3.13169

A88 3.15562 -0.00255 -0.00413 0.00000 -0.00413 3.15149

A89 3.06360 0.00312 0.07307 0.00000 0.07307 3.13668

A90 3.21958 -0.00312 -0.07307 0.00000 -0.07307 3.14651

A91 3.12756 0.00255 0.00413 0.00000 0.00413 3.13169

A92 3.06360 0.00312 0.07307 0.00000 0.07307 3.13668

A93 3.15562 -0.00255 -0.00413 0.00000 -0.00413 3.15149

A94 3.21958 -0.00312 -0.07307 0.00000 -0.07307 3.14651

D1 -0.02394 0.00088 0.01917 0.00000 0.01917 -0.00477

D2 3.12619 0.00021 -0.00595 0.00000 -0.00595 3.12024

D3 3.11313 0.00076 0.02599 0.00000 0.02599 3.13911

D4 -0.01993 0.00010 0.00087 0.00000 0.00086 -0.01907

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 3.13690 -0.00011 0.00704 0.00000 0.00705 -3.13923

D7 -3.13690 0.00011 -0.00704 0.00000 -0.00705 3.13923

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.03875 -0.00140 -0.03104 0.00000 -0.03104 0.00771

D10 -3.09450 -0.00083 0.03020 0.00000 0.03020 -3.06430

D11 -3.11143 -0.00073 -0.00575 0.00000 -0.00575 -3.11719

D12 0.03850 -0.00015 0.05549 0.00000 0.05549 0.09399

D13 3.11924 0.00099 0.05012 0.00000 0.05013 -3.11382

D14 0.01260 -0.00035 0.00052 0.00000 0.00052 0.01312

D15 -0.01243 0.00021 0.02095 0.00000 0.02094 0.00852

D16 -3.11906 -0.00113 -0.02865 0.00000 -0.02866 3.13546

D17 -0.03875 0.00140 0.03104 0.00000 0.03104 -0.00771

D18 3.11143 0.00073 0.00575 0.00000 0.00575 3.11719

D19 3.09450 0.00083 -0.03020 0.00000 -0.03020 3.06430

D20 -0.03850 0.00015 -0.05549 0.00000 -0.05549 -0.09399

D21 -3.10562 -0.00074 0.01809 0.00000 0.01816 -3.08746

D22 -0.04583 0.00007 -0.09051 0.00000 -0.09056 -0.13639

D23 -1.57572 -0.00034 -0.03621 0.00000 -0.03620 -1.61193

D24 0.04583 -0.00007 0.09051 0.00000 0.09056 0.13639

D25 3.10562 0.00074 -0.01809 0.00000 -0.01816 3.08746

D26 1.57572 0.00034 0.03621 0.00000 0.03620 1.61193

D27 0.02394 -0.00088 -0.01917 0.00000 -0.01917 0.00477

D28 -3.11313 -0.00076 -0.02599 0.00000 -0.02599 -3.13911

D29 -3.12619 -0.00021 0.00595 0.00000 0.00595 -3.12024

D30 0.01993 -0.00010 -0.00087 0.00000 -0.00086 0.01907

D31 0.01243 -0.00021 -0.02095 0.00000 -0.02094 -0.00852

D32 3.11906 0.00113 0.02865 0.00000 0.02866 -3.13546

D33 -3.11924 -0.00099 -0.05012 0.00000 -0.05013 3.11382

D34 -0.01260 0.00035 -0.00052 0.00000 -0.00052 -0.01312

D35 -0.01243 0.00021 0.02095 0.00000 0.02094 0.00852

D36 3.11924 0.00099 0.05012 0.00000 0.05013 -3.11382

D37 -3.11906 -0.00114 -0.02865 0.00000 -0.02866 3.13546

D38 0.01260 -0.00036 0.00052 0.00000 0.00052 0.01312

D39 -3.11143 -0.00073 -0.00575 0.00000 -0.00575 -3.11719

D40 0.03850 -0.00015 0.05549 0.00000 0.05549 0.09399

D41 0.03875 -0.00140 -0.03104 0.00000 -0.03104 0.00771

D42 -3.09450 -0.00083 0.03020 0.00000 0.03020 -3.06430

D43 3.12619 0.00021 -0.00595 0.00000 -0.00595 3.12024

D44 -0.01993 0.00010 0.00087 0.00000 0.00086 -0.01907

D45 -0.02394 0.00088 0.01917 0.00000 0.01917 -0.00477

D46 3.11313 0.00076 0.02599 0.00000 0.02599 3.13911

D47 -0.03875 0.00140 0.03104 0.00000 0.03104 -0.00771

D48 3.11143 0.00073 0.00575 0.00000 0.00575 3.11719

D49 3.09450 0.00083 -0.03020 0.00000 -0.03020 3.06430

D50 -0.03850 0.00015 -0.05549 0.00000 -0.05549 -0.09399

D51 -0.04583 0.00007 -0.09051 0.00000 -0.09056 -0.13639

D52 -1.57572 -0.00034 -0.03621 0.00000 -0.03620 -1.61193

D53 -3.10562 -0.00074 0.01809 0.00000 0.01816 -3.08746

D54 3.10562 0.00074 -0.01809 0.00000 -0.01816 3.08746

D55 1.57572 0.00034 0.03621 0.00000 0.03620 1.61193

D56 0.04583 -0.00007 0.09051 0.00000 0.09056 0.13639

D57 0.02394 -0.00088 -0.01917 0.00000 -0.01917 0.00477

D58 -3.11313 -0.00076 -0.02599 0.00000 -0.02599 -3.13911

D59 -3.12619 -0.00021 0.00595 0.00000 0.00595 -3.12024

D60 0.01993 -0.00010 -0.00087 0.00000 -0.00086 0.01907

D61 0.01243 -0.00021 -0.02095 0.00000 -0.02094 -0.00852

D62 3.11906 0.00113 0.02865 0.00000 0.02866 -3.13546

D63 -3.11924 -0.00099 -0.05012 0.00000 -0.05013 3.11382

D64 -0.01260 0.00035 -0.00052 0.00000 -0.00052 -0.01312

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 -3.13690 0.00011 -0.00704 0.00000 -0.00705 3.13923

D67 3.13690 -0.00011 0.00704 0.00000 0.00705 -3.13923

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 -3.11924 -0.00099 -0.05012 0.00000 -0.05013 3.11382

D70 0.01243 -0.00021 -0.02095 0.00000 -0.02094 -0.00852

D71 -0.01260 0.00036 -0.00052 0.00000 -0.00052 -0.01312

D72 3.11906 0.00114 0.02865 0.00000 0.02866 -3.13546

D73 -3.12619 -0.00021 0.00595 0.00000 0.00595 -3.12024

D74 0.01993 -0.00010 -0.00087 0.00000 -0.00086 0.01907

D75 0.02394 -0.00088 -0.01917 0.00000 -0.01917 0.00477

D76 -3.11313 -0.00076 -0.02599 0.00000 -0.02599 -3.13911

D77 3.11143 0.00073 0.00575 0.00000 0.00575 3.11719

D78 -0.03850 0.00015 -0.05549 0.00000 -0.05549 -0.09399

D79 -0.03875 0.00140 0.03104 0.00000 0.03104 -0.00771

D80 3.09450 0.00083 -0.03020 0.00000 -0.03020 3.06430

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 -3.13690 0.00011 -0.00704 0.00000 -0.00705 3.13923

D83 3.13690 -0.00011 0.00704 0.00000 0.00705 -3.13923

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 -0.02394 0.00088 0.01917 0.00000 0.01917 -0.00477

D86 3.12619 0.00021 -0.00595 0.00000 -0.00595 3.12024

D87 3.11313 0.00076 0.02599 0.00000 0.02599 3.13911

D88 -0.01993 0.00010 0.00087 0.00000 0.00086 -0.01907

D89 0.03875 -0.00140 -0.03104 0.00000 -0.03104 0.00771

D90 -3.09450 -0.00083 0.03020 0.00000 0.03020 -3.06430

D91 -3.11143 -0.00073 -0.00575 0.00000 -0.00575 -3.11719

D92 0.03850 -0.00015 0.05549 0.00000 0.05549 0.09399

D93 3.11924 0.00099 0.05012 0.00000 0.05013 -3.11382

D94 0.01260 -0.00035 0.00052 0.00000 0.00052 0.01312

D95 -0.01243 0.00021 0.02095 0.00000 0.02094 0.00852

D96 -3.11906 -0.00113 -0.02865 0.00000 -0.02866 3.13546

D97 0.04583 -0.00007 0.09051 0.00000 0.09056 0.13639

D98 1.57572 0.00034 0.03621 0.00000 0.03620 1.61193

D99 3.10562 0.00074 -0.01809 0.00000 -0.01816 3.08746

D100 -3.10562 -0.00074 0.01809 0.00000 0.01816 -3.08746

D101 -1.57572 -0.00034 -0.03621 0.00000 -0.03620 -1.61193

D102 -0.04583 0.00007 -0.09051 0.00000 -0.09056 -0.13639

D103 -3.11924 -0.00099 -0.05012 0.00000 -0.05013 3.11382

D104 0.01243 -0.00021 -0.02095 0.00000 -0.02094 -0.00852

D105 -0.01260 0.00036 -0.00052 0.00000 -0.00052 -0.01312

D106 3.11906 0.00114 0.02865 0.00000 0.02866 -3.13546

D107 -3.12619 -0.00021 0.00595 0.00000 0.00595 -3.12024

D108 0.01993 -0.00010 -0.00087 0.00000 -0.00086 0.01907

D109 0.02394 -0.00088 -0.01917 0.00000 -0.01917 0.00477

D110 -3.11313 -0.00076 -0.02599 0.00000 -0.02599 -3.13911

D111 3.11143 0.00073 0.00575 0.00000 0.00575 3.11719

D112 -0.03850 0.00015 -0.05549 0.00000 -0.05549 -0.09399

D113 -0.03875 0.00140 0.03104 0.00000 0.03104 -0.00771

D114 3.09450 0.00083 -0.03020 0.00000 -0.03020 3.06430

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 -3.13690 0.00011 -0.00704 0.00000 -0.00705 3.13923

D117 3.13690 -0.00011 0.00704 0.00000 0.00705 -3.13923

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 -0.02394 0.00088 0.01917 0.00000 0.01917 -0.00477

D120 3.12619 0.00021 -0.00595 0.00000 -0.00595 3.12024

D121 3.11313 0.00076 0.02599 0.00000 0.02599 3.13911

D122 -0.01993 0.00010 0.00087 0.00000 0.00086 -0.01907

D123 0.03875 -0.00140 -0.03104 0.00000 -0.03104 0.00771

D124 -3.09450 -0.00083 0.03020 0.00000 0.03020 -3.06430

D125 -3.11143 -0.00073 -0.00575 0.00000 -0.00575 -3.11719

D126 0.03850 -0.00015 0.05549 0.00000 0.05549 0.09399

D127 3.11924 0.00099 0.05012 0.00000 0.05013 -3.11382

D128 0.01260 -0.00036 0.00052 0.00000 0.00052 0.01312

D129 -0.01243 0.00021 0.02095 0.00000 0.02094 0.00852

D130 -3.11906 -0.00114 -0.02865 0.00000 -0.02866 3.13546

D131 1.57572 0.00034 0.03621 0.00000 0.03620 1.61193

D132 3.10562 0.00074 -0.01809 0.00000 -0.01816 3.08746

D133 0.04583 -0.00007 0.09051 0.00000 0.09056 0.13639

D134 -1.57572 -0.00034 -0.03621 0.00000 -0.03620 -1.61193

D135 -0.04583 0.00007 -0.09051 0.00000 -0.09056 -0.13639

D136 -3.10562 -0.00074 0.01809 0.00000 0.01816 -3.08746

Item Value Threshold Converged?

Maximum Force 0.003654 0.000450 NO

RMS Force 0.001079 0.000300 NO

Maximum Displacement 0.284206 0.001800 NO

RMS Displacement 0.030776 0.001200 NO

Predicted change in Energy=-7.090144D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:19:28 2019, MaxMem= 1342177280 cpu: 1.0

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 0.681560 4.273191 -0.035853

2 6 0 1.103299 2.890790 0.008329

3 7 0 0.000000 2.082223 0.040331

4 6 0 -1.103299 2.890790 0.008329

5 6 0 -0.681560 4.273191 -0.035853

6 6 0 -2.449402 2.449402 -0.002331

7 6 0 -2.890790 1.103299 0.008329

8 7 0 -2.082223 0.000000 0.040331

9 6 0 -2.890790 -1.103299 0.008329

10 6 0 -4.273191 -0.681560 -0.035853

11 6 0 -4.273191 0.681560 -0.035853

12 6 0 2.449402 2.449402 -0.002331

13 6 0 2.890790 1.103299 0.008329

14 6 0 4.273191 0.681560 -0.035853

15 6 0 4.273191 -0.681560 -0.035853

16 6 0 2.890790 -1.103299 0.008329

17 7 0 2.082223 0.000000 0.040331

18 6 0 2.449402 -2.449402 -0.002331

19 6 0 1.103299 -2.890790 0.008329

20 6 0 0.681560 -4.273191 -0.035853

21 6 0 -0.681560 -4.273191 -0.035853

22 6 0 -1.103299 -2.890790 0.008329

23 7 0 0.000000 -2.082223 0.040331

24 1 0 1.341325 5.127157 -0.065162

25 1 0 -1.341325 5.127157 -0.065162

26 1 0 -5.127157 -1.341325 -0.065162

27 1 0 -5.127157 1.341325 -0.065162

28 1 0 5.127157 1.341325 -0.065162

29 1 0 5.127157 -1.341325 -0.065162

30 1 0 1.341325 -5.127157 -0.065162

31 1 0 -1.341325 -5.127157 -0.065162

32 30 0 0.000000 0.000000 0.240204

33 6 0 -2.449402 -2.449402 -0.002331

34 6 0 -3.456923 -3.456923 -0.044706

35 6 0 3.456923 3.456923 -0.044706

36 6 0 -4.308927 -4.308927 -0.092401

37 6 0 4.308927 4.308927 -0.092401

38 6 0 -3.456923 3.456923 -0.044706

39 6 0 -4.308927 4.308927 -0.092401

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41 6 0 4.308927 -4.308927 -0.092401

42 1 0 5.062896 -5.062896 -0.139173

43 1 0 -5.062896 -5.062896 -0.139173

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45 1 0 5.062896 5.062896 -0.139173

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.445977 0.000000

3 N 2.295794 1.368238 0.000000

4 C 2.258032 2.206599 1.368238 0.000000

5 C 1.363120 2.258032 2.295794 1.445977 0.000000

6 C 3.623569 3.580032 2.477138 1.416662 2.540196

7 C 4.776176 4.375829 3.052210 2.527894 3.864048

8 N 5.089643 4.301773 2.944708 3.052210 4.497536

9 C 6.455253 5.648496 4.301773 4.375829 5.812857

10 C 7.007077 6.455253 5.089643 4.776176 6.119590

11 C 6.119590 5.812857 4.497536 3.864048 5.079334

12 C 2.540196 1.416662 2.477138 3.580032 3.623569

13 C 3.864048 2.527894 3.052210 4.375829 4.776176

14 C 5.079334 3.864048 4.497536 5.812857 6.119590

15 C 6.119590 4.776176 5.089643 6.455253 7.007077

16 C 5.812857 4.375829 4.301773 5.648496 6.455253

17 N 4.497536 3.052210 2.944708 4.301773 5.089643

18 C 6.951234 5.507247 5.151410 6.414005 7.416018

19 C 7.176521 5.781581 5.094032 6.188356 7.383110

20 C 8.546383 7.176521 6.392310 7.383110 8.654407

21 C 8.654407 7.383110 6.392310 7.176521 8.546383

22 C 7.383110 6.188356 5.094032 5.781581 7.176521

23 N 6.392310 5.094032 4.164446 5.094032 6.392310

24 H 1.079540 2.250198 3.328949 3.314050 2.195946

25 H 2.195946 3.314050 3.328949 2.250198 1.079540

26 H 8.078666 7.532250 6.165999 5.840174 7.161493

27 H 6.506757 6.420657 5.181486 4.312502 5.325414

28 H 5.325414 4.312502 5.181486 6.420657 6.506757

29 H 7.161493 5.840174 6.165999 7.532250 8.078666

30 H 9.423518 8.021816 7.333856 8.382665 9.615585

31 H 9.615585 8.382665 7.333856 8.021816 9.423518

32 Zn 4.336000 3.102854 2.091794 3.102854 4.336000

33 C 7.416018 6.414005 5.151410 5.507247 6.951234

34 C 8.768226 7.816131 6.529907 6.770215 8.213244

35 C 2.892924 2.421335 3.721202 4.595535 4.218224

36 C 9.927785 9.007679 7.709168 7.881759 9.317390

37 C 3.627984 3.506752 4.852080 5.595843 4.990936

38 C 4.218224 4.595535 3.721202 2.421335 2.892924

39 C 4.990936 5.595843 4.852080 3.506752 3.627984

40 C 8.213244 6.770215 6.529907 7.816131 8.768226

41 C 9.317390 7.881759 7.709168 9.007679 9.927785

42 H 10.313550 8.886017 8.758874 10.065032 10.962298

43 H 10.962298 10.065032 8.758874 8.886017 10.313550

44 H 5.799404 6.539248 5.877887 4.518651 4.453136

45 H 4.453136 4.518651 5.877887 6.539248 5.799404

6 7 8 9 10

6 C 0.000000

7 C 1.416662 0.000000

8 N 2.477138 1.368238 0.000000

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14 C 6.951234 7.176521 6.392310 7.383110 8.654407

15 C 7.416018 7.383110 6.392310 7.176521 8.546383

16 C 6.414005 6.188356 5.094032 5.781581 7.176521

17 N 5.151410 5.094032 4.164446 5.094032 6.392310

18 C 6.927956 6.414005 5.151410 5.507247 6.951234

19 C 6.414005 5.648496 4.301773 4.375829 5.812857

20 C 7.416018 6.455253 5.089643 4.776176 6.119590

21 C 6.951234 5.812857 4.497536 3.864048 5.079334

22 C 5.507247 4.375829 3.052210 2.527894 3.864048

23 N 5.151410 4.301773 2.944708 3.052210 4.497536

24 H 4.641544 5.840174 6.165999 7.532250 8.078666

25 H 2.898647 4.312502 5.181486 6.420657 6.506757

26 H 4.641544 3.314050 3.328949 2.250198 1.079540

27 H 2.898647 2.250198 3.328949 3.314050 2.195946

28 H 7.657417 8.021816 7.333856 8.382665 9.615585

29 H 8.472179 8.382665 7.333856 8.021816 9.423518

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32 Zn 3.472458 3.102854 2.091794 3.102854 4.336000

33 C 4.898805 3.580032 2.477138 1.416662 2.540196

34 C 5.991792 4.595535 3.721202 2.421335 2.892924

35 C 5.991792 6.770215 6.529907 7.816131 8.768226

36 C 7.010062 5.595843 4.852080 3.506752 3.627984

37 C 7.010062 7.881759 7.709168 9.007679 9.927785

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40 C 8.352912 7.816131 6.529907 6.770215 8.213244

41 C 9.558146 9.007679 7.709168 7.881759 9.317390

42 H 10.624876 10.065032 8.758874 8.886017 10.313550

43 H 7.955106 6.539248 5.877887 4.518651 4.453136

44 H 3.698571 4.518651 5.877887 6.539248 5.799404

45 H 7.955106 8.886017 8.758874 10.065032 10.962298

11 12 13 14 15

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17 N 6.392310 2.477138 1.368238 2.295794 2.295794

18 C 7.416018 4.898805 3.580032 3.623569 2.540196

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23 N 5.089643 5.151410 4.301773 5.089643 4.497536

24 H 7.161493 2.898647 4.312502 5.325414 6.506757

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26 H 2.195946 8.472179 8.382665 9.615585 9.423518

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32 Zn 4.336000 3.472458 3.102854 4.336000 4.336000

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42 H 10.962298 7.955106 6.539248 5.799404 4.453136

43 H 5.799404 10.624876 10.065032 10.962298 10.313550

44 H 4.453136 7.955106 8.886017 10.313550 10.962298

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16 17 18 19 20

16 C 0.000000

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21 C 4.776176 5.089643 3.623569 2.258032 1.363120

22 C 4.375829 4.301773 3.580032 2.206599 2.258032

23 N 3.052210 2.944708 2.477138 1.368238 2.295794

24 H 6.420657 5.181486 7.657417 8.021816 9.423518

25 H 7.532250 6.165999 8.472179 8.382665 9.615585

26 H 8.021816 7.333856 7.657417 6.420657 6.506757

27 H 8.382665 7.333856 8.472179 7.532250 8.078666

28 H 3.314050 3.328949 4.641544 5.840174 7.161493

29 H 2.250198 3.328949 2.898647 4.312502 5.325414

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31 H 5.840174 6.165999 4.641544 3.314050 2.195946

32 Zn 3.102854 2.091794 3.472458 3.102854 4.336000

33 C 5.507247 5.151410 4.898805 3.580032 3.623569

34 C 6.770215 6.529907 5.991792 4.595535 4.218224

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36 C 7.881759 7.709168 7.010062 5.595843 4.990936

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44 H 10.065032 8.758874 10.624876 10.065032 10.962298

45 H 6.539248 5.877887 7.955106 8.886017 10.313550

21 22 23 24 25

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22 C 1.445977 0.000000

23 N 2.295794 1.368238 0.000000

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25 H 9.423518 8.021816 7.333856 2.682650 0.000000

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28 H 8.078666 7.532250 6.165999 5.353975 7.494917

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35 C 8.768226 7.816131 6.529907 2.695525 5.080677

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37 C 9.927785 9.007679 7.709168 3.078458 5.709255

38 C 8.213244 6.770215 6.529907 5.080677 2.695525

39 C 9.317390 7.881759 7.709168 5.709255 3.078458

40 C 4.218224 4.595535 3.721202 8.840961 9.834125

41 C 4.990936 5.595843 4.852080 9.891769 10.998444

42 H 5.799404 6.539248 5.877887 10.848629 12.035643

43 H 4.453136 4.518651 5.877887 12.035643 10.848629

44 H 10.313550 8.886017 8.758874 6.404971 3.722862

45 H 10.962298 10.065032 8.758874 3.722862 6.404971

26 27 28 29 30

26 H 0.000000

27 H 2.682650 0.000000

28 H 10.599413 10.254314 0.000000

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33 C 2.898647 4.641544 8.472179 7.657417 4.641544

34 C 2.695525 5.080677 9.834125 8.840961 5.080677

35 C 9.834125 8.840961 2.695525 5.080677 8.840961

36 C 3.078458 5.709255 10.998444 9.891769 5.709255

37 C 10.998444 9.891769 3.078458 5.709255 9.891769

38 C 5.080677 2.695525 8.840961 9.834125 9.834125

39 C 5.709255 3.078458 9.891769 10.998444 10.998444

40 C 8.840961 9.834125 5.080677 2.695525 2.695525

41 C 9.891769 10.998444 5.709255 3.078458 3.078458

42 H 10.848629 12.035643 6.404971 3.722862 3.722862

43 H 3.722862 6.404971 12.035643 10.848629 6.404971

44 H 6.404971 3.722862 10.848629 12.035643 12.035643

45 H 12.035643 10.848629 3.722862 6.404971 10.848629

31 32 33 34 35

31 H 0.000000

32 Zn 5.308497 0.000000

33 C 2.898647 3.472458 0.000000

34 C 2.695525 4.897122 1.425479 0.000000

35 C 9.834125 4.897122 8.352912 9.777654 0.000000

36 C 3.078458 6.102814 2.631307 1.205860 10.982674

37 C 10.998444 6.102814 9.558146 10.982674 1.205860

38 C 8.840961 4.897122 5.991792 6.913845 6.913845

39 C 9.891769 6.102814 7.010062 7.812593 7.812593

40 C 5.080677 4.897122 5.991792 6.913845 6.913845

41 C 5.709255 6.102814 7.010062 7.812593 7.812593

42 H 6.404971 7.170060 7.955106 8.670374 8.670374

43 H 3.722862 7.170060 3.698571 2.273153 12.049214

44 H 10.848629 7.170060 7.955106 8.670374 8.670374

45 H 12.035643 7.170060 10.624876 12.049214 2.273153

36 37 38 39 40

36 C 0.000000

37 C 12.187487 0.000000

38 C 7.812593 7.812593 0.000000

39 C 8.617855 8.617855 1.205860 0.000000

40 C 7.812593 7.812593 9.777654 10.982674 0.000000

41 C 8.617855 8.617855 10.982674 12.187487 1.205860

42 H 9.402220 9.402220 12.049214 13.253843 2.273153

43 H 1.067299 13.253843 8.670374 9.402220 8.670374

44 H 9.402220 9.402220 2.273153 1.067299 12.049214

45 H 13.253843 1.067299 8.670374 9.402220 8.670374

41 42 43 44 45

41 C 0.000000

42 H 1.067299 0.000000

43 H 9.402220 10.125793 0.000000

44 H 13.253843 14.320033 10.125793 0.000000

45 H 9.402220 10.125793 14.320033 10.125793 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

RotChk: IX=3 Diff= 2.87D-19

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681560 -4.273191 -0.046734

2 6 0 -1.103299 -2.890790 -0.002553

3 7 0 0.000000 -2.082223 0.029450

4 6 0 1.103299 -2.890790 -0.002553

5 6 0 0.681560 -4.273191 -0.046734

6 6 0 2.449402 -2.449402 -0.013212

7 6 0 2.890790 -1.103299 -0.002553

8 7 0 2.082223 0.000000 0.029450

9 6 0 2.890790 1.103299 -0.002553

10 6 0 4.273191 0.681560 -0.046734

11 6 0 4.273191 -0.681560 -0.046734

12 6 0 -2.449402 -2.449402 -0.013212

13 6 0 -2.890790 -1.103299 -0.002553

14 6 0 -4.273191 -0.681560 -0.046734

15 6 0 -4.273191 0.681560 -0.046734

16 6 0 -2.890790 1.103299 -0.002553

17 7 0 -2.082223 0.000000 0.029450

18 6 0 -2.449402 2.449402 -0.013212

19 6 0 -1.103299 2.890790 -0.002553

20 6 0 -0.681560 4.273191 -0.046734

21 6 0 0.681560 4.273191 -0.046734

22 6 0 1.103299 2.890790 -0.002553

23 7 0 0.000000 2.082223 0.029450

24 1 0 -1.341325 -5.127157 -0.076043

25 1 0 1.341325 -5.127157 -0.076043

26 1 0 5.127157 1.341325 -0.076043

27 1 0 5.127157 -1.341325 -0.076043

28 1 0 -5.127157 -1.341325 -0.076043

29 1 0 -5.127157 1.341325 -0.076043

30 1 0 -1.341325 5.127157 -0.076043

31 1 0 1.341325 5.127157 -0.076043

32 30 0 0.000000 0.000000 0.229323

33 6 0 2.449402 2.449402 -0.013212

34 6 0 3.456923 3.456923 -0.055587

35 6 0 -3.456923 -3.456923 -0.055587

36 6 0 4.308927 4.308927 -0.103282

37 6 0 -4.308927 -4.308927 -0.103282

38 6 0 3.456923 -3.456923 -0.055587

39 6 0 4.308927 -4.308927 -0.103282

40 6 0 -3.456923 3.456923 -0.055587

41 6 0 -4.308927 4.308927 -0.103282

42 1 0 -5.062896 5.062896 -0.150054

43 1 0 5.062896 5.062896 -0.150054

44 1 0 5.062896 -5.062896 -0.150054

45 1 0 -5.062896 -5.062896 -0.150054

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

Rotational constants (GHZ): 0.1463365 0.1463365 0.0732620

Leave Link 202 at Fri Jul 26 14:19:29 2019, MaxMem= 1342177280 cpu: 0.1

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 184 symmetry adapted cartesian basis functions of A1 symmetry.

There are 155 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3059.1010383522 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= 9 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= -0.1305118153 Hartrees.

Nuclear repulsion after empirical dispersion term = 3058.9705265368 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: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3850

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.28D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 132

GePol: Fraction of low-weight points (<1% of avg) = 3.43%

GePol: Cavity surface area = 416.405 Ang\*\*2

GePol: Cavity volume = 420.327 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0084126376 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3058.9789391744 Hartrees.

Leave Link 301 at Fri Jul 26 14:19:29 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44800.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.40D-05 NBF= 172 148 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 172 148 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:19:29 2019, MaxMem= 1342177280 cpu: 6.6

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:19:29 2019, MaxMem= 1342177280 cpu: 0.8

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

Lowest energy guess from the checkpoint file: "ZnTSPsim0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 1.62D-01

Max alpha theta= 1.535 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

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

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

(A1) (E) (E) (B1) (A1) (A1) (B1) (E) (E) (E) (E)

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

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

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

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

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

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

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

(A2) (E) (E) (B2)

Virtual (A2) (E) (E) (B1) (E) (E) (B2) (A1) (E) (E) (A1)

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

(A1) (E) (E) (B1) (A1) (A1) (B1) (E) (E) (E) (E)

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The electronic state of the initial guess is 1-A1.

Leave Link 401 at Fri Jul 26 14:19:31 2019, MaxMem= 1342177280 cpu: 16.8

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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.

An orbital has undefined symmetry, so N\*\*3 symmetry is turned off.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 660000000 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= 0 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= 44467500.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.99D-15 for 629.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.03D-15 for 2412 978.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.44D-15 for 1280.

Iteration 1 A^-1\*A deviation from orthogonality is 3.12D-12 for 2355 2319.

E= -1359.06287151224

DIIS: error= 8.82D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.06287151224 IErMin= 1 ErrMin= 8.82D-05

ErrMax= 8.82D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.14D-06 BMatP= 1.14D-06

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

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 14.195 Goal= None Shift= 0.000

RMSDP=1.26D-05 MaxDP=4.26D-04 OVMax= 3.76D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.24D-05 CP: 1.00D+00

E= -1359.06287262441 Delta-E= -0.000001112177 Rises=F Damp=F

DIIS: error= 1.28D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.06287262441 IErMin= 1 ErrMin= 8.82D-05

ErrMax= 1.28D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.61D-07 BMatP= 1.14D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.28D-03

Coeff-Com: 0.432D+00 0.568D+00

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

Coeff: 0.432D+00 0.568D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.74D-06 MaxDP=5.42D-05 DE=-1.11D-06 OVMax= 1.16D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.68D-06 CP: 1.00D+00 9.65D-01

E= -1359.06287301494 Delta-E= -0.000000390525 Rises=F Damp=F

DIIS: error= 4.28D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.06287301494 IErMin= 3 ErrMin= 4.28D-05

ErrMax= 4.28D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.12D-08 BMatP= 7.61D-07

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

Coeff-Com: 0.238D-02 0.241D+00 0.757D+00

Coeff: 0.238D-02 0.241D+00 0.757D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=4.18D-07 MaxDP=1.21D-05 DE=-3.91D-07 OVMax= 3.71D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.54D-07 CP: 1.00D+00 9.79D-01 8.36D-01

E= -1359.06287304723 Delta-E= -0.000000032288 Rises=F Damp=F

DIIS: error= 5.33D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.06287304723 IErMin= 4 ErrMin= 5.33D-06

ErrMax= 5.33D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.84D-09 BMatP= 8.12D-08

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

Coeff-Com: -0.884D-02 0.127D+00 0.423D+00 0.458D+00

Coeff: -0.884D-02 0.127D+00 0.423D+00 0.458D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.25D-07 MaxDP=8.88D-06 DE=-3.23D-08 OVMax= 2.16D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 9.74D-08 CP: 1.00D+00 9.80D-01 8.26D-01 6.98D-01

E= -1359.06287305398 Delta-E= -0.000000006752 Rises=F Damp=F

DIIS: error= 2.12D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.06287305398 IErMin= 5 ErrMin= 2.12D-06

ErrMax= 2.12D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-09 BMatP= 7.84D-09

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

Coeff-Com: -0.551D-02 0.438D-01 0.140D+00 0.284D+00 0.537D+00

Coeff: -0.551D-02 0.438D-01 0.140D+00 0.284D+00 0.537D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=3.99D-08 MaxDP=3.22D-06 DE=-6.75D-09 OVMax= 7.22D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.04D-08 CP: 1.00D+00 9.80D-01 8.16D-01 7.40D-01 8.33D-01

E= -1359.06287305521 Delta-E= -0.000000001232 Rises=F Damp=F

DIIS: error= 8.18D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.06287305521 IErMin= 6 ErrMin= 8.18D-07

ErrMax= 8.18D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.38D-11 BMatP= 1.03D-09

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

Coeff-Com: -0.113D-02 0.341D-02 0.457D-02 0.802D-01 0.272D+00 0.641D+00

Coeff: -0.113D-02 0.341D-02 0.457D-02 0.802D-01 0.272D+00 0.641D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.57D-08 MaxDP=5.92D-07 DE=-1.23D-09 OVMax= 1.71D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.13D-08 CP: 1.00D+00 9.80D-01 8.17D-01 7.53D-01 8.20D-01

CP: 6.72D-01

E= -1359.06287305542 Delta-E= -0.000000000206 Rises=F Damp=F

DIIS: error= 1.19D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.06287305542 IErMin= 7 ErrMin= 1.19D-07

ErrMax= 1.19D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.90D-12 BMatP= 7.38D-11

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

Coeff-Com: -0.204D-03-0.117D-02-0.649D-02 0.219D-01 0.102D+00 0.325D+00

Coeff-Com: 0.559D+00

Coeff: -0.204D-03-0.117D-02-0.649D-02 0.219D-01 0.102D+00 0.325D+00

Coeff: 0.559D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=4.85D-09 MaxDP=1.62D-07 DE=-2.06D-10 OVMax= 6.35D-07

Error on total polarization charges = 0.06214

SCF Done: E(RB3LYP) = -1359.06287306 A.U. after 7 cycles

NFock= 7 Conv=0.49D-08 -V/T= 1.9682

KE= 1.403687097158D+03 PE=-9.360047085221D+03 EE= 3.538318175834D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.28

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:20:03 2019, MaxMem= 1342177280 cpu: 353.4

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44800.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 251

Leave Link 701 at Fri Jul 26 14:20:06 2019, MaxMem= 1342177280 cpu: 42.8

(Enter /apps/gaussian/g09d01/g09/l702.exe)

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

Leave Link 702 at Fri Jul 26 14:20:06 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Fri Jul 26 14:20:10 2019, MaxMem= 1342177280 cpu: 43.0

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-1.13686838D-13 1.70530257D-13 3.50565324D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000546080 0.000391255 0.000106011

2 6 -0.000653216 -0.001061186 0.000135675

3 7 0.000000000 0.000272515 0.000173153

4 6 0.000653216 -0.001061186 0.000135675

5 6 0.000546080 0.000391255 0.000106011

6 6 0.001848764 -0.001848764 0.000709112

7 6 0.001061186 -0.000653216 0.000135675

8 7 -0.000272515 0.000000000 0.000173153

9 6 0.001061186 0.000653216 0.000135675

10 6 -0.000391255 0.000546080 0.000106011

11 6 -0.000391255 -0.000546080 0.000106011

12 6 -0.001848764 -0.001848764 0.000709112

13 6 -0.001061186 -0.000653216 0.000135675

14 6 0.000391255 -0.000546080 0.000106011

15 6 0.000391255 0.000546080 0.000106011

16 6 -0.001061186 0.000653216 0.000135675

17 7 0.000272515 0.000000000 0.000173153

18 6 -0.001848764 0.001848764 0.000709112

19 6 -0.000653216 0.001061186 0.000135675

20 6 -0.000546080 -0.000391255 0.000106011

21 6 0.000546080 -0.000391255 0.000106011

22 6 0.000653216 0.001061186 0.000135675

23 7 0.000000000 -0.000272515 0.000173153

24 1 -0.000094412 0.000263392 -0.000147970

25 1 0.000094412 0.000263392 -0.000147970

26 1 -0.000263392 0.000094412 -0.000147970

27 1 -0.000263392 -0.000094412 -0.000147970

28 1 0.000263392 -0.000094412 -0.000147970

29 1 0.000263392 0.000094412 -0.000147970

30 1 -0.000094412 -0.000263392 -0.000147970

31 1 0.000094412 -0.000263392 -0.000147970

32 30 0.000000000 0.000000000 -0.003091863

33 6 0.001848764 0.001848764 0.000709112

34 6 -0.000546792 -0.000546792 -0.000357334

35 6 0.000546792 0.000546792 -0.000357334

36 6 0.000044522 0.000044522 -0.000183532

37 6 -0.000044522 -0.000044522 -0.000183532

38 6 -0.000546792 0.000546792 -0.000357334

39 6 0.000044522 -0.000044522 -0.000183532

40 6 0.000546792 -0.000546792 -0.000357334

41 6 -0.000044522 0.000044522 -0.000183532

42 1 0.000017174 -0.000017174 0.000244135

43 1 -0.000017174 -0.000017174 0.000244135

44 1 -0.000017174 0.000017174 0.000244135

45 1 0.000017174 0.000017174 0.000244135

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

Cartesian Forces: Max 0.003091863 RMS 0.000664980

Leave Link 716 at Fri Jul 26 14:20:10 2019, MaxMem= 1342177280 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001575885 RMS 0.000444701

Search for a local minimum.

Step number 10 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .44470D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 2 3 4 5

7 9 8 10

ITU= 0 -1 0 0 -1 1 0 -1 -1 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.00410 0.00534 0.00534 0.00534 0.00534

Eigenvalues --- 0.00534 0.00534 0.00535 0.01169 0.01259

Eigenvalues --- 0.01259 0.01453 0.01453 0.01616 0.01647

Eigenvalues --- 0.01675 0.01756 0.01756 0.01791 0.01806

Eigenvalues --- 0.01806 0.01825 0.01832 0.01860 0.01860

Eigenvalues --- 0.01868 0.01868 0.01868 0.01870 0.01909

Eigenvalues --- 0.01921 0.01930 0.01930 0.01934 0.01936

Eigenvalues --- 0.01965 0.01965 0.02180 0.02182 0.02187

Eigenvalues --- 0.02187 0.02533 0.03315 0.03664 0.04654

Eigenvalues --- 0.04654 0.04654 0.04654 0.04654 0.04654

Eigenvalues --- 0.04655 0.06002 0.13847 0.15018 0.15018

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16301 0.19631 0.22826

Eigenvalues --- 0.22865 0.22869 0.22869 0.24750 0.24756

Eigenvalues --- 0.24756 0.24802 0.24841 0.24975 0.24975

Eigenvalues --- 0.24997 0.24998 0.24998 0.24998 0.24999

Eigenvalues --- 0.26776 0.35043 0.35043 0.35181 0.35467

Eigenvalues --- 0.35503 0.36024 0.36034 0.36034 0.36034

Eigenvalues --- 0.36034 0.36034 0.36034 0.36034 0.36770

Eigenvalues --- 0.36861 0.36861 0.37559 0.37563 0.37563

Eigenvalues --- 0.37563 0.38976 0.38976 0.39538 0.39698

Eigenvalues --- 0.41397 0.41397 0.41397 0.41512 0.41512

Eigenvalues --- 0.41617 0.41791 0.42515 0.43516 0.43781

Eigenvalues --- 0.43781 0.47074 0.47901 0.49086 0.49086

Eigenvalues --- 0.50131 0.51398 0.51901 0.51901 0.70435

Eigenvalues --- 1.01729 1.01831 1.01831 1.01831

RFO step: Lambda=-2.39153578D-04 EMin= 4.09536874D-03

Quartic linear search produced a step of 0.22856.

Maximum step size ( 0.050) exceeded in Quadratic search.

-- Step size scaled by 0.845

Iteration 1 RMS(Cart)= 0.00691120 RMS(Int)= 0.00006046

Iteration 2 RMS(Cart)= 0.00008118 RMS(Int)= 0.00002799

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002799

ITry= 1 IFail=0 DXMaxC= 4.69D-02 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 7.04D-03 for atom 44.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73250 0.00055 -0.00012 0.00040 0.00027 2.73277

R2 2.57592 -0.00091 0.00012 -0.00042 -0.00034 2.57558

R3 2.04003 0.00015 0.00003 -0.00001 0.00001 2.04005

R4 2.58559 -0.00158 0.00017 -0.00073 -0.00054 2.58506

R5 2.67710 -0.00095 0.00014 -0.00058 -0.00016 2.67694

R6 2.58559 -0.00158 0.00017 -0.00073 -0.00054 2.58506

R7 3.95292 -0.00111 -0.00048 -0.00404 -0.00391 3.94901

R8 2.73250 0.00055 -0.00012 0.00040 0.00027 2.73277

R9 2.67710 -0.00095 0.00014 -0.00058 -0.00016 2.67694

R10 2.04003 0.00015 0.00003 -0.00001 0.00001 2.04005

R11 2.67710 -0.00095 0.00014 -0.00058 -0.00016 2.67694

R12 2.69376 0.00074 -0.00002 0.00039 -0.00038 2.69338

R13 2.58559 -0.00158 0.00017 -0.00073 -0.00054 2.58506

R14 2.73250 0.00055 -0.00012 0.00041 0.00027 2.73277

R15 2.58559 -0.00158 0.00017 -0.00073 -0.00054 2.58506

R16 3.95292 -0.00111 -0.00048 -0.00404 -0.00391 3.94901

R17 2.73250 0.00055 -0.00012 0.00040 0.00027 2.73277

R18 2.67710 -0.00095 0.00014 -0.00058 -0.00016 2.67694

R19 2.57592 -0.00091 0.00012 -0.00042 -0.00034 2.57558

R20 2.04003 0.00015 0.00003 -0.00001 0.00001 2.04005

R21 2.04003 0.00015 0.00003 0.00000 0.00001 2.04005

R22 2.67710 -0.00095 0.00014 -0.00058 -0.00016 2.67694

R23 2.69376 0.00074 -0.00002 0.00039 -0.00038 2.69338

R24 2.73250 0.00055 -0.00012 0.00041 0.00027 2.73277

R25 2.58559 -0.00158 0.00017 -0.00073 -0.00054 2.58506

R26 2.57592 -0.00091 0.00012 -0.00042 -0.00034 2.57558

R27 2.04003 0.00015 0.00003 0.00000 0.00001 2.04005

R28 2.73250 0.00055 -0.00012 0.00040 0.00027 2.73277

R29 2.04003 0.00015 0.00003 -0.00001 0.00001 2.04005

R30 2.58559 -0.00158 0.00017 -0.00073 -0.00054 2.58506

R31 2.67710 -0.00095 0.00014 -0.00058 -0.00016 2.67694

R32 3.95292 -0.00111 -0.00048 -0.00404 -0.00391 3.94901

R33 2.67710 -0.00095 0.00014 -0.00058 -0.00016 2.67694

R34 2.69376 0.00074 -0.00002 0.00039 -0.00038 2.69338

R35 2.73250 0.00055 -0.00012 0.00041 0.00027 2.73277

R36 2.58559 -0.00158 0.00017 -0.00073 -0.00054 2.58506

R37 2.57592 -0.00091 0.00012 -0.00042 -0.00034 2.57558

R38 2.04003 0.00015 0.00003 0.00000 0.00001 2.04005

R39 2.73250 0.00055 -0.00012 0.00041 0.00027 2.73277

R40 2.04003 0.00015 0.00003 0.00000 0.00001 2.04005

R41 2.58559 -0.00158 0.00017 -0.00073 -0.00054 2.58506

R42 2.67710 -0.00095 0.00014 -0.00058 -0.00016 2.67694

R43 3.95292 -0.00111 -0.00048 -0.00404 -0.00391 3.94901

R44 2.69376 0.00074 -0.00002 0.00039 -0.00038 2.69338

R45 2.27875 -0.00004 -0.00002 0.00003 0.00001 2.27875

R46 2.27875 -0.00004 -0.00002 0.00003 0.00001 2.27875

R47 2.01690 0.00001 0.00001 -0.00011 -0.00011 2.01679

R48 2.01690 0.00001 0.00001 -0.00011 -0.00011 2.01679

R49 2.27875 -0.00004 -0.00002 0.00003 0.00001 2.27875

R50 2.01690 0.00001 0.00001 -0.00011 -0.00011 2.01679

R51 2.27875 -0.00004 -0.00002 0.00003 0.00001 2.27875

R52 2.01690 0.00001 0.00001 -0.00011 -0.00011 2.01679

A1 1.86676 -0.00038 0.00009 -0.00026 -0.00018 1.86658

A2 2.18811 0.00044 -0.00022 0.00056 0.00034 2.18845

A3 2.22831 -0.00005 0.00013 -0.00029 -0.00016 2.22815

A4 1.90763 0.00040 -0.00017 0.00040 0.00027 1.90790

A5 2.18313 0.00000 0.00011 0.00000 0.00014 2.18327

A6 2.19230 -0.00041 0.00008 -0.00046 -0.00046 2.19183

A7 1.87596 -0.00004 0.00016 -0.00024 -0.00016 1.87580

A8 2.20246 0.00002 0.00002 0.00056 0.00054 2.20300

A9 2.20246 0.00002 0.00002 0.00056 0.00054 2.20300

A10 1.90763 0.00040 -0.00017 0.00040 0.00027 1.90790

A11 2.19230 -0.00041 0.00008 -0.00046 -0.00046 2.19183

A12 2.18313 0.00000 0.00011 0.00000 0.00014 2.18327

A13 1.86676 -0.00038 0.00009 -0.00026 -0.00018 1.86658

A14 2.22831 -0.00005 0.00013 -0.00029 -0.00016 2.22815

A15 2.18811 0.00044 -0.00022 0.00056 0.00034 2.18845

A16 2.20439 0.00076 0.00000 0.00072 0.00080 2.20520

A17 2.03935 -0.00038 0.00002 -0.00036 -0.00042 2.03894

A18 2.03935 -0.00038 0.00002 -0.00041 -0.00042 2.03894

A19 2.19230 -0.00041 0.00008 -0.00046 -0.00046 2.19183

A20 2.18313 0.00000 0.00011 -0.00001 0.00014 2.18327

A21 1.90763 0.00040 -0.00017 0.00040 0.00027 1.90790

A22 1.87596 -0.00004 0.00016 -0.00024 -0.00016 1.87580

A23 2.20246 0.00002 0.00002 0.00055 0.00054 2.20300

A24 2.20246 0.00002 0.00002 0.00056 0.00054 2.20300

A25 1.90763 0.00040 -0.00017 0.00040 0.00027 1.90790

A26 2.19230 -0.00041 0.00008 -0.00046 -0.00046 2.19183

A27 2.18313 0.00000 0.00011 0.00000 0.00014 2.18327

A28 1.86676 -0.00038 0.00009 -0.00026 -0.00018 1.86658

A29 2.18811 0.00044 -0.00022 0.00055 0.00034 2.18845

A30 2.22831 -0.00005 0.00013 -0.00030 -0.00016 2.22815

A31 1.86676 -0.00038 0.00009 -0.00026 -0.00018 1.86658

A32 2.18811 0.00044 -0.00022 0.00057 0.00034 2.18845

A33 2.22831 -0.00005 0.00013 -0.00030 -0.00016 2.22815

A34 2.20439 0.00076 0.00000 0.00072 0.00080 2.20520

A35 2.03935 -0.00038 0.00002 -0.00036 -0.00042 2.03894

A36 2.03935 -0.00038 0.00002 -0.00041 -0.00042 2.03894

A37 2.18313 0.00000 0.00011 -0.00001 0.00014 2.18327

A38 2.19230 -0.00041 0.00008 -0.00046 -0.00046 2.19183

A39 1.90763 0.00040 -0.00017 0.00040 0.00027 1.90790

A40 1.86676 -0.00038 0.00009 -0.00026 -0.00018 1.86658

A41 2.18811 0.00044 -0.00022 0.00057 0.00034 2.18845

A42 2.22831 -0.00005 0.00013 -0.00030 -0.00016 2.22815

A43 1.86676 -0.00038 0.00009 -0.00026 -0.00018 1.86658

A44 2.22831 -0.00005 0.00013 -0.00030 -0.00016 2.22815

A45 2.18811 0.00044 -0.00022 0.00055 0.00034 2.18845

A46 1.90763 0.00040 -0.00017 0.00040 0.00027 1.90790

A47 2.18313 0.00000 0.00011 0.00000 0.00014 2.18327

A48 2.19230 -0.00041 0.00008 -0.00046 -0.00046 2.19183

A49 1.87596 -0.00004 0.00016 -0.00024 -0.00016 1.87580

A50 2.20246 0.00002 0.00002 0.00055 0.00054 2.20300

A51 2.20246 0.00002 0.00002 0.00056 0.00054 2.20300

A52 2.20439 0.00076 0.00000 0.00072 0.00080 2.20520

A53 2.03935 -0.00038 0.00002 -0.00036 -0.00042 2.03894

A54 2.03935 -0.00038 0.00002 -0.00041 -0.00042 2.03894

A55 2.18313 0.00000 0.00011 -0.00001 0.00014 2.18327

A56 2.19230 -0.00041 0.00008 -0.00046 -0.00046 2.19183

A57 1.90763 0.00040 -0.00017 0.00040 0.00027 1.90790

A58 1.86676 -0.00038 0.00009 -0.00026 -0.00018 1.86658

A59 2.18811 0.00044 -0.00022 0.00056 0.00034 2.18845

A60 2.22831 -0.00005 0.00013 -0.00030 -0.00016 2.22815

A61 1.86676 -0.00038 0.00009 -0.00026 -0.00018 1.86658

A62 2.22831 -0.00005 0.00013 -0.00030 -0.00016 2.22815

A63 2.18811 0.00044 -0.00022 0.00056 0.00034 2.18845

A64 1.90763 0.00040 -0.00017 0.00040 0.00027 1.90790

A65 2.18313 0.00000 0.00011 -0.00001 0.00014 2.18327

A66 2.19230 -0.00041 0.00008 -0.00046 -0.00046 2.19183

A67 1.87596 -0.00004 0.00016 -0.00024 -0.00016 1.87580

A68 2.20246 0.00002 0.00002 0.00056 0.00054 2.20300

A69 2.20246 0.00002 0.00002 0.00056 0.00054 2.20300

A70 1.56167 0.00006 0.00049 0.00171 0.00205 1.56371

A71 1.56167 0.00006 0.00049 0.00171 0.00205 1.56371

A72 2.95020 0.00066 0.00485 0.01801 0.02287 2.97307

A73 2.95020 0.00066 0.00485 0.01801 0.02287 2.97307

A74 1.56167 0.00006 0.00049 0.00171 0.00205 1.56371

A75 1.56167 0.00006 0.00049 0.00171 0.00205 1.56371

A76 2.20439 0.00076 0.00000 0.00072 0.00080 2.20520

A77 2.03935 -0.00038 0.00002 -0.00036 -0.00042 2.03894

A78 2.03935 -0.00038 0.00002 -0.00041 -0.00042 2.03894

A79 3.14148 0.00001 0.00001 0.00044 0.00009 3.14157

A80 3.14148 0.00001 0.00001 0.00044 0.00009 3.14157

A81 3.14153 0.00001 -0.00004 0.00301 0.00016 3.14169

A82 3.14153 0.00001 -0.00004 0.00301 0.00016 3.14169

A83 3.14148 0.00001 0.00001 0.00044 0.00009 3.14157

A84 3.14153 0.00001 -0.00004 0.00301 0.00016 3.14169

A85 3.14148 0.00001 0.00001 0.00044 0.00009 3.14157

A86 3.14153 0.00001 -0.00004 0.00301 0.00016 3.14169

A87 3.13169 0.00062 -0.00018 0.00835 0.00819 3.13989

A88 3.15149 -0.00062 0.00018 -0.00835 -0.00819 3.14330

A89 3.13668 0.00043 -0.00323 0.01848 0.01527 3.15195

A90 3.14651 -0.00043 0.00323 -0.01848 -0.01527 3.13124

A91 3.13169 0.00062 -0.00018 0.00835 0.00819 3.13989

A92 3.13668 0.00043 -0.00323 0.01848 0.01527 3.15195

A93 3.15149 -0.00062 0.00018 -0.00835 -0.00819 3.14330

A94 3.14651 -0.00043 0.00323 -0.01848 -0.01527 3.13124

D1 -0.00477 0.00013 -0.00085 0.00246 0.00161 -0.00316

D2 3.12024 0.00014 0.00026 -0.00175 -0.00149 3.11875

D3 3.13911 0.00012 -0.00115 0.00205 0.00090 3.14001

D4 -0.01907 0.00013 -0.00004 -0.00216 -0.00220 -0.02127

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13923 -0.00001 -0.00031 -0.00042 -0.00073 -3.13997

D7 3.13923 0.00001 0.00031 0.00042 0.00073 3.13997

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00771 -0.00021 0.00137 -0.00397 -0.00260 0.00511

D10 -3.06430 -0.00016 -0.00133 -0.01704 -0.01839 -3.08269

D11 -3.11719 -0.00022 0.00025 0.00026 0.00051 -3.11668

D12 0.09399 -0.00017 -0.00245 -0.01281 -0.01528 0.07871

D13 -3.11382 -0.00010 -0.00222 0.00676 0.00454 -3.10928

D14 0.01312 -0.00003 -0.00002 0.00202 0.00197 0.01510

D15 0.00852 -0.00008 -0.00093 0.00188 0.00095 0.00947

D16 3.13546 -0.00001 0.00127 -0.00286 -0.00161 3.13385

D17 -0.00771 0.00021 -0.00137 0.00397 0.00260 -0.00511

D18 3.11719 0.00022 -0.00025 -0.00026 -0.00051 3.11668

D19 3.06430 0.00016 0.00133 0.01704 0.01839 3.08269

D20 -0.09399 0.00017 0.00245 0.01281 0.01528 -0.07871

D21 -3.08746 -0.00036 -0.00078 -0.00117 -0.00198 -3.08944

D22 -0.13639 0.00029 0.00399 0.01659 0.02062 -0.11577

D23 -1.61193 -0.00003 0.00160 0.00771 0.00932 -1.60260

D24 0.13639 -0.00029 -0.00399 -0.01659 -0.02062 0.11577

D25 3.08746 0.00036 0.00078 0.00117 0.00198 3.08944

D26 1.61193 0.00003 -0.00160 -0.00771 -0.00932 1.60260

D27 0.00477 -0.00013 0.00085 -0.00246 -0.00161 0.00316

D28 -3.13911 -0.00012 0.00115 -0.00205 -0.00090 -3.14001

D29 -3.12024 -0.00014 -0.00026 0.00175 0.00149 -3.11875

D30 0.01907 -0.00013 0.00004 0.00216 0.00220 0.02127

D31 -0.00852 0.00008 0.00093 -0.00188 -0.00095 -0.00947

D32 -3.13546 0.00001 -0.00127 0.00286 0.00161 -3.13385

D33 3.11382 0.00010 0.00222 -0.00676 -0.00454 3.10928

D34 -0.01312 0.00003 0.00002 -0.00202 -0.00197 -0.01510

D35 0.00852 -0.00008 -0.00093 0.00188 0.00095 0.00947

D36 -3.11382 -0.00010 -0.00222 0.00676 0.00454 -3.10928

D37 3.13546 -0.00001 0.00127 -0.00286 -0.00161 3.13385

D38 0.01312 -0.00003 -0.00002 0.00202 0.00197 0.01510

D39 -3.11719 -0.00022 0.00025 0.00026 0.00051 -3.11668

D40 0.09399 -0.00017 -0.00245 -0.01281 -0.01528 0.07871

D41 0.00771 -0.00021 0.00137 -0.00397 -0.00260 0.00511

D42 -3.06430 -0.00016 -0.00133 -0.01704 -0.01839 -3.08269

D43 3.12024 0.00014 0.00026 -0.00175 -0.00149 3.11875

D44 -0.01907 0.00013 -0.00004 -0.00216 -0.00220 -0.02127

D45 -0.00477 0.00013 -0.00085 0.00246 0.00161 -0.00316

D46 3.13911 0.00012 -0.00115 0.00205 0.00090 3.14001

D47 -0.00771 0.00021 -0.00137 0.00397 0.00260 -0.00511

D48 3.11719 0.00022 -0.00025 -0.00026 -0.00051 3.11668

D49 3.06430 0.00016 0.00133 0.01704 0.01839 3.08269

D50 -0.09399 0.00017 0.00245 0.01281 0.01528 -0.07871

D51 -0.13639 0.00029 0.00399 0.01659 0.02062 -0.11577

D52 -1.61193 -0.00003 0.00160 0.00771 0.00932 -1.60260

D53 -3.08746 -0.00036 -0.00078 -0.00117 -0.00198 -3.08944

D54 3.08746 0.00036 0.00078 0.00117 0.00198 3.08944

D55 1.61193 0.00003 -0.00160 -0.00771 -0.00932 1.60260

D56 0.13639 -0.00029 -0.00399 -0.01659 -0.02062 0.11577

D57 0.00477 -0.00013 0.00085 -0.00246 -0.00161 0.00316

D58 -3.13911 -0.00012 0.00115 -0.00205 -0.00090 -3.14001

D59 -3.12024 -0.00014 -0.00026 0.00175 0.00149 -3.11875

D60 0.01907 -0.00013 0.00004 0.00216 0.00220 0.02127

D61 -0.00852 0.00008 0.00093 -0.00188 -0.00095 -0.00947

D62 -3.13546 0.00001 -0.00127 0.00286 0.00161 -3.13385

D63 3.11382 0.00010 0.00222 -0.00676 -0.00454 3.10928

D64 -0.01312 0.00003 0.00002 -0.00202 -0.00197 -0.01510

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13923 0.00001 0.00031 0.00042 0.00073 3.13997

D67 -3.13923 -0.00001 -0.00031 -0.00042 -0.00073 -3.13997

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.11382 0.00010 0.00222 -0.00676 -0.00454 3.10928

D70 -0.00852 0.00008 0.00093 -0.00188 -0.00095 -0.00947

D71 -0.01312 0.00003 0.00002 -0.00202 -0.00197 -0.01510

D72 -3.13546 0.00001 -0.00127 0.00286 0.00161 -3.13385

D73 -3.12024 -0.00014 -0.00026 0.00175 0.00149 -3.11875

D74 0.01907 -0.00013 0.00004 0.00216 0.00220 0.02127

D75 0.00477 -0.00013 0.00085 -0.00246 -0.00161 0.00316

D76 -3.13911 -0.00012 0.00115 -0.00205 -0.00090 -3.14001

D77 3.11719 0.00022 -0.00025 -0.00026 -0.00051 3.11668

D78 -0.09399 0.00017 0.00245 0.01281 0.01528 -0.07871

D79 -0.00771 0.00021 -0.00137 0.00397 0.00260 -0.00511

D80 3.06430 0.00016 0.00133 0.01704 0.01839 3.08269

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 3.13923 0.00001 0.00031 0.00042 0.00073 3.13997

D83 -3.13923 -0.00001 -0.00031 -0.00042 -0.00073 -3.13997

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 -0.00477 0.00013 -0.00085 0.00246 0.00161 -0.00316

D86 3.12024 0.00014 0.00026 -0.00175 -0.00149 3.11875

D87 3.13911 0.00012 -0.00115 0.00205 0.00090 3.14001

D88 -0.01907 0.00013 -0.00004 -0.00216 -0.00220 -0.02127

D89 0.00771 -0.00021 0.00137 -0.00397 -0.00260 0.00511

D90 -3.06430 -0.00016 -0.00133 -0.01704 -0.01839 -3.08269

D91 -3.11719 -0.00022 0.00025 0.00026 0.00051 -3.11668

D92 0.09399 -0.00017 -0.00245 -0.01281 -0.01528 0.07871

D93 -3.11382 -0.00010 -0.00222 0.00676 0.00454 -3.10928

D94 0.01312 -0.00003 -0.00002 0.00202 0.00197 0.01510

D95 0.00852 -0.00008 -0.00093 0.00188 0.00095 0.00947

D96 3.13546 -0.00001 0.00127 -0.00286 -0.00161 3.13385

D97 0.13639 -0.00029 -0.00399 -0.01659 -0.02062 0.11577

D98 1.61193 0.00003 -0.00160 -0.00771 -0.00932 1.60260

D99 3.08746 0.00036 0.00078 0.00117 0.00198 3.08944

D100 -3.08746 -0.00036 -0.00078 -0.00117 -0.00198 -3.08944

D101 -1.61193 -0.00003 0.00160 0.00771 0.00932 -1.60260

D102 -0.13639 0.00029 0.00399 0.01659 0.02062 -0.11577

D103 3.11382 0.00010 0.00222 -0.00676 -0.00454 3.10928

D104 -0.00852 0.00008 0.00093 -0.00188 -0.00095 -0.00947

D105 -0.01312 0.00003 0.00002 -0.00202 -0.00197 -0.01510

D106 -3.13546 0.00001 -0.00127 0.00286 0.00161 -3.13385

D107 -3.12024 -0.00014 -0.00026 0.00175 0.00149 -3.11875

D108 0.01907 -0.00013 0.00004 0.00216 0.00220 0.02127

D109 0.00477 -0.00013 0.00085 -0.00246 -0.00161 0.00316

D110 -3.13911 -0.00012 0.00115 -0.00205 -0.00090 -3.14001

D111 3.11719 0.00022 -0.00025 -0.00026 -0.00051 3.11668

D112 -0.09399 0.00017 0.00245 0.01281 0.01528 -0.07871

D113 -0.00771 0.00021 -0.00137 0.00397 0.00260 -0.00511

D114 3.06430 0.00016 0.00133 0.01704 0.01839 3.08269

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.13923 0.00001 0.00031 0.00042 0.00073 3.13997

D117 -3.13923 -0.00001 -0.00031 -0.00042 -0.00073 -3.13997

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 -0.00477 0.00013 -0.00085 0.00246 0.00161 -0.00316

D120 3.12024 0.00014 0.00026 -0.00175 -0.00149 3.11875

D121 3.13911 0.00012 -0.00115 0.00205 0.00090 3.14001

D122 -0.01907 0.00013 -0.00004 -0.00216 -0.00220 -0.02127

D123 0.00771 -0.00021 0.00137 -0.00397 -0.00260 0.00511

D124 -3.06430 -0.00016 -0.00133 -0.01704 -0.01839 -3.08269

D125 -3.11719 -0.00022 0.00025 0.00026 0.00051 -3.11668

D126 0.09399 -0.00017 -0.00245 -0.01281 -0.01528 0.07871

D127 -3.11382 -0.00010 -0.00222 0.00676 0.00454 -3.10928

D128 0.01312 -0.00003 -0.00002 0.00202 0.00197 0.01510

D129 0.00852 -0.00008 -0.00093 0.00188 0.00095 0.00947

D130 3.13546 -0.00001 0.00127 -0.00286 -0.00161 3.13385

D131 1.61193 0.00003 -0.00160 -0.00771 -0.00932 1.60260

D132 3.08746 0.00036 0.00078 0.00117 0.00198 3.08944

D133 0.13639 -0.00029 -0.00399 -0.01659 -0.02062 0.11577

D134 -1.61193 -0.00003 0.00160 0.00771 0.00932 -1.60260

D135 -0.13639 0.00029 0.00399 0.01659 0.02062 -0.11577

D136 -3.08746 -0.00036 -0.00078 -0.00117 -0.00198 -3.08944

Item Value Threshold Converged?

Maximum Force 0.001576 0.000450 NO

RMS Force 0.000445 0.000300 NO

Maximum Displacement 0.046845 0.001800 NO

RMS Displacement 0.006858 0.001200 NO

Predicted change in Energy=-1.220578D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:20:10 2019, MaxMem= 1342177280 cpu: 1.1

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.681470 4.273185 -0.040613

2 6 0 1.103005 2.890753 0.008941

3 7 0 0.000000 2.082310 0.042003

4 6 0 -1.103005 2.890753 0.008941

5 6 0 -0.681470 4.273185 -0.040613

6 6 0 -2.448850 2.448850 -0.001713

7 6 0 -2.890753 1.103005 0.008941

8 7 0 -2.082310 0.000000 0.042003

9 6 0 -2.890753 -1.103005 0.008941

10 6 0 -4.273185 -0.681470 -0.040613

11 6 0 -4.273185 0.681470 -0.040613

12 6 0 2.448850 2.448850 -0.001713

13 6 0 2.890753 1.103005 0.008941

14 6 0 4.273185 0.681470 -0.040613

15 6 0 4.273185 -0.681470 -0.040613

16 6 0 2.890753 -1.103005 0.008941

17 7 0 2.082310 0.000000 0.042003

18 6 0 2.448850 -2.448850 -0.001713

19 6 0 1.103005 -2.890753 0.008941

20 6 0 0.681470 -4.273185 -0.040613

21 6 0 -0.681470 -4.273185 -0.040613

22 6 0 -1.103005 -2.890753 0.008941

23 7 0 0.000000 -2.082310 0.042003

24 1 0 1.341100 5.127168 -0.072615

25 1 0 -1.341100 5.127168 -0.072615

26 1 0 -5.127168 -1.341100 -0.072615

27 1 0 -5.127168 1.341100 -0.072615

28 1 0 5.127168 1.341100 -0.072615

29 1 0 5.127168 -1.341100 -0.072615

30 1 0 1.341100 -5.127168 -0.072615

31 1 0 -1.341100 -5.127168 -0.072615

32 30 0 0.000000 0.000000 0.217876

33 6 0 -2.448850 -2.448850 -0.001713

34 6 0 -3.456156 -3.456156 -0.047351

35 6 0 3.456156 3.456156 -0.047351

36 6 0 -4.308346 -4.308346 -0.088008

37 6 0 4.308346 4.308346 -0.088008

38 6 0 -3.456156 3.456156 -0.047351

39 6 0 -4.308346 4.308346 -0.088008

40 6 0 3.456156 -3.456156 -0.047351

41 6 0 4.308346 -4.308346 -0.088008

42 1 0 5.062769 -5.062769 -0.114384

43 1 0 -5.062769 -5.062769 -0.114384

44 1 0 -5.062769 5.062769 -0.114384

45 1 0 5.062769 5.062769 -0.114384

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.446121 0.000000

3 N 2.295901 1.367952 0.000000

4 C 2.257858 2.206010 1.367952 0.000000

5 C 1.362940 2.257858 2.295901 1.446121 0.000000

6 C 3.623343 3.579255 2.476516 1.416577 2.540343

7 C 4.776325 4.375631 3.052308 2.528258 3.864380

8 N 5.089736 4.301602 2.944831 3.052308 4.497698

9 C 6.454971 5.648027 4.301602 4.375631 5.812642

10 C 7.006941 6.454971 5.089736 4.776325 6.119561

11 C 6.119561 5.812642 4.497698 3.864380 5.079452

12 C 2.540343 1.416577 2.476516 3.579255 3.623343

13 C 3.864380 2.528258 3.052308 4.375631 4.776325

14 C 5.079452 3.864380 4.497698 5.812642 6.119561

15 C 6.119561 4.776325 5.089736 6.454971 7.006941

16 C 5.812642 4.375631 4.301602 5.648027 6.454971

17 N 4.497698 3.052308 2.944831 4.301602 5.089736

18 C 6.950605 5.506612 5.150747 6.413046 7.415267

19 C 7.176501 5.781507 5.094023 6.188077 7.383009

20 C 8.546370 7.176501 6.392460 7.383009 8.654366

21 C 8.654366 7.383009 6.392460 7.176501 8.546370

22 C 7.383009 6.188077 5.094023 5.781507 7.176501

23 N 6.392460 5.094023 4.164620 5.094023 6.392460

24 H 1.079547 2.250531 3.329091 3.313887 2.195700

25 H 2.195700 3.313887 3.329091 2.250531 1.079547

26 H 8.078458 7.531951 6.166094 5.840301 7.161386

27 H 6.506798 6.420524 5.181735 4.312999 5.325634

28 H 5.325634 4.312999 5.181735 6.420524 6.506798

29 H 7.161386 5.840301 6.166094 7.531951 8.078458

30 H 9.423522 8.021870 7.334047 8.382563 9.615531

31 H 9.615531 8.382563 7.334047 8.021870 9.423522

32 Zn 4.334897 3.101085 2.089724 3.101085 4.334897

33 C 7.415267 6.413046 5.150747 5.506612 6.950605

34 C 8.767138 7.814882 6.528982 6.769324 8.212286

35 C 2.892484 2.420779 3.720276 4.594431 4.217527

36 C 9.926892 9.006616 7.708386 7.881030 9.316606

37 C 3.627356 3.506163 4.851183 5.594790 4.990164

38 C 4.217527 4.594431 3.720276 2.420779 2.892484

39 C 4.990164 5.594790 4.851183 3.506163 3.627356

40 C 8.212286 6.769324 6.528982 7.814882 8.767138

41 C 9.316606 7.881030 7.708386 9.006616 9.926892

42 H 10.313159 8.885575 8.758323 10.064317 10.961832

43 H 10.961832 10.064317 8.758323 8.885575 10.313159

44 H 5.798721 6.538320 5.877008 4.518029 4.452490

45 H 4.452490 4.518029 5.877008 6.538320 5.798721

6 7 8 9 10

6 C 0.000000

7 C 1.416577 0.000000

8 N 2.476516 1.367952 0.000000

9 C 3.579255 2.206010 1.367952 0.000000

10 C 3.623343 2.257858 2.295901 1.446121 0.000000

11 C 2.540343 1.446121 2.295901 2.257858 1.362940

12 C 4.897700 5.506612 5.150747 6.413046 7.415267

13 C 5.506612 5.781507 5.094023 6.188077 7.383009

14 C 6.950605 7.176501 6.392460 7.383009 8.654366

15 C 7.415267 7.383009 6.392460 7.176501 8.546370

16 C 6.413046 6.188077 5.094023 5.781507 7.176501

17 N 5.150747 5.094023 4.164620 5.094023 6.392460

18 C 6.926394 6.413046 5.150747 5.506612 6.950605

19 C 6.413046 5.648027 4.301602 4.375631 5.812642

20 C 7.415267 6.454971 5.089736 4.776325 6.119561

21 C 6.950605 5.812642 4.497698 3.864380 5.079452

22 C 5.506612 4.375631 3.052308 2.528258 3.864380

23 N 5.150747 4.301602 2.944831 3.052308 4.497698

24 H 4.641350 5.840301 6.166094 7.531951 8.078458

25 H 2.899228 4.312999 5.181735 6.420524 6.506798

26 H 4.641350 3.313887 3.329091 2.250531 1.079547

27 H 2.899228 2.250531 3.329091 3.313887 2.195700

28 H 7.656904 8.021870 7.334047 8.382563 9.615531

29 H 8.471410 8.382563 7.334047 8.021870 9.423522

30 H 8.471410 7.531951 6.166094 5.840301 7.161386

31 H 7.656904 6.420524 5.181735 4.312999 5.325634

32 Zn 3.470152 3.101085 2.089724 3.101085 4.334897

33 C 4.897700 3.579255 2.476516 1.416577 2.540343

34 C 5.990480 4.594431 3.720276 2.420779 2.892484

35 C 5.990480 6.769324 6.528982 7.814882 8.767138

36 C 7.008913 5.594790 4.851183 3.506163 3.627356

37 C 7.008913 7.881030 7.708386 9.006616 9.926892

38 C 1.425276 2.420779 3.720276 4.594431 4.217527

39 C 2.631139 3.506163 4.851183 5.594790 4.990164

40 C 8.351065 7.814882 6.528982 6.769324 8.212286

41 C 9.556508 9.006616 7.708386 7.881030 9.316606

42 H 10.623631 10.064317 8.758323 8.885575 10.313159

43 H 7.954224 6.538320 5.877008 4.518029 4.452490

44 H 3.698356 4.518029 5.877008 6.538320 5.798721

45 H 7.954224 8.885575 8.758323 10.064317 10.961832

11 12 13 14 15

11 C 0.000000

12 C 6.950605 0.000000

13 C 7.176501 1.416577 0.000000

14 C 8.546370 2.540343 1.446121 0.000000

15 C 8.654366 3.623343 2.257858 1.362940 0.000000

16 C 7.383009 3.579255 2.206010 2.257858 1.446121

17 N 6.392460 2.476516 1.367952 2.295901 2.295901

18 C 7.415267 4.897700 3.579255 3.623343 2.540343

19 C 6.454971 5.506612 4.375631 4.776325 3.864380

20 C 7.006941 6.950605 5.812642 6.119561 5.079452

21 C 6.119561 7.415267 6.454971 7.006941 6.119561

22 C 4.776325 6.413046 5.648027 6.454971 5.812642

23 N 5.089736 5.150747 4.301602 5.089736 4.497698

24 H 7.161386 2.899228 4.312999 5.325634 6.506798

25 H 5.325634 4.641350 5.840301 7.161386 8.078458

26 H 2.195700 8.471410 8.382563 9.615531 9.423522

27 H 1.079547 7.656904 8.021870 9.423522 9.615531

28 H 9.423522 2.899228 2.250531 1.079547 2.195700

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31 H 6.506798 8.471410 7.531951 8.078458 7.161386

32 Zn 4.334897 3.470152 3.101085 4.334897 4.334897

33 C 3.623343 6.926394 6.413046 7.415267 6.950605

34 C 4.217527 8.351065 7.814882 8.767138 8.212286

35 C 8.212286 1.425276 2.420779 2.892484 4.217527

36 C 4.990164 9.556508 9.006616 9.926892 9.316606

37 C 9.316606 2.631139 3.506163 3.627356 4.990164

38 C 2.892484 5.990480 6.769324 8.212286 8.767138

39 C 3.627356 7.008913 7.881030 9.316606 9.926892

40 C 8.767138 5.990480 4.594431 4.217527 2.892484

41 C 9.926892 7.008913 5.594790 4.990164 3.627356

42 H 10.961832 7.954224 6.538320 5.798721 4.452490

43 H 5.798721 10.623631 10.064317 10.961832 10.313159

44 H 4.452490 7.954224 8.885575 10.313159 10.961832

45 H 10.313159 3.698356 4.518029 4.452490 5.798721

16 17 18 19 20

16 C 0.000000

17 N 1.367952 0.000000

18 C 1.416577 2.476516 0.000000

19 C 2.528258 3.052308 1.416577 0.000000

20 C 3.864380 4.497698 2.540343 1.446121 0.000000

21 C 4.776325 5.089736 3.623343 2.257858 1.362940

22 C 4.375631 4.301602 3.579255 2.206010 2.257858

23 N 3.052308 2.944831 2.476516 1.367952 2.295901

24 H 6.420524 5.181735 7.656904 8.021870 9.423522

25 H 7.531951 6.166094 8.471410 8.382563 9.615531

26 H 8.021870 7.334047 7.656904 6.420524 6.506798

27 H 8.382563 7.334047 8.471410 7.531951 8.078458

28 H 3.313887 3.329091 4.641350 5.840301 7.161386

29 H 2.250531 3.329091 2.899228 4.312999 5.325634

30 H 4.312999 5.181735 2.899228 2.250531 1.079547

31 H 5.840301 6.166094 4.641350 3.313887 2.195700

32 Zn 3.101085 2.089724 3.470152 3.101085 4.334897

33 C 5.506612 5.150747 4.897700 3.579255 3.623343

34 C 6.769324 6.528982 5.990480 4.594431 4.217527

35 C 4.594431 3.720276 5.990480 6.769324 8.212286

36 C 7.881030 7.708386 7.008913 5.594790 4.990164

37 C 5.594790 4.851183 7.008913 7.881030 9.316606

38 C 7.814882 6.528982 8.351065 7.814882 8.767138

39 C 9.006616 7.708386 9.556508 9.006616 9.926892

40 C 2.420779 3.720276 1.425276 2.420779 2.892484

41 C 3.506163 4.851183 2.631139 3.506163 3.627356

42 H 4.518029 5.877008 3.698356 4.518029 4.452490

43 H 8.885575 8.758323 7.954224 6.538320 5.798721

44 H 10.064317 8.758323 10.623631 10.064317 10.961832

45 H 6.538320 5.877008 7.954224 8.885575 10.313159

21 22 23 24 25

21 C 0.000000

22 C 1.446121 0.000000

23 N 2.295901 1.367952 0.000000

24 H 9.615531 8.382563 7.334047 0.000000

25 H 9.423522 8.021870 7.334047 2.682200 0.000000

26 H 5.325634 4.312999 5.181735 9.147511 7.494851

27 H 7.161386 5.840301 6.166094 7.494851 5.354308

28 H 8.078458 7.531951 6.166094 5.354308 7.494851

29 H 6.506798 6.420524 5.181735 7.494851 9.147511

30 H 2.195700 3.313887 3.329091 10.254335 10.599320

31 H 1.079547 2.250531 3.329091 10.599320 10.254335

32 Zn 4.334897 3.101085 2.089724 5.307615 5.307615

33 C 2.540343 1.416577 2.476516 8.471410 7.656904

34 C 2.892484 2.420779 3.720276 9.832993 8.840110

35 C 8.767138 7.814882 6.528982 2.695622 5.080018

36 C 3.627356 3.506163 4.851183 10.997517 9.891091

37 C 9.926892 9.006616 7.708386 3.078190 5.708497

38 C 8.212286 6.769324 6.528982 5.080018 2.695622

39 C 9.316606 7.881030 7.708386 5.708497 3.078190

40 C 4.217527 4.594431 3.720276 8.840110 9.832993

41 C 4.990164 5.594790 4.851183 9.891091 10.997517

42 H 5.798721 6.538320 5.877008 10.848381 12.035202

43 H 4.452490 4.518029 5.877008 12.035202 10.848381

44 H 10.313159 8.885575 8.758323 6.404329 3.722460

45 H 10.961832 10.064317 8.758323 3.722460 6.404329

26 27 28 29 30

26 H 0.000000

27 H 2.682200 0.000000

28 H 10.599320 10.254335 0.000000

29 H 10.254335 10.599320 2.682200 0.000000

30 H 7.494851 9.147511 7.494851 5.354308 0.000000

31 H 5.354308 7.494851 9.147511 7.494851 2.682200

32 Zn 5.307615 5.307615 5.307615 5.307615 5.307615

33 C 2.899228 4.641350 8.471410 7.656904 4.641350

34 C 2.695622 5.080018 9.832993 8.840110 5.080018

35 C 9.832993 8.840110 2.695622 5.080018 8.840110

36 C 3.078190 5.708497 10.997517 9.891091 5.708497

37 C 10.997517 9.891091 3.078190 5.708497 9.891091

38 C 5.080018 2.695622 8.840110 9.832993 9.832993

39 C 5.708497 3.078190 9.891091 10.997517 10.997517

40 C 8.840110 9.832993 5.080018 2.695622 2.695622

41 C 9.891091 10.997517 5.708497 3.078190 3.078190

42 H 10.848381 12.035202 6.404329 3.722460 3.722460

43 H 3.722460 6.404329 12.035202 10.848381 6.404329

44 H 6.404329 3.722460 10.848381 12.035202 12.035202

45 H 12.035202 10.848381 3.722460 6.404329 10.848381

31 32 33 34 35

31 H 0.000000

32 Zn 5.307615 0.000000

33 C 2.899228 3.470152 0.000000

34 C 2.695622 4.894934 1.425276 0.000000

35 C 9.832993 4.894934 8.351065 9.775485 0.000000

36 C 3.078190 6.100594 2.631139 1.205864 10.980739

37 C 10.997517 6.100594 9.556508 10.980739 1.205864

38 C 8.840110 4.894934 5.990480 6.912312 6.912312

39 C 9.891091 6.100594 7.008913 7.811233 7.811233

40 C 5.080018 4.894934 5.990480 6.912312 6.912312

41 C 5.708497 6.100594 7.008913 7.811233 7.811233

42 H 6.404329 7.167541 7.954224 8.669358 8.669358

43 H 3.722460 7.167541 3.698356 2.273082 12.047765

44 H 10.848381 7.167541 7.954224 8.669358 8.669358

45 H 12.035202 7.167541 10.623631 12.047765 2.273082

36 37 38 39 40

36 C 0.000000

37 C 12.185841 0.000000

38 C 7.811233 7.811233 0.000000

39 C 8.616691 8.616691 1.205864 0.000000

40 C 7.811233 7.811233 9.775485 10.980739 0.000000

41 C 8.616691 8.616691 10.980739 12.185841 1.205864

42 H 9.401470 9.401470 12.047765 13.252783 2.273082

43 H 1.067241 13.252783 8.669358 9.401470 8.669358

44 H 9.401470 9.401470 2.273082 1.067241 12.047765

45 H 13.252783 1.067241 8.669358 9.401470 8.669358

41 42 43 44 45

41 C 0.000000

42 H 1.067241 0.000000

43 H 9.401470 10.125537 0.000000

44 H 13.252783 14.319672 10.125537 0.000000

45 H 9.401470 10.125537 14.319672 10.125537 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

RotChk: IX=3 Diff= 1.32D-20

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681470 -4.273185 -0.048444

2 6 0 -1.103005 -2.890753 0.001110

3 7 0 0.000000 -2.082310 0.034171

4 6 0 1.103005 -2.890753 0.001110

5 6 0 0.681470 -4.273185 -0.048444

6 6 0 2.448850 -2.448850 -0.009544

7 6 0 2.890753 -1.103005 0.001110

8 7 0 2.082310 0.000000 0.034171

9 6 0 2.890753 1.103005 0.001110

10 6 0 4.273185 0.681470 -0.048444

11 6 0 4.273185 -0.681470 -0.048444

12 6 0 -2.448850 -2.448850 -0.009544

13 6 0 -2.890753 -1.103005 0.001110

14 6 0 -4.273185 -0.681470 -0.048444

15 6 0 -4.273185 0.681470 -0.048444

16 6 0 -2.890753 1.103005 0.001110

17 7 0 -2.082310 0.000000 0.034171

18 6 0 -2.448850 2.448850 -0.009544

19 6 0 -1.103005 2.890753 0.001110

20 6 0 -0.681470 4.273185 -0.048444

21 6 0 0.681470 4.273185 -0.048444

22 6 0 1.103005 2.890753 0.001110

23 7 0 0.000000 2.082310 0.034171

24 1 0 -1.341100 -5.127168 -0.080447

25 1 0 1.341100 -5.127168 -0.080447

26 1 0 5.127168 1.341100 -0.080447

27 1 0 5.127168 -1.341100 -0.080447

28 1 0 -5.127168 -1.341100 -0.080447

29 1 0 -5.127168 1.341100 -0.080447

30 1 0 -1.341100 5.127168 -0.080447

31 1 0 1.341100 5.127168 -0.080447

32 30 0 0.000000 0.000000 0.210044

33 6 0 2.448850 2.448850 -0.009544

34 6 0 3.456156 3.456156 -0.055183

35 6 0 -3.456156 -3.456156 -0.055183

36 6 0 4.308346 4.308346 -0.095840

37 6 0 -4.308346 -4.308346 -0.095840

38 6 0 3.456156 -3.456156 -0.055183

39 6 0 4.308346 -4.308346 -0.095840

40 6 0 -3.456156 3.456156 -0.055183

41 6 0 -4.308346 4.308346 -0.095840

42 1 0 -5.062769 5.062769 -0.122215

43 1 0 5.062769 5.062769 -0.122215

44 1 0 5.062769 -5.062769 -0.122215

45 1 0 -5.062769 -5.062769 -0.122215

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

Rotational constants (GHZ): 0.1463908 0.1463908 0.0732762

Leave Link 202 at Fri Jul 26 14:20:10 2019, MaxMem= 1342177280 cpu: 0.1

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 184 symmetry adapted cartesian basis functions of A1 symmetry.

There are 155 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3059.5346506915 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= 9 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= -0.1305211862 Hartrees.

Nuclear repulsion after empirical dispersion term = 3059.4041295052 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: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3874

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.93D-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) = 3.61%

GePol: Cavity surface area = 416.328 Ang\*\*2

GePol: Cavity volume = 420.318 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0083944000 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3059.4125239053 Hartrees.

Leave Link 301 at Fri Jul 26 14:20:10 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44808.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.40D-05 NBF= 172 148 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 172 148 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:20:11 2019, MaxMem= 1342177280 cpu: 6.6

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:20:11 2019, MaxMem= 1342177280 cpu: 0.8

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

Initial guess from the checkpoint file: "ZnTSPsim0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Occupied (E) (E) (B2) (A1) (E) (E) (B1) (A1) (B2) (E) (E)

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

(E) (E) (A1) (A2) (E) (E) (B1) (B1) (E) (E) (A1)

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

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

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(E) (E) (A2) (A1)

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(E) (E) (E) (E) (E) (E) (E) (E) (E) (E) (E) (E)

(E) (E) (E)

The electronic state of the initial guess is 1-A1.

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= -1359.45252986602

Leave Link 401 at Fri Jul 26 14:20:13 2019, MaxMem= 1342177280 cpu: 21.2

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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.

An orbital has undefined symmetry, so N\*\*3 symmetry is turned off.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 660000000 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= 0 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= 45023628.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.44D-15 for 3868.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.04D-15 for 3830 557.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.10D-15 for 1604.

Iteration 1 A^-1\*A deviation from orthogonality is 6.55D-13 for 2359 2323.

E= -1359.06268033099

DIIS: error= 8.21D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.06268033099 IErMin= 1 ErrMin= 8.21D-04

ErrMax= 8.21D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.02D-04 BMatP= 2.02D-04

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.21D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 3.225 Goal= None Shift= 0.000

RMSDP=7.97D-05 MaxDP=3.09D-03 OVMax= 4.05D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 7.97D-05 CP: 1.00D+00

E= -1359.06295827787 Delta-E= -0.000277946880 Rises=F Damp=F

DIIS: error= 2.23D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.06295827787 IErMin= 2 ErrMin= 2.23D-04

ErrMax= 2.23D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.26D-06 BMatP= 2.02D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.23D-03

Coeff-Com: 0.152D-02 0.998D+00

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

Coeff: 0.152D-02 0.998D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=7.54D-06 MaxDP=2.56D-04 DE=-2.78D-04 OVMax= 7.43D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 7.49D-06 CP: 1.00D+00 1.00D+00

E= -1359.06295864510 Delta-E= -0.000000367234 Rises=F Damp=F

DIIS: error= 3.06D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.06295864510 IErMin= 2 ErrMin= 2.23D-04

ErrMax= 3.06D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.35D-06 BMatP= 5.26D-06

IDIUse=3 WtCom= 3.64D-01 WtEn= 6.36D-01

Coeff-Com: -0.213D-01 0.577D+00 0.445D+00

Coeff-En: 0.000D+00 0.479D+00 0.521D+00

Coeff: -0.775D-02 0.514D+00 0.493D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=4.79D-06 MaxDP=2.33D-04 DE=-3.67D-07 OVMax= 6.29D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.08D-06 CP: 1.00D+00 1.01D+00 5.15D-01

E= -1359.06296330360 Delta-E= -0.000004658502 Rises=F Damp=F

DIIS: error= 6.60D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.06296330360 IErMin= 4 ErrMin= 6.60D-05

ErrMax= 6.60D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D-06 BMatP= 5.26D-06

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

Coeff-Com: -0.107D-01 0.168D+00 0.292D+00 0.551D+00

Coeff: -0.107D-01 0.168D+00 0.292D+00 0.551D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.52D-06 MaxDP=8.32D-05 DE=-4.66D-06 OVMax= 2.41D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 8.38D-07 CP: 1.00D+00 1.00D+00 6.42D-01 7.39D-01

E= -1359.06296416564 Delta-E= -0.000000862041 Rises=F Damp=F

DIIS: error= 3.08D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.06296416564 IErMin= 5 ErrMin= 3.08D-05

ErrMax= 3.08D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.89D-08 BMatP= 1.09D-06

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

Coeff-Com: -0.409D-02 0.403D-01 0.121D+00 0.313D+00 0.530D+00

Coeff: -0.409D-02 0.403D-01 0.121D+00 0.313D+00 0.530D+00

Gap= 0.091 Goal= None Shift= 0.000

RMSDP=4.30D-07 MaxDP=1.33D-05 DE=-8.62D-07 OVMax= 4.42D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.63D-07 CP: 1.00D+00 1.00D+00 6.44D-01 8.06D-01 6.80D-01

E= -1359.06296420785 Delta-E= -0.000000042211 Rises=F Damp=F

DIIS: error= 5.33D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.06296420785 IErMin= 6 ErrMin= 5.33D-06

ErrMax= 5.33D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.08D-09 BMatP= 6.89D-08

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

Coeff-Com: 0.758D-04-0.863D-02-0.783D-03 0.235D-01 0.166D+00 0.820D+00

Coeff: 0.758D-04-0.863D-02-0.783D-03 0.235D-01 0.166D+00 0.820D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.03D-07 MaxDP=4.85D-06 DE=-4.22D-08 OVMax= 9.00D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.61D-08 CP: 1.00D+00 1.00D+00 6.48D-01 8.16D-01 7.43D-01

CP: 8.89D-01

E= -1359.06296420869 Delta-E= -0.000000000830 Rises=F Damp=F

DIIS: error= 1.83D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.06296420869 IErMin= 7 ErrMin= 1.83D-06

ErrMax= 1.83D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.19D-10 BMatP= 2.08D-09

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

Coeff-Com: 0.191D-03-0.694D-02-0.493D-02 0.340D-02 0.858D-01 0.524D+00

Coeff-Com: 0.398D+00

Coeff: 0.191D-03-0.694D-02-0.493D-02 0.340D-02 0.858D-01 0.524D+00

Coeff: 0.398D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=3.06D-08 MaxDP=1.97D-06 DE=-8.30D-10 OVMax= 6.19D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.17D-08 CP: 1.00D+00 1.00D+00 6.48D-01 8.17D-01 7.47D-01

CP: 9.08D-01 6.38D-01

E= -1359.06296420919 Delta-E= -0.000000000502 Rises=F Damp=F

DIIS: error= 3.31D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.06296420919 IErMin= 8 ErrMin= 3.31D-07

ErrMax= 3.31D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.15D-11 BMatP= 7.19D-10

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

Coeff-Com: 0.810D-04-0.228D-02-0.236D-02-0.167D-02 0.194D-01 0.151D+00

Coeff-Com: 0.208D+00 0.627D+00

Coeff: 0.810D-04-0.228D-02-0.236D-02-0.167D-02 0.194D-01 0.151D+00

Coeff: 0.208D+00 0.627D+00

Gap= 0.091 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=8.84D-09 MaxDP=3.02D-07 DE=-5.02D-10 OVMax= 1.02D-06

Error on total polarization charges = 0.06211

SCF Done: E(RB3LYP) = -1359.06296421 A.U. after 8 cycles

NFock= 8 Conv=0.88D-08 -V/T= 1.9682

KE= 1.403697868379D+03 PE=-9.360913357098D+03 EE= 3.538740000605D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.27

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:20:48 2019, MaxMem= 1342177280 cpu: 392.9

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44808.

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 Fri Jul 26 14:20:52 2019, MaxMem= 1342177280 cpu: 42.9

(Enter /apps/gaussian/g09d01/g09/l702.exe)

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

Leave Link 702 at Fri Jul 26 14:20:52 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Fri Jul 26 14:20:56 2019, MaxMem= 1342177280 cpu: 43.2

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-9.23705556D-14 7.10542736D-15 3.22120537D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000412839 0.000310154 0.000285902

2 6 -0.000407058 -0.001048082 -0.000203977

3 7 0.000000000 0.000796533 -0.000191973

4 6 0.000407058 -0.001048082 -0.000203977

5 6 0.000412839 0.000310154 0.000285902

6 6 0.001745658 -0.001745658 0.000202707

7 6 0.001048082 -0.000407058 -0.000203977

8 7 -0.000796533 0.000000000 -0.000191973

9 6 0.001048082 0.000407058 -0.000203977

10 6 -0.000310154 0.000412839 0.000285902

11 6 -0.000310154 -0.000412839 0.000285902

12 6 -0.001745658 -0.001745658 0.000202707

13 6 -0.001048082 -0.000407058 -0.000203977

14 6 0.000310154 -0.000412839 0.000285902

15 6 0.000310154 0.000412839 0.000285902

16 6 -0.001048082 0.000407058 -0.000203977

17 7 0.000796533 0.000000000 -0.000191973

18 6 -0.001745658 0.001745658 0.000202707

19 6 -0.000407058 0.001048082 -0.000203977

20 6 -0.000412839 -0.000310154 0.000285902

21 6 0.000412839 -0.000310154 0.000285902

22 6 0.000407058 0.001048082 -0.000203977

23 7 0.000000000 -0.000796533 -0.000191973

24 1 -0.000075499 0.000230174 -0.000146434

25 1 0.000075499 0.000230174 -0.000146434

26 1 -0.000230174 0.000075499 -0.000146434

27 1 -0.000230174 -0.000075499 -0.000146434

28 1 0.000230174 -0.000075499 -0.000146434

29 1 0.000230174 0.000075499 -0.000146434

30 1 -0.000075499 -0.000230174 -0.000146434

31 1 0.000075499 -0.000230174 -0.000146434

32 30 0.000000000 0.000000000 -0.000199132

33 6 0.001745658 0.001745658 0.000202707

34 6 -0.000702490 -0.000702490 0.000199764

35 6 0.000702490 0.000702490 0.000199764

36 6 0.000077668 0.000077668 0.000145092

37 6 -0.000077668 -0.000077668 0.000145092

38 6 -0.000702490 0.000702490 0.000199764

39 6 0.000077668 -0.000077668 0.000145092

40 6 0.000702490 -0.000702490 0.000199764

41 6 -0.000077668 0.000077668 0.000145092

42 1 0.000049046 -0.000049046 -0.000176788

43 1 -0.000049046 -0.000049046 -0.000176788

44 1 -0.000049046 0.000049046 -0.000176788

45 1 0.000049046 0.000049046 -0.000176788

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

Cartesian Forces: Max 0.001745658 RMS 0.000580717

Leave Link 716 at Fri Jul 26 14:20:56 2019, MaxMem= 1342177280 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001320950 RMS 0.000349392

Search for a local minimum.

Step number 11 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .34939D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 2 3 4 5 7

9 8 10 11

DE= -9.12D-05 DEPred=-1.22D-04 R= 7.47D-01

TightC=F SS= 1.41D+00 RLast= 1.07D-01 DXNew= 8.4090D-02 3.2043D-01

Trust test= 7.47D-01 RLast= 1.07D-01 DXMaxT set to 8.41D-02

ITU= 1 0 -1 0 0 -1 1 0 -1 -1 0

Eigenvalues --- 0.00440 0.00534 0.00534 0.00534 0.00534

Eigenvalues --- 0.00534 0.00534 0.00535 0.01165 0.01173

Eigenvalues --- 0.01173 0.01383 0.01383 0.01595 0.01645

Eigenvalues --- 0.01674 0.01730 0.01730 0.01806 0.01806

Eigenvalues --- 0.01826 0.01832 0.01833 0.01846 0.01860

Eigenvalues --- 0.01860 0.01868 0.01868 0.01868 0.01908

Eigenvalues --- 0.01921 0.01928 0.01928 0.01934 0.01936

Eigenvalues --- 0.01962 0.01962 0.02179 0.02182 0.02186

Eigenvalues --- 0.02186 0.02845 0.03314 0.03435 0.04654

Eigenvalues --- 0.04654 0.04654 0.04654 0.04654 0.04654

Eigenvalues --- 0.04655 0.06914 0.13848 0.15001 0.15001

Eigenvalues --- 0.15366 0.15894 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.22831

Eigenvalues --- 0.22866 0.22870 0.22870 0.24764 0.24782

Eigenvalues --- 0.24782 0.24868 0.24890 0.24977 0.24977

Eigenvalues --- 0.24995 0.24997 0.24997 0.24997 0.24998

Eigenvalues --- 0.25236 0.35038 0.35038 0.35097 0.35474

Eigenvalues --- 0.35502 0.36007 0.36034 0.36034 0.36034

Eigenvalues --- 0.36034 0.36034 0.36034 0.36034 0.36773

Eigenvalues --- 0.36864 0.36864 0.37241 0.37563 0.37563

Eigenvalues --- 0.37563 0.37644 0.38976 0.38976 0.39538

Eigenvalues --- 0.41397 0.41397 0.41397 0.41520 0.41522

Eigenvalues --- 0.41522 0.41796 0.42524 0.43516 0.43781

Eigenvalues --- 0.43781 0.44798 0.47925 0.49089 0.49089

Eigenvalues --- 0.50131 0.51399 0.51902 0.51902 0.52437

Eigenvalues --- 1.01755 1.01831 1.01831 1.01831

En-DIIS/RFO-DIIS IScMMF= 0 using points: 11 10

RFO step: Lambda=-6.35691228D-05.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 9.12D-05 SmlDif= 1.00D-05

RMS Error= 0.8262683327D-03 NUsed= 2 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.91004 0.08996

Iteration 1 RMS(Cart)= 0.02366066 RMS(Int)= 0.00017052

Iteration 2 RMS(Cart)= 0.00037584 RMS(Int)= 0.00002379

Iteration 3 RMS(Cart)= 0.00000002 RMS(Int)= 0.00002379

ITry= 1 IFail=0 DXMaxC= 1.39D-01 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 8.59D-03 for atom 44.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73277 0.00046 -0.00002 0.00195 0.00191 2.73468

R2 2.57558 -0.00066 0.00003 -0.00201 -0.00202 2.57357

R3 2.04005 0.00014 0.00000 0.00074 0.00074 2.04078

R4 2.58506 -0.00132 0.00005 -0.00366 -0.00359 2.58147

R5 2.67694 -0.00080 0.00001 -0.00489 -0.00450 2.67245

R6 2.58506 -0.00132 0.00005 -0.00366 -0.00359 2.58147

R7 3.94901 -0.00057 0.00035 -0.00889 -0.00789 3.94112

R8 2.73277 0.00046 -0.00002 0.00195 0.00191 2.73468

R9 2.67694 -0.00080 0.00001 -0.00489 -0.00450 2.67245

R10 2.04005 0.00014 0.00000 0.00074 0.00074 2.04078

R11 2.67694 -0.00080 0.00001 -0.00489 -0.00450 2.67245

R12 2.69338 0.00095 0.00003 0.00305 0.00220 2.69559

R13 2.58506 -0.00132 0.00005 -0.00366 -0.00359 2.58147

R14 2.73277 0.00046 -0.00002 0.00195 0.00191 2.73468

R15 2.58506 -0.00132 0.00005 -0.00366 -0.00359 2.58147

R16 3.94901 -0.00057 0.00035 -0.00889 -0.00789 3.94112

R17 2.73277 0.00046 -0.00002 0.00195 0.00191 2.73468

R18 2.67694 -0.00080 0.00001 -0.00489 -0.00450 2.67245

R19 2.57558 -0.00066 0.00003 -0.00201 -0.00202 2.57357

R20 2.04005 0.00014 0.00000 0.00074 0.00074 2.04078

R21 2.04005 0.00014 0.00000 0.00075 0.00074 2.04078

R22 2.67694 -0.00080 0.00001 -0.00489 -0.00450 2.67245

R23 2.69338 0.00095 0.00003 0.00305 0.00220 2.69559

R24 2.73277 0.00046 -0.00002 0.00195 0.00191 2.73468

R25 2.58506 -0.00132 0.00005 -0.00366 -0.00359 2.58147

R26 2.57558 -0.00066 0.00003 -0.00201 -0.00202 2.57357

R27 2.04005 0.00014 0.00000 0.00075 0.00074 2.04078

R28 2.73277 0.00046 -0.00002 0.00195 0.00191 2.73468

R29 2.04005 0.00014 0.00000 0.00074 0.00074 2.04078

R30 2.58506 -0.00132 0.00005 -0.00366 -0.00359 2.58147

R31 2.67694 -0.00080 0.00001 -0.00489 -0.00450 2.67245

R32 3.94901 -0.00057 0.00035 -0.00889 -0.00789 3.94112

R33 2.67694 -0.00080 0.00001 -0.00489 -0.00450 2.67245

R34 2.69338 0.00095 0.00003 0.00305 0.00220 2.69559

R35 2.73277 0.00046 -0.00002 0.00195 0.00191 2.73468

R36 2.58506 -0.00132 0.00005 -0.00366 -0.00359 2.58147

R37 2.57558 -0.00066 0.00003 -0.00201 -0.00202 2.57357

R38 2.04005 0.00014 0.00000 0.00075 0.00074 2.04078

R39 2.73277 0.00046 -0.00002 0.00195 0.00191 2.73468

R40 2.04005 0.00014 0.00000 0.00075 0.00074 2.04078

R41 2.58506 -0.00132 0.00005 -0.00366 -0.00359 2.58147

R42 2.67694 -0.00080 0.00001 -0.00489 -0.00450 2.67245

R43 3.94901 -0.00057 0.00035 -0.00889 -0.00789 3.94112

R44 2.69338 0.00095 0.00003 0.00305 0.00220 2.69559

R45 2.27875 -0.00004 0.00000 -0.00035 -0.00035 2.27840

R46 2.27875 -0.00004 0.00000 -0.00035 -0.00035 2.27840

R47 2.01679 0.00007 0.00001 0.00012 0.00012 2.01691

R48 2.01679 0.00007 0.00001 0.00012 0.00012 2.01691

R49 2.27875 -0.00004 0.00000 -0.00035 -0.00035 2.27840

R50 2.01679 0.00007 0.00001 0.00012 0.00012 2.01691

R51 2.27875 -0.00004 0.00000 -0.00035 -0.00035 2.27840

R52 2.01679 0.00007 0.00001 0.00012 0.00012 2.01691

A1 1.86658 -0.00030 0.00002 -0.00159 -0.00157 1.86501

A2 2.18845 0.00036 -0.00003 0.00270 0.00266 2.19111

A3 2.22815 -0.00006 0.00001 -0.00112 -0.00111 2.22704

A4 1.90790 0.00023 -0.00002 0.00267 0.00267 1.91057

A5 2.18327 0.00002 -0.00001 -0.00043 -0.00043 2.18284

A6 2.19183 -0.00025 0.00004 -0.00210 -0.00213 2.18970

A7 1.87580 0.00013 0.00001 -0.00215 -0.00219 1.87361

A8 2.20300 -0.00007 -0.00005 0.00052 0.00038 2.20339

A9 2.20300 -0.00007 -0.00005 0.00052 0.00038 2.20339

A10 1.90790 0.00023 -0.00002 0.00267 0.00267 1.91057

A11 2.19183 -0.00025 0.00004 -0.00210 -0.00213 2.18970

A12 2.18327 0.00002 -0.00001 -0.00043 -0.00043 2.18284

A13 1.86658 -0.00030 0.00002 -0.00159 -0.00157 1.86501

A14 2.22815 -0.00006 0.00001 -0.00112 -0.00111 2.22704

A15 2.18845 0.00036 -0.00003 0.00270 0.00266 2.19111

A16 2.20520 0.00062 -0.00007 0.00161 0.00169 2.20688

A17 2.03894 -0.00031 0.00004 -0.00068 -0.00079 2.03815

A18 2.03894 -0.00031 0.00004 -0.00073 -0.00079 2.03815

A19 2.19183 -0.00025 0.00004 -0.00210 -0.00213 2.18970

A20 2.18327 0.00002 -0.00001 -0.00043 -0.00043 2.18284

A21 1.90790 0.00023 -0.00002 0.00267 0.00267 1.91057

A22 1.87580 0.00013 0.00001 -0.00215 -0.00219 1.87361

A23 2.20300 -0.00007 -0.00005 0.00052 0.00038 2.20339

A24 2.20300 -0.00007 -0.00005 0.00052 0.00038 2.20339

A25 1.90790 0.00023 -0.00002 0.00267 0.00267 1.91057

A26 2.19183 -0.00025 0.00004 -0.00210 -0.00213 2.18970

A27 2.18327 0.00002 -0.00001 -0.00043 -0.00043 2.18284

A28 1.86658 -0.00030 0.00002 -0.00159 -0.00157 1.86501

A29 2.18845 0.00036 -0.00003 0.00270 0.00266 2.19111

A30 2.22815 -0.00006 0.00001 -0.00112 -0.00111 2.22704

A31 1.86658 -0.00030 0.00002 -0.00159 -0.00157 1.86501

A32 2.18845 0.00036 -0.00003 0.00271 0.00266 2.19111

A33 2.22815 -0.00006 0.00001 -0.00113 -0.00111 2.22704

A34 2.20520 0.00062 -0.00007 0.00161 0.00169 2.20688

A35 2.03894 -0.00031 0.00004 -0.00068 -0.00079 2.03815

A36 2.03894 -0.00031 0.00004 -0.00073 -0.00079 2.03815

A37 2.18327 0.00002 -0.00001 -0.00043 -0.00043 2.18284

A38 2.19183 -0.00025 0.00004 -0.00210 -0.00213 2.18970

A39 1.90790 0.00023 -0.00002 0.00267 0.00267 1.91057

A40 1.86658 -0.00030 0.00002 -0.00159 -0.00157 1.86501

A41 2.18845 0.00036 -0.00003 0.00271 0.00266 2.19111

A42 2.22815 -0.00006 0.00001 -0.00113 -0.00111 2.22704

A43 1.86658 -0.00030 0.00002 -0.00159 -0.00157 1.86501

A44 2.22815 -0.00006 0.00001 -0.00112 -0.00111 2.22704

A45 2.18845 0.00036 -0.00003 0.00270 0.00266 2.19111

A46 1.90790 0.00023 -0.00002 0.00267 0.00267 1.91057

A47 2.18327 0.00002 -0.00001 -0.00043 -0.00043 2.18284

A48 2.19183 -0.00025 0.00004 -0.00210 -0.00213 2.18970

A49 1.87580 0.00013 0.00001 -0.00215 -0.00219 1.87361

A50 2.20300 -0.00007 -0.00005 0.00052 0.00038 2.20339

A51 2.20300 -0.00007 -0.00005 0.00052 0.00038 2.20339

A52 2.20520 0.00062 -0.00007 0.00161 0.00169 2.20688

A53 2.03894 -0.00031 0.00004 -0.00068 -0.00079 2.03815

A54 2.03894 -0.00031 0.00004 -0.00072 -0.00079 2.03815

A55 2.18327 0.00002 -0.00001 -0.00043 -0.00043 2.18284

A56 2.19183 -0.00025 0.00004 -0.00210 -0.00213 2.18970

A57 1.90790 0.00023 -0.00002 0.00267 0.00267 1.91057

A58 1.86658 -0.00030 0.00002 -0.00159 -0.00157 1.86501

A59 2.18845 0.00036 -0.00003 0.00271 0.00266 2.19111

A60 2.22815 -0.00006 0.00001 -0.00113 -0.00111 2.22704

A61 1.86658 -0.00030 0.00002 -0.00159 -0.00157 1.86501

A62 2.22815 -0.00006 0.00001 -0.00113 -0.00111 2.22704

A63 2.18845 0.00036 -0.00003 0.00271 0.00266 2.19111

A64 1.90790 0.00023 -0.00002 0.00267 0.00267 1.91057

A65 2.18327 0.00002 -0.00001 -0.00043 -0.00043 2.18284

A66 2.19183 -0.00025 0.00004 -0.00210 -0.00213 2.18970

A67 1.87580 0.00013 0.00001 -0.00215 -0.00219 1.87361

A68 2.20300 -0.00007 -0.00005 0.00052 0.00038 2.20339

A69 2.20300 -0.00007 -0.00005 0.00052 0.00038 2.20339

A70 1.56371 0.00001 -0.00018 -0.00071 -0.00091 1.56281

A71 1.56371 0.00001 -0.00018 -0.00071 -0.00091 1.56281

A72 2.97307 0.00012 -0.00206 -0.00847 -0.01049 2.96258

A73 2.97307 0.00012 -0.00206 -0.00847 -0.01049 2.96258

A74 1.56371 0.00001 -0.00018 -0.00071 -0.00091 1.56281

A75 1.56371 0.00001 -0.00018 -0.00071 -0.00091 1.56281

A76 2.20520 0.00062 -0.00007 0.00161 0.00169 2.20688

A77 2.03894 -0.00031 0.00004 -0.00068 -0.00079 2.03815

A78 2.03894 -0.00031 0.00004 -0.00072 -0.00079 2.03815

A79 3.14157 0.00000 -0.00001 0.00047 0.00015 3.14172

A80 3.14157 0.00000 -0.00001 0.00047 0.00015 3.14172

A81 3.14169 0.00000 -0.00001 0.00366 -0.00006 3.14163

A82 3.14169 0.00000 -0.00001 0.00366 -0.00006 3.14163

A83 3.14157 0.00000 -0.00001 0.00047 0.00015 3.14172

A84 3.14169 0.00000 -0.00001 0.00366 -0.00006 3.14163

A85 3.14157 0.00000 -0.00001 0.00047 0.00015 3.14172

A86 3.14169 0.00000 -0.00001 0.00366 -0.00006 3.14163

A87 3.13989 -0.00043 -0.00074 0.01098 0.01026 3.15015

A88 3.14330 0.00043 0.00074 -0.01098 -0.01026 3.13304

A89 3.15195 -0.00031 -0.00137 -0.00583 -0.00715 3.14480

A90 3.13124 0.00031 0.00137 0.00583 0.00715 3.13839

A91 3.13989 -0.00043 -0.00074 0.01098 0.01026 3.15015

A92 3.15195 -0.00031 -0.00137 -0.00583 -0.00715 3.14480

A93 3.14330 0.00043 0.00074 -0.01098 -0.01026 3.13304

A94 3.13124 0.00031 0.00137 0.00583 0.00715 3.13839

D1 -0.00316 0.00001 -0.00014 0.00119 0.00103 -0.00213

D2 3.11875 0.00009 0.00013 0.00831 0.00845 3.12719

D3 3.14001 0.00005 -0.00008 0.00611 0.00603 -3.13714

D4 -0.02127 0.00013 0.00020 0.01324 0.01345 -0.00782

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13997 0.00004 0.00007 0.00507 0.00513 -3.13484

D7 3.13997 -0.00004 -0.00007 -0.00507 -0.00513 3.13484

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00511 -0.00002 0.00023 -0.00192 -0.00168 0.00343

D10 -3.08269 0.00007 0.00165 0.01956 0.02119 -3.06150

D11 -3.11668 -0.00010 -0.00005 -0.00912 -0.00915 -3.12583

D12 0.07871 -0.00002 0.00137 0.01236 0.01372 0.09243

D13 -3.10928 -0.00007 -0.00041 -0.00882 -0.00922 -3.11851

D14 0.01510 -0.00002 -0.00018 0.00594 0.00575 0.02085

D15 0.00947 0.00003 -0.00009 -0.00049 -0.00059 0.00888

D16 3.13385 0.00007 0.00015 0.01427 0.01439 -3.13495

D17 -0.00511 0.00002 -0.00023 0.00192 0.00168 -0.00343

D18 3.11668 0.00010 0.00005 0.00912 0.00915 3.12583

D19 3.08269 -0.00007 -0.00165 -0.01956 -0.02119 3.06150

D20 -0.07871 0.00002 -0.00137 -0.01236 -0.01372 -0.09243

D21 -3.08944 -0.00011 0.00018 -0.00855 -0.00839 -3.09783

D22 -0.11577 0.00001 -0.00185 -0.01693 -0.01876 -0.13453

D23 -1.60260 -0.00005 -0.00084 -0.01274 -0.01357 -1.61618

D24 0.11577 -0.00001 0.00185 0.01693 0.01876 0.13453

D25 3.08944 0.00011 -0.00018 0.00855 0.00839 3.09783

D26 1.60260 0.00005 0.00084 0.01274 0.01357 1.61618

D27 0.00316 -0.00001 0.00014 -0.00119 -0.00103 0.00213

D28 -3.14001 -0.00005 0.00008 -0.00611 -0.00603 3.13714

D29 -3.11875 -0.00009 -0.00013 -0.00831 -0.00845 -3.12719

D30 0.02127 -0.00013 -0.00020 -0.01324 -0.01345 0.00782

D31 -0.00947 -0.00003 0.00009 0.00049 0.00059 -0.00888

D32 -3.13385 -0.00007 -0.00015 -0.01427 -0.01439 3.13495

D33 3.10928 0.00007 0.00041 0.00882 0.00922 3.11851

D34 -0.01510 0.00002 0.00018 -0.00594 -0.00575 -0.02085

D35 0.00947 0.00003 -0.00009 -0.00049 -0.00059 0.00888

D36 -3.10928 -0.00007 -0.00041 -0.00882 -0.00922 -3.11851

D37 3.13385 0.00007 0.00015 0.01427 0.01439 -3.13495

D38 0.01510 -0.00002 -0.00018 0.00594 0.00575 0.02085

D39 -3.11668 -0.00010 -0.00005 -0.00912 -0.00915 -3.12583

D40 0.07871 -0.00002 0.00137 0.01236 0.01372 0.09243

D41 0.00511 -0.00002 0.00023 -0.00192 -0.00168 0.00343

D42 -3.08269 0.00007 0.00165 0.01956 0.02119 -3.06150

D43 3.11875 0.00009 0.00013 0.00831 0.00845 3.12719

D44 -0.02127 0.00013 0.00020 0.01324 0.01345 -0.00782

D45 -0.00316 0.00001 -0.00014 0.00119 0.00103 -0.00213

D46 3.14001 0.00005 -0.00008 0.00611 0.00603 -3.13714

D47 -0.00511 0.00002 -0.00023 0.00192 0.00168 -0.00343

D48 3.11668 0.00010 0.00005 0.00912 0.00915 3.12583

D49 3.08269 -0.00007 -0.00165 -0.01956 -0.02119 3.06150

D50 -0.07871 0.00002 -0.00137 -0.01236 -0.01372 -0.09243

D51 -0.11577 0.00001 -0.00185 -0.01693 -0.01876 -0.13453

D52 -1.60260 -0.00005 -0.00084 -0.01274 -0.01357 -1.61618

D53 -3.08944 -0.00011 0.00018 -0.00855 -0.00839 -3.09783

D54 3.08944 0.00011 -0.00018 0.00855 0.00839 3.09783

D55 1.60260 0.00005 0.00084 0.01274 0.01357 1.61618

D56 0.11577 -0.00001 0.00185 0.01693 0.01876 0.13453

D57 0.00316 -0.00001 0.00014 -0.00119 -0.00103 0.00213

D58 -3.14001 -0.00005 0.00008 -0.00611 -0.00603 3.13714

D59 -3.11875 -0.00009 -0.00013 -0.00831 -0.00845 -3.12719

D60 0.02127 -0.00013 -0.00020 -0.01324 -0.01345 0.00782

D61 -0.00947 -0.00003 0.00009 0.00049 0.00059 -0.00888

D62 -3.13385 -0.00007 -0.00015 -0.01427 -0.01439 3.13495

D63 3.10928 0.00007 0.00041 0.00882 0.00922 3.11851

D64 -0.01510 0.00002 0.00018 -0.00594 -0.00575 -0.02085

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13997 -0.00004 -0.00007 -0.00507 -0.00513 3.13484

D67 -3.13997 0.00004 0.00007 0.00507 0.00513 -3.13484

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.10928 0.00007 0.00041 0.00882 0.00922 3.11851

D70 -0.00947 -0.00003 0.00009 0.00049 0.00059 -0.00888

D71 -0.01510 0.00002 0.00018 -0.00594 -0.00575 -0.02085

D72 -3.13385 -0.00007 -0.00015 -0.01427 -0.01439 3.13495

D73 -3.11875 -0.00009 -0.00013 -0.00831 -0.00845 -3.12719

D74 0.02127 -0.00013 -0.00020 -0.01324 -0.01345 0.00782

D75 0.00316 -0.00001 0.00014 -0.00119 -0.00103 0.00213

D76 -3.14001 -0.00005 0.00008 -0.00611 -0.00603 3.13714

D77 3.11668 0.00010 0.00005 0.00912 0.00915 3.12583

D78 -0.07871 0.00002 -0.00137 -0.01236 -0.01372 -0.09243

D79 -0.00511 0.00002 -0.00023 0.00192 0.00168 -0.00343

D80 3.08269 -0.00007 -0.00165 -0.01956 -0.02119 3.06150

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 3.13997 -0.00004 -0.00007 -0.00507 -0.00513 3.13484

D83 -3.13997 0.00004 0.00007 0.00507 0.00513 -3.13484

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 -0.00316 0.00001 -0.00014 0.00119 0.00103 -0.00213

D86 3.11875 0.00009 0.00013 0.00831 0.00845 3.12719

D87 3.14001 0.00005 -0.00008 0.00611 0.00603 -3.13714

D88 -0.02127 0.00013 0.00020 0.01324 0.01345 -0.00782

D89 0.00511 -0.00002 0.00023 -0.00192 -0.00168 0.00343

D90 -3.08269 0.00007 0.00165 0.01956 0.02119 -3.06150

D91 -3.11668 -0.00010 -0.00005 -0.00912 -0.00915 -3.12583

D92 0.07871 -0.00002 0.00137 0.01236 0.01372 0.09243

D93 -3.10928 -0.00007 -0.00041 -0.00882 -0.00922 -3.11851

D94 0.01510 -0.00002 -0.00018 0.00594 0.00575 0.02085

D95 0.00947 0.00003 -0.00009 -0.00049 -0.00059 0.00888

D96 3.13385 0.00007 0.00015 0.01427 0.01439 -3.13495

D97 0.11577 -0.00001 0.00185 0.01693 0.01876 0.13453

D98 1.60260 0.00005 0.00084 0.01274 0.01357 1.61618

D99 3.08944 0.00011 -0.00018 0.00855 0.00839 3.09783

D100 -3.08944 -0.00011 0.00018 -0.00855 -0.00839 -3.09783

D101 -1.60260 -0.00005 -0.00084 -0.01274 -0.01357 -1.61618

D102 -0.11577 0.00001 -0.00185 -0.01693 -0.01876 -0.13453

D103 3.10928 0.00007 0.00041 0.00882 0.00922 3.11851

D104 -0.00947 -0.00003 0.00009 0.00049 0.00059 -0.00888

D105 -0.01510 0.00002 0.00018 -0.00594 -0.00575 -0.02085

D106 -3.13385 -0.00007 -0.00015 -0.01427 -0.01439 3.13495

D107 -3.11875 -0.00009 -0.00013 -0.00831 -0.00845 -3.12719

D108 0.02127 -0.00013 -0.00020 -0.01324 -0.01345 0.00782

D109 0.00316 -0.00001 0.00014 -0.00119 -0.00103 0.00213

D110 -3.14001 -0.00005 0.00008 -0.00611 -0.00603 3.13714

D111 3.11668 0.00010 0.00005 0.00912 0.00915 3.12583

D112 -0.07871 0.00002 -0.00137 -0.01236 -0.01372 -0.09243

D113 -0.00511 0.00002 -0.00023 0.00192 0.00168 -0.00343

D114 3.08269 -0.00007 -0.00165 -0.01956 -0.02119 3.06150

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.13997 -0.00004 -0.00007 -0.00507 -0.00513 3.13484

D117 -3.13997 0.00004 0.00007 0.00507 0.00513 -3.13484

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 -0.00316 0.00001 -0.00014 0.00119 0.00103 -0.00213

D120 3.11875 0.00009 0.00013 0.00831 0.00845 3.12719

D121 3.14001 0.00005 -0.00008 0.00611 0.00603 -3.13714

D122 -0.02127 0.00013 0.00020 0.01324 0.01345 -0.00782

D123 0.00511 -0.00002 0.00023 -0.00192 -0.00168 0.00343

D124 -3.08269 0.00007 0.00165 0.01956 0.02119 -3.06150

D125 -3.11668 -0.00010 -0.00005 -0.00912 -0.00915 -3.12583

D126 0.07871 -0.00002 0.00137 0.01236 0.01372 0.09243

D127 -3.10928 -0.00007 -0.00041 -0.00882 -0.00922 -3.11851

D128 0.01510 -0.00002 -0.00018 0.00594 0.00575 0.02085

D129 0.00947 0.00003 -0.00009 -0.00049 -0.00059 0.00888

D130 3.13385 0.00007 0.00015 0.01427 0.01439 -3.13495

D131 1.60260 0.00005 0.00084 0.01274 0.01357 1.61618

D132 3.08944 0.00011 -0.00018 0.00855 0.00839 3.09783

D133 0.11577 -0.00001 0.00185 0.01693 0.01876 0.13453

D134 -1.60260 -0.00005 -0.00084 -0.01274 -0.01357 -1.61618

D135 -0.11577 0.00001 -0.00185 -0.01693 -0.01876 -0.13453

D136 -3.08944 -0.00011 0.00018 -0.00855 -0.00839 -3.09783

Item Value Threshold Converged?

Maximum Force 0.001321 0.000450 NO

RMS Force 0.000349 0.000300 NO

Maximum Displacement 0.139430 0.001800 NO

RMS Displacement 0.023692 0.001200 NO

Predicted change in Energy=-9.505957D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:20:56 2019, MaxMem= 1342177280 cpu: 1.2

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.680936 4.270633 -0.048934

2 6 0 1.100587 2.886094 -0.015259

3 7 0 0.000000 2.077200 0.007153

4 6 0 -1.100587 2.886094 -0.015259

5 6 0 -0.680936 4.270633 -0.048934

6 6 0 -2.443841 2.443841 -0.021172

7 6 0 -2.886094 1.100587 -0.015259

8 7 0 -2.077200 0.000000 0.007153

9 6 0 -2.886094 -1.100587 -0.015259

10 6 0 -4.270633 -0.680936 -0.048934

11 6 0 -4.270633 0.680936 -0.048934

12 6 0 2.443841 2.443841 -0.021172

13 6 0 2.886094 1.100587 -0.015259

14 6 0 4.270633 0.680936 -0.048934

15 6 0 4.270633 -0.680936 -0.048934

16 6 0 2.886094 -1.100587 -0.015259

17 7 0 2.077200 0.000000 0.007153

18 6 0 2.443841 -2.443841 -0.021172

19 6 0 1.100587 -2.886094 -0.015259

20 6 0 0.680936 -4.270633 -0.048934

21 6 0 -0.680936 -4.270633 -0.048934

22 6 0 -1.100587 -2.886094 -0.015259

23 7 0 0.000000 -2.077200 0.007153

24 1 0 1.339854 5.125843 -0.075516

25 1 0 -1.339854 5.125843 -0.075516

26 1 0 -5.125843 -1.339854 -0.075516

27 1 0 -5.125843 1.339854 -0.075516

28 1 0 5.125843 1.339854 -0.075516

29 1 0 5.125843 -1.339854 -0.075516

30 1 0 1.339854 -5.125843 -0.075516

31 1 0 -1.339854 -5.125843 -0.075516

32 30 0 0.000000 0.000000 0.193570

33 6 0 -2.443841 -2.443841 -0.021172

34 6 0 -3.452424 -3.452424 -0.037259

35 6 0 3.452424 3.452424 -0.037259

36 6 0 -4.304964 -4.304964 -0.040610

37 6 0 4.304964 4.304964 -0.040610

38 6 0 -3.452424 3.452424 -0.037259

39 6 0 -4.304964 4.304964 -0.040610

40 6 0 3.452424 -3.452424 -0.037259

41 6 0 4.304964 -4.304964 -0.040610

42 1 0 5.059661 -5.059661 -0.040601

43 1 0 -5.059661 -5.059661 -0.040601

44 1 0 -5.059661 5.059661 -0.040601

45 1 0 5.059661 5.059661 -0.040601

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.447132 0.000000

3 N 2.297383 1.366054 0.000000

4 C 2.256526 2.201174 1.366054 0.000000

5 C 1.361872 2.256526 2.297383 1.447132 0.000000

6 C 3.619693 3.571918 2.471354 1.414197 2.538853

7 C 4.772214 4.368256 3.046935 2.525087 3.861741

8 N 5.084169 4.292828 2.937605 3.046935 4.493441

9 C 6.447856 5.638018 4.292828 4.368256 5.806364

10 C 7.002577 6.447856 5.084169 4.772214 6.115878

11 C 6.115878 5.806364 4.493441 3.861741 5.076598

12 C 2.538853 1.414197 2.471354 3.571918 3.619693

13 C 3.861741 2.525087 3.046935 4.368256 4.772214

14 C 5.076598 3.861741 4.493441 5.806364 6.115878

15 C 6.115878 4.772214 5.084169 6.447856 7.002577

16 C 5.806364 4.368256 4.292828 5.638018 6.447856

17 N 4.493441 3.046935 2.937605 4.292828 5.084169

18 C 6.942102 5.496597 5.139356 6.400876 7.406023

19 C 7.169099 5.772187 5.083904 6.177646 7.375209

20 C 8.541267 7.169099 6.384498 7.375209 8.649158

21 C 8.649158 7.375209 6.384498 7.169099 8.541267

22 C 7.375209 6.177646 5.083904 5.772187 7.169099

23 N 6.384498 5.083904 4.154401 5.083904 6.384498

24 H 1.079937 2.253299 3.331106 3.312984 2.194466

25 H 2.194466 3.312984 3.331106 2.253299 1.079937

26 H 8.074464 7.525337 6.160955 5.836519 7.157896

27 H 6.504527 6.415834 5.179265 4.312444 5.324225

28 H 5.324225 4.312444 5.179265 6.415834 6.504527

29 H 7.157896 5.836519 6.160955 7.525337 8.074464

30 H 9.419589 8.015735 7.327065 8.375591 9.611351

31 H 9.611351 8.375591 7.327065 8.015735 9.419589

32 Zn 4.331373 3.095874 2.085549 3.095874 4.331373

33 C 7.406023 6.400876 5.139356 5.496597 6.942102

34 C 8.759591 7.804307 6.519046 6.760801 8.205297

35 C 2.889766 2.419164 3.716510 4.588151 4.213582

36 C 9.919684 8.996218 7.698507 7.872736 9.309915

37 C 3.624200 3.504549 4.847466 5.588722 4.986025

38 C 4.213582 4.588151 3.716510 2.419164 2.889766

39 C 4.986025 5.588722 4.847466 3.504549 3.624200

40 C 8.205297 6.760801 6.519046 7.804307 8.759591

41 C 9.309915 7.872736 7.698507 8.996218 9.919684

42 H 10.306683 8.877496 8.748557 10.054070 10.954859

43 H 10.954859 10.054070 8.748557 8.877496 10.306683

44 H 5.794575 6.532511 5.873460 4.516559 4.449255

45 H 4.449255 4.516559 5.873460 6.532511 5.794575

6 7 8 9 10

6 C 0.000000

7 C 1.414197 0.000000

8 N 2.471354 1.366054 0.000000

9 C 3.571918 2.201174 1.366054 0.000000

10 C 3.619693 2.256526 2.297383 1.447132 0.000000

11 C 2.538853 1.447132 2.297383 2.256526 1.361872

12 C 4.887683 5.496597 5.139356 6.400876 7.406023

13 C 5.496597 5.772187 5.083904 6.177646 7.375209

14 C 6.942102 7.169099 6.384498 7.375209 8.649158

15 C 7.406023 7.375209 6.384498 7.169099 8.541267

16 C 6.400876 6.177646 5.083904 5.772187 7.169099

17 N 5.139356 5.083904 4.154401 5.083904 6.384498

18 C 6.912227 6.400876 5.139356 5.496597 6.942102

19 C 6.400876 5.638018 4.292828 4.368256 5.806364

20 C 7.406023 6.447856 5.084169 4.772214 6.115878

21 C 6.942102 5.806364 4.493441 3.861741 5.076598

22 C 5.496597 4.368256 3.046935 2.525087 3.861741

23 N 5.139356 4.292828 2.937605 3.046935 4.493441

24 H 4.638150 5.836519 6.160955 7.525337 8.074464

25 H 2.900841 4.312444 5.179265 6.415834 6.504527

26 H 4.638150 3.312984 3.331106 2.253299 1.079937

27 H 2.900841 2.253299 3.331106 3.312984 2.194466

28 H 7.649959 8.015735 7.327065 8.375591 9.611351

29 H 8.462826 8.375591 7.327065 8.015735 9.419589

30 H 8.462826 7.525337 6.160955 5.836519 7.157896

31 H 7.649959 6.415834 5.179265 4.312444 5.324225

32 Zn 3.462779 3.095874 2.085549 3.095874 4.331373

33 C 4.887683 3.571918 2.471354 1.414197 2.538853

34 C 5.981927 4.588151 3.716510 2.419164 2.889766

35 C 5.981927 6.760801 6.519046 7.804307 8.759591

36 C 7.000752 5.588722 4.847466 3.504549 3.624200

37 C 7.000752 7.872736 7.698507 8.996218 9.919684

38 C 1.426442 2.419164 3.716510 4.588151 4.213582

39 C 2.632096 3.504549 4.847466 5.588722 4.986025

40 C 8.338595 7.804307 6.519046 6.760801 8.205297

41 C 9.544272 8.996218 7.698507 7.872736 9.309915

42 H 10.611573 10.054070 8.748557 8.877496 10.306683

43 H 7.946411 6.532511 5.873460 4.516559 4.449255

44 H 3.699379 4.516559 5.873460 6.532511 5.794575

45 H 7.946411 8.877496 8.748557 10.054070 10.954859

11 12 13 14 15

11 C 0.000000

12 C 6.942102 0.000000

13 C 7.169099 1.414197 0.000000

14 C 8.541267 2.538853 1.447132 0.000000

15 C 8.649158 3.619693 2.256526 1.361872 0.000000

16 C 7.375209 3.571918 2.201174 2.256526 1.447132

17 N 6.384498 2.471354 1.366054 2.297383 2.297383

18 C 7.406023 4.887683 3.571918 3.619693 2.538853

19 C 6.447856 5.496597 4.368256 4.772214 3.861741

20 C 7.002577 6.942102 5.806364 6.115878 5.076598

21 C 6.115878 7.406023 6.447856 7.002577 6.115878

22 C 4.772214 6.400876 5.638018 6.447856 5.806364

23 N 5.084169 5.139356 4.292828 5.084169 4.493441

24 H 7.157896 2.900841 4.312444 5.324225 6.504527

25 H 5.324225 4.638150 5.836519 7.157896 8.074464

26 H 2.194466 8.462826 8.375591 9.611351 9.419589

27 H 1.079937 7.649959 8.015735 9.419589 9.611351

28 H 9.419589 2.900841 2.253299 1.079937 2.194466

29 H 9.611351 4.638150 3.312984 2.194466 1.079937

30 H 8.074464 7.649959 6.415834 6.504527 5.324225

31 H 6.504527 8.462826 7.525337 8.074464 7.157896

32 Zn 4.331373 3.462779 3.095874 4.331373 4.331373

33 C 3.619693 6.912227 6.400876 7.406023 6.942102

34 C 4.213582 8.338595 7.804307 8.759591 8.205297

35 C 8.205297 1.426442 2.419164 2.889766 4.213582

36 C 4.986025 9.544272 8.996218 9.919684 9.309915

37 C 9.309915 2.632096 3.504549 3.624200 4.986025

38 C 2.889766 5.981927 6.760801 8.205297 8.759591

39 C 3.624200 7.000752 7.872736 9.309915 9.919684

40 C 8.759591 5.981927 4.588151 4.213582 2.889766

41 C 9.919684 7.000752 5.588722 4.986025 3.624200

42 H 10.954859 7.946411 6.532511 5.794575 4.449255

43 H 5.794575 10.611573 10.054070 10.954859 10.306683

44 H 4.449255 7.946411 8.877496 10.306683 10.954859

45 H 10.306683 3.699379 4.516559 4.449255 5.794575

16 17 18 19 20

16 C 0.000000

17 N 1.366054 0.000000

18 C 1.414197 2.471354 0.000000

19 C 2.525087 3.046935 1.414197 0.000000

20 C 3.861741 4.493441 2.538853 1.447132 0.000000

21 C 4.772214 5.084169 3.619693 2.256526 1.361872

22 C 4.368256 4.292828 3.571918 2.201174 2.256526

23 N 3.046935 2.937605 2.471354 1.366054 2.297383

24 H 6.415834 5.179265 7.649959 8.015735 9.419589

25 H 7.525337 6.160955 8.462826 8.375591 9.611351

26 H 8.015735 7.327065 7.649959 6.415834 6.504527

27 H 8.375591 7.327065 8.462826 7.525337 8.074464

28 H 3.312984 3.331106 4.638150 5.836519 7.157896

29 H 2.253299 3.331106 2.900841 4.312444 5.324225

30 H 4.312444 5.179265 2.900841 2.253299 1.079937

31 H 5.836519 6.160955 4.638150 3.312984 2.194466

32 Zn 3.095874 2.085549 3.462779 3.095874 4.331373

33 C 5.496597 5.139356 4.887683 3.571918 3.619693

34 C 6.760801 6.519046 5.981927 4.588151 4.213582

35 C 4.588151 3.716510 5.981927 6.760801 8.205297

36 C 7.872736 7.698507 7.000752 5.588722 4.986025

37 C 5.588722 4.847466 7.000752 7.872736 9.309915

38 C 7.804307 6.519046 8.338595 7.804307 8.759591

39 C 8.996218 7.698507 9.544272 8.996218 9.919684

40 C 2.419164 3.716510 1.426442 2.419164 2.889766

41 C 3.504549 4.847466 2.632096 3.504549 3.624200

42 H 4.516559 5.873460 3.699379 4.516559 4.449255

43 H 8.877496 8.748557 7.946411 6.532511 5.794575

44 H 10.054070 8.748557 10.611573 10.054070 10.954859

45 H 6.532511 5.873460 7.946411 8.877496 10.306683

21 22 23 24 25

21 C 0.000000

22 C 1.447132 0.000000

23 N 2.297383 1.366054 0.000000

24 H 9.611351 8.375591 7.327065 0.000000

25 H 9.419589 8.015735 7.327065 2.679707 0.000000

26 H 5.324225 4.312444 5.179265 9.143877 7.492594

27 H 7.157896 5.836519 6.160955 7.492594 5.354198

28 H 8.074464 7.525337 6.160955 5.354198 7.492594

29 H 6.504527 6.415834 5.179265 7.492594 9.143877

30 H 2.194466 3.312984 3.331106 10.251687 10.596127

31 H 1.079937 2.253299 3.331106 10.596127 10.251687

32 Zn 4.331373 3.095874 2.085549 5.304893 5.304893

33 C 2.538853 1.414197 2.471354 8.462826 7.649959

34 C 2.889766 2.419164 3.716510 9.826193 8.834653

35 C 8.759591 7.804307 6.519046 2.695320 5.076192

36 C 3.624200 3.504549 4.847466 10.991147 9.886011

37 C 9.919684 8.996218 7.698507 3.076839 5.704299

38 C 8.205297 6.760801 6.519046 5.076192 2.695320

39 C 9.309915 7.872736 7.698507 5.704299 3.076839

40 C 4.213582 4.588151 3.716510 8.834653 9.826193

41 C 4.986025 5.588722 4.847466 9.886011 10.991147

42 H 5.794575 6.532511 5.873460 10.843556 12.029111

43 H 4.449255 4.516559 5.873460 12.029111 10.843556

44 H 10.306683 8.877496 8.748557 6.399953 3.720560

45 H 10.954859 10.054070 8.748557 3.720560 6.399953

26 27 28 29 30

26 H 0.000000

27 H 2.679707 0.000000

28 H 10.596127 10.251687 0.000000

29 H 10.251687 10.596127 2.679707 0.000000

30 H 7.492594 9.143877 7.492594 5.354198 0.000000

31 H 5.354198 7.492594 9.143877 7.492594 2.679707

32 Zn 5.304893 5.304893 5.304893 5.304893 5.304893

33 C 2.900841 4.638150 8.462826 7.649959 4.638150

34 C 2.695320 5.076192 9.826193 8.834653 5.076192

35 C 9.826193 8.834653 2.695320 5.076192 8.834653

36 C 3.076839 5.704299 10.991147 9.886011 5.704299

37 C 10.991147 9.886011 3.076839 5.704299 9.886011

38 C 5.076192 2.695320 8.834653 9.826193 9.826193

39 C 5.704299 3.076839 9.886011 10.991147 10.991147

40 C 8.834653 9.826193 5.076192 2.695320 2.695320

41 C 9.886011 10.991147 5.704299 3.076839 3.076839

42 H 10.843556 12.029111 6.399953 3.720560 3.720560

43 H 3.720560 6.399953 12.029111 10.843556 6.399953

44 H 6.399953 3.720560 10.843556 12.029111 12.029111

45 H 12.029111 10.843556 3.720560 6.399953 10.843556

31 32 33 34 35

31 H 0.000000

32 Zn 5.304893 0.000000

33 C 2.900841 3.462779 0.000000

34 C 2.695320 4.887919 1.426442 0.000000

35 C 9.826193 4.887919 8.338595 9.764931 0.000000

36 C 3.076839 6.092640 2.632096 1.205677 10.970604

37 C 10.991147 6.092640 9.544272 10.970604 1.205677

38 C 8.834653 4.887919 5.981927 6.904849 6.904849

39 C 9.886011 6.092640 7.000752 7.804095 7.804095

40 C 5.076192 4.887919 5.981927 6.904849 6.904849

41 C 5.704299 6.092640 7.000752 7.804095 7.804095

42 H 6.399953 7.159272 7.946411 8.662495 8.662495

43 H 3.720560 7.159272 3.699379 2.272979 12.037908

44 H 10.843556 7.159272 7.946411 8.662495 8.662495

45 H 12.029111 7.159272 10.611573 12.037908 2.272979

36 37 38 39 40

36 C 0.000000

37 C 12.176276 0.000000

38 C 7.804095 7.804095 0.000000

39 C 8.609927 8.609927 1.205677 0.000000

40 C 7.804095 7.804095 9.764931 10.970604 0.000000

41 C 8.609927 8.609927 10.970604 12.176276 1.205677

42 H 9.394987 9.394987 12.037908 13.243580 2.272979

43 H 1.067304 13.243580 8.662495 9.394987 8.662495

44 H 9.394987 9.394987 2.272979 1.067304 12.037908

45 H 13.243580 1.067304 8.662495 9.394987 8.662495

41 42 43 44 45

41 C 0.000000

42 H 1.067304 0.000000

43 H 9.394987 10.119323 0.000000

44 H 13.243580 14.310883 10.119323 0.000000

45 H 9.394987 10.119323 14.310883 10.119323 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

RotChk: IX=3 Diff= 3.23D-19

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.680936 -4.270633 -0.048020

2 6 0 -1.100587 -2.886094 -0.014345

3 7 0 0.000000 -2.077200 0.008066

4 6 0 1.100587 -2.886094 -0.014345

5 6 0 0.680936 -4.270633 -0.048020

6 6 0 2.443841 -2.443841 -0.020259

7 6 0 2.886094 -1.100587 -0.014345

8 7 0 2.077200 0.000000 0.008066

9 6 0 2.886094 1.100587 -0.014345

10 6 0 4.270633 0.680936 -0.048020

11 6 0 4.270633 -0.680936 -0.048020

12 6 0 -2.443841 -2.443841 -0.020259

13 6 0 -2.886094 -1.100587 -0.014345

14 6 0 -4.270633 -0.680936 -0.048020

15 6 0 -4.270633 0.680936 -0.048020

16 6 0 -2.886094 1.100587 -0.014345

17 7 0 -2.077200 0.000000 0.008066

18 6 0 -2.443841 2.443841 -0.020259

19 6 0 -1.100587 2.886094 -0.014345

20 6 0 -0.680936 4.270633 -0.048020

21 6 0 0.680936 4.270633 -0.048020

22 6 0 1.100587 2.886094 -0.014345

23 7 0 0.000000 2.077200 0.008066

24 1 0 -1.339854 -5.125843 -0.074603

25 1 0 1.339854 -5.125843 -0.074603

26 1 0 5.125843 1.339854 -0.074603

27 1 0 5.125843 -1.339854 -0.074603

28 1 0 -5.125843 -1.339854 -0.074603

29 1 0 -5.125843 1.339854 -0.074603

30 1 0 -1.339854 5.125843 -0.074603

31 1 0 1.339854 5.125843 -0.074603

32 30 0 0.000000 0.000000 0.194483

33 6 0 2.443841 2.443841 -0.020259

34 6 0 3.452424 3.452424 -0.036345

35 6 0 -3.452424 -3.452424 -0.036345

36 6 0 4.304964 4.304964 -0.039697

37 6 0 -4.304964 -4.304964 -0.039697

38 6 0 3.452424 -3.452424 -0.036345

39 6 0 4.304964 -4.304964 -0.039697

40 6 0 -3.452424 3.452424 -0.036345

41 6 0 -4.304964 4.304964 -0.039697

42 1 0 -5.059661 5.059661 -0.039687

43 1 0 5.059661 5.059661 -0.039687

44 1 0 5.059661 -5.059661 -0.039687

45 1 0 -5.059661 -5.059661 -0.039687

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

Rotational constants (GHZ): 0.1467381 0.1467381 0.0734302

Leave Link 202 at Fri Jul 26 14:20:56 2019, MaxMem= 1342177280 cpu: 0.1

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 184 symmetry adapted cartesian basis functions of A1 symmetry.

There are 155 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3062.6737166618 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= 9 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= -0.1305747179 Hartrees.

Nuclear repulsion after empirical dispersion term = 3062.5431419439 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: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3898

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.50D-05

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 140

GePol: Fraction of low-weight points (<1% of avg) = 3.59%

GePol: Cavity surface area = 414.877 Ang\*\*2

GePol: Cavity volume = 419.520 Ang\*\*3

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

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

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PCM non-electrostatic energy = 0.0083958809 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3062.5515378248 Hartrees.

Leave Link 301 at Fri Jul 26 14:20:56 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16223 LenP2D= 44848.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.38D-05 NBF= 172 148 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 172 148 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:20:56 2019, MaxMem= 1342177280 cpu: 6.5

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:20:57 2019, MaxMem= 1342177280 cpu: 0.8

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

Initial guess from the checkpoint file: "ZnTSPsim0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Occupied (E) (E) (B2) (A1) (E) (E) (B1) (A1) (B2) (E) (E)

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

(E) (E) (A1) (A2) (E) (E) (B1) (B1) (E) (E) (A1)

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

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

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

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

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

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

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(E) (E) (E)

The electronic state of the initial guess is 1-A1.

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= -1359.45363647030

Leave Link 401 at Fri Jul 26 14:20:58 2019, MaxMem= 1342177280 cpu: 21.1

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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.

An orbital has undefined symmetry, so N\*\*3 symmetry is turned off.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 660000000 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= 0 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= 45583212.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.10D-15 for 643.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.72D-15 for 2261 1943.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.66D-15 for 3879.

Iteration 1 A^-1\*A deviation from orthogonality is 1.26D-14 for 2171 2125.

E= -1359.05942878698

DIIS: error= 2.90D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.05942878698 IErMin= 1 ErrMin= 2.90D-03

ErrMax= 2.90D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.70D-03 BMatP= 2.70D-03

IDIUse=3 WtCom= 9.71D-01 WtEn= 2.90D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 3.231 Goal= None Shift= 0.000

GapD= 3.231 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.05D-04 MaxDP=3.06D-03 OVMax= 1.28D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.05D-04 CP: 1.00D+00

E= -1359.06291658403 Delta-E= -0.003487797054 Rises=F Damp=F

DIIS: error= 3.31D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.06291658403 IErMin= 2 ErrMin= 3.31D-04

ErrMax= 3.31D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.56D-05 BMatP= 2.70D-03

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.31D-03

Coeff-Com: -0.447D-01 0.104D+01

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

Coeff: -0.446D-01 0.104D+01

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.67D-05 MaxDP=6.04D-04 DE=-3.49D-03 OVMax= 1.80D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.45D-05 CP: 1.00D+00 1.08D+00

E= -1359.06293505641 Delta-E= -0.000018472374 Rises=F Damp=F

DIIS: error= 3.19D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.06293505641 IErMin= 3 ErrMin= 3.19D-04

ErrMax= 3.19D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.14D-05 BMatP= 2.56D-05

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

Coeff-Com: -0.308D-01 0.590D+00 0.441D+00

Coeff-En: 0.000D+00 0.244D+00 0.756D+00

Coeff: -0.111D-01 0.369D+00 0.642D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=1.38D-05 MaxDP=6.89D-04 DE=-1.85D-05 OVMax= 2.28D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 9.43D-06 CP: 1.00D+00 1.09D+00 3.15D-01

E= -1359.06294120799 Delta-E= -0.000006151585 Rises=F Damp=F

DIIS: error= 2.96D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.06294120799 IErMin= 4 ErrMin= 2.96D-04

ErrMax= 2.96D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.45D-05 BMatP= 2.56D-05

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.96D-03

Coeff-Com: -0.634D-02 0.840D-01 0.456D+00 0.466D+00

Coeff-En: 0.000D+00 0.000D+00 0.451D+00 0.549D+00

Coeff: -0.632D-02 0.837D-01 0.456D+00 0.466D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=6.60D-06 MaxDP=3.25D-04 DE=-6.15D-06 OVMax= 1.05D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.89D-06 CP: 1.00D+00 1.09D+00 6.28D-01 5.35D-01

E= -1359.06296222950 Delta-E= -0.000021021510 Rises=F Damp=F

DIIS: error= 2.77D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.06296222950 IErMin= 5 ErrMin= 2.77D-05

ErrMax= 2.77D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.09D-07 BMatP= 2.45D-05

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

Coeff-Com: -0.878D-03-0.243D-02 0.184D+00 0.222D+00 0.598D+00

Coeff: -0.878D-03-0.243D-02 0.184D+00 0.222D+00 0.598D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=8.79D-07 MaxDP=3.85D-05 DE=-2.10D-05 OVMax= 9.58D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 5.40D-07 CP: 1.00D+00 1.09D+00 6.51D-01 5.62D-01 7.11D-01

E= -1359.06296237812 Delta-E= -0.000000148614 Rises=F Damp=F

DIIS: error= 1.47D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.06296237812 IErMin= 6 ErrMin= 1.47D-05

ErrMax= 1.47D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.90D-08 BMatP= 2.09D-07

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

Coeff-Com: 0.323D-03-0.140D-01 0.527D-01 0.756D-01 0.378D+00 0.507D+00

Coeff: 0.323D-03-0.140D-01 0.527D-01 0.756D-01 0.378D+00 0.507D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=3.19D-07 MaxDP=1.74D-05 DE=-1.49D-07 OVMax= 4.76D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.69D-07 CP: 1.00D+00 1.09D+00 6.51D-01 5.71D-01 7.34D-01

CP: 5.43D-01

E= -1359.06296243017 Delta-E= -0.000000052055 Rises=F Damp=F

DIIS: error= 3.70D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.06296243017 IErMin= 7 ErrMin= 3.70D-06

ErrMax= 3.70D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.97D-09 BMatP= 5.90D-08

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

Coeff-Com: 0.267D-03-0.824D-02 0.149D-01 0.255D-01 0.173D+00 0.298D+00

Coeff-Com: 0.497D+00

Coeff: 0.267D-03-0.824D-02 0.149D-01 0.255D-01 0.173D+00 0.298D+00

Coeff: 0.497D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=9.33D-08 MaxDP=6.52D-06 DE=-5.21D-08 OVMax= 1.37D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.03D-08 CP: 1.00D+00 1.09D+00 6.51D-01 5.70D-01 7.52D-01

CP: 5.84D-01 6.52D-01

E= -1359.06296243474 Delta-E= -0.000000004568 Rises=F Damp=F

DIIS: error= 1.18D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.06296243474 IErMin= 8 ErrMin= 1.18D-06

ErrMax= 1.18D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.78D-10 BMatP= 4.97D-09

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

Coeff-Com: 0.103D-03-0.288D-02 0.280D-02 0.610D-02 0.541D-01 0.106D+00

Coeff-Com: 0.255D+00 0.579D+00

Coeff: 0.103D-03-0.288D-02 0.280D-02 0.610D-02 0.541D-01 0.106D+00

Coeff: 0.255D+00 0.579D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 305122 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.39D-08 MaxDP=1.16D-06 DE=-4.57D-09 OVMax= 2.78D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.13D-08 CP: 1.00D+00 1.09D+00 6.51D-01 5.70D-01 7.54D-01

CP: 5.87D-01 6.84D-01 8.67D-01

E= -1359.06296243467 Delta-E= 0.000000000066 Rises=F Damp=F

DIIS: error= 1.55D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 8 EnMin= -1359.06296243474 IErMin= 9 ErrMin= 1.55D-07

ErrMax= 1.55D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.14D-11 BMatP= 2.78D-10

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

Coeff-Com: 0.768D-05-0.101D-03-0.626D-03-0.613D-03 0.141D-03 0.551D-02

Coeff-Com: 0.376D-01 0.203D+00 0.755D+00

Coeff: 0.768D-05-0.101D-03-0.626D-03-0.613D-03 0.141D-03 0.551D-02

Coeff: 0.376D-01 0.203D+00 0.755D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=7.32D-09 MaxDP=2.31D-07 DE= 6.64D-11 OVMax= 7.04D-07

Error on total polarization charges = 0.06212

SCF Done: E(RB3LYP) = -1359.06296243 A.U. after 9 cycles

NFock= 9 Conv=0.73D-08 -V/T= 1.9681

KE= 1.403775461799D+03 PE=-9.367235920735D+03 EE= 3.541845958677D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.27

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:21:37 2019, MaxMem= 1342177280 cpu: 426.6

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16223 LenP2D= 44848.

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 Fri Jul 26 14:21:40 2019, MaxMem= 1342177280 cpu: 43.5

(Enter /apps/gaussian/g09d01/g09/l702.exe)

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

Leave Link 702 at Fri Jul 26 14:21:40 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Fri Jul 26 14:21:44 2019, MaxMem= 1342177280 cpu: 43.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 4.61852778D-14-2.77111667D-13 3.98173794D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000227158 -0.000098350 -0.000079053

2 6 0.000486276 0.000217924 -0.000095280

3 7 0.000000000 0.001284869 0.000036764

4 6 -0.000486276 0.000217924 -0.000095280

5 6 -0.000227158 -0.000098350 -0.000079053

6 6 -0.000251125 0.000251125 0.000445911

7 6 -0.000217924 0.000486276 -0.000095280

8 7 -0.001284869 0.000000000 0.000036764

9 6 -0.000217924 -0.000486276 -0.000095280

10 6 0.000098350 -0.000227158 -0.000079053

11 6 0.000098350 0.000227158 -0.000079053

12 6 0.000251125 0.000251125 0.000445911

13 6 0.000217924 0.000486276 -0.000095280

14 6 -0.000098350 0.000227158 -0.000079053

15 6 -0.000098350 -0.000227158 -0.000079053

16 6 0.000217924 -0.000486276 -0.000095280

17 7 0.001284869 0.000000000 0.000036764

18 6 0.000251125 -0.000251125 0.000445911

19 6 0.000486276 -0.000217924 -0.000095280

20 6 0.000227158 0.000098350 -0.000079053

21 6 -0.000227158 0.000098350 -0.000079053

22 6 -0.000486276 -0.000217924 -0.000095280

23 7 0.000000000 -0.001284869 0.000036764

24 1 -0.000046917 -0.000170245 0.000019895

25 1 0.000046917 -0.000170245 0.000019895

26 1 0.000170245 0.000046917 0.000019895

27 1 0.000170245 -0.000046917 0.000019895

28 1 -0.000170245 -0.000046917 0.000019895

29 1 -0.000170245 0.000046917 0.000019895

30 1 -0.000046917 0.000170245 0.000019895

31 1 0.000046917 0.000170245 0.000019895

32 30 0.000000000 0.000000000 -0.001061098

33 6 -0.000251125 -0.000251125 0.000445911

34 6 -0.000210312 -0.000210312 0.000284937

35 6 0.000210312 0.000210312 0.000284937

36 6 -0.000156192 -0.000156192 -0.000041280

37 6 0.000156192 0.000156192 -0.000041280

38 6 -0.000210312 0.000210312 0.000284937

39 6 -0.000156192 0.000156192 -0.000041280

40 6 0.000210312 -0.000210312 0.000284937

41 6 0.000156192 -0.000156192 -0.000041280

42 1 0.000018946 -0.000018946 -0.000152181

43 1 -0.000018946 -0.000018946 -0.000152181

44 1 -0.000018946 0.000018946 -0.000152181

45 1 0.000018946 0.000018946 -0.000152181

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

Cartesian Forces: Max 0.001284869 RMS 0.000312077

Leave Link 716 at Fri Jul 26 14:21:44 2019, MaxMem= 1342177280 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001223991 RMS 0.000283224

Search for a local minimum.

Step number 12 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .28322D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

7 9 8 10 11

12

DE= 1.77D-06 DEPred=-9.51D-05 R=-1.87D-02

Trust test=-1.87D-02 RLast= 1.32D-01 DXMaxT set to 5.00D-02

ITU= -1 1 0 -1 0 0 -1 1 0 -1 -1 0

Eigenvalues --- 0.00534 0.00534 0.00534 0.00534 0.00534

Eigenvalues --- 0.00534 0.00534 0.00557 0.01169 0.01218

Eigenvalues --- 0.01218 0.01251 0.01415 0.01415 0.01647

Eigenvalues --- 0.01674 0.01737 0.01737 0.01805 0.01805

Eigenvalues --- 0.01806 0.01825 0.01831 0.01859 0.01859

Eigenvalues --- 0.01868 0.01868 0.01868 0.01899 0.01908

Eigenvalues --- 0.01920 0.01927 0.01927 0.01933 0.01962

Eigenvalues --- 0.01962 0.01964 0.02062 0.02178 0.02180

Eigenvalues --- 0.02185 0.02185 0.03320 0.04268 0.04654

Eigenvalues --- 0.04654 0.04654 0.04654 0.04654 0.04654

Eigenvalues --- 0.04654 0.08164 0.13851 0.15011 0.15011

Eigenvalues --- 0.15755 0.15999 0.15999 0.15999 0.15999

Eigenvalues --- 0.16000 0.16000 0.16000 0.18814 0.22830

Eigenvalues --- 0.22868 0.22872 0.22872 0.24749 0.24756

Eigenvalues --- 0.24756 0.24792 0.24833 0.24976 0.24976

Eigenvalues --- 0.24997 0.25000 0.25000 0.25000 0.25001

Eigenvalues --- 0.26816 0.35031 0.35031 0.35455 0.35491

Eigenvalues --- 0.35522 0.36034 0.36034 0.36034 0.36034

Eigenvalues --- 0.36034 0.36034 0.36034 0.36093 0.36787

Eigenvalues --- 0.36867 0.36867 0.37535 0.37563 0.37563

Eigenvalues --- 0.37563 0.38009 0.38965 0.38965 0.39534

Eigenvalues --- 0.41397 0.41397 0.41397 0.41507 0.41508

Eigenvalues --- 0.41508 0.41785 0.42514 0.43517 0.43782

Eigenvalues --- 0.43782 0.45610 0.47883 0.49079 0.49079

Eigenvalues --- 0.50124 0.51396 0.51900 0.51900 0.54498

Eigenvalues --- 1.01831 1.01831 1.01831 1.01865

En-DIIS/RFO-DIIS IScMMF= 0 using points: 12 11 10

RFO step: Lambda=-4.87526821D-05.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=F DC= 9.12D-05 SmlDif= 1.00D-05

RMS Error= 0.7439007047D-03 NUsed= 3 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.51569 0.59852 -0.11421

Iteration 1 RMS(Cart)= 0.01006593 RMS(Int)= 0.00005079

Iteration 2 RMS(Cart)= 0.00009064 RMS(Int)= 0.00001247

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001247

ITry= 1 IFail=0 DXMaxC= 6.61D-02 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.53D-03 for atom 45.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73468 -0.00017 -0.00089 0.00050 -0.00040 2.73429

R2 2.57357 0.00046 0.00094 -0.00004 0.00090 2.57447

R3 2.04078 -0.00016 -0.00036 0.00004 -0.00031 2.04047

R4 2.58147 0.00064 0.00168 -0.00086 0.00082 2.58228

R5 2.67245 0.00056 0.00216 -0.00022 0.00208 2.67453

R6 2.58147 0.00064 0.00168 -0.00086 0.00082 2.58228

R7 3.94112 0.00122 0.00337 0.00059 0.00424 3.94536

R8 2.73468 -0.00017 -0.00089 0.00050 -0.00040 2.73429

R9 2.67245 0.00056 0.00216 -0.00022 0.00208 2.67453

R10 2.04078 -0.00016 -0.00036 0.00004 -0.00031 2.04047

R11 2.67245 0.00056 0.00216 -0.00022 0.00208 2.67453

R12 2.69559 0.00054 -0.00111 0.00171 0.00023 2.69582

R13 2.58147 0.00064 0.00168 -0.00086 0.00082 2.58228

R14 2.73468 -0.00017 -0.00089 0.00050 -0.00040 2.73429

R15 2.58147 0.00064 0.00168 -0.00086 0.00082 2.58228

R16 3.94112 0.00122 0.00337 0.00058 0.00424 3.94536

R17 2.73468 -0.00017 -0.00089 0.00050 -0.00040 2.73429

R18 2.67245 0.00056 0.00216 -0.00022 0.00208 2.67453

R19 2.57357 0.00046 0.00094 -0.00004 0.00090 2.57447

R20 2.04078 -0.00016 -0.00036 0.00004 -0.00031 2.04047

R21 2.04078 -0.00016 -0.00036 0.00004 -0.00031 2.04047

R22 2.67245 0.00056 0.00216 -0.00022 0.00208 2.67453

R23 2.69559 0.00054 -0.00111 0.00171 0.00023 2.69582

R24 2.73468 -0.00017 -0.00089 0.00050 -0.00040 2.73429

R25 2.58147 0.00064 0.00168 -0.00086 0.00082 2.58228

R26 2.57357 0.00046 0.00094 -0.00004 0.00090 2.57447

R27 2.04078 -0.00016 -0.00036 0.00004 -0.00031 2.04047

R28 2.73468 -0.00017 -0.00089 0.00050 -0.00040 2.73429

R29 2.04078 -0.00016 -0.00036 0.00004 -0.00031 2.04047

R30 2.58147 0.00064 0.00168 -0.00086 0.00082 2.58228

R31 2.67245 0.00056 0.00216 -0.00022 0.00208 2.67453

R32 3.94112 0.00122 0.00337 0.00058 0.00424 3.94536

R33 2.67245 0.00056 0.00216 -0.00022 0.00208 2.67453

R34 2.69559 0.00054 -0.00111 0.00171 0.00023 2.69582

R35 2.73468 -0.00017 -0.00089 0.00050 -0.00040 2.73429

R36 2.58147 0.00064 0.00168 -0.00086 0.00082 2.58228

R37 2.57357 0.00046 0.00094 -0.00004 0.00090 2.57447

R38 2.04078 -0.00016 -0.00036 0.00004 -0.00031 2.04047

R39 2.73468 -0.00017 -0.00089 0.00050 -0.00040 2.73429

R40 2.04078 -0.00016 -0.00036 0.00004 -0.00031 2.04047

R41 2.58147 0.00064 0.00168 -0.00086 0.00082 2.58228

R42 2.67245 0.00056 0.00216 -0.00022 0.00208 2.67453

R43 3.94112 0.00122 0.00337 0.00058 0.00424 3.94536

R44 2.69559 0.00054 -0.00111 0.00171 0.00023 2.69582

R45 2.27840 0.00025 0.00017 0.00004 0.00021 2.27861

R46 2.27840 0.00025 0.00017 0.00004 0.00021 2.27861

R47 2.01691 0.00003 -0.00007 0.00010 0.00003 2.01694

R48 2.01691 0.00003 -0.00007 0.00010 0.00003 2.01694

R49 2.27840 0.00025 0.00017 0.00004 0.00021 2.27861

R50 2.01691 0.00003 -0.00007 0.00010 0.00003 2.01694

R51 2.27840 0.00025 0.00017 0.00004 0.00021 2.27861

R52 2.01691 0.00003 -0.00007 0.00010 0.00003 2.01694

A1 1.86501 0.00023 0.00074 0.00004 0.00078 1.86579

A2 2.19111 -0.00019 -0.00125 0.00042 -0.00083 2.19028

A3 2.22704 -0.00005 0.00052 -0.00046 0.00006 2.22710

A4 1.91057 -0.00042 -0.00126 -0.00064 -0.00190 1.90867

A5 2.18284 0.00011 0.00023 0.00067 0.00094 2.18378

A6 2.18970 0.00031 0.00098 0.00002 0.00095 2.19066

A7 1.87361 0.00036 0.00104 0.00120 0.00224 1.87585

A8 2.20339 -0.00018 -0.00012 -0.00056 -0.00066 2.20273

A9 2.20339 -0.00018 -0.00012 -0.00056 -0.00066 2.20273

A10 1.91057 -0.00042 -0.00126 -0.00064 -0.00190 1.90867

A11 2.18970 0.00031 0.00098 0.00002 0.00095 2.19066

A12 2.18284 0.00011 0.00023 0.00067 0.00094 2.18378

A13 1.86501 0.00023 0.00074 0.00004 0.00078 1.86579

A14 2.22704 -0.00005 0.00052 -0.00046 0.00006 2.22710

A15 2.19111 -0.00019 -0.00125 0.00042 -0.00083 2.19028

A16 2.20688 -0.00025 -0.00073 0.00105 0.00036 2.20725

A17 2.03815 0.00013 0.00033 -0.00052 -0.00020 2.03795

A18 2.03815 0.00013 0.00033 -0.00053 -0.00020 2.03795

A19 2.18970 0.00031 0.00098 0.00002 0.00095 2.19066

A20 2.18284 0.00011 0.00023 0.00067 0.00094 2.18378

A21 1.91057 -0.00042 -0.00126 -0.00064 -0.00190 1.90867

A22 1.87361 0.00036 0.00104 0.00120 0.00224 1.87585

A23 2.20339 -0.00018 -0.00012 -0.00056 -0.00066 2.20273

A24 2.20339 -0.00018 -0.00012 -0.00056 -0.00066 2.20273

A25 1.91057 -0.00042 -0.00126 -0.00064 -0.00190 1.90867

A26 2.18970 0.00031 0.00098 0.00002 0.00095 2.19066

A27 2.18284 0.00011 0.00023 0.00067 0.00094 2.18378

A28 1.86501 0.00023 0.00074 0.00004 0.00078 1.86579

A29 2.19111 -0.00019 -0.00125 0.00042 -0.00083 2.19028

A30 2.22704 -0.00005 0.00052 -0.00046 0.00006 2.22710

A31 1.86501 0.00023 0.00074 0.00004 0.00078 1.86579

A32 2.19111 -0.00019 -0.00125 0.00042 -0.00083 2.19028

A33 2.22704 -0.00005 0.00052 -0.00046 0.00006 2.22710

A34 2.20688 -0.00025 -0.00073 0.00105 0.00036 2.20725

A35 2.03815 0.00013 0.00033 -0.00052 -0.00020 2.03795

A36 2.03815 0.00013 0.00033 -0.00053 -0.00020 2.03795

A37 2.18284 0.00011 0.00023 0.00067 0.00094 2.18378

A38 2.18970 0.00031 0.00098 0.00002 0.00095 2.19066

A39 1.91057 -0.00042 -0.00126 -0.00064 -0.00190 1.90867

A40 1.86501 0.00023 0.00074 0.00004 0.00078 1.86579

A41 2.19111 -0.00019 -0.00125 0.00042 -0.00083 2.19028

A42 2.22704 -0.00005 0.00052 -0.00046 0.00006 2.22710

A43 1.86501 0.00023 0.00074 0.00004 0.00078 1.86579

A44 2.22704 -0.00005 0.00052 -0.00046 0.00006 2.22710

A45 2.19111 -0.00019 -0.00125 0.00042 -0.00083 2.19028

A46 1.91057 -0.00042 -0.00126 -0.00064 -0.00190 1.90867

A47 2.18284 0.00011 0.00023 0.00067 0.00094 2.18378

A48 2.18970 0.00031 0.00098 0.00002 0.00095 2.19066

A49 1.87361 0.00036 0.00104 0.00120 0.00224 1.87585

A50 2.20339 -0.00018 -0.00012 -0.00056 -0.00066 2.20273

A51 2.20339 -0.00018 -0.00012 -0.00056 -0.00066 2.20273

A52 2.20688 -0.00025 -0.00073 0.00105 0.00036 2.20725

A53 2.03815 0.00013 0.00033 -0.00052 -0.00020 2.03795

A54 2.03815 0.00013 0.00033 -0.00053 -0.00020 2.03795

A55 2.18284 0.00011 0.00023 0.00067 0.00094 2.18378

A56 2.18970 0.00031 0.00098 0.00002 0.00095 2.19066

A57 1.91057 -0.00042 -0.00126 -0.00064 -0.00190 1.90867

A58 1.86501 0.00023 0.00074 0.00004 0.00078 1.86579

A59 2.19111 -0.00019 -0.00125 0.00042 -0.00083 2.19028

A60 2.22704 -0.00005 0.00052 -0.00046 0.00006 2.22710

A61 1.86501 0.00023 0.00074 0.00004 0.00078 1.86579

A62 2.22704 -0.00005 0.00052 -0.00046 0.00006 2.22710

A63 2.19111 -0.00019 -0.00125 0.00042 -0.00083 2.19028

A64 1.91057 -0.00042 -0.00126 -0.00064 -0.00190 1.90867

A65 2.18284 0.00011 0.00023 0.00067 0.00094 2.18378

A66 2.18970 0.00031 0.00098 0.00002 0.00095 2.19066

A67 1.87361 0.00036 0.00104 0.00120 0.00224 1.87585

A68 2.20339 -0.00018 -0.00012 -0.00056 -0.00066 2.20273

A69 2.20339 -0.00018 -0.00012 -0.00056 -0.00066 2.20273

A70 1.56281 0.00003 0.00067 0.00093 0.00153 1.56434

A71 1.56281 0.00003 0.00067 0.00093 0.00153 1.56434

A72 2.96258 0.00031 0.00769 0.01040 0.01811 2.98069

A73 2.96258 0.00031 0.00769 0.01040 0.01811 2.98069

A74 1.56281 0.00003 0.00067 0.00093 0.00153 1.56434

A75 1.56281 0.00003 0.00067 0.00093 0.00153 1.56434

A76 2.20688 -0.00025 -0.00073 0.00105 0.00036 2.20725

A77 2.03815 0.00013 0.00033 -0.00052 -0.00020 2.03795

A78 2.03815 0.00013 0.00033 -0.00053 -0.00020 2.03795

A79 3.14172 -0.00001 -0.00006 0.00008 -0.00014 3.14158

A80 3.14172 -0.00001 -0.00006 0.00008 -0.00014 3.14158

A81 3.14163 0.00000 0.00005 0.00140 -0.00003 3.14160

A82 3.14163 0.00000 0.00005 0.00140 -0.00003 3.14160

A83 3.14172 -0.00001 -0.00006 0.00008 -0.00014 3.14158

A84 3.14163 0.00000 0.00005 0.00140 -0.00003 3.14160

A85 3.14172 -0.00001 -0.00006 0.00008 -0.00014 3.14158

A86 3.14163 0.00000 0.00005 0.00140 -0.00003 3.14160

A87 3.15015 -0.00074 -0.00403 -0.00514 -0.00917 3.14097

A88 3.13304 0.00074 0.00403 0.00514 0.00917 3.14221

A89 3.14480 -0.00027 0.00521 -0.00805 -0.00282 3.14198

A90 3.13839 0.00027 -0.00521 0.00805 0.00282 3.14121

A91 3.15015 -0.00074 -0.00403 -0.00514 -0.00917 3.14097

A92 3.14480 -0.00027 0.00521 -0.00805 -0.00282 3.14198

A93 3.13304 0.00074 0.00403 0.00514 0.00917 3.14221

A94 3.13839 0.00027 -0.00521 0.00805 0.00282 3.14121

D1 -0.00213 0.00008 -0.00032 0.00031 -0.00001 -0.00213

D2 3.12719 0.00010 -0.00426 0.00406 -0.00021 3.12699

D3 -3.13714 0.00001 -0.00282 0.00077 -0.00205 -3.13919

D4 -0.00782 0.00003 -0.00676 0.00452 -0.00225 -0.01007

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13484 -0.00007 -0.00257 0.00047 -0.00209 -3.13693

D7 3.13484 0.00007 0.00257 -0.00047 0.00209 3.13693

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00343 -0.00013 0.00052 -0.00050 0.00002 0.00345

D10 -3.06150 -0.00011 -0.01236 -0.00154 -0.01391 -3.07541

D11 -3.12583 -0.00015 0.00449 -0.00427 0.00022 -3.12561

D12 0.09243 -0.00012 -0.00839 -0.00531 -0.01370 0.07872

D13 -3.11851 0.00002 0.00499 -0.00184 0.00314 -3.11536

D14 0.02085 -0.00011 -0.00256 -0.00165 -0.00421 0.01664

D15 0.00888 0.00004 0.00039 0.00249 0.00289 0.01177

D16 -3.13495 -0.00010 -0.00715 0.00269 -0.00447 -3.13941

D17 -0.00343 0.00013 -0.00052 0.00050 -0.00002 -0.00345

D18 3.12583 0.00015 -0.00449 0.00427 -0.00022 3.12561

D19 3.06150 0.00011 0.01236 0.00154 0.01391 3.07541

D20 -0.09243 0.00012 0.00839 0.00531 0.01370 -0.07872

D21 -3.09783 -0.00015 0.00384 -0.00449 -0.00067 -3.09849

D22 -0.13453 0.00015 0.01144 0.00579 0.01725 -0.11728

D23 -1.61618 0.00000 0.00764 0.00065 0.00829 -1.60789

D24 0.13453 -0.00015 -0.01144 -0.00579 -0.01725 0.11728

D25 3.09783 0.00015 -0.00384 0.00449 0.00067 3.09849

D26 1.61618 0.00000 -0.00764 -0.00065 -0.00829 1.60789

D27 0.00213 -0.00008 0.00032 -0.00031 0.00001 0.00213

D28 3.13714 -0.00001 0.00282 -0.00077 0.00205 3.13919

D29 -3.12719 -0.00010 0.00426 -0.00406 0.00021 -3.12699

D30 0.00782 -0.00003 0.00676 -0.00452 0.00225 0.01007

D31 -0.00888 -0.00004 -0.00039 -0.00249 -0.00289 -0.01177

D32 3.13495 0.00010 0.00715 -0.00269 0.00447 3.13941

D33 3.11851 -0.00002 -0.00499 0.00184 -0.00314 3.11536

D34 -0.02085 0.00011 0.00256 0.00165 0.00421 -0.01664

D35 0.00888 0.00004 0.00039 0.00249 0.00289 0.01177

D36 -3.11851 0.00002 0.00499 -0.00184 0.00314 -3.11536

D37 -3.13495 -0.00010 -0.00715 0.00269 -0.00447 -3.13941

D38 0.02085 -0.00011 -0.00256 -0.00165 -0.00421 0.01664

D39 -3.12583 -0.00015 0.00449 -0.00427 0.00022 -3.12561

D40 0.09243 -0.00012 -0.00839 -0.00531 -0.01370 0.07872

D41 0.00343 -0.00013 0.00052 -0.00050 0.00002 0.00345

D42 -3.06150 -0.00011 -0.01236 -0.00154 -0.01391 -3.07541

D43 3.12719 0.00010 -0.00426 0.00406 -0.00021 3.12699

D44 -0.00782 0.00003 -0.00676 0.00452 -0.00225 -0.01007

D45 -0.00213 0.00008 -0.00032 0.00031 -0.00001 -0.00213

D46 -3.13714 0.00001 -0.00282 0.00077 -0.00205 -3.13919

D47 -0.00343 0.00013 -0.00052 0.00050 -0.00002 -0.00345

D48 3.12583 0.00015 -0.00449 0.00427 -0.00022 3.12561

D49 3.06150 0.00011 0.01236 0.00154 0.01391 3.07541

D50 -0.09243 0.00012 0.00839 0.00531 0.01370 -0.07872

D51 -0.13453 0.00015 0.01144 0.00579 0.01725 -0.11728

D52 -1.61618 0.00000 0.00764 0.00065 0.00829 -1.60789

D53 -3.09783 -0.00015 0.00384 -0.00449 -0.00067 -3.09849

D54 3.09783 0.00015 -0.00384 0.00449 0.00067 3.09849

D55 1.61618 0.00000 -0.00764 -0.00065 -0.00829 1.60789

D56 0.13453 -0.00015 -0.01144 -0.00579 -0.01725 0.11728

D57 0.00213 -0.00008 0.00032 -0.00031 0.00001 0.00213

D58 3.13714 -0.00001 0.00282 -0.00077 0.00205 3.13919

D59 -3.12719 -0.00010 0.00426 -0.00406 0.00021 -3.12699

D60 0.00782 -0.00003 0.00676 -0.00452 0.00225 0.01007

D61 -0.00888 -0.00004 -0.00039 -0.00249 -0.00289 -0.01177

D62 3.13495 0.00010 0.00715 -0.00269 0.00447 3.13941

D63 3.11851 -0.00002 -0.00499 0.00184 -0.00314 3.11536

D64 -0.02085 0.00011 0.00256 0.00165 0.00421 -0.01664

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13484 0.00007 0.00257 -0.00047 0.00209 3.13693

D67 -3.13484 -0.00007 -0.00257 0.00047 -0.00209 -3.13693

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.11851 -0.00002 -0.00499 0.00184 -0.00314 3.11536

D70 -0.00888 -0.00004 -0.00039 -0.00249 -0.00289 -0.01177

D71 -0.02085 0.00011 0.00256 0.00165 0.00421 -0.01664

D72 3.13495 0.00010 0.00715 -0.00269 0.00447 3.13941

D73 -3.12719 -0.00010 0.00426 -0.00406 0.00021 -3.12699

D74 0.00782 -0.00003 0.00676 -0.00452 0.00225 0.01007

D75 0.00213 -0.00008 0.00032 -0.00031 0.00001 0.00213

D76 3.13714 -0.00001 0.00282 -0.00077 0.00205 3.13919

D77 3.12583 0.00015 -0.00449 0.00427 -0.00022 3.12561

D78 -0.09243 0.00012 0.00839 0.00531 0.01370 -0.07872

D79 -0.00343 0.00013 -0.00052 0.00050 -0.00002 -0.00345

D80 3.06150 0.00011 0.01236 0.00154 0.01391 3.07541

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 3.13484 0.00007 0.00257 -0.00047 0.00209 3.13693

D83 -3.13484 -0.00007 -0.00257 0.00047 -0.00209 -3.13693

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 -0.00213 0.00008 -0.00032 0.00031 -0.00001 -0.00213

D86 3.12719 0.00010 -0.00426 0.00406 -0.00021 3.12699

D87 -3.13714 0.00001 -0.00282 0.00077 -0.00205 -3.13919

D88 -0.00782 0.00003 -0.00676 0.00452 -0.00225 -0.01007

D89 0.00343 -0.00013 0.00052 -0.00050 0.00002 0.00345

D90 -3.06150 -0.00011 -0.01236 -0.00154 -0.01391 -3.07541

D91 -3.12583 -0.00015 0.00449 -0.00427 0.00022 -3.12561

D92 0.09243 -0.00012 -0.00839 -0.00531 -0.01370 0.07872

D93 -3.11851 0.00002 0.00499 -0.00184 0.00314 -3.11536

D94 0.02085 -0.00011 -0.00256 -0.00165 -0.00421 0.01664

D95 0.00888 0.00004 0.00039 0.00249 0.00289 0.01177

D96 -3.13495 -0.00010 -0.00715 0.00269 -0.00447 -3.13941

D97 0.13453 -0.00015 -0.01144 -0.00579 -0.01725 0.11728

D98 1.61618 0.00000 -0.00764 -0.00065 -0.00829 1.60789

D99 3.09783 0.00015 -0.00384 0.00449 0.00067 3.09849

D100 -3.09783 -0.00015 0.00384 -0.00449 -0.00067 -3.09849

D101 -1.61618 0.00000 0.00764 0.00065 0.00829 -1.60789

D102 -0.13453 0.00015 0.01144 0.00579 0.01725 -0.11728

D103 3.11851 -0.00002 -0.00499 0.00184 -0.00314 3.11536

D104 -0.00888 -0.00004 -0.00039 -0.00249 -0.00289 -0.01177

D105 -0.02085 0.00011 0.00256 0.00165 0.00421 -0.01664

D106 3.13495 0.00010 0.00715 -0.00269 0.00447 3.13941

D107 -3.12719 -0.00010 0.00426 -0.00406 0.00021 -3.12699

D108 0.00782 -0.00003 0.00676 -0.00452 0.00225 0.01007

D109 0.00213 -0.00008 0.00032 -0.00031 0.00001 0.00213

D110 3.13714 -0.00001 0.00282 -0.00077 0.00205 3.13919

D111 3.12583 0.00015 -0.00449 0.00427 -0.00022 3.12561

D112 -0.09243 0.00012 0.00839 0.00531 0.01370 -0.07872

D113 -0.00343 0.00013 -0.00052 0.00050 -0.00002 -0.00345

D114 3.06150 0.00011 0.01236 0.00154 0.01391 3.07541

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.13484 0.00007 0.00257 -0.00047 0.00209 3.13693

D117 -3.13484 -0.00007 -0.00257 0.00047 -0.00209 -3.13693

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 -0.00213 0.00008 -0.00032 0.00031 -0.00001 -0.00213

D120 3.12719 0.00010 -0.00426 0.00406 -0.00021 3.12699

D121 -3.13714 0.00001 -0.00282 0.00077 -0.00205 -3.13919

D122 -0.00782 0.00003 -0.00676 0.00452 -0.00225 -0.01007

D123 0.00343 -0.00013 0.00052 -0.00050 0.00002 0.00345

D124 -3.06150 -0.00011 -0.01236 -0.00154 -0.01391 -3.07541

D125 -3.12583 -0.00015 0.00449 -0.00427 0.00022 -3.12561

D126 0.09243 -0.00012 -0.00839 -0.00531 -0.01370 0.07872

D127 -3.11851 0.00002 0.00499 -0.00184 0.00314 -3.11536

D128 0.02085 -0.00011 -0.00256 -0.00165 -0.00421 0.01664

D129 0.00888 0.00004 0.00039 0.00249 0.00289 0.01177

D130 -3.13495 -0.00010 -0.00715 0.00269 -0.00447 -3.13941

D131 1.61618 0.00000 -0.00764 -0.00065 -0.00829 1.60789

D132 3.09783 0.00015 -0.00384 0.00449 0.00067 3.09849

D133 0.13453 -0.00015 -0.01144 -0.00579 -0.01725 0.11728

D134 -1.61618 0.00000 0.00764 0.00065 0.00829 -1.60789

D135 -0.13453 0.00015 0.01144 0.00579 0.01725 -0.11728

D136 -3.09783 -0.00015 0.00384 -0.00449 -0.00067 -3.09849

Item Value Threshold Converged?

Maximum Force 0.001224 0.000450 NO

RMS Force 0.000283 0.000300 YES

Maximum Displacement 0.066059 0.001800 NO

RMS Displacement 0.010058 0.001200 NO

Predicted change in Energy=-7.715731D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:21:44 2019, MaxMem= 1342177280 cpu: 1.1

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.681175 4.272842 -0.044033

2 6 0 1.101843 2.888905 -0.007434

3 7 0 0.000000 2.081041 0.016680

4 6 0 -1.101843 2.888905 -0.007434

5 6 0 -0.681175 4.272842 -0.044033

6 6 0 -2.446068 2.446068 -0.012638

7 6 0 -2.888905 1.101843 -0.007434

8 7 0 -2.081041 0.000000 0.016680

9 6 0 -2.888905 -1.101843 -0.007434

10 6 0 -4.272842 -0.681175 -0.044033

11 6 0 -4.272842 0.681175 -0.044033

12 6 0 2.446068 2.446068 -0.012638

13 6 0 2.888905 1.101843 -0.007434

14 6 0 4.272842 0.681175 -0.044033

15 6 0 4.272842 -0.681175 -0.044033

16 6 0 2.888905 -1.101843 -0.007434

17 7 0 2.081041 0.000000 0.016680

18 6 0 2.446068 -2.446068 -0.012638

19 6 0 1.101843 -2.888905 -0.007434

20 6 0 0.681175 -4.272842 -0.044033

21 6 0 -0.681175 -4.272842 -0.044033

22 6 0 -1.101843 -2.888905 -0.007434

23 7 0 0.000000 -2.081041 0.016680

24 1 0 1.340047 5.127878 -0.070637

25 1 0 -1.340047 5.127878 -0.070637

26 1 0 -5.127878 -1.340047 -0.070637

27 1 0 -5.127878 1.340047 -0.070637

28 1 0 5.127878 1.340047 -0.070637

29 1 0 5.127878 -1.340047 -0.070637

30 1 0 1.340047 -5.127878 -0.070637

31 1 0 -1.340047 -5.127878 -0.070637

32 30 0 0.000000 0.000000 0.184465

33 6 0 -2.446068 -2.446068 -0.012638

34 6 0 -3.454661 -3.454661 -0.036499

35 6 0 3.454661 3.454661 -0.036499

36 6 0 -4.307154 -4.307154 -0.057407

37 6 0 4.307154 4.307154 -0.057407

38 6 0 -3.454661 3.454661 -0.036499

39 6 0 -4.307154 4.307154 -0.057407

40 6 0 3.454661 -3.454661 -0.036499

41 6 0 4.307154 -4.307154 -0.057407

42 1 0 5.061754 -5.061754 -0.075557

43 1 0 -5.061754 -5.061754 -0.075557

44 1 0 -5.061754 5.061754 -0.075557

45 1 0 5.061754 5.061754 -0.075557

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.446922 0.000000

3 N 2.296014 1.366486 0.000000

4 C 2.257382 2.203685 1.366486 0.000000

5 C 1.362351 2.257382 2.296014 1.446922 0.000000

6 C 3.621842 3.575444 2.473328 1.415299 2.540262

7 C 4.775149 4.372603 3.050439 2.527287 3.864019

8 N 5.088290 4.298499 2.943036 3.050439 4.496719

9 C 6.452445 5.643769 4.298499 4.372603 5.810563

10 C 7.006038 6.452445 5.088290 4.775149 6.119016

11 C 6.119016 5.810563 4.496719 3.864019 5.079383

12 C 2.540262 1.415299 2.473328 3.575444 3.621842

13 C 3.864019 2.527287 3.050439 4.372603 4.775149

14 C 5.079383 3.864019 4.496719 5.810563 6.119016

15 C 6.119016 4.775149 5.088290 6.452445 7.006038

16 C 5.810563 4.372603 4.298499 5.643769 6.452445

17 N 4.496719 3.050439 2.943036 4.298499 5.088290

18 C 6.946911 5.501717 5.145757 6.406998 7.411098

19 C 7.174184 5.777809 5.090677 6.183794 7.380454

20 C 8.545683 7.174184 6.390579 7.380454 8.653595

21 C 8.653595 7.380454 6.390579 7.174184 8.545683

22 C 7.380454 6.183794 5.090677 5.777809 7.174184

23 N 6.390579 5.090677 4.162081 5.090677 6.390579

24 H 1.079771 2.252495 3.329649 3.313581 2.194797

25 H 2.194797 3.313581 3.329649 2.252495 1.079771

26 H 8.077767 7.529770 6.164949 5.839262 7.160893

27 H 6.507464 6.419686 5.181875 4.314152 5.326833

28 H 5.326833 4.314152 5.181875 6.419686 6.507464

29 H 7.160893 5.839262 6.164949 7.529770 8.077767

30 H 9.423818 8.020569 7.332929 8.380669 9.615590

31 H 9.615590 8.380669 7.332929 8.020569 9.423818

32 Zn 4.332827 3.097846 2.087793 3.097846 4.332827

33 C 7.411098 6.406998 5.145757 5.501717 6.946911

34 C 8.764674 7.810467 6.525451 6.765902 8.210151

35 C 2.891660 2.420058 3.718111 4.591585 4.215996

36 C 9.924713 9.002389 7.704939 7.877803 9.314731

37 C 3.626165 3.505417 4.848984 5.592063 4.988465

38 C 4.215996 4.591585 3.718111 2.420058 2.891660

39 C 4.988465 5.592063 4.848984 3.505417 3.626165

40 C 8.210151 6.765902 6.525451 7.810467 8.764674

41 C 9.314731 7.877803 7.704939 9.002389 9.924713

42 H 10.311408 8.882483 8.754963 10.060195 10.959786

43 H 10.959786 10.060195 8.754963 8.882483 10.311408

44 H 5.796949 6.535735 5.874905 4.517390 4.451162

45 H 4.451162 4.517390 5.874905 6.535735 5.796949

6 7 8 9 10

6 C 0.000000

7 C 1.415299 0.000000

8 N 2.473328 1.366486 0.000000

9 C 3.575444 2.203685 1.366486 0.000000

10 C 3.621842 2.257382 2.296014 1.446922 0.000000

11 C 2.540262 1.446922 2.296014 2.257382 1.362351

12 C 4.892135 5.501717 5.145757 6.406998 7.411098

13 C 5.501717 5.777809 5.090677 6.183794 7.380454

14 C 6.946911 7.174184 6.390579 7.380454 8.653595

15 C 7.411098 7.380454 6.390579 7.174184 8.545683

16 C 6.406998 6.183794 5.090677 5.777809 7.174184

17 N 5.145757 5.090677 4.162081 5.090677 6.390579

18 C 6.918524 6.406998 5.145757 5.501717 6.946911

19 C 6.406998 5.643769 4.298499 4.372603 5.810563

20 C 7.411098 6.452445 5.088290 4.775149 6.119016

21 C 6.946911 5.810563 4.496719 3.864019 5.079383

22 C 5.501717 4.372603 3.050439 2.527287 3.864019

23 N 5.145757 4.298499 2.943036 3.050439 4.496719

24 H 4.640057 5.839262 6.164949 7.529770 8.077767

25 H 2.901508 4.314152 5.181875 6.419686 6.507464

26 H 4.640057 3.313581 3.329649 2.252495 1.079771

27 H 2.901508 2.252495 3.329649 3.313581 2.194797

28 H 7.654495 8.020569 7.332929 8.380669 9.615590

29 H 8.467743 8.380669 7.332929 8.020569 9.423818

30 H 8.467743 7.529770 6.164949 5.839262 7.160893

31 H 7.654495 6.419686 5.181875 4.314152 5.326833

32 Zn 3.464873 3.097846 2.087793 3.097846 4.332827

33 C 4.892135 3.575444 2.473328 1.415299 2.540262

34 C 5.986354 4.591585 3.718111 2.420058 2.891660

35 C 5.986354 6.765902 6.525451 7.810467 8.764674

36 C 7.005116 5.592063 4.848984 3.505417 3.626165

37 C 7.005116 7.877803 7.704939 9.002389 9.924713

38 C 1.426567 2.420058 3.718111 4.591585 4.215996

39 C 2.632354 3.505417 4.848984 5.592063 4.988465

40 C 8.344925 7.810467 6.525451 6.765902 8.210151

41 C 9.550602 9.002389 7.704939 7.877803 9.314731

42 H 10.617849 10.060195 8.754963 8.882483 10.311408

43 H 7.950670 6.535735 5.874905 4.517390 4.451162

44 H 3.699674 4.517390 5.874905 6.535735 5.796949

45 H 7.950670 8.882483 8.754963 10.060195 10.959786

11 12 13 14 15

11 C 0.000000

12 C 6.946911 0.000000

13 C 7.174184 1.415299 0.000000

14 C 8.545683 2.540262 1.446922 0.000000

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17 N 6.390579 2.473328 1.366486 2.296014 2.296014

18 C 7.411098 4.892135 3.575444 3.621842 2.540262

19 C 6.452445 5.501717 4.372603 4.775149 3.864019

20 C 7.006038 6.946911 5.810563 6.119016 5.079383

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22 C 4.775149 6.406998 5.643769 6.452445 5.810563

23 N 5.088290 5.145757 4.298499 5.088290 4.496719

24 H 7.160893 2.901508 4.314152 5.326833 6.507464

25 H 5.326833 4.640057 5.839262 7.160893 8.077767

26 H 2.194797 8.467743 8.380669 9.615590 9.423818

27 H 1.079771 7.654495 8.020569 9.423818 9.615590

28 H 9.423818 2.901508 2.252495 1.079771 2.194797

29 H 9.615590 4.640057 3.313581 2.194797 1.079771

30 H 8.077767 7.654495 6.419686 6.507464 5.326833

31 H 6.507464 8.467743 7.529770 8.077767 7.160893

32 Zn 4.332827 3.464873 3.097846 4.332827 4.332827

33 C 3.621842 6.918524 6.406998 7.411098 6.946911

34 C 4.215996 8.344925 7.810467 8.764674 8.210151

35 C 8.210151 1.426567 2.420058 2.891660 4.215996

36 C 4.988465 9.550602 9.002389 9.924713 9.314731

37 C 9.314731 2.632354 3.505417 3.626165 4.988465

38 C 2.891660 5.986354 6.765902 8.210151 8.764674

39 C 3.626165 7.005116 7.877803 9.314731 9.924713

40 C 8.764674 5.986354 4.591585 4.215996 2.891660

41 C 9.924713 7.005116 5.592063 4.988465 3.626165

42 H 10.959786 7.950670 6.535735 5.796949 4.451162

43 H 5.796949 10.617849 10.060195 10.959786 10.311408

44 H 4.451162 7.950670 8.882483 10.311408 10.959786

45 H 10.311408 3.699674 4.517390 4.451162 5.796949

16 17 18 19 20

16 C 0.000000

17 N 1.366486 0.000000

18 C 1.415299 2.473328 0.000000

19 C 2.527287 3.050439 1.415299 0.000000

20 C 3.864019 4.496719 2.540262 1.446922 0.000000

21 C 4.775149 5.088290 3.621842 2.257382 1.362351

22 C 4.372603 4.298499 3.575444 2.203685 2.257382

23 N 3.050439 2.943036 2.473328 1.366486 2.296014

24 H 6.419686 5.181875 7.654495 8.020569 9.423818

25 H 7.529770 6.164949 8.467743 8.380669 9.615590

26 H 8.020569 7.332929 7.654495 6.419686 6.507464

27 H 8.380669 7.332929 8.467743 7.529770 8.077767

28 H 3.313581 3.329649 4.640057 5.839262 7.160893

29 H 2.252495 3.329649 2.901508 4.314152 5.326833

30 H 4.314152 5.181875 2.901508 2.252495 1.079771

31 H 5.839262 6.164949 4.640057 3.313581 2.194797

32 Zn 3.097846 2.087793 3.464873 3.097846 4.332827

33 C 5.501717 5.145757 4.892135 3.575444 3.621842

34 C 6.765902 6.525451 5.986354 4.591585 4.215996

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36 C 7.877803 7.704939 7.005116 5.592063 4.988465

37 C 5.592063 4.848984 7.005116 7.877803 9.314731

38 C 7.810467 6.525451 8.344925 7.810467 8.764674

39 C 9.002389 7.704939 9.550602 9.002389 9.924713

40 C 2.420058 3.718111 1.426567 2.420058 2.891660

41 C 3.505417 4.848984 2.632354 3.505417 3.626165

42 H 4.517390 5.874905 3.699674 4.517390 4.451162

43 H 8.882483 8.754963 7.950670 6.535735 5.796949

44 H 10.060195 8.754963 10.617849 10.060195 10.959786

45 H 6.535735 5.874905 7.950670 8.882483 10.311408

21 22 23 24 25

21 C 0.000000

22 C 1.446922 0.000000

23 N 2.296014 1.366486 0.000000

24 H 9.615590 8.380669 7.332929 0.000000

25 H 9.423818 8.020569 7.332929 2.680094 0.000000

26 H 5.326833 4.314152 5.181875 9.147026 7.495446

27 H 7.160893 5.839262 6.164949 7.495446 5.356802

28 H 8.077767 7.529770 6.164949 5.356802 7.495446

29 H 6.507464 6.419686 5.181875 7.495446 9.147026

30 H 2.194797 3.313581 3.329649 10.255755 10.600161

31 H 1.079771 2.252495 3.329649 10.600161 10.255755

32 Zn 4.332827 3.097846 2.087793 5.306216 5.306216

33 C 2.540262 1.415299 2.473328 8.467743 7.654495

34 C 2.891660 2.420058 3.718111 9.831092 8.839272

35 C 8.764674 7.810467 6.525451 2.696741 5.078390

36 C 3.626165 3.505417 4.848984 10.995948 9.890587

37 C 9.924713 9.002389 7.704939 3.078553 5.706543

38 C 8.210151 6.765902 6.525451 5.078390 2.696741

39 C 9.314731 7.877803 7.704939 5.706543 3.078553

40 C 4.215996 4.591585 3.718111 8.839272 9.831092

41 C 4.988465 5.592063 4.848984 9.890587 10.995948

42 H 5.796949 6.535735 5.874905 10.848028 12.033772

43 H 4.451162 4.517390 5.874905 12.033772 10.848028

44 H 10.311408 8.882483 8.754963 6.402144 3.722298

45 H 10.959786 10.060195 8.754963 3.722298 6.402144

26 27 28 29 30

26 H 0.000000

27 H 2.680094 0.000000

28 H 10.600161 10.255755 0.000000

29 H 10.255755 10.600161 2.680094 0.000000

30 H 7.495446 9.147026 7.495446 5.356802 0.000000

31 H 5.356802 7.495446 9.147026 7.495446 2.680094

32 Zn 5.306216 5.306216 5.306216 5.306216 5.306216

33 C 2.901508 4.640057 8.467743 7.654495 4.640057

34 C 2.696741 5.078390 9.831092 8.839272 5.078390

35 C 9.831092 8.839272 2.696741 5.078390 8.839272

36 C 3.078553 5.706543 10.995948 9.890587 5.706543

37 C 10.995948 9.890587 3.078553 5.706543 9.890587

38 C 5.078390 2.696741 8.839272 9.831092 9.831092

39 C 5.706543 3.078553 9.890587 10.995948 10.995948

40 C 8.839272 9.831092 5.078390 2.696741 2.696741

41 C 9.890587 10.995948 5.706543 3.078553 3.078553

42 H 10.848028 12.033772 6.402144 3.722298 3.722298

43 H 3.722298 6.402144 12.033772 10.848028 6.402144

44 H 6.402144 3.722298 10.848028 12.033772 12.033772

45 H 12.033772 10.848028 3.722298 6.402144 10.848028

31 32 33 34 35

31 H 0.000000

32 Zn 5.306216 0.000000

33 C 2.901508 3.464873 0.000000

34 C 2.696741 4.890623 1.426567 0.000000

35 C 9.831092 4.890623 8.344925 9.771258 0.000000

36 C 3.078553 6.096036 2.632354 1.205788 10.976884

37 C 10.995948 6.096036 9.550602 10.976884 1.205788

38 C 8.839272 4.890623 5.986354 6.909323 6.909323

39 C 9.890587 6.096036 7.005116 7.808518 7.808518

40 C 5.078390 4.890623 5.986354 6.909323 6.909323

41 C 5.706543 6.096036 7.005116 7.808518 7.808518

42 H 6.402144 7.163122 7.950670 8.666810 8.666810

43 H 3.722298 7.163122 3.699674 2.273108 12.044093

44 H 10.848028 7.163122 7.950670 8.666810 8.666810

45 H 12.033772 7.163122 10.617849 12.044093 2.273108

36 37 38 39 40

36 C 0.000000

37 C 12.182471 0.000000

38 C 7.808518 7.808518 0.000000

39 C 8.614308 8.614308 1.205788 0.000000

40 C 7.808518 7.808518 9.771258 10.976884 0.000000

41 C 8.614308 8.614308 10.976884 12.182471 1.205788

42 H 9.399265 9.399265 12.044093 13.249649 2.273108

43 H 1.067320 13.249649 8.666810 9.399265 8.666810

44 H 9.399265 9.399265 2.273108 1.067320 12.044093

45 H 13.249649 1.067320 8.666810 9.399265 8.666810

41 42 43 44 45

41 C 0.000000

42 H 1.067320 0.000000

43 H 9.399265 10.123508 0.000000

44 H 13.249649 14.316802 10.123508 0.000000

45 H 9.399265 10.123508 14.316802 10.123508 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

RotChk: IX=3 Diff= 2.17D-19

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681175 -4.272842 -0.044479

2 6 0 -1.101843 -2.888905 -0.007880

3 7 0 0.000000 -2.081041 0.016234

4 6 0 1.101843 -2.888905 -0.007880

5 6 0 0.681175 -4.272842 -0.044479

6 6 0 2.446068 -2.446068 -0.013084

7 6 0 2.888905 -1.101843 -0.007880

8 7 0 2.081041 0.000000 0.016234

9 6 0 2.888905 1.101843 -0.007880

10 6 0 4.272842 0.681175 -0.044479

11 6 0 4.272842 -0.681175 -0.044479

12 6 0 -2.446068 -2.446068 -0.013084

13 6 0 -2.888905 -1.101843 -0.007880

14 6 0 -4.272842 -0.681175 -0.044479

15 6 0 -4.272842 0.681175 -0.044479

16 6 0 -2.888905 1.101843 -0.007880

17 7 0 -2.081041 0.000000 0.016234

18 6 0 -2.446068 2.446068 -0.013084

19 6 0 -1.101843 2.888905 -0.007880

20 6 0 -0.681175 4.272842 -0.044479

21 6 0 0.681175 4.272842 -0.044479

22 6 0 1.101843 2.888905 -0.007880

23 7 0 0.000000 2.081041 0.016234

24 1 0 -1.340047 -5.127878 -0.071083

25 1 0 1.340047 -5.127878 -0.071083

26 1 0 5.127878 1.340047 -0.071083

27 1 0 5.127878 -1.340047 -0.071083

28 1 0 -5.127878 -1.340047 -0.071083

29 1 0 -5.127878 1.340047 -0.071083

30 1 0 -1.340047 5.127878 -0.071083

31 1 0 1.340047 5.127878 -0.071083

32 30 0 0.000000 0.000000 0.184019

33 6 0 2.446068 2.446068 -0.013084

34 6 0 3.454661 3.454661 -0.036945

35 6 0 -3.454661 -3.454661 -0.036945

36 6 0 4.307154 4.307154 -0.057853

37 6 0 -4.307154 -4.307154 -0.057853

38 6 0 3.454661 -3.454661 -0.036945

39 6 0 4.307154 -4.307154 -0.057853

40 6 0 -3.454661 3.454661 -0.036945

41 6 0 -4.307154 4.307154 -0.057853

42 1 0 -5.061754 5.061754 -0.076004

43 1 0 5.061754 5.061754 -0.076004

44 1 0 5.061754 -5.061754 -0.076004

45 1 0 -5.061754 -5.061754 -0.076004

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

Rotational constants (GHZ): 0.1465500 0.1465500 0.0733317

Leave Link 202 at Fri Jul 26 14:21:44 2019, MaxMem= 1342177280 cpu: 0.1

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 184 symmetry adapted cartesian basis functions of A1 symmetry.

There are 155 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3060.9008488493 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= 9 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= -0.1305385034 Hartrees.

Nuclear repulsion after empirical dispersion term = 3060.7703103459 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: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3898

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.56D-05

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 156

GePol: Fraction of low-weight points (<1% of avg) = 4.00%

GePol: Cavity surface area = 415.360 Ang\*\*2

GePol: Cavity volume = 419.840 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0084011902 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3060.7787115361 Hartrees.

Leave Link 301 at Fri Jul 26 14:21:44 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44808.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.40D-05 NBF= 172 148 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 172 148 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:21:45 2019, MaxMem= 1342177280 cpu: 6.6

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:21:45 2019, MaxMem= 1342177280 cpu: 0.8

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

Initial guess from the checkpoint file: "ZnTSPsim0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Occupied (E) (E) (B2) (A1) (E) (E) (B1) (A1) (B2) (E) (E)

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

(E) (E) (A1) (A2) (E) (E) (B1) (B1) (E) (E) (A1)

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

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

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

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

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

(E) (E) (A2) (A1)

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(E) (E) (E)

The electronic state of the initial guess is 1-A1.

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= -1359.45313457860

Leave Link 401 at Fri Jul 26 14:21:47 2019, MaxMem= 1342177280 cpu: 21.2

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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.

An orbital has undefined symmetry, so N\*\*3 symmetry is turned off.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 660000000 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= 0 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= 45583212.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.66D-15 for 634.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.90D-15 for 2259 673.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.22D-15 for 303.

Iteration 1 A^-1\*A deviation from orthogonality is 1.25D-14 for 918 866.

E= -1359.06242155266

DIIS: error= 1.25D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.06242155266 IErMin= 1 ErrMin= 1.25D-03

ErrMax= 1.25D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.11D-04 BMatP= 5.11D-04

IDIUse=3 WtCom= 9.88D-01 WtEn= 1.25D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 3.228 Goal= None Shift= 0.000

GapD= 3.228 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=5.83D-05 MaxDP=1.90D-03 OVMax= 5.81D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.82D-05 CP: 1.00D+00

E= -1359.06302901986 Delta-E= -0.000607467202 Rises=F Damp=F

DIIS: error= 1.60D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.06302901986 IErMin= 2 ErrMin= 1.60D-04

ErrMax= 1.60D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.31D-06 BMatP= 5.11D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.60D-03

Coeff-Com: -0.390D-01 0.104D+01

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

Coeff: -0.389D-01 0.104D+01

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=6.43D-06 MaxDP=3.37D-04 DE=-6.07D-04 OVMax= 7.37D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 5.98D-06 CP: 1.00D+00 1.04D+00

E= -1359.06303425441 Delta-E= -0.000005234549 Rises=F Damp=F

DIIS: error= 7.72D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.06303425441 IErMin= 3 ErrMin= 7.72D-05

ErrMax= 7.72D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.63D-06 BMatP= 4.31D-06

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

Coeff-Com: -0.228D-01 0.472D+00 0.550D+00

Coeff: -0.228D-01 0.472D+00 0.550D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=3.40D-06 MaxDP=1.43D-04 DE=-5.23D-06 OVMax= 5.40D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.96D-06 CP: 1.00D+00 1.04D+00 7.24D-01

E= -1359.06303601828 Delta-E= -0.000001763874 Rises=F Damp=F

DIIS: error= 4.63D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.06303601828 IErMin= 4 ErrMin= 4.63D-05

ErrMax= 4.63D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.04D-07 BMatP= 2.63D-06

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

Coeff-Com: -0.702D-02 0.108D+00 0.343D+00 0.555D+00

Coeff: -0.702D-02 0.108D+00 0.343D+00 0.555D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.35D-06 MaxDP=5.72D-05 DE=-1.76D-06 OVMax= 2.10D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 6.79D-07 CP: 1.00D+00 1.04D+00 8.24D-01 6.63D-01

E= -1359.06303663527 Delta-E= -0.000000616986 Rises=F Damp=F

DIIS: error= 9.56D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.06303663527 IErMin= 5 ErrMin= 9.56D-06

ErrMax= 9.56D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.12D-08 BMatP= 7.04D-07

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

Coeff-Com: -0.115D-02 0.652D-02 0.103D+00 0.245D+00 0.646D+00

Coeff: -0.115D-02 0.652D-02 0.103D+00 0.245D+00 0.646D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=2.97D-07 MaxDP=1.69D-05 DE=-6.17D-07 OVMax= 3.65D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.20D-07 CP: 1.00D+00 1.04D+00 8.40D-01 6.97D-01 7.93D-01

E= -1359.06303665656 Delta-E= -0.000000021293 Rises=F Damp=F

DIIS: error= 4.81D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.06303665656 IErMin= 6 ErrMin= 4.81D-06

ErrMax= 4.81D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.59D-09 BMatP= 3.12D-08

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

Coeff-Com: 0.287D-03-0.111D-01 0.833D-02 0.580D-01 0.359D+00 0.586D+00

Coeff: 0.287D-03-0.111D-01 0.833D-02 0.580D-01 0.359D+00 0.586D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=1.09D-07 MaxDP=5.68D-06 DE=-2.13D-08 OVMax= 1.29D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.67D-08 CP: 1.00D+00 1.04D+00 8.44D-01 7.09D-01 8.47D-01

CP: 6.62D-01

E= -1359.06303666237 Delta-E= -0.000000005804 Rises=F Damp=F

DIIS: error= 8.23D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.06303666237 IErMin= 7 ErrMin= 8.23D-07

ErrMax= 8.23D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.37D-10 BMatP= 6.59D-09

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

Coeff-Com: 0.179D-03-0.541D-02-0.108D-02 0.154D-01 0.136D+00 0.274D+00

Coeff-Com: 0.581D+00

Coeff: 0.179D-03-0.541D-02-0.108D-02 0.154D-01 0.136D+00 0.274D+00

Coeff: 0.581D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.53D-08 MaxDP=9.85D-07 DE=-5.80D-09 OVMax= 2.65D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.61D-08 CP: 1.00D+00 1.04D+00 8.44D-01 7.09D-01 8.59D-01

CP: 6.93D-01 7.16D-01

E= -1359.06303666249 Delta-E= -0.000000000123 Rises=F Damp=F

DIIS: error= 1.72D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.06303666249 IErMin= 8 ErrMin= 1.72D-07

ErrMax= 1.72D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.08D-11 BMatP= 2.37D-10

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

Coeff-Com: 0.567D-04-0.159D-02-0.921D-03 0.303D-02 0.356D-01 0.795D-01

Coeff-Com: 0.241D+00 0.643D+00

Coeff: 0.567D-04-0.159D-02-0.921D-03 0.303D-02 0.356D-01 0.795D-01

Coeff: 0.241D+00 0.643D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=6.83D-09 MaxDP=3.47D-07 DE=-1.23D-10 OVMax= 7.48D-07

Error on total polarization charges = 0.06211

SCF Done: E(RB3LYP) = -1359.06303666 A.U. after 8 cycles

NFock= 8 Conv=0.68D-08 -V/T= 1.9682

KE= 1.403734688724D+03 PE=-9.363651652997D+03 EE= 3.540075216075D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.27

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:22:22 2019, MaxMem= 1342177280 cpu: 391.6

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44808.

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 = 258

Leave Link 701 at Fri Jul 26 14:22:26 2019, MaxMem= 1342177280 cpu: 43.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

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

Leave Link 702 at Fri Jul 26 14:22:26 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Fri Jul 26 14:22:29 2019, MaxMem= 1342177280 cpu: 43.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.24344979D-13 9.23705556D-14 3.19593802D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000007571 0.000055572 0.000053256

2 6 0.000088028 -0.000145401 0.000011869

3 7 0.000000000 0.000499682 -0.000351382

4 6 -0.000088028 -0.000145401 0.000011869

5 6 0.000007571 0.000055572 0.000053256

6 6 0.000225955 -0.000225955 0.000236716

7 6 0.000145401 0.000088028 0.000011869

8 7 -0.000499682 0.000000000 -0.000351382

9 6 0.000145401 -0.000088028 0.000011869

10 6 -0.000055572 0.000007571 0.000053256

11 6 -0.000055572 -0.000007571 0.000053256

12 6 -0.000225955 -0.000225955 0.000236716

13 6 -0.000145401 0.000088028 0.000011869

14 6 0.000055572 -0.000007571 0.000053256

15 6 0.000055572 0.000007571 0.000053256

16 6 -0.000145401 -0.000088028 0.000011869

17 7 0.000499682 0.000000000 -0.000351382

18 6 -0.000225955 0.000225955 0.000236716

19 6 0.000088028 0.000145401 0.000011869

20 6 -0.000007571 -0.000055572 0.000053256

21 6 0.000007571 -0.000055572 0.000053256

22 6 -0.000088028 0.000145401 0.000011869

23 7 0.000000000 -0.000499682 -0.000351382

24 1 -0.000041859 -0.000010586 -0.000030184

25 1 0.000041859 -0.000010586 -0.000030184

26 1 0.000010586 0.000041859 -0.000030184

27 1 0.000010586 -0.000041859 -0.000030184

28 1 -0.000010586 -0.000041859 -0.000030184

29 1 -0.000010586 0.000041859 -0.000030184

30 1 -0.000041859 0.000010586 -0.000030184

31 1 0.000041859 0.000010586 -0.000030184

32 30 0.000000000 0.000000000 0.000533547

33 6 0.000225955 0.000225955 0.000236716

34 6 -0.000189533 -0.000189533 -0.000022333

35 6 0.000189533 0.000189533 -0.000022333

36 6 -0.000019161 -0.000019161 -0.000081995

37 6 0.000019161 0.000019161 -0.000081995

38 6 -0.000189533 0.000189533 -0.000022333

39 6 -0.000019161 0.000019161 -0.000081995

40 6 0.000189533 -0.000189533 -0.000022333

41 6 0.000019161 -0.000019161 -0.000081995

42 1 0.000011605 -0.000011605 0.000015725

43 1 -0.000011605 -0.000011605 0.000015725

44 1 -0.000011605 0.000011605 0.000015725

45 1 0.000011605 0.000011605 0.000015725

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

Cartesian Forces: Max 0.000533547 RMS 0.000149900

Leave Link 716 at Fri Jul 26 14:22:29 2019, MaxMem= 1342177280 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000312987 RMS 0.000065076

Search for a local minimum.

Step number 13 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .65076D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 2 3 4 5 7

9 8 10 11 12

13

DE= -7.42D-05 DEPred=-7.72D-05 R= 9.62D-01

TightC=F SS= 1.41D+00 RLast= 8.81D-02 DXNew= 8.4090D-02 2.6440D-01

Trust test= 9.62D-01 RLast= 8.81D-02 DXMaxT set to 8.41D-02

ITU= 1 -1 1 0 -1 0 0 -1 1 0 -1 -1 0

Eigenvalues --- 0.00534 0.00534 0.00534 0.00534 0.00534

Eigenvalues --- 0.00534 0.00535 0.00713 0.01134 0.01134

Eigenvalues --- 0.01166 0.01376 0.01376 0.01531 0.01645

Eigenvalues --- 0.01673 0.01723 0.01723 0.01800 0.01805

Eigenvalues --- 0.01805 0.01825 0.01831 0.01859 0.01859

Eigenvalues --- 0.01868 0.01868 0.01868 0.01908 0.01920

Eigenvalues --- 0.01927 0.01927 0.01933 0.01936 0.01961

Eigenvalues --- 0.01961 0.02158 0.02178 0.02181 0.02185

Eigenvalues --- 0.02185 0.02283 0.03317 0.03776 0.04654

Eigenvalues --- 0.04654 0.04654 0.04654 0.04654 0.04654

Eigenvalues --- 0.04654 0.08279 0.13848 0.14996 0.14996

Eigenvalues --- 0.15408 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.17858 0.22833

Eigenvalues --- 0.22868 0.22872 0.22872 0.24762 0.24780

Eigenvalues --- 0.24780 0.24852 0.24877 0.24980 0.24980

Eigenvalues --- 0.24998 0.24999 0.24999 0.24999 0.25000

Eigenvalues --- 0.26656 0.35034 0.35034 0.35468 0.35498

Eigenvalues --- 0.35667 0.36028 0.36034 0.36034 0.36034

Eigenvalues --- 0.36034 0.36034 0.36034 0.36037 0.36782

Eigenvalues --- 0.36865 0.36865 0.37380 0.37563 0.37563

Eigenvalues --- 0.37563 0.37652 0.38968 0.38968 0.39538

Eigenvalues --- 0.40639 0.41397 0.41397 0.41397 0.41519

Eigenvalues --- 0.41519 0.41791 0.42523 0.43515 0.43779

Eigenvalues --- 0.43779 0.45496 0.47917 0.49087 0.49087

Eigenvalues --- 0.50129 0.51398 0.51901 0.51901 0.53864

Eigenvalues --- 1.01812 1.01831 1.01831 1.01831

En-DIIS/RFO-DIIS IScMMF= 0 using points: 13 12 11 10

RFO step: Lambda=-3.61369347D-06.

NNeg= 0 NP= 4 Switch= 2.50D-03 Rises=F DC= 9.12D-05 SmlDif= 1.00D-05

RMS Error= 0.2364057214D-03 NUsed= 4 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.97272 -0.02526 -0.07791 0.13044

Iteration 1 RMS(Cart)= 0.00309402 RMS(Int)= 0.00000577

Iteration 2 RMS(Cart)= 0.00000748 RMS(Int)= 0.00000440

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000440

ITry= 1 IFail=0 DXMaxC= 1.89D-02 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 8.61D-04 for atom 44.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73429 0.00006 -0.00013 0.00030 0.00018 2.73446

R2 2.57447 0.00001 0.00013 -0.00007 0.00006 2.57453

R3 2.04047 -0.00003 -0.00003 -0.00006 -0.00009 2.04038

R4 2.58228 -0.00004 0.00024 -0.00036 -0.00012 2.58216

R5 2.67453 0.00001 0.00020 -0.00013 0.00004 2.67457

R6 2.58228 -0.00004 0.00024 -0.00036 -0.00012 2.58216

R7 3.94536 0.00028 0.00081 0.00117 0.00190 3.94725

R8 2.73429 0.00006 -0.00013 0.00030 0.00018 2.73446

R9 2.67453 0.00001 0.00020 -0.00013 0.00004 2.67457

R10 2.04047 -0.00003 -0.00003 -0.00006 -0.00009 2.04038

R11 2.67453 0.00001 0.00020 -0.00013 0.00004 2.67457

R12 2.69582 0.00031 -0.00007 0.00091 0.00093 2.69675

R13 2.58228 -0.00004 0.00024 -0.00036 -0.00012 2.58216

R14 2.73429 0.00006 -0.00013 0.00030 0.00018 2.73446

R15 2.58228 -0.00004 0.00024 -0.00036 -0.00012 2.58216

R16 3.94536 0.00028 0.00081 0.00117 0.00190 3.94725

R17 2.73429 0.00006 -0.00013 0.00030 0.00018 2.73446

R18 2.67453 0.00001 0.00020 -0.00013 0.00004 2.67457

R19 2.57447 0.00001 0.00013 -0.00007 0.00006 2.57453

R20 2.04047 -0.00003 -0.00003 -0.00006 -0.00009 2.04038

R21 2.04047 -0.00003 -0.00003 -0.00006 -0.00009 2.04038

R22 2.67453 0.00001 0.00020 -0.00013 0.00004 2.67457

R23 2.69582 0.00031 -0.00007 0.00091 0.00093 2.69675

R24 2.73429 0.00006 -0.00013 0.00030 0.00018 2.73446

R25 2.58228 -0.00004 0.00024 -0.00036 -0.00012 2.58216

R26 2.57447 0.00001 0.00013 -0.00007 0.00006 2.57453

R27 2.04047 -0.00003 -0.00003 -0.00006 -0.00009 2.04038

R28 2.73429 0.00006 -0.00013 0.00030 0.00018 2.73446

R29 2.04047 -0.00003 -0.00003 -0.00006 -0.00009 2.04038

R30 2.58228 -0.00004 0.00024 -0.00036 -0.00012 2.58216

R31 2.67453 0.00001 0.00020 -0.00013 0.00004 2.67457

R32 3.94536 0.00028 0.00081 0.00117 0.00190 3.94725

R33 2.67453 0.00001 0.00020 -0.00013 0.00004 2.67457

R34 2.69582 0.00031 -0.00007 0.00091 0.00093 2.69675

R35 2.73429 0.00006 -0.00013 0.00030 0.00018 2.73446

R36 2.58228 -0.00004 0.00024 -0.00036 -0.00012 2.58216

R37 2.57447 0.00001 0.00013 -0.00007 0.00006 2.57453

R38 2.04047 -0.00003 -0.00003 -0.00006 -0.00009 2.04038

R39 2.73429 0.00006 -0.00013 0.00030 0.00018 2.73446

R40 2.04047 -0.00003 -0.00003 -0.00006 -0.00009 2.04038

R41 2.58228 -0.00004 0.00024 -0.00036 -0.00012 2.58216

R42 2.67453 0.00001 0.00020 -0.00013 0.00004 2.67457

R43 3.94536 0.00028 0.00081 0.00117 0.00190 3.94725

R44 2.69582 0.00031 -0.00007 0.00091 0.00093 2.69675

R45 2.27861 0.00004 0.00001 0.00003 0.00004 2.27865

R46 2.27861 0.00004 0.00001 0.00003 0.00004 2.27865

R47 2.01694 0.00002 0.00001 0.00003 0.00004 2.01698

R48 2.01694 0.00002 0.00001 0.00003 0.00004 2.01698

R49 2.27861 0.00004 0.00001 0.00003 0.00004 2.27865

R50 2.01694 0.00002 0.00001 0.00003 0.00004 2.01698

R51 2.27861 0.00004 0.00001 0.00003 0.00004 2.27865

R52 2.01694 0.00002 0.00001 0.00003 0.00004 2.01698

A1 1.86579 0.00002 0.00008 0.00002 0.00011 1.86590

A2 2.19028 0.00002 -0.00016 0.00031 0.00015 2.19043

A3 2.22710 -0.00004 0.00008 -0.00034 -0.00027 2.22684

A4 1.90867 -0.00008 -0.00012 -0.00029 -0.00042 1.90826

A5 2.18378 0.00003 -0.00002 0.00022 0.00019 2.18397

A6 2.19066 0.00005 0.00015 0.00007 0.00023 2.19088

A7 1.87585 0.00013 0.00007 0.00053 0.00061 1.87646

A8 2.20273 -0.00006 -0.00007 -0.00032 -0.00040 2.20233

A9 2.20273 -0.00006 -0.00007 -0.00032 -0.00040 2.20233

A10 1.90867 -0.00008 -0.00012 -0.00029 -0.00042 1.90826

A11 2.19066 0.00005 0.00015 0.00007 0.00023 2.19088

A12 2.18378 0.00003 -0.00002 0.00022 0.00019 2.18397

A13 1.86579 0.00002 0.00008 0.00002 0.00011 1.86590

A14 2.22710 -0.00004 0.00008 -0.00034 -0.00027 2.22684

A15 2.19028 0.00002 -0.00016 0.00031 0.00015 2.19043

A16 2.20725 0.00003 -0.00020 0.00035 0.00014 2.20739

A17 2.03795 -0.00002 0.00010 -0.00020 -0.00009 2.03786

A18 2.03795 -0.00002 0.00010 -0.00019 -0.00009 2.03786

A19 2.19066 0.00005 0.00015 0.00007 0.00023 2.19088

A20 2.18378 0.00003 -0.00002 0.00022 0.00019 2.18397

A21 1.90867 -0.00008 -0.00012 -0.00029 -0.00042 1.90826

A22 1.87585 0.00013 0.00007 0.00053 0.00061 1.87646

A23 2.20273 -0.00006 -0.00007 -0.00032 -0.00040 2.20233

A24 2.20273 -0.00006 -0.00007 -0.00032 -0.00040 2.20233

A25 1.90867 -0.00008 -0.00012 -0.00029 -0.00042 1.90826

A26 2.19066 0.00005 0.00015 0.00007 0.00023 2.19088

A27 2.18378 0.00003 -0.00002 0.00022 0.00019 2.18397

A28 1.86579 0.00002 0.00008 0.00002 0.00011 1.86590

A29 2.19028 0.00002 -0.00016 0.00031 0.00015 2.19043

A30 2.22710 -0.00004 0.00008 -0.00034 -0.00027 2.22684

A31 1.86579 0.00002 0.00008 0.00003 0.00011 1.86590

A32 2.19028 0.00002 -0.00016 0.00031 0.00015 2.19043

A33 2.22710 -0.00004 0.00008 -0.00034 -0.00027 2.22684

A34 2.20725 0.00003 -0.00020 0.00035 0.00014 2.20739

A35 2.03795 -0.00002 0.00010 -0.00020 -0.00009 2.03786

A36 2.03795 -0.00002 0.00010 -0.00019 -0.00009 2.03786

A37 2.18378 0.00003 -0.00002 0.00022 0.00019 2.18397

A38 2.19066 0.00005 0.00015 0.00007 0.00023 2.19088

A39 1.90867 -0.00008 -0.00012 -0.00029 -0.00042 1.90826

A40 1.86579 0.00002 0.00008 0.00003 0.00011 1.86590

A41 2.19028 0.00002 -0.00016 0.00031 0.00015 2.19043

A42 2.22710 -0.00004 0.00008 -0.00034 -0.00027 2.22684

A43 1.86579 0.00002 0.00008 0.00002 0.00011 1.86590

A44 2.22710 -0.00004 0.00008 -0.00034 -0.00027 2.22684

A45 2.19028 0.00002 -0.00016 0.00031 0.00015 2.19043

A46 1.90867 -0.00008 -0.00012 -0.00029 -0.00042 1.90826

A47 2.18378 0.00003 -0.00002 0.00022 0.00019 2.18397

A48 2.19066 0.00005 0.00015 0.00007 0.00023 2.19088

A49 1.87585 0.00013 0.00007 0.00053 0.00061 1.87646

A50 2.20273 -0.00006 -0.00007 -0.00032 -0.00040 2.20233

A51 2.20273 -0.00006 -0.00007 -0.00032 -0.00040 2.20233

A52 2.20725 0.00003 -0.00020 0.00035 0.00014 2.20739

A53 2.03795 -0.00002 0.00010 -0.00020 -0.00009 2.03786

A54 2.03795 -0.00002 0.00010 -0.00019 -0.00009 2.03786

A55 2.18378 0.00003 -0.00002 0.00022 0.00019 2.18397

A56 2.19066 0.00005 0.00015 0.00007 0.00023 2.19088

A57 1.90867 -0.00008 -0.00012 -0.00029 -0.00042 1.90826

A58 1.86579 0.00002 0.00008 0.00002 0.00011 1.86590

A59 2.19028 0.00002 -0.00016 0.00031 0.00015 2.19043

A60 2.22710 -0.00004 0.00008 -0.00034 -0.00027 2.22684

A61 1.86579 0.00002 0.00008 0.00002 0.00011 1.86590

A62 2.22710 -0.00004 0.00008 -0.00034 -0.00027 2.22684

A63 2.19028 0.00002 -0.00016 0.00031 0.00015 2.19043

A64 1.90867 -0.00008 -0.00012 -0.00029 -0.00042 1.90826

A65 2.18378 0.00003 -0.00002 0.00022 0.00019 2.18397

A66 2.19066 0.00005 0.00015 0.00007 0.00023 2.19088

A67 1.87585 0.00013 0.00007 0.00053 0.00061 1.87646

A68 2.20273 -0.00006 -0.00007 -0.00032 -0.00040 2.20233

A69 2.20273 -0.00006 -0.00007 -0.00032 -0.00040 2.20233

A70 1.56434 -0.00001 -0.00026 -0.00010 -0.00034 1.56400

A71 1.56434 -0.00001 -0.00026 -0.00010 -0.00034 1.56400

A72 2.98069 -0.00008 -0.00293 -0.00122 -0.00415 2.97654

A73 2.98069 -0.00008 -0.00293 -0.00122 -0.00415 2.97654

A74 1.56434 -0.00001 -0.00026 -0.00010 -0.00034 1.56400

A75 1.56434 -0.00001 -0.00026 -0.00010 -0.00034 1.56400

A76 2.20725 0.00003 -0.00020 0.00035 0.00014 2.20739

A77 2.03795 -0.00002 0.00010 -0.00020 -0.00009 2.03786

A78 2.03795 -0.00002 0.00010 -0.00019 -0.00009 2.03786

A79 3.14158 0.00000 -0.00002 -0.00007 -0.00003 3.14155

A80 3.14158 0.00000 -0.00002 -0.00007 -0.00003 3.14155

A81 3.14160 0.00000 -0.00002 -0.00028 0.00002 3.14162

A82 3.14160 0.00000 -0.00002 -0.00028 0.00002 3.14162

A83 3.14158 0.00000 -0.00002 -0.00007 -0.00003 3.14155

A84 3.14160 0.00000 -0.00002 -0.00028 0.00002 3.14162

A85 3.14158 0.00000 -0.00002 -0.00007 -0.00003 3.14155

A86 3.14160 0.00000 -0.00002 -0.00028 0.00002 3.14162

A87 3.14097 -0.00012 -0.00136 -0.00101 -0.00237 3.13861

A88 3.14221 0.00012 0.00136 0.00101 0.00237 3.14458

A89 3.14198 0.00003 -0.00154 0.00334 0.00180 3.14378

A90 3.14121 -0.00003 0.00154 -0.00334 -0.00180 3.13941

A91 3.14097 -0.00012 -0.00136 -0.00101 -0.00237 3.13861

A92 3.14198 0.00003 -0.00154 0.00334 0.00180 3.14378

A93 3.14221 0.00012 0.00136 0.00101 0.00237 3.14458

A94 3.14121 -0.00003 0.00154 -0.00334 -0.00180 3.13941

D1 -0.00213 0.00001 -0.00026 0.00052 0.00026 -0.00187

D2 3.12699 0.00000 -0.00024 0.00080 0.00056 3.12755

D3 -3.13919 0.00002 -0.00038 0.00134 0.00097 -3.13822

D4 -0.01007 0.00001 -0.00036 0.00162 0.00127 -0.00880

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13693 0.00001 -0.00012 0.00084 0.00072 -3.13620

D7 3.13693 -0.00001 0.00012 -0.00084 -0.00072 3.13620

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00345 -0.00002 0.00043 -0.00085 -0.00042 0.00303

D10 -3.07541 0.00002 0.00166 0.00105 0.00271 -3.07269

D11 -3.12561 -0.00001 0.00041 -0.00113 -0.00072 -3.12633

D12 0.07872 0.00003 0.00165 0.00077 0.00241 0.08114

D13 -3.11536 0.00004 -0.00019 0.00070 0.00051 -3.11486

D14 0.01664 -0.00007 -0.00044 -0.00288 -0.00333 0.01331

D15 0.01177 0.00003 -0.00017 0.00102 0.00085 0.01262

D16 -3.13941 -0.00008 -0.00042 -0.00256 -0.00298 3.14079

D17 -0.00345 0.00002 -0.00043 0.00085 0.00042 -0.00303

D18 3.12561 0.00001 -0.00041 0.00113 0.00072 3.12633

D19 3.07541 -0.00002 -0.00166 -0.00105 -0.00271 3.07269

D20 -0.07872 -0.00003 -0.00165 -0.00077 -0.00241 -0.08114

D21 -3.09849 0.00002 0.00072 -0.00050 0.00022 -3.09827

D22 -0.11728 -0.00006 -0.00217 -0.00171 -0.00389 -0.12117

D23 -1.60789 -0.00002 -0.00073 -0.00111 -0.00183 -1.60972

D24 0.11728 0.00006 0.00217 0.00171 0.00389 0.12117

D25 3.09849 -0.00002 -0.00072 0.00050 -0.00022 3.09827

D26 1.60789 0.00002 0.00073 0.00111 0.00183 1.60972

D27 0.00213 -0.00001 0.00026 -0.00052 -0.00026 0.00187

D28 3.13919 -0.00002 0.00038 -0.00134 -0.00097 3.13822

D29 -3.12699 0.00000 0.00024 -0.00080 -0.00056 -3.12755

D30 0.01007 -0.00001 0.00036 -0.00162 -0.00127 0.00880

D31 -0.01177 -0.00003 0.00017 -0.00102 -0.00085 -0.01262

D32 3.13941 0.00008 0.00042 0.00256 0.00298 -3.14079

D33 3.11536 -0.00004 0.00019 -0.00070 -0.00051 3.11486

D34 -0.01664 0.00007 0.00044 0.00288 0.00333 -0.01331

D35 0.01177 0.00003 -0.00017 0.00102 0.00085 0.01262

D36 -3.11536 0.00004 -0.00019 0.00070 0.00051 -3.11486

D37 -3.13941 -0.00008 -0.00042 -0.00256 -0.00298 3.14079

D38 0.01664 -0.00007 -0.00044 -0.00288 -0.00333 0.01331

D39 -3.12561 -0.00001 0.00041 -0.00113 -0.00072 -3.12633

D40 0.07872 0.00003 0.00165 0.00077 0.00241 0.08114

D41 0.00345 -0.00002 0.00043 -0.00085 -0.00042 0.00303

D42 -3.07541 0.00002 0.00166 0.00105 0.00271 -3.07269

D43 3.12699 0.00000 -0.00024 0.00080 0.00056 3.12755

D44 -0.01007 0.00001 -0.00036 0.00162 0.00127 -0.00880

D45 -0.00213 0.00001 -0.00026 0.00052 0.00026 -0.00187

D46 -3.13919 0.00002 -0.00038 0.00134 0.00097 -3.13822

D47 -0.00345 0.00002 -0.00043 0.00085 0.00042 -0.00303

D48 3.12561 0.00001 -0.00041 0.00113 0.00072 3.12633

D49 3.07541 -0.00002 -0.00166 -0.00105 -0.00271 3.07269

D50 -0.07872 -0.00003 -0.00165 -0.00077 -0.00241 -0.08114

D51 -0.11728 -0.00006 -0.00217 -0.00171 -0.00389 -0.12117

D52 -1.60789 -0.00002 -0.00073 -0.00111 -0.00183 -1.60972

D53 -3.09849 0.00002 0.00072 -0.00050 0.00022 -3.09827

D54 3.09849 -0.00002 -0.00072 0.00050 -0.00022 3.09827

D55 1.60789 0.00002 0.00073 0.00111 0.00183 1.60972

D56 0.11728 0.00006 0.00217 0.00171 0.00389 0.12117

D57 0.00213 -0.00001 0.00026 -0.00052 -0.00026 0.00187

D58 3.13919 -0.00002 0.00038 -0.00134 -0.00097 3.13822

D59 -3.12699 0.00000 0.00024 -0.00080 -0.00056 -3.12755

D60 0.01007 -0.00001 0.00036 -0.00162 -0.00127 0.00880

D61 -0.01177 -0.00003 0.00017 -0.00102 -0.00085 -0.01262

D62 3.13941 0.00008 0.00042 0.00256 0.00298 -3.14079

D63 3.11536 -0.00004 0.00019 -0.00070 -0.00051 3.11486

D64 -0.01664 0.00007 0.00044 0.00288 0.00333 -0.01331

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13693 -0.00001 0.00012 -0.00084 -0.00072 3.13620

D67 -3.13693 0.00001 -0.00012 0.00084 0.00072 -3.13620

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.11536 -0.00004 0.00019 -0.00070 -0.00051 3.11486

D70 -0.01177 -0.00003 0.00017 -0.00102 -0.00085 -0.01262

D71 -0.01664 0.00007 0.00044 0.00288 0.00333 -0.01331

D72 3.13941 0.00008 0.00042 0.00256 0.00298 -3.14079

D73 -3.12699 0.00000 0.00024 -0.00080 -0.00056 -3.12755

D74 0.01007 -0.00001 0.00036 -0.00162 -0.00127 0.00880

D75 0.00213 -0.00001 0.00026 -0.00052 -0.00026 0.00187

D76 3.13919 -0.00002 0.00038 -0.00134 -0.00097 3.13822

D77 3.12561 0.00001 -0.00041 0.00113 0.00072 3.12633

D78 -0.07872 -0.00003 -0.00165 -0.00077 -0.00241 -0.08114

D79 -0.00345 0.00002 -0.00043 0.00085 0.00042 -0.00303

D80 3.07541 -0.00002 -0.00166 -0.00105 -0.00271 3.07269

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 3.13693 -0.00001 0.00012 -0.00084 -0.00072 3.13620

D83 -3.13693 0.00001 -0.00012 0.00084 0.00072 -3.13620

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 -0.00213 0.00001 -0.00026 0.00052 0.00026 -0.00187

D86 3.12699 0.00000 -0.00024 0.00080 0.00056 3.12755

D87 -3.13919 0.00002 -0.00038 0.00134 0.00097 -3.13822

D88 -0.01007 0.00001 -0.00036 0.00162 0.00127 -0.00880

D89 0.00345 -0.00002 0.00043 -0.00085 -0.00042 0.00303

D90 -3.07541 0.00002 0.00166 0.00105 0.00271 -3.07269

D91 -3.12561 -0.00001 0.00041 -0.00113 -0.00072 -3.12633

D92 0.07872 0.00003 0.00165 0.00077 0.00241 0.08114

D93 -3.11536 0.00004 -0.00019 0.00070 0.00051 -3.11486

D94 0.01664 -0.00007 -0.00044 -0.00288 -0.00333 0.01331

D95 0.01177 0.00003 -0.00017 0.00102 0.00085 0.01262

D96 -3.13941 -0.00008 -0.00042 -0.00256 -0.00298 3.14079

D97 0.11728 0.00006 0.00217 0.00171 0.00389 0.12117

D98 1.60789 0.00002 0.00073 0.00111 0.00183 1.60972

D99 3.09849 -0.00002 -0.00072 0.00050 -0.00022 3.09827

D100 -3.09849 0.00002 0.00072 -0.00050 0.00022 -3.09827

D101 -1.60789 -0.00002 -0.00073 -0.00111 -0.00183 -1.60972

D102 -0.11728 -0.00006 -0.00217 -0.00171 -0.00389 -0.12117

D103 3.11536 -0.00004 0.00019 -0.00070 -0.00051 3.11486

D104 -0.01177 -0.00003 0.00017 -0.00102 -0.00085 -0.01262

D105 -0.01664 0.00007 0.00044 0.00288 0.00333 -0.01331

D106 3.13941 0.00008 0.00042 0.00256 0.00298 -3.14079

D107 -3.12699 0.00000 0.00024 -0.00080 -0.00056 -3.12755

D108 0.01007 -0.00001 0.00036 -0.00162 -0.00127 0.00880

D109 0.00213 -0.00001 0.00026 -0.00052 -0.00026 0.00187

D110 3.13919 -0.00002 0.00038 -0.00134 -0.00097 3.13822

D111 3.12561 0.00001 -0.00041 0.00113 0.00072 3.12633

D112 -0.07872 -0.00003 -0.00165 -0.00077 -0.00241 -0.08114

D113 -0.00345 0.00002 -0.00043 0.00085 0.00042 -0.00303

D114 3.07541 -0.00002 -0.00166 -0.00105 -0.00271 3.07269

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.13693 -0.00001 0.00012 -0.00084 -0.00072 3.13620

D117 -3.13693 0.00001 -0.00012 0.00084 0.00072 -3.13620

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 -0.00213 0.00001 -0.00026 0.00052 0.00026 -0.00187

D120 3.12699 0.00000 -0.00024 0.00080 0.00056 3.12755

D121 -3.13919 0.00002 -0.00038 0.00134 0.00097 -3.13822

D122 -0.01007 0.00001 -0.00036 0.00162 0.00127 -0.00880

D123 0.00345 -0.00002 0.00043 -0.00085 -0.00042 0.00303

D124 -3.07541 0.00002 0.00166 0.00105 0.00271 -3.07269

D125 -3.12561 -0.00001 0.00041 -0.00113 -0.00072 -3.12633

D126 0.07872 0.00003 0.00165 0.00077 0.00241 0.08114

D127 -3.11536 0.00004 -0.00019 0.00070 0.00051 -3.11486

D128 0.01664 -0.00007 -0.00044 -0.00288 -0.00333 0.01331

D129 0.01177 0.00003 -0.00017 0.00102 0.00085 0.01262

D130 -3.13941 -0.00008 -0.00042 -0.00256 -0.00298 3.14079

D131 1.60789 0.00002 0.00073 0.00111 0.00183 1.60972

D132 3.09849 -0.00002 -0.00072 0.00050 -0.00022 3.09827

D133 0.11728 0.00006 0.00217 0.00171 0.00389 0.12117

D134 -1.60789 -0.00002 -0.00073 -0.00111 -0.00183 -1.60972

D135 -0.11728 -0.00006 -0.00217 -0.00171 -0.00389 -0.12117

D136 -3.09849 0.00002 0.00072 -0.00050 0.00022 -3.09827

Item Value Threshold Converged?

Maximum Force 0.000313 0.000450 YES

RMS Force 0.000065 0.000300 YES

Maximum Displacement 0.018931 0.001800 NO

RMS Displacement 0.003090 0.001200 NO

Predicted change in Energy=-7.696730D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:22:30 2019, MaxMem= 1342177280 cpu: 1.1

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.681190 4.273170 -0.041898

2 6 0 1.102037 2.889188 -0.005373

3 7 0 0.000000 2.081688 0.018352

4 6 0 -1.102037 2.889188 -0.005373

5 6 0 -0.681190 4.273170 -0.041898

6 6 0 -2.446254 2.446254 -0.009948

7 6 0 -2.889188 1.102037 -0.005373

8 7 0 -2.081688 0.000000 0.018352

9 6 0 -2.889188 -1.102037 -0.005373

10 6 0 -4.273170 -0.681190 -0.041898

11 6 0 -4.273170 0.681190 -0.041898

12 6 0 2.446254 2.446254 -0.009948

13 6 0 2.889188 1.102037 -0.005373

14 6 0 4.273170 0.681190 -0.041898

15 6 0 4.273170 -0.681190 -0.041898

16 6 0 2.889188 -1.102037 -0.005373

17 7 0 2.081688 0.000000 0.018352

18 6 0 2.446254 -2.446254 -0.009948

19 6 0 1.102037 -2.889188 -0.005373

20 6 0 0.681190 -4.273170 -0.041898

21 6 0 -0.681190 -4.273170 -0.041898

22 6 0 -1.102037 -2.889188 -0.005373

23 7 0 0.000000 -2.081688 0.018352

24 1 0 1.339805 5.128325 -0.069078

25 1 0 -1.339805 5.128325 -0.069078

26 1 0 -5.128325 -1.339805 -0.069078

27 1 0 -5.128325 1.339805 -0.069078

28 1 0 5.128325 1.339805 -0.069078

29 1 0 5.128325 -1.339805 -0.069078

30 1 0 1.339805 -5.128325 -0.069078

31 1 0 -1.339805 -5.128325 -0.069078

32 30 0 0.000000 0.000000 0.190538

33 6 0 -2.446254 -2.446254 -0.009948

34 6 0 -3.455153 -3.455153 -0.037297

35 6 0 3.455153 3.455153 -0.037297

36 6 0 -4.307580 -4.307580 -0.063981

37 6 0 4.307580 4.307580 -0.063981

38 6 0 -3.455153 3.455153 -0.037297

39 6 0 -4.307580 4.307580 -0.063981

40 6 0 3.455153 -3.455153 -0.037297

41 6 0 4.307580 -4.307580 -0.063981

42 1 0 5.062148 -5.062148 -0.085575

43 1 0 -5.062148 -5.062148 -0.085575

44 1 0 -5.062148 5.062148 -0.085575

45 1 0 5.062148 5.062148 -0.085575

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.447015 0.000000

3 N 2.295701 1.366421 0.000000

4 C 2.257574 2.204075 1.366421 0.000000

5 C 1.362380 2.257574 2.295701 1.447015 0.000000

6 C 3.622092 3.575833 2.473433 1.415320 2.540491

7 C 4.775460 4.373075 3.050850 2.527413 3.864282

8 N 5.088920 4.299311 2.943952 3.050850 4.497222

9 C 6.453045 5.644445 4.299311 4.373075 5.811148

10 C 7.006524 6.453045 5.088920 4.775460 6.119478

11 C 6.119478 5.811148 4.497222 3.864282 5.079827

12 C 2.540491 1.415320 2.473433 3.575833 3.622092

13 C 3.864282 2.527413 3.050850 4.373075 4.775460

14 C 5.079827 3.864282 4.497222 5.811148 6.119478

15 C 6.119478 4.775460 5.088920 6.453045 7.006524

16 C 5.811148 4.373075 4.299311 5.644445 6.453045

17 N 4.497222 3.050850 2.943952 4.299311 5.088920

18 C 6.947455 5.502171 5.146574 6.407600 7.411652

19 C 7.174805 5.778376 5.091626 6.184463 7.381098

20 C 8.546340 7.174805 6.391547 7.381098 8.654248

21 C 8.654248 7.381098 6.391547 7.174805 8.546340

22 C 7.381098 6.184463 5.091626 5.778376 7.174805

23 N 6.391547 5.091626 4.163376 5.091626 6.391547

24 H 1.079723 2.252626 3.329372 3.313667 2.194641

25 H 2.194641 3.313667 3.329372 2.252626 1.079723

26 H 8.078161 7.530329 6.165547 5.839472 7.161231

27 H 6.508136 6.420440 5.182446 4.314584 5.327511

28 H 5.327511 4.314584 5.182446 6.420440 6.508136

29 H 7.161231 5.839472 6.165547 7.530329 8.078161

30 H 9.424575 8.021290 7.333962 8.381358 9.616302

31 H 9.616302 8.381358 7.333962 8.021290 9.424575

32 Zn 4.333362 3.098431 2.088797 3.098431 4.333362

33 C 7.411652 6.407600 5.146574 5.502171 6.947455

34 C 8.765634 7.811509 6.526698 6.766745 8.211082

35 C 2.892065 2.420431 3.718546 4.592311 4.216457

36 C 9.925602 9.003381 7.706151 7.878604 9.315603

37 C 3.626620 3.505820 4.849393 5.592784 4.988938

38 C 4.216457 4.592311 3.718546 2.420431 2.892065

39 C 4.988938 5.592784 4.849393 3.505820 3.626620

40 C 8.211082 6.766745 6.526698 7.811509 8.765634

41 C 9.315603 7.878604 7.706151 9.003381 9.925602

42 H 10.312268 8.883280 8.756172 10.061181 10.960658

43 H 10.960658 10.061181 8.756172 8.883280 10.312268

44 H 5.797442 6.536465 5.875312 4.517817 4.451650

45 H 4.451650 4.517817 5.875312 6.536465 5.797442

6 7 8 9 10

6 C 0.000000

7 C 1.415320 0.000000

8 N 2.473433 1.366421 0.000000

9 C 3.575833 2.204075 1.366421 0.000000

10 C 3.622092 2.257574 2.295701 1.447015 0.000000

11 C 2.540491 1.447015 2.295701 2.257574 1.362380

12 C 4.892508 5.502171 5.146574 6.407600 7.411652

13 C 5.502171 5.778376 5.091626 6.184463 7.381098

14 C 6.947455 7.174805 6.391547 7.381098 8.654248

15 C 7.411652 7.381098 6.391547 7.174805 8.546340

16 C 6.407600 6.184463 5.091626 5.778376 7.174805

17 N 5.146574 5.091626 4.163376 5.091626 6.391547

18 C 6.919051 6.407600 5.146574 5.502171 6.947455

19 C 6.407600 5.644445 4.299311 4.373075 5.811148

20 C 7.411652 6.453045 5.088920 4.775460 6.119478

21 C 6.947455 5.811148 4.497222 3.864282 5.079827

22 C 5.502171 4.373075 3.050850 2.527413 3.864282

23 N 5.146574 4.299311 2.943952 3.050850 4.497222

24 H 4.640177 5.839472 6.165547 7.530329 8.078161

25 H 2.901935 4.314584 5.182446 6.420440 6.508136

26 H 4.640177 3.313667 3.329372 2.252626 1.079723

27 H 2.901935 2.252626 3.329372 3.313667 2.194641

28 H 7.655192 8.021290 7.333962 8.381358 9.616302

29 H 8.468293 8.381358 7.333962 8.021290 9.424575

30 H 8.468293 7.530329 6.165547 5.839472 7.161231

31 H 7.655192 6.420440 5.182446 4.314584 5.327511

32 Zn 3.465330 3.098431 2.088797 3.098431 4.333362

33 C 4.892508 3.575833 2.473433 1.415320 2.540491

34 C 5.987089 4.592311 3.718546 2.420431 2.892065

35 C 5.987089 6.766745 6.526698 7.811509 8.765634

36 C 7.005835 5.592784 4.849393 3.505820 3.626620

37 C 7.005835 7.878604 7.706151 9.003381 9.925602

38 C 1.427061 2.420431 3.718546 4.592311 4.216457

39 C 2.632867 3.505820 4.849393 5.592784 4.988938

40 C 8.345895 7.811509 6.526698 6.766745 8.211082

41 C 9.551516 9.003381 7.706151 7.878604 9.315603

42 H 10.618754 10.061181 8.756172 8.883280 10.312268

43 H 7.951398 6.536465 5.875312 4.517817 4.451650

44 H 3.700206 4.517817 5.875312 6.536465 5.797442

45 H 7.951398 8.883280 8.756172 10.061181 10.960658

11 12 13 14 15

11 C 0.000000

12 C 6.947455 0.000000

13 C 7.174805 1.415320 0.000000

14 C 8.546340 2.540491 1.447015 0.000000

15 C 8.654248 3.622092 2.257574 1.362380 0.000000

16 C 7.381098 3.575833 2.204075 2.257574 1.447015

17 N 6.391547 2.473433 1.366421 2.295701 2.295701

18 C 7.411652 4.892508 3.575833 3.622092 2.540491

19 C 6.453045 5.502171 4.373075 4.775460 3.864282

20 C 7.006524 6.947455 5.811148 6.119478 5.079827

21 C 6.119478 7.411652 6.453045 7.006524 6.119478

22 C 4.775460 6.407600 5.644445 6.453045 5.811148

23 N 5.088920 5.146574 4.299311 5.088920 4.497222

24 H 7.161231 2.901935 4.314584 5.327511 6.508136

25 H 5.327511 4.640177 5.839472 7.161231 8.078161

26 H 2.194641 8.468293 8.381358 9.616302 9.424575

27 H 1.079723 7.655192 8.021290 9.424575 9.616302

28 H 9.424575 2.901935 2.252626 1.079723 2.194641

29 H 9.616302 4.640177 3.313667 2.194641 1.079723

30 H 8.078161 7.655192 6.420440 6.508136 5.327511

31 H 6.508136 8.468293 7.530329 8.078161 7.161231

32 Zn 4.333362 3.465330 3.098431 4.333362 4.333362

33 C 3.622092 6.919051 6.407600 7.411652 6.947455

34 C 4.216457 8.345895 7.811509 8.765634 8.211082

35 C 8.211082 1.427061 2.420431 2.892065 4.216457

36 C 4.988938 9.551516 9.003381 9.925602 9.315603

37 C 9.315603 2.632867 3.505820 3.626620 4.988938

38 C 2.892065 5.987089 6.766745 8.211082 8.765634

39 C 3.626620 7.005835 7.878604 9.315603 9.925602

40 C 8.765634 5.987089 4.592311 4.216457 2.892065

41 C 9.925602 7.005835 5.592784 4.988938 3.626620

42 H 10.960658 7.951398 6.536465 5.797442 4.451650

43 H 5.797442 10.618754 10.061181 10.960658 10.312268

44 H 4.451650 7.951398 8.883280 10.312268 10.960658

45 H 10.312268 3.700206 4.517817 4.451650 5.797442

16 17 18 19 20

16 C 0.000000

17 N 1.366421 0.000000

18 C 1.415320 2.473433 0.000000

19 C 2.527413 3.050850 1.415320 0.000000

20 C 3.864282 4.497222 2.540491 1.447015 0.000000

21 C 4.775460 5.088920 3.622092 2.257574 1.362380

22 C 4.373075 4.299311 3.575833 2.204075 2.257574

23 N 3.050850 2.943952 2.473433 1.366421 2.295701

24 H 6.420440 5.182446 7.655192 8.021290 9.424575

25 H 7.530329 6.165547 8.468293 8.381358 9.616302

26 H 8.021290 7.333962 7.655192 6.420440 6.508136

27 H 8.381358 7.333962 8.468293 7.530329 8.078161

28 H 3.313667 3.329372 4.640177 5.839472 7.161231

29 H 2.252626 3.329372 2.901935 4.314584 5.327511

30 H 4.314584 5.182446 2.901935 2.252626 1.079723

31 H 5.839472 6.165547 4.640177 3.313667 2.194641

32 Zn 3.098431 2.088797 3.465330 3.098431 4.333362

33 C 5.502171 5.146574 4.892508 3.575833 3.622092

34 C 6.766745 6.526698 5.987089 4.592311 4.216457

35 C 4.592311 3.718546 5.987089 6.766745 8.211082

36 C 7.878604 7.706151 7.005835 5.592784 4.988938

37 C 5.592784 4.849393 7.005835 7.878604 9.315603

38 C 7.811509 6.526698 8.345895 7.811509 8.765634

39 C 9.003381 7.706151 9.551516 9.003381 9.925602

40 C 2.420431 3.718546 1.427061 2.420431 2.892065

41 C 3.505820 4.849393 2.632867 3.505820 3.626620

42 H 4.517817 5.875312 3.700206 4.517817 4.451650

43 H 8.883280 8.756172 7.951398 6.536465 5.797442

44 H 10.061181 8.756172 10.618754 10.061181 10.960658

45 H 6.536465 5.875312 7.951398 8.883280 10.312268

21 22 23 24 25

21 C 0.000000

22 C 1.447015 0.000000

23 N 2.295701 1.366421 0.000000

24 H 9.616302 8.381358 7.333962 0.000000

25 H 9.424575 8.021290 7.333962 2.679611 0.000000

26 H 5.327511 4.314584 5.182446 9.147317 7.495971

27 H 7.161231 5.839472 6.165547 7.495971 5.357775

28 H 8.078161 7.530329 6.165547 5.357775 7.495971

29 H 6.508136 6.420440 5.182446 7.495971 9.147317

30 H 2.194641 3.313667 3.329372 10.256649 10.600904

31 H 1.079723 2.252626 3.329372 10.600904 10.256649

32 Zn 4.333362 3.098431 2.088797 5.306806 5.306806

33 C 2.540491 1.415320 2.473433 8.468293 7.655192

34 C 2.892065 2.420431 3.718546 9.832025 8.840350

35 C 8.765634 7.811509 6.526698 2.697260 5.078596

36 C 3.626620 3.505820 4.849393 10.996785 9.891613

37 C 9.925602 9.003381 7.706151 3.079177 5.706716

38 C 8.211082 6.766745 6.526698 5.078596 2.697260

39 C 9.315603 7.878604 7.706151 5.706716 3.079177

40 C 4.216457 4.592311 3.718546 8.840350 9.832025

41 C 4.988938 5.592784 4.849393 9.891613 10.996785

42 H 5.797442 6.536465 5.875312 10.849048 12.034576

43 H 4.451650 4.517817 5.875312 12.034576 10.849048

44 H 10.312268 8.883280 8.756172 6.402317 3.722968

45 H 10.960658 10.061181 8.756172 3.722968 6.402317

26 27 28 29 30

26 H 0.000000

27 H 2.679611 0.000000

28 H 10.600904 10.256649 0.000000

29 H 10.256649 10.600904 2.679611 0.000000

30 H 7.495971 9.147317 7.495971 5.357775 0.000000

31 H 5.357775 7.495971 9.147317 7.495971 2.679611

32 Zn 5.306806 5.306806 5.306806 5.306806 5.306806

33 C 2.901935 4.640177 8.468293 7.655192 4.640177

34 C 2.697260 5.078596 9.832025 8.840350 5.078596

35 C 9.832025 8.840350 2.697260 5.078596 8.840350

36 C 3.079177 5.706716 10.996785 9.891613 5.706716

37 C 10.996785 9.891613 3.079177 5.706716 9.891613

38 C 5.078596 2.697260 8.840350 9.832025 9.832025

39 C 5.706716 3.079177 9.891613 10.996785 10.996785

40 C 8.840350 9.832025 5.078596 2.697260 2.697260

41 C 9.891613 10.996785 5.706716 3.079177 3.079177

42 H 10.849048 12.034576 6.402317 3.722968 3.722968

43 H 3.722968 6.402317 12.034576 10.849048 6.402317

44 H 6.402317 3.722968 10.849048 12.034576 12.034576

45 H 12.034576 10.849048 3.722968 6.402317 10.849048

31 32 33 34 35

31 H 0.000000

32 Zn 5.306806 0.000000

33 C 2.901935 3.465330 0.000000

34 C 2.697260 4.891633 1.427061 0.000000

35 C 9.832025 4.891633 8.345895 9.772648 0.000000

36 C 3.079177 6.097152 2.632867 1.205809 10.978194

37 C 10.996785 6.097152 9.551516 10.978194 1.205809

38 C 8.840350 4.891633 5.987089 6.910306 6.910306

39 C 9.891613 6.097152 7.005835 7.809441 7.809441

40 C 5.078596 4.891633 5.987089 6.910306 6.910306

41 C 5.706716 6.097152 7.005835 7.809441 7.809441

42 H 6.402317 7.164282 7.951398 8.667709 8.667709

43 H 3.722968 7.164282 3.700206 2.273147 12.045380

44 H 10.849048 7.164282 7.951398 8.667709 8.667709

45 H 12.034576 7.164282 10.618754 12.045380 2.273147

36 37 38 39 40

36 C 0.000000

37 C 12.183676 0.000000

38 C 7.809441 7.809441 0.000000

39 C 8.615160 8.615160 1.205809 0.000000

40 C 7.809441 7.809441 9.772648 10.978194 0.000000

41 C 8.615160 8.615160 10.978194 12.183676 1.205809

42 H 9.400088 9.400088 12.045380 13.250814 2.273147

43 H 1.067339 13.250814 8.667709 9.400088 8.667709

44 H 9.400088 9.400088 2.273147 1.067339 12.045380

45 H 13.250814 1.067339 8.667709 9.400088 8.667709

41 42 43 44 45

41 C 0.000000

42 H 1.067339 0.000000

43 H 9.400088 10.124297 0.000000

44 H 13.250814 14.317918 10.124297 0.000000

45 H 9.400088 10.124297 14.317918 10.124297 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

RotChk: IX=3 Diff= 4.09D-20

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681190 -4.273170 -0.043565

2 6 0 -1.102037 -2.889188 -0.007040

3 7 0 0.000000 -2.081688 0.016686

4 6 0 1.102037 -2.889188 -0.007040

5 6 0 0.681190 -4.273170 -0.043565

6 6 0 2.446254 -2.446254 -0.011615

7 6 0 2.889188 -1.102037 -0.007040

8 7 0 2.081688 0.000000 0.016686

9 6 0 2.889188 1.102037 -0.007040

10 6 0 4.273170 0.681190 -0.043565

11 6 0 4.273170 -0.681190 -0.043565

12 6 0 -2.446254 -2.446254 -0.011615

13 6 0 -2.889188 -1.102037 -0.007040

14 6 0 -4.273170 -0.681190 -0.043565

15 6 0 -4.273170 0.681190 -0.043565

16 6 0 -2.889188 1.102037 -0.007040

17 7 0 -2.081688 0.000000 0.016686

18 6 0 -2.446254 2.446254 -0.011615

19 6 0 -1.102037 2.889188 -0.007040

20 6 0 -0.681190 4.273170 -0.043565

21 6 0 0.681190 4.273170 -0.043565

22 6 0 1.102037 2.889188 -0.007040

23 7 0 0.000000 2.081688 0.016686

24 1 0 -1.339805 -5.128325 -0.070745

25 1 0 1.339805 -5.128325 -0.070745

26 1 0 5.128325 1.339805 -0.070745

27 1 0 5.128325 -1.339805 -0.070745

28 1 0 -5.128325 -1.339805 -0.070745

29 1 0 -5.128325 1.339805 -0.070745

30 1 0 -1.339805 5.128325 -0.070745

31 1 0 1.339805 5.128325 -0.070745

32 30 0 0.000000 0.000000 0.188871

33 6 0 2.446254 2.446254 -0.011615

34 6 0 3.455153 3.455153 -0.038963

35 6 0 -3.455153 -3.455153 -0.038963

36 6 0 4.307580 4.307580 -0.065648

37 6 0 -4.307580 -4.307580 -0.065648

38 6 0 3.455153 -3.455153 -0.038963

39 6 0 4.307580 -4.307580 -0.065648

40 6 0 -3.455153 3.455153 -0.038963

41 6 0 -4.307580 4.307580 -0.065648

42 1 0 -5.062148 5.062148 -0.087241

43 1 0 5.062148 5.062148 -0.087241

44 1 0 5.062148 -5.062148 -0.087241

45 1 0 -5.062148 -5.062148 -0.087241

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

Rotational constants (GHZ): 0.1465121 0.1465121 0.0733163

Leave Link 202 at Fri Jul 26 14:22:30 2019, MaxMem= 1342177280 cpu: 0.1

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 184 symmetry adapted cartesian basis functions of A1 symmetry.

There are 155 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3060.5687965902 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= 9 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= -0.1305295253 Hartrees.

Nuclear repulsion after empirical dispersion term = 3060.4382670650 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: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3898

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.26D-05

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 156

GePol: Fraction of low-weight points (<1% of avg) = 4.00%

GePol: Cavity surface area = 415.543 Ang\*\*2

GePol: Cavity volume = 419.937 Ang\*\*3

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

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

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PCM non-electrostatic energy = 0.0084012916 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3060.4466683566 Hartrees.

Leave Link 301 at Fri Jul 26 14:22:30 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44808.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.40D-05 NBF= 172 148 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 172 148 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:22:30 2019, MaxMem= 1342177280 cpu: 6.6

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:22:30 2019, MaxMem= 1342177280 cpu: 0.8

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

Initial guess from the checkpoint file: "ZnTSPsim0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Occupied (E) (E) (B2) (A1) (E) (E) (B1) (A1) (B2) (E) (E)

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

(E) (E) (A1) (A2) (E) (E) (B1) (B1) (E) (E) (A1)

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

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

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(E) (E) (A2) (A1)

Virtual (A1) (A1) (B2) (A1) (B2) (A1) (A1) (B2) (A1) (B2)

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The electronic state of the initial guess is 1-A1.

Leave Link 401 at Fri Jul 26 14:22:31 2019, MaxMem= 1342177280 cpu: 10.3

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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.

An orbital has undefined symmetry, so N\*\*3 symmetry is turned off.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 660000000 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= 0 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= 45583212.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.44D-15 for 647.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.38D-15 for 3163 982.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.99D-15 for 626.

Iteration 1 A^-1\*A deviation from orthogonality is 1.50D-14 for 882 866.

E= -1359.06298432499

DIIS: error= 3.86D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.06298432499 IErMin= 1 ErrMin= 3.86D-04

ErrMax= 3.86D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.23D-05 BMatP= 5.23D-05

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.86D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 3.229 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.58D-05 MaxDP=6.59D-04 OVMax= 1.80D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.58D-05 CP: 1.00D+00

E= -1359.06304390767 Delta-E= -0.000059582680 Rises=F Damp=F

DIIS: error= 5.09D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.06304390767 IErMin= 2 ErrMin= 5.09D-05

ErrMax= 5.09D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.02D-07 BMatP= 5.23D-05

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

Coeff-Com: -0.374D-01 0.104D+01

Coeff: -0.374D-01 0.104D+01

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.61D-06 MaxDP=8.20D-05 DE=-5.96D-05 OVMax= 2.33D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.32D-06 CP: 1.00D+00 1.05D+00

E= -1359.06304400993 Delta-E= -0.000000102258 Rises=F Damp=F

DIIS: error= 7.42D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.06304400993 IErMin= 2 ErrMin= 5.09D-05

ErrMax= 7.42D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.12D-07 BMatP= 5.02D-07

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

Coeff-Com: -0.286D-01 0.614D+00 0.415D+00

Coeff: -0.286D-01 0.614D+00 0.415D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.25D-06 MaxDP=4.79D-05 DE=-1.02D-07 OVMax= 1.62D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 7.30D-07 CP: 1.00D+00 1.05D+00 5.72D-01

E= -1359.06304462981 Delta-E= -0.000000619888 Rises=F Damp=F

DIIS: error= 1.04D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.06304462981 IErMin= 4 ErrMin= 1.04D-05

ErrMax= 1.04D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.85D-08 BMatP= 5.02D-07

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

Coeff-Com: -0.800D-02 0.140D+00 0.195D+00 0.673D+00

Coeff: -0.800D-02 0.140D+00 0.195D+00 0.673D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 305122 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.86D-07 MaxDP=1.75D-05 DE=-6.20D-07 OVMax= 4.65D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.34D-07 CP: 1.00D+00 1.05D+00 6.17D-01 8.25D-01

E= -1359.06304466011 Delta-E= -0.000000030299 Rises=F Damp=F

DIIS: error= 1.10D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.06304466011 IErMin= 4 ErrMin= 1.04D-05

ErrMax= 1.10D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-08 BMatP= 3.85D-08

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

Coeff-Com: -0.131D-02 0.799D-02 0.650D-01 0.405D+00 0.524D+00

Coeff: -0.131D-02 0.799D-02 0.650D-01 0.405D+00 0.524D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.27D-07 MaxDP=6.46D-06 DE=-3.03D-08 OVMax= 1.86D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 7.48D-08 CP: 1.00D+00 1.05D+00 6.25D-01 8.90D-01 6.19D-01

E= -1359.06304466699 Delta-E= -0.000000006876 Rises=F Damp=F

DIIS: error= 1.38D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.06304466699 IErMin= 6 ErrMin= 1.38D-06

ErrMax= 1.38D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.27D-10 BMatP= 1.03D-08

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

Coeff-Com: 0.178D-03-0.109D-01 0.117D-01 0.127D+00 0.257D+00 0.615D+00

Coeff: 0.178D-03-0.109D-01 0.117D-01 0.127D+00 0.257D+00 0.615D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=4.31D-08 MaxDP=1.54D-06 DE=-6.88D-09 OVMax= 6.28D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.61D-08 CP: 1.00D+00 1.05D+00 6.24D-01 9.01D-01 6.61D-01

CP: 7.61D-01

E= -1359.06304466717 Delta-E= -0.000000000178 Rises=F Damp=F

DIIS: error= 8.74D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.06304466717 IErMin= 7 ErrMin= 8.74D-07

ErrMax= 8.74D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.09D-10 BMatP= 6.27D-10

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

Coeff-Com: 0.250D-03-0.802D-02 0.383D-03 0.363D-01 0.109D+00 0.417D+00

Coeff-Com: 0.445D+00

Coeff: 0.250D-03-0.802D-02 0.383D-03 0.363D-01 0.109D+00 0.417D+00

Coeff: 0.445D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.07D-08 MaxDP=7.83D-07 DE=-1.78D-10 OVMax= 2.59D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.30D-09 CP: 1.00D+00 1.05D+00 6.27D-01 9.00D-01 6.75D-01

CP: 7.80D-01 5.09D-01

E= -1359.06304466740 Delta-E= -0.000000000234 Rises=F Damp=F

DIIS: error= 7.87D-08 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.06304466740 IErMin= 8 ErrMin= 7.87D-08

ErrMax= 7.87D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.52D-12 BMatP= 2.09D-10

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

Coeff-Com: 0.764D-04-0.222D-02-0.359D-03 0.666D-02 0.244D-01 0.115D+00

Coeff-Com: 0.148D+00 0.708D+00

Coeff: 0.764D-04-0.222D-02-0.359D-03 0.666D-02 0.244D-01 0.115D+00

Coeff: 0.148D+00 0.708D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.56D-09 MaxDP=9.14D-08 DE=-2.34D-10 OVMax= 2.74D-07

Error on total polarization charges = 0.06212

SCF Done: E(RB3LYP) = -1359.06304467 A.U. after 8 cycles

NFock= 8 Conv=0.26D-08 -V/T= 1.9682

KE= 1.403727450055D+03 PE=-9.362978034089D+03 EE= 3.539740871010D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.27

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:23:07 2019, MaxMem= 1342177280 cpu: 399.7

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44808.

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 = 260

Leave Link 701 at Fri Jul 26 14:23:11 2019, MaxMem= 1342177280 cpu: 43.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

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

Leave Link 702 at Fri Jul 26 14:23:11 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Fri Jul 26 14:23:15 2019, MaxMem= 1342177280 cpu: 42.9

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 0.00000000D+00 7.17648163D-13 3.25175567D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000037336 0.000035839 0.000013702

2 6 -0.000022932 -0.000029320 0.000066084

3 7 0.000000000 0.000012234 -0.000110207

4 6 0.000022932 -0.000029320 0.000066084

5 6 0.000037336 0.000035839 0.000013702

6 6 0.000033845 -0.000033845 -0.000022914

7 6 0.000029320 -0.000022932 0.000066084

8 7 -0.000012234 0.000000000 -0.000110207

9 6 0.000029320 0.000022932 0.000066084

10 6 -0.000035839 0.000037336 0.000013702

11 6 -0.000035839 -0.000037336 0.000013702

12 6 -0.000033845 -0.000033845 -0.000022914

13 6 -0.000029320 -0.000022932 0.000066084

14 6 0.000035839 -0.000037336 0.000013702

15 6 0.000035839 0.000037336 0.000013702

16 6 -0.000029320 0.000022932 0.000066084

17 7 0.000012234 0.000000000 -0.000110207

18 6 -0.000033845 0.000033845 -0.000022914

19 6 -0.000022932 0.000029320 0.000066084

20 6 -0.000037336 -0.000035839 0.000013702

21 6 0.000037336 -0.000035839 0.000013702

22 6 0.000022932 0.000029320 0.000066084

23 7 0.000000000 -0.000012234 -0.000110207

24 1 -0.000009678 0.000011314 -0.000004041

25 1 0.000009678 0.000011314 -0.000004041

26 1 -0.000011314 0.000009678 -0.000004041

27 1 -0.000011314 -0.000009678 -0.000004041

28 1 0.000011314 -0.000009678 -0.000004041

29 1 0.000011314 0.000009678 -0.000004041

30 1 -0.000009678 -0.000011314 -0.000004041

31 1 0.000009678 -0.000011314 -0.000004041

32 30 0.000000000 0.000000000 0.000060855

33 6 0.000033845 0.000033845 -0.000022914

34 6 0.000017049 0.000017049 -0.000023829

35 6 -0.000017049 -0.000017049 -0.000023829

36 6 0.000011484 0.000011484 -0.000014619

37 6 -0.000011484 -0.000011484 -0.000014619

38 6 0.000017049 -0.000017049 -0.000023829

39 6 0.000011484 -0.000011484 -0.000014619

40 6 -0.000017049 0.000017049 -0.000023829

41 6 -0.000011484 0.000011484 -0.000014619

42 1 0.000000898 -0.000000898 0.000004866

43 1 -0.000000898 -0.000000898 0.000004866

44 1 -0.000000898 0.000000898 0.000004866

45 1 0.000000898 0.000000898 0.000004866

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

Cartesian Forces: Max 0.000110207 RMS 0.000032388

Leave Link 716 at Fri Jul 26 14:23:15 2019, MaxMem= 1342177280 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000050500 RMS 0.000018808

Search for a local minimum.

Step number 14 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .18808D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 2 3 4 5 7

9 8 10 11 12

13 14

DE= -8.00D-06 DEPred=-7.70D-06 R= 1.04D+00

TightC=F SS= 1.41D+00 RLast= 2.34D-02 DXNew= 1.4142D-01 7.0292D-02

Trust test= 1.04D+00 RLast= 2.34D-02 DXMaxT set to 8.41D-02

ITU= 1 1 -1 1 0 -1 0 0 -1 1 0 -1 -1 0

Eigenvalues --- 0.00534 0.00534 0.00534 0.00534 0.00534

Eigenvalues --- 0.00534 0.00535 0.00665 0.01156 0.01156

Eigenvalues --- 0.01167 0.01383 0.01383 0.01562 0.01624

Eigenvalues --- 0.01646 0.01674 0.01726 0.01726 0.01805

Eigenvalues --- 0.01805 0.01825 0.01831 0.01859 0.01859

Eigenvalues --- 0.01868 0.01868 0.01868 0.01908 0.01920

Eigenvalues --- 0.01927 0.01927 0.01934 0.01941 0.01961

Eigenvalues --- 0.01961 0.02178 0.02180 0.02185 0.02185

Eigenvalues --- 0.02222 0.02627 0.03317 0.03685 0.04654

Eigenvalues --- 0.04654 0.04654 0.04654 0.04654 0.04654

Eigenvalues --- 0.04654 0.08540 0.13847 0.14999 0.14999

Eigenvalues --- 0.15057 0.15999 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.18042 0.22832

Eigenvalues --- 0.22868 0.22872 0.22872 0.24760 0.24776

Eigenvalues --- 0.24776 0.24840 0.24867 0.24979 0.24979

Eigenvalues --- 0.24998 0.24998 0.24998 0.24998 0.24999

Eigenvalues --- 0.27458 0.35035 0.35035 0.35468 0.35499

Eigenvalues --- 0.35728 0.35916 0.36034 0.36034 0.36034

Eigenvalues --- 0.36034 0.36034 0.36034 0.36035 0.36780

Eigenvalues --- 0.36864 0.36864 0.36884 0.37563 0.37563

Eigenvalues --- 0.37563 0.37602 0.38968 0.38968 0.39538

Eigenvalues --- 0.41397 0.41397 0.41397 0.41517 0.41517

Eigenvalues --- 0.41770 0.41790 0.42522 0.43514 0.43779

Eigenvalues --- 0.43779 0.45620 0.47914 0.49087 0.49087

Eigenvalues --- 0.50131 0.51399 0.51901 0.51901 0.54284

Eigenvalues --- 1.01831 1.01831 1.01831 1.01919

En-DIIS/RFO-DIIS IScMMF= 0 using points: 14 13 12 11 10

RFO step: Lambda=-2.60925058D-07.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 9.12D-05 SmlDif= 1.00D-05

RMS Error= 0.6766916108D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.15030 -0.15611 0.01995 -0.00866 -0.00549

Iteration 1 RMS(Cart)= 0.00116971 RMS(Int)= 0.00000040

Iteration 2 RMS(Cart)= 0.00000064 RMS(Int)= 0.00000029

ITry= 1 IFail=0 DXMaxC= 6.37D-03 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.36D-04 for atom 45.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73446 0.00004 0.00006 0.00007 0.00013 2.73459

R2 2.57453 -0.00005 -0.00003 -0.00004 -0.00007 2.57446

R3 2.04038 0.00000 0.00000 0.00000 0.00000 2.04038

R4 2.58216 -0.00005 -0.00008 0.00000 -0.00008 2.58208

R5 2.67457 -0.00002 -0.00007 0.00002 -0.00004 2.67452

R6 2.58216 -0.00005 -0.00008 0.00000 -0.00008 2.58208

R7 3.94725 -0.00001 0.00013 0.00003 0.00017 3.94743

R8 2.73446 0.00004 0.00006 0.00007 0.00013 2.73459

R9 2.67457 -0.00002 -0.00007 0.00002 -0.00004 2.67452

R10 2.04038 0.00000 0.00000 0.00000 0.00000 2.04038

R11 2.67457 -0.00002 -0.00007 0.00002 -0.00004 2.67452

R12 2.69675 -0.00004 0.00017 -0.00015 0.00000 2.69675

R13 2.58216 -0.00005 -0.00008 0.00000 -0.00008 2.58208

R14 2.73446 0.00004 0.00006 0.00007 0.00013 2.73459

R15 2.58216 -0.00005 -0.00008 0.00000 -0.00008 2.58208

R16 3.94725 -0.00001 0.00013 0.00003 0.00017 3.94743

R17 2.73446 0.00004 0.00006 0.00007 0.00013 2.73459

R18 2.67457 -0.00002 -0.00007 0.00002 -0.00004 2.67452

R19 2.57453 -0.00005 -0.00003 -0.00004 -0.00007 2.57446

R20 2.04038 0.00000 0.00000 0.00000 0.00000 2.04038

R21 2.04038 0.00000 0.00000 0.00000 0.00000 2.04038

R22 2.67457 -0.00002 -0.00007 0.00002 -0.00004 2.67452

R23 2.69675 -0.00004 0.00017 -0.00015 0.00000 2.69675

R24 2.73446 0.00004 0.00006 0.00007 0.00013 2.73459

R25 2.58216 -0.00005 -0.00008 0.00000 -0.00008 2.58208

R26 2.57453 -0.00005 -0.00003 -0.00004 -0.00007 2.57446

R27 2.04038 0.00000 0.00000 0.00000 0.00000 2.04038

R28 2.73446 0.00004 0.00006 0.00007 0.00013 2.73459

R29 2.04038 0.00000 0.00000 0.00000 0.00000 2.04038

R30 2.58216 -0.00005 -0.00008 0.00000 -0.00008 2.58208

R31 2.67457 -0.00002 -0.00007 0.00002 -0.00004 2.67452

R32 3.94725 -0.00001 0.00013 0.00003 0.00017 3.94743

R33 2.67457 -0.00002 -0.00007 0.00002 -0.00004 2.67452

R34 2.69675 -0.00004 0.00017 -0.00015 0.00000 2.69675

R35 2.73446 0.00004 0.00006 0.00007 0.00013 2.73459

R36 2.58216 -0.00005 -0.00008 0.00000 -0.00008 2.58208

R37 2.57453 -0.00005 -0.00003 -0.00004 -0.00007 2.57446

R38 2.04038 0.00000 0.00000 0.00000 0.00000 2.04038

R39 2.73446 0.00004 0.00006 0.00007 0.00013 2.73459

R40 2.04038 0.00000 0.00000 0.00000 0.00000 2.04038

R41 2.58216 -0.00005 -0.00008 0.00000 -0.00008 2.58208

R42 2.67457 -0.00002 -0.00007 0.00002 -0.00004 2.67452

R43 3.94725 -0.00001 0.00013 0.00003 0.00017 3.94743

R44 2.69675 -0.00004 0.00017 -0.00015 0.00000 2.69675

R45 2.27865 -0.00001 0.00000 -0.00002 -0.00002 2.27863

R46 2.27865 -0.00001 0.00000 -0.00002 -0.00002 2.27863

R47 2.01698 0.00000 0.00001 0.00000 0.00001 2.01699

R48 2.01698 0.00000 0.00001 0.00000 0.00001 2.01699

R49 2.27865 -0.00001 0.00000 -0.00002 -0.00002 2.27863

R50 2.01698 0.00000 0.00001 0.00000 0.00001 2.01699

R51 2.27865 -0.00001 0.00000 -0.00002 -0.00002 2.27863

R52 2.01698 0.00000 0.00001 0.00000 0.00001 2.01699

A1 1.86590 -0.00001 -0.00001 0.00000 -0.00002 1.86588

A2 2.19043 0.00002 0.00007 0.00004 0.00011 2.19054

A3 2.22684 -0.00001 -0.00006 -0.00004 -0.00009 2.22675

A4 1.90826 0.00002 -0.00001 0.00001 0.00000 1.90825

A5 2.18397 0.00001 0.00002 0.00005 0.00007 2.18404

A6 2.19088 -0.00003 0.00000 -0.00006 -0.00007 2.19082

A7 1.87646 -0.00001 0.00005 -0.00001 0.00004 1.87650

A8 2.20233 0.00000 -0.00005 -0.00001 -0.00006 2.20227

A9 2.20233 0.00000 -0.00005 -0.00001 -0.00006 2.20227

A10 1.90826 0.00002 -0.00001 0.00001 0.00000 1.90825

A11 2.19088 -0.00003 0.00000 -0.00006 -0.00007 2.19082

A12 2.18397 0.00001 0.00002 0.00005 0.00007 2.18404

A13 1.86590 -0.00001 -0.00001 0.00000 -0.00002 1.86588

A14 2.22684 -0.00001 -0.00006 -0.00004 -0.00009 2.22675

A15 2.19043 0.00002 0.00007 0.00004 0.00011 2.19054

A16 2.20739 0.00004 0.00005 0.00011 0.00016 2.20755

A17 2.03786 -0.00002 -0.00003 -0.00005 -0.00008 2.03778

A18 2.03786 -0.00002 -0.00003 -0.00006 -0.00008 2.03778

A19 2.19088 -0.00003 0.00000 -0.00006 -0.00007 2.19082

A20 2.18397 0.00001 0.00002 0.00005 0.00007 2.18404

A21 1.90826 0.00002 -0.00001 0.00001 0.00000 1.90825

A22 1.87646 -0.00001 0.00005 -0.00001 0.00004 1.87650

A23 2.20233 0.00000 -0.00005 -0.00001 -0.00006 2.20227

A24 2.20233 0.00000 -0.00005 -0.00001 -0.00006 2.20227

A25 1.90826 0.00002 -0.00001 0.00001 0.00000 1.90825

A26 2.19088 -0.00003 0.00000 -0.00006 -0.00007 2.19082

A27 2.18397 0.00001 0.00002 0.00005 0.00007 2.18404

A28 1.86590 -0.00001 -0.00001 0.00000 -0.00002 1.86588

A29 2.19043 0.00002 0.00007 0.00004 0.00011 2.19054

A30 2.22684 -0.00001 -0.00006 -0.00004 -0.00009 2.22675

A31 1.86590 -0.00001 -0.00001 0.00000 -0.00002 1.86588

A32 2.19043 0.00002 0.00007 0.00004 0.00011 2.19054

A33 2.22684 -0.00001 -0.00006 -0.00004 -0.00009 2.22675

A34 2.20739 0.00004 0.00005 0.00011 0.00016 2.20755

A35 2.03786 -0.00002 -0.00003 -0.00005 -0.00008 2.03778

A36 2.03786 -0.00002 -0.00003 -0.00006 -0.00008 2.03778

A37 2.18397 0.00001 0.00002 0.00005 0.00007 2.18404

A38 2.19088 -0.00003 0.00000 -0.00006 -0.00007 2.19082

A39 1.90826 0.00002 -0.00001 0.00001 0.00000 1.90825

A40 1.86590 -0.00001 -0.00001 0.00000 -0.00002 1.86588

A41 2.19043 0.00002 0.00007 0.00004 0.00011 2.19054

A42 2.22684 -0.00001 -0.00006 -0.00004 -0.00009 2.22675

A43 1.86590 -0.00001 -0.00001 0.00000 -0.00002 1.86588

A44 2.22684 -0.00001 -0.00006 -0.00004 -0.00009 2.22675

A45 2.19043 0.00002 0.00007 0.00004 0.00011 2.19054

A46 1.90826 0.00002 -0.00001 0.00001 0.00000 1.90825

A47 2.18397 0.00001 0.00002 0.00005 0.00007 2.18404

A48 2.19088 -0.00003 0.00000 -0.00006 -0.00007 2.19082

A49 1.87646 -0.00001 0.00005 -0.00001 0.00004 1.87650

A50 2.20233 0.00000 -0.00005 -0.00001 -0.00006 2.20227

A51 2.20233 0.00000 -0.00005 -0.00001 -0.00006 2.20227

A52 2.20739 0.00004 0.00005 0.00011 0.00016 2.20755

A53 2.03786 -0.00002 -0.00003 -0.00005 -0.00008 2.03778

A54 2.03786 -0.00002 -0.00003 -0.00006 -0.00008 2.03778

A55 2.18397 0.00001 0.00002 0.00005 0.00007 2.18404

A56 2.19088 -0.00003 0.00000 -0.00006 -0.00007 2.19082

A57 1.90826 0.00002 -0.00001 0.00001 0.00000 1.90825

A58 1.86590 -0.00001 -0.00001 0.00000 -0.00002 1.86588

A59 2.19043 0.00002 0.00007 0.00004 0.00011 2.19054

A60 2.22684 -0.00001 -0.00006 -0.00004 -0.00009 2.22675

A61 1.86590 -0.00001 -0.00001 0.00000 -0.00002 1.86588

A62 2.22684 -0.00001 -0.00006 -0.00004 -0.00009 2.22675

A63 2.19043 0.00002 0.00007 0.00004 0.00011 2.19054

A64 1.90826 0.00002 -0.00001 0.00001 0.00000 1.90825

A65 2.18397 0.00001 0.00002 0.00005 0.00007 2.18404

A66 2.19088 -0.00003 0.00000 -0.00006 -0.00007 2.19082

A67 1.87646 -0.00001 0.00005 -0.00001 0.00004 1.87650

A68 2.20233 0.00000 -0.00005 -0.00001 -0.00006 2.20227

A69 2.20233 0.00000 -0.00005 -0.00001 -0.00006 2.20227

A70 1.56400 0.00000 -0.00006 0.00002 -0.00004 1.56396

A71 1.56400 0.00000 -0.00006 0.00002 -0.00004 1.56396

A72 2.97654 0.00000 -0.00075 0.00028 -0.00047 2.97607

A73 2.97654 0.00000 -0.00075 0.00028 -0.00047 2.97607

A74 1.56400 0.00000 -0.00006 0.00002 -0.00004 1.56396

A75 1.56400 0.00000 -0.00006 0.00002 -0.00004 1.56396

A76 2.20739 0.00004 0.00005 0.00011 0.00016 2.20755

A77 2.03786 -0.00002 -0.00003 -0.00005 -0.00008 2.03778

A78 2.03786 -0.00002 -0.00003 -0.00006 -0.00008 2.03778

A79 3.14155 0.00000 0.00000 0.00000 0.00000 3.14155

A80 3.14155 0.00000 0.00000 0.00000 0.00000 3.14155

A81 3.14162 0.00000 0.00000 0.00010 0.00000 3.14162

A82 3.14162 0.00000 0.00000 0.00010 0.00000 3.14162

A83 3.14155 0.00000 0.00000 0.00000 0.00000 3.14155

A84 3.14162 0.00000 0.00000 0.00010 0.00000 3.14162

A85 3.14155 0.00000 0.00000 0.00000 0.00000 3.14155

A86 3.14162 0.00000 0.00000 0.00010 0.00000 3.14162

A87 3.13861 -0.00001 -0.00011 -0.00044 -0.00056 3.13805

A88 3.14458 0.00001 0.00011 0.00044 0.00056 3.14513

A89 3.14378 0.00001 0.00027 0.00002 0.00029 3.14406

A90 3.13941 -0.00001 -0.00027 -0.00002 -0.00029 3.13912

A91 3.13861 -0.00001 -0.00011 -0.00044 -0.00056 3.13805

A92 3.14378 0.00001 0.00027 0.00002 0.00029 3.14406

A93 3.14458 0.00001 0.00011 0.00044 0.00056 3.14513

A94 3.13941 -0.00001 -0.00027 -0.00002 -0.00029 3.13912

D1 -0.00187 0.00000 0.00006 0.00008 0.00014 -0.00173

D2 3.12755 -0.00001 0.00020 -0.00022 -0.00003 3.12752

D3 -3.13822 0.00001 0.00025 0.00006 0.00031 -3.13791

D4 -0.00880 0.00000 0.00038 -0.00024 0.00014 -0.00866

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13620 0.00000 0.00019 -0.00002 0.00017 -3.13603

D7 3.13620 0.00000 -0.00019 0.00002 -0.00017 3.13603

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00303 -0.00001 -0.00010 -0.00013 -0.00023 0.00280

D10 -3.07269 0.00000 0.00069 0.00043 0.00112 -3.07157

D11 -3.12633 0.00000 -0.00024 0.00017 -0.00006 -3.12639

D12 0.08114 0.00001 0.00055 0.00074 0.00129 0.08242

D13 -3.11486 -0.00001 -0.00005 -0.00097 -0.00102 -3.11587

D14 0.01331 -0.00002 -0.00038 -0.00084 -0.00123 0.01209

D15 0.01262 -0.00002 0.00011 -0.00132 -0.00121 0.01141

D16 3.14079 -0.00003 -0.00023 -0.00119 -0.00142 3.13937

D17 -0.00303 0.00001 0.00010 0.00013 0.00023 -0.00280

D18 3.12633 0.00000 0.00024 -0.00017 0.00006 3.12639

D19 3.07269 0.00000 -0.00069 -0.00043 -0.00112 3.07157

D20 -0.08114 -0.00001 -0.00055 -0.00074 -0.00129 -0.08242

D21 -3.09827 -0.00001 -0.00009 -0.00047 -0.00056 -3.09884

D22 -0.12117 -0.00001 -0.00084 -0.00019 -0.00103 -0.12220

D23 -1.60972 -0.00001 -0.00046 -0.00033 -0.00080 -1.61052

D24 0.12117 0.00001 0.00084 0.00019 0.00103 0.12220

D25 3.09827 0.00001 0.00009 0.00047 0.00056 3.09884

D26 1.60972 0.00001 0.00046 0.00033 0.00080 1.61052

D27 0.00187 0.00000 -0.00006 -0.00008 -0.00014 0.00173

D28 3.13822 -0.00001 -0.00025 -0.00006 -0.00031 3.13791

D29 -3.12755 0.00001 -0.00020 0.00022 0.00003 -3.12752

D30 0.00880 0.00000 -0.00038 0.00024 -0.00014 0.00866

D31 -0.01262 0.00002 -0.00011 0.00132 0.00121 -0.01141

D32 -3.14079 0.00003 0.00023 0.00119 0.00142 -3.13937

D33 3.11486 0.00001 0.00005 0.00097 0.00102 3.11587

D34 -0.01331 0.00002 0.00038 0.00084 0.00123 -0.01209

D35 0.01262 -0.00002 0.00011 -0.00132 -0.00121 0.01141

D36 -3.11486 -0.00001 -0.00005 -0.00097 -0.00102 -3.11587

D37 3.14079 -0.00003 -0.00023 -0.00119 -0.00142 3.13937

D38 0.01331 -0.00002 -0.00038 -0.00084 -0.00123 0.01209

D39 -3.12633 0.00000 -0.00024 0.00017 -0.00006 -3.12639

D40 0.08114 0.00001 0.00055 0.00074 0.00129 0.08242

D41 0.00303 -0.00001 -0.00010 -0.00013 -0.00023 0.00280

D42 -3.07269 0.00000 0.00069 0.00043 0.00112 -3.07157

D43 3.12755 -0.00001 0.00020 -0.00022 -0.00003 3.12752

D44 -0.00880 0.00000 0.00038 -0.00024 0.00014 -0.00866

D45 -0.00187 0.00000 0.00006 0.00008 0.00014 -0.00173

D46 -3.13822 0.00001 0.00025 0.00006 0.00031 -3.13791

D47 -0.00303 0.00001 0.00010 0.00013 0.00023 -0.00280

D48 3.12633 0.00000 0.00024 -0.00017 0.00006 3.12639

D49 3.07269 0.00000 -0.00069 -0.00043 -0.00112 3.07157

D50 -0.08114 -0.00001 -0.00055 -0.00074 -0.00129 -0.08242

D51 -0.12117 -0.00001 -0.00084 -0.00019 -0.00103 -0.12220

D52 -1.60972 -0.00001 -0.00046 -0.00033 -0.00080 -1.61052

D53 -3.09827 -0.00001 -0.00009 -0.00047 -0.00056 -3.09884

D54 3.09827 0.00001 0.00009 0.00047 0.00056 3.09884

D55 1.60972 0.00001 0.00046 0.00033 0.00080 1.61052

D56 0.12117 0.00001 0.00084 0.00019 0.00103 0.12220

D57 0.00187 0.00000 -0.00006 -0.00008 -0.00014 0.00173

D58 3.13822 -0.00001 -0.00025 -0.00006 -0.00031 3.13791

D59 -3.12755 0.00001 -0.00020 0.00022 0.00003 -3.12752

D60 0.00880 0.00000 -0.00038 0.00024 -0.00014 0.00866

D61 -0.01262 0.00002 -0.00011 0.00132 0.00121 -0.01141

D62 -3.14079 0.00003 0.00023 0.00119 0.00142 -3.13937

D63 3.11486 0.00001 0.00005 0.00097 0.00102 3.11587

D64 -0.01331 0.00002 0.00038 0.00084 0.00123 -0.01209

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13620 0.00000 -0.00019 0.00002 -0.00017 3.13603

D67 -3.13620 0.00000 0.00019 -0.00002 0.00017 -3.13603

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.11486 0.00001 0.00005 0.00097 0.00102 3.11587

D70 -0.01262 0.00002 -0.00011 0.00132 0.00121 -0.01141

D71 -0.01331 0.00002 0.00038 0.00084 0.00123 -0.01209

D72 -3.14079 0.00003 0.00023 0.00119 0.00142 -3.13937

D73 -3.12755 0.00001 -0.00020 0.00022 0.00003 -3.12752

D74 0.00880 0.00000 -0.00038 0.00024 -0.00014 0.00866

D75 0.00187 0.00000 -0.00006 -0.00008 -0.00014 0.00173

D76 3.13822 -0.00001 -0.00025 -0.00006 -0.00031 3.13791

D77 3.12633 0.00000 0.00024 -0.00017 0.00006 3.12639

D78 -0.08114 -0.00001 -0.00055 -0.00074 -0.00129 -0.08242

D79 -0.00303 0.00001 0.00010 0.00013 0.00023 -0.00280

D80 3.07269 0.00000 -0.00069 -0.00043 -0.00112 3.07157

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 3.13620 0.00000 -0.00019 0.00002 -0.00017 3.13603

D83 -3.13620 0.00000 0.00019 -0.00002 0.00017 -3.13603

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 -0.00187 0.00000 0.00006 0.00008 0.00014 -0.00173

D86 3.12755 -0.00001 0.00020 -0.00022 -0.00003 3.12752

D87 -3.13822 0.00001 0.00025 0.00006 0.00031 -3.13791

D88 -0.00880 0.00000 0.00038 -0.00024 0.00014 -0.00866

D89 0.00303 -0.00001 -0.00010 -0.00013 -0.00023 0.00280

D90 -3.07269 0.00000 0.00069 0.00043 0.00112 -3.07157

D91 -3.12633 0.00000 -0.00024 0.00017 -0.00006 -3.12639

D92 0.08114 0.00001 0.00055 0.00074 0.00129 0.08242

D93 -3.11486 -0.00001 -0.00005 -0.00097 -0.00102 -3.11587

D94 0.01331 -0.00002 -0.00038 -0.00084 -0.00123 0.01209

D95 0.01262 -0.00002 0.00011 -0.00132 -0.00121 0.01141

D96 3.14079 -0.00003 -0.00023 -0.00119 -0.00142 3.13937

D97 0.12117 0.00001 0.00084 0.00019 0.00103 0.12220

D98 1.60972 0.00001 0.00046 0.00033 0.00080 1.61052

D99 3.09827 0.00001 0.00009 0.00047 0.00056 3.09884

D100 -3.09827 -0.00001 -0.00009 -0.00047 -0.00056 -3.09884

D101 -1.60972 -0.00001 -0.00046 -0.00033 -0.00080 -1.61052

D102 -0.12117 -0.00001 -0.00084 -0.00019 -0.00103 -0.12220

D103 3.11486 0.00001 0.00005 0.00097 0.00102 3.11587

D104 -0.01262 0.00002 -0.00011 0.00132 0.00121 -0.01141

D105 -0.01331 0.00002 0.00038 0.00084 0.00123 -0.01209

D106 -3.14079 0.00003 0.00023 0.00119 0.00142 -3.13937

D107 -3.12755 0.00001 -0.00020 0.00022 0.00003 -3.12752

D108 0.00880 0.00000 -0.00038 0.00024 -0.00014 0.00866

D109 0.00187 0.00000 -0.00006 -0.00008 -0.00014 0.00173

D110 3.13822 -0.00001 -0.00025 -0.00006 -0.00031 3.13791

D111 3.12633 0.00000 0.00024 -0.00017 0.00006 3.12639

D112 -0.08114 -0.00001 -0.00055 -0.00074 -0.00129 -0.08242

D113 -0.00303 0.00001 0.00010 0.00013 0.00023 -0.00280

D114 3.07269 0.00000 -0.00069 -0.00043 -0.00112 3.07157

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.13620 0.00000 -0.00019 0.00002 -0.00017 3.13603

D117 -3.13620 0.00000 0.00019 -0.00002 0.00017 -3.13603

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 -0.00187 0.00000 0.00006 0.00008 0.00014 -0.00173

D120 3.12755 -0.00001 0.00020 -0.00022 -0.00003 3.12752

D121 -3.13822 0.00001 0.00025 0.00006 0.00031 -3.13791

D122 -0.00880 0.00000 0.00038 -0.00024 0.00014 -0.00866

D123 0.00303 -0.00001 -0.00010 -0.00013 -0.00023 0.00280

D124 -3.07269 0.00000 0.00069 0.00043 0.00112 -3.07157

D125 -3.12633 0.00000 -0.00024 0.00017 -0.00006 -3.12639

D126 0.08114 0.00001 0.00055 0.00074 0.00129 0.08242

D127 -3.11486 -0.00001 -0.00005 -0.00097 -0.00102 -3.11587

D128 0.01331 -0.00002 -0.00038 -0.00084 -0.00123 0.01209

D129 0.01262 -0.00002 0.00011 -0.00132 -0.00121 0.01141

D130 3.14079 -0.00003 -0.00023 -0.00119 -0.00142 3.13937

D131 1.60972 0.00001 0.00046 0.00033 0.00080 1.61052

D132 3.09827 0.00001 0.00009 0.00047 0.00056 3.09884

D133 0.12117 0.00001 0.00084 0.00019 0.00103 0.12220

D134 -1.60972 -0.00001 -0.00046 -0.00033 -0.00080 -1.61052

D135 -0.12117 -0.00001 -0.00084 -0.00019 -0.00103 -0.12220

D136 -3.09827 -0.00001 -0.00009 -0.00047 -0.00056 -3.09884

Item Value Threshold Converged?

Maximum Force 0.000050 0.000450 YES

RMS Force 0.000019 0.000300 YES

Maximum Displacement 0.006367 0.001800 NO

RMS Displacement 0.001170 0.001200 YES

Predicted change in Energy=-6.444011D-07

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:23:15 2019, MaxMem= 1342177280 cpu: 1.1

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.681173 4.273291 -0.040622

2 6 0 1.102019 2.889214 -0.004969

3 7 0 0.000000 2.081738 0.018063

4 6 0 -1.102019 2.889214 -0.004969

5 6 0 -0.681173 4.273291 -0.040622

6 6 0 -2.446176 2.446176 -0.009850

7 6 0 -2.889214 1.102019 -0.004969

8 7 0 -2.081738 0.000000 0.018063

9 6 0 -2.889214 -1.102019 -0.004969

10 6 0 -4.273291 -0.681173 -0.040622

11 6 0 -4.273291 0.681173 -0.040622

12 6 0 2.446176 2.446176 -0.009850

13 6 0 2.889214 1.102019 -0.004969

14 6 0 4.273291 0.681173 -0.040622

15 6 0 4.273291 -0.681173 -0.040622

16 6 0 2.889214 -1.102019 -0.004969

17 7 0 2.081738 0.000000 0.018063

18 6 0 2.446176 -2.446176 -0.009850

19 6 0 1.102019 -2.889214 -0.004969

20 6 0 0.681173 -4.273291 -0.040622

21 6 0 -0.681173 -4.273291 -0.040622

22 6 0 -1.102019 -2.889214 -0.004969

23 7 0 0.000000 -2.081738 0.018063

24 1 0 1.339708 5.128520 -0.067409

25 1 0 -1.339708 5.128520 -0.067409

26 1 0 -5.128520 -1.339708 -0.067409

27 1 0 -5.128520 1.339708 -0.067409

28 1 0 5.128520 1.339708 -0.067409

29 1 0 5.128520 -1.339708 -0.067409

30 1 0 1.339708 -5.128520 -0.067409

31 1 0 -1.339708 -5.128520 -0.067409

32 30 0 0.000000 0.000000 0.190742

33 6 0 -2.446176 -2.446176 -0.009850

34 6 0 -3.455061 -3.455061 -0.038156

35 6 0 3.455061 3.455061 -0.038156

36 6 0 -4.307457 -4.307457 -0.066314

37 6 0 4.307457 4.307457 -0.066314

38 6 0 -3.455061 3.455061 -0.038156

39 6 0 -4.307457 4.307457 -0.066314

40 6 0 3.455061 -3.455061 -0.038156

41 6 0 4.307457 -4.307457 -0.066314

42 1 0 5.062013 -5.062013 -0.088944

43 1 0 -5.062013 -5.062013 -0.088944

44 1 0 -5.062013 5.062013 -0.088944

45 1 0 5.062013 5.062013 -0.088944

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.447084 0.000000

3 N 2.295723 1.366379 0.000000

4 C 2.257590 2.204037 1.366379 0.000000

5 C 1.362345 2.257590 2.295723 1.447084 0.000000

6 C 3.622100 3.575750 2.473332 1.415297 2.540577

7 C 4.775552 4.373100 3.050891 2.527476 3.864413

8 N 5.089021 4.299348 2.944022 3.050891 4.497337

9 C 6.453130 5.644455 4.299348 4.373100 5.811254

10 C 7.006669 6.453130 5.089021 4.775552 6.119642

11 C 6.119642 5.811254 4.497337 3.864413 5.080023

12 C 2.540577 1.415297 2.473332 3.575750 3.622100

13 C 3.864413 2.527476 3.050891 4.373100 4.775552

14 C 5.080023 3.864413 4.497337 5.811254 6.119642

15 C 6.119642 4.775552 5.089021 6.453130 7.006669

16 C 5.811254 4.373100 4.299348 5.644455 6.453130

17 N 4.497337 3.050891 2.944022 4.299348 5.089021

18 C 6.947476 5.502106 5.146510 6.407503 7.411646

19 C 7.174946 5.778428 5.091693 6.184497 7.381227

20 C 8.546582 7.174946 6.391700 7.381227 8.654481

21 C 8.654481 7.381227 6.391700 7.174946 8.546582

22 C 7.381227 6.184497 5.091693 5.778428 7.174946

23 N 6.391700 5.091693 4.163476 5.091693 6.391700

24 H 1.079723 2.252751 3.329415 3.313671 2.194560

25 H 2.194560 3.313671 3.329415 2.252751 1.079723

26 H 8.078304 7.530424 6.165656 5.839554 7.161381

27 H 6.508391 6.420629 5.182627 4.314809 5.327806

28 H 5.327806 4.314809 5.182627 6.420629 6.508391

29 H 7.161381 5.839554 6.165656 7.530424 8.078304

30 H 9.424883 8.021499 7.334162 8.381526 9.616586

31 H 9.616586 8.381526 7.334162 8.021499 9.424883

32 Zn 4.333421 3.098436 2.088887 3.098436 4.333421

33 C 7.411646 6.407503 5.146510 5.502106 6.947476

34 C 8.765606 7.811395 6.526618 6.766663 8.211083

35 C 2.892052 2.420350 3.718417 4.592195 4.216389

36 C 9.925539 9.003236 7.706045 7.878495 9.315570

37 C 3.626537 3.505712 4.849241 5.592639 4.988813

38 C 4.216389 4.592195 3.718417 2.420350 2.892052

39 C 4.988813 5.592639 4.849241 3.505712 3.626537

40 C 8.211083 6.766663 6.526618 7.811395 8.765606

41 C 9.315570 7.878495 7.706045 9.003236 9.925539

42 H 10.312226 8.883165 8.756061 10.061031 10.960585

43 H 10.960585 10.061031 8.756061 8.883165 10.312226

44 H 5.797293 6.536314 5.875157 4.517706 4.451537

45 H 4.451537 4.517706 5.875157 6.536314 5.797293

6 7 8 9 10

6 C 0.000000

7 C 1.415297 0.000000

8 N 2.473332 1.366379 0.000000

9 C 3.575750 2.204037 1.366379 0.000000

10 C 3.622100 2.257590 2.295723 1.447084 0.000000

11 C 2.540577 1.447084 2.295723 2.257590 1.362345

12 C 4.892352 5.502106 5.146510 6.407503 7.411646

13 C 5.502106 5.778428 5.091693 6.184497 7.381227

14 C 6.947476 7.174946 6.391700 7.381227 8.654481

15 C 7.411646 7.381227 6.391700 7.174946 8.546582

16 C 6.407503 6.184497 5.091693 5.778428 7.174946

17 N 5.146510 5.091693 4.163476 5.091693 6.391700

18 C 6.918831 6.407503 5.146510 5.502106 6.947476

19 C 6.407503 5.644455 4.299348 4.373100 5.811254

20 C 7.411646 6.453130 5.089021 4.775552 6.119642

21 C 6.947476 5.811254 4.497337 3.864413 5.080023

22 C 5.502106 4.373100 3.050891 2.527476 3.864413

23 N 5.146510 4.299348 2.944022 3.050891 4.497337

24 H 4.640172 5.839554 6.165656 7.530424 8.078304

25 H 2.902163 4.314809 5.182627 6.420629 6.508391

26 H 4.640172 3.313671 3.329415 2.252751 1.079723

27 H 2.902163 2.252751 3.329415 3.313671 2.194560

28 H 7.655299 8.021499 7.334162 8.381526 9.616586

29 H 8.468308 8.381526 7.334162 8.021499 9.424883

30 H 8.468308 7.530424 6.165656 5.839554 7.161381

31 H 7.655299 6.420629 5.182627 4.314809 5.327806

32 Zn 3.465226 3.098436 2.088887 3.098436 4.333421

33 C 4.892352 3.575750 2.473332 1.415297 2.540577

34 C 5.986923 4.592195 3.718417 2.420350 2.892052

35 C 5.986923 6.766663 6.526618 7.811395 8.765606

36 C 7.005649 5.592639 4.849241 3.505712 3.626537

37 C 7.005649 7.878495 7.706045 9.003236 9.925539

38 C 1.427059 2.420350 3.718417 4.592195 4.216389

39 C 2.632855 3.505712 4.849241 5.592639 4.988813

40 C 8.345658 7.811395 6.526618 6.766663 8.211083

41 C 9.551247 9.003236 7.706045 7.878495 9.315570

42 H 10.618478 10.061031 8.756061 8.883165 10.312226

43 H 7.951212 6.536314 5.875157 4.517706 4.451537

44 H 3.700198 4.517706 5.875157 6.536314 5.797293

45 H 7.951212 8.883165 8.756061 10.061031 10.960585

11 12 13 14 15

11 C 0.000000

12 C 6.947476 0.000000

13 C 7.174946 1.415297 0.000000

14 C 8.546582 2.540577 1.447084 0.000000

15 C 8.654481 3.622100 2.257590 1.362345 0.000000

16 C 7.381227 3.575750 2.204037 2.257590 1.447084

17 N 6.391700 2.473332 1.366379 2.295723 2.295723

18 C 7.411646 4.892352 3.575750 3.622100 2.540577

19 C 6.453130 5.502106 4.373100 4.775552 3.864413

20 C 7.006669 6.947476 5.811254 6.119642 5.080023

21 C 6.119642 7.411646 6.453130 7.006669 6.119642

22 C 4.775552 6.407503 5.644455 6.453130 5.811254

23 N 5.089021 5.146510 4.299348 5.089021 4.497337

24 H 7.161381 2.902163 4.314809 5.327806 6.508391

25 H 5.327806 4.640172 5.839554 7.161381 8.078304

26 H 2.194560 8.468308 8.381526 9.616586 9.424883

27 H 1.079723 7.655299 8.021499 9.424883 9.616586

28 H 9.424883 2.902163 2.252751 1.079723 2.194560

29 H 9.616586 4.640172 3.313671 2.194560 1.079723

30 H 8.078304 7.655299 6.420629 6.508391 5.327806

31 H 6.508391 8.468308 7.530424 8.078304 7.161381

32 Zn 4.333421 3.465226 3.098436 4.333421 4.333421

33 C 3.622100 6.918831 6.407503 7.411646 6.947476

34 C 4.216389 8.345658 7.811395 8.765606 8.211083

35 C 8.211083 1.427059 2.420350 2.892052 4.216389

36 C 4.988813 9.551247 9.003236 9.925539 9.315570

37 C 9.315570 2.632855 3.505712 3.626537 4.988813

38 C 2.892052 5.986923 6.766663 8.211083 8.765606

39 C 3.626537 7.005649 7.878495 9.315570 9.925539

40 C 8.765606 5.986923 4.592195 4.216389 2.892052

41 C 9.925539 7.005649 5.592639 4.988813 3.626537

42 H 10.960585 7.951212 6.536314 5.797293 4.451537

43 H 5.797293 10.618478 10.061031 10.960585 10.312226

44 H 4.451537 7.951212 8.883165 10.312226 10.960585

45 H 10.312226 3.700198 4.517706 4.451537 5.797293

16 17 18 19 20

16 C 0.000000

17 N 1.366379 0.000000

18 C 1.415297 2.473332 0.000000

19 C 2.527476 3.050891 1.415297 0.000000

20 C 3.864413 4.497337 2.540577 1.447084 0.000000

21 C 4.775552 5.089021 3.622100 2.257590 1.362345

22 C 4.373100 4.299348 3.575750 2.204037 2.257590

23 N 3.050891 2.944022 2.473332 1.366379 2.295723

24 H 6.420629 5.182627 7.655299 8.021499 9.424883

25 H 7.530424 6.165656 8.468308 8.381526 9.616586

26 H 8.021499 7.334162 7.655299 6.420629 6.508391

27 H 8.381526 7.334162 8.468308 7.530424 8.078304

28 H 3.313671 3.329415 4.640172 5.839554 7.161381

29 H 2.252751 3.329415 2.902163 4.314809 5.327806

30 H 4.314809 5.182627 2.902163 2.252751 1.079723

31 H 5.839554 6.165656 4.640172 3.313671 2.194560

32 Zn 3.098436 2.088887 3.465226 3.098436 4.333421

33 C 5.502106 5.146510 4.892352 3.575750 3.622100

34 C 6.766663 6.526618 5.986923 4.592195 4.216389

35 C 4.592195 3.718417 5.986923 6.766663 8.211083

36 C 7.878495 7.706045 7.005649 5.592639 4.988813

37 C 5.592639 4.849241 7.005649 7.878495 9.315570

38 C 7.811395 6.526618 8.345658 7.811395 8.765606

39 C 9.003236 7.706045 9.551247 9.003236 9.925539

40 C 2.420350 3.718417 1.427059 2.420350 2.892052

41 C 3.505712 4.849241 2.632855 3.505712 3.626537

42 H 4.517706 5.875157 3.700198 4.517706 4.451537

43 H 8.883165 8.756061 7.951212 6.536314 5.797293

44 H 10.061031 8.756061 10.618478 10.061031 10.960585

45 H 6.536314 5.875157 7.951212 8.883165 10.312226

21 22 23 24 25

21 C 0.000000

22 C 1.447084 0.000000

23 N 2.295723 1.366379 0.000000

24 H 9.616586 8.381526 7.334162 0.000000

25 H 9.424883 8.021499 7.334162 2.679416 0.000000

26 H 5.327806 4.314809 5.182627 9.147455 7.496203

27 H 7.161381 5.839554 6.165656 7.496203 5.358188

28 H 8.078304 7.530424 6.165656 5.358188 7.496203

29 H 6.508391 6.420629 5.182627 7.496203 9.147455

30 H 2.194560 3.313671 3.329415 10.257039 10.601232

31 H 1.079723 2.252751 3.329415 10.601232 10.257039

32 Zn 4.333421 3.098436 2.088887 5.306899 5.306899

33 C 2.540577 1.415297 2.473332 8.468308 7.655299

34 C 2.892052 2.420350 3.718417 9.832015 8.840443

35 C 8.765606 7.811395 6.526618 2.697413 5.078497

36 C 3.626537 3.505712 4.849241 10.996733 9.891673

37 C 9.925539 9.003236 7.706045 3.079234 5.706542

38 C 8.211083 6.766663 6.526618 5.078497 2.697413

39 C 9.315570 7.878495 7.706045 5.706542 3.079234

40 C 4.216389 4.592195 3.718417 8.840443 9.832015

41 C 4.988813 5.592639 4.849241 9.891673 10.996733

42 H 5.797293 6.536314 5.875157 10.849100 12.034511

43 H 4.451537 4.517706 5.875157 12.034511 10.849100

44 H 10.312226 8.883165 8.756061 6.402103 3.722962

45 H 10.960585 10.061031 8.756061 3.722962 6.402103

26 27 28 29 30

26 H 0.000000

27 H 2.679416 0.000000

28 H 10.601232 10.257039 0.000000

29 H 10.257039 10.601232 2.679416 0.000000

30 H 7.496203 9.147455 7.496203 5.358188 0.000000

31 H 5.358188 7.496203 9.147455 7.496203 2.679416

32 Zn 5.306899 5.306899 5.306899 5.306899 5.306899

33 C 2.902163 4.640172 8.468308 7.655299 4.640172

34 C 2.697413 5.078497 9.832015 8.840443 5.078497

35 C 9.832015 8.840443 2.697413 5.078497 8.840443

36 C 3.079234 5.706542 10.996733 9.891673 5.706542

37 C 10.996733 9.891673 3.079234 5.706542 9.891673

38 C 5.078497 2.697413 8.840443 9.832015 9.832015

39 C 5.706542 3.079234 9.891673 10.996733 10.996733

40 C 8.840443 9.832015 5.078497 2.697413 2.697413

41 C 9.891673 10.996733 5.706542 3.079234 3.079234

42 H 10.849100 12.034511 6.402103 3.722962 3.722962

43 H 3.722962 6.402103 12.034511 10.849100 6.402103

44 H 6.402103 3.722962 10.849100 12.034511 12.034511

45 H 12.034511 10.849100 3.722962 6.402103 10.849100

31 32 33 34 35

31 H 0.000000

32 Zn 5.306899 0.000000

33 C 2.902163 3.465226 0.000000

34 C 2.697413 4.891553 1.427059 0.000000

35 C 9.832015 4.891553 8.345658 9.772388 0.000000

36 C 3.079234 6.097086 2.632855 1.205799 10.977895

37 C 10.996733 6.097086 9.551247 10.977895 1.205799

38 C 8.840443 4.891553 5.986923 6.910122 6.910122

39 C 9.891673 6.097086 7.005649 7.809229 7.809229

40 C 5.078497 4.891553 5.986923 6.910122 6.910122

41 C 5.706542 6.097086 7.005649 7.809229 7.809229

42 H 6.402103 7.164229 7.951212 8.667493 8.667493

43 H 3.722962 7.164229 3.700198 2.273141 12.045069

44 H 10.849100 7.164229 7.951212 8.667493 8.667493

45 H 12.034511 7.164229 10.618478 12.045069 2.273141

36 37 38 39 40

36 C 0.000000

37 C 12.183329 0.000000

38 C 7.809229 7.809229 0.000000

39 C 8.614915 8.614915 1.205799 0.000000

40 C 7.809229 7.809229 9.772388 10.977895 0.000000

41 C 8.614915 8.614915 10.977895 12.183329 1.205799

42 H 9.399832 9.399832 12.045069 13.250452 2.273141

43 H 1.067343 13.250452 8.667493 9.399832 8.667493

44 H 9.399832 9.399832 2.273141 1.067343 12.045069

45 H 13.250452 1.067343 8.667493 9.399832 8.667493

41 42 43 44 45

41 C 0.000000

42 H 1.067343 0.000000

43 H 9.399832 10.124027 0.000000

44 H 13.250452 14.317536 10.124027 0.000000

45 H 9.399832 10.124027 14.317536 10.124027 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

RotChk: IX=3 Diff= 1.40D-20

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681173 -4.273291 -0.042306

2 6 0 -1.102019 -2.889214 -0.006653

3 7 0 0.000000 -2.081738 0.016379

4 6 0 1.102019 -2.889214 -0.006653

5 6 0 0.681173 -4.273291 -0.042306

6 6 0 2.446176 -2.446176 -0.011535

7 6 0 2.889214 -1.102019 -0.006653

8 7 0 2.081738 0.000000 0.016379

9 6 0 2.889214 1.102019 -0.006653

10 6 0 4.273291 0.681173 -0.042306

11 6 0 4.273291 -0.681173 -0.042306

12 6 0 -2.446176 -2.446176 -0.011535

13 6 0 -2.889214 -1.102019 -0.006653

14 6 0 -4.273291 -0.681173 -0.042306

15 6 0 -4.273291 0.681173 -0.042306

16 6 0 -2.889214 1.102019 -0.006653

17 7 0 -2.081738 0.000000 0.016379

18 6 0 -2.446176 2.446176 -0.011535

19 6 0 -1.102019 2.889214 -0.006653

20 6 0 -0.681173 4.273291 -0.042306

21 6 0 0.681173 4.273291 -0.042306

22 6 0 1.102019 2.889214 -0.006653

23 7 0 0.000000 2.081738 0.016379

24 1 0 -1.339708 -5.128520 -0.069094

25 1 0 1.339708 -5.128520 -0.069094

26 1 0 5.128520 1.339708 -0.069094

27 1 0 5.128520 -1.339708 -0.069094

28 1 0 -5.128520 -1.339708 -0.069094

29 1 0 -5.128520 1.339708 -0.069094

30 1 0 -1.339708 5.128520 -0.069094

31 1 0 1.339708 5.128520 -0.069094

32 30 0 0.000000 0.000000 0.189057

33 6 0 2.446176 2.446176 -0.011535

34 6 0 3.455061 3.455061 -0.039840

35 6 0 -3.455061 -3.455061 -0.039840

36 6 0 4.307457 4.307457 -0.067999

37 6 0 -4.307457 -4.307457 -0.067999

38 6 0 3.455061 -3.455061 -0.039840

39 6 0 4.307457 -4.307457 -0.067999

40 6 0 -3.455061 3.455061 -0.039840

41 6 0 -4.307457 4.307457 -0.067999

42 1 0 -5.062013 5.062013 -0.090629

43 1 0 5.062013 5.062013 -0.090629

44 1 0 5.062013 -5.062013 -0.090629

45 1 0 -5.062013 -5.062013 -0.090629

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

Rotational constants (GHZ): 0.1465132 0.1465132 0.0733171

Leave Link 202 at Fri Jul 26 14:23:15 2019, MaxMem= 1342177280 cpu: 0.1

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 184 symmetry adapted cartesian basis functions of A1 symmetry.

There are 155 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3060.5731992996 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= 9 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= -0.1305292439 Hartrees.

Nuclear repulsion after empirical dispersion term = 3060.4426700557 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: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3898

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.11D-05

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 156

GePol: Fraction of low-weight points (<1% of avg) = 4.00%

GePol: Cavity surface area = 415.569 Ang\*\*2

GePol: Cavity volume = 419.949 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0083994943 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3060.4510695500 Hartrees.

Leave Link 301 at Fri Jul 26 14:23:15 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44808.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.40D-05 NBF= 172 148 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 172 148 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:23:16 2019, MaxMem= 1342177280 cpu: 6.5

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:23:16 2019, MaxMem= 1342177280 cpu: 0.8

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

Initial guess from the checkpoint file: "ZnTSPsim0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Occupied (E) (E) (B2) (A1) (E) (E) (B1) (A1) (B2) (E) (E)

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

(E) (E) (A1) (A2) (E) (E) (B1) (B1) (E) (E) (A1)

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

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

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

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(E) (E) (A2) (A1)

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(E) (E) (E)

The electronic state of the initial guess is 1-A1.

Leave Link 401 at Fri Jul 26 14:23:17 2019, MaxMem= 1342177280 cpu: 10.4

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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.

An orbital has undefined symmetry, so N\*\*3 symmetry is turned off.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 660000000 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= 0 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= 45583212.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.55D-15 for 3889.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.32D-15 for 1370 1236.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.04D-14 for 643.

Iteration 1 A^-1\*A deviation from orthogonality is 1.82D-14 for 1971 1953.

E= -1359.06303896190

DIIS: error= 1.08D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.06303896190 IErMin= 1 ErrMin= 1.08D-04

ErrMax= 1.08D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.71D-06 BMatP= 4.71D-06

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.08D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 3.228 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=6.56D-06 MaxDP=1.92D-04 OVMax= 4.93D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.56D-06 CP: 1.00D+00

E= -1359.06304547227 Delta-E= -0.000006510375 Rises=F Damp=F

DIIS: error= 1.36D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.06304547227 IErMin= 2 ErrMin= 1.36D-05

ErrMax= 1.36D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.64D-08 BMatP= 4.71D-06

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

Coeff-Com: -0.529D-01 0.105D+01

Coeff: -0.529D-01 0.105D+01

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=6.44D-07 MaxDP=2.48D-05 DE=-6.51D-06 OVMax= 6.48D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.80D-07 CP: 1.00D+00 1.07D+00

E= -1359.06304554894 Delta-E= -0.000000076670 Rises=F Damp=F

DIIS: error= 4.70D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.06304554894 IErMin= 3 ErrMin= 4.70D-06

ErrMax= 4.70D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.50D-09 BMatP= 3.64D-08

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

Coeff-Com: -0.138D-01 0.223D+00 0.791D+00

Coeff: -0.138D-01 0.223D+00 0.791D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=1.48D-07 MaxDP=6.29D-06 DE=-7.67D-08 OVMax= 1.32D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.44D-07 CP: 1.00D+00 1.07D+00 9.43D-01

E= -1359.06304555089 Delta-E= -0.000000001950 Rises=F Damp=F

DIIS: error= 3.81D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.06304555089 IErMin= 4 ErrMin= 3.81D-06

ErrMax= 3.81D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.68D-09 BMatP= 3.50D-09

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

Coeff-Com: -0.325D-02 0.354D-01 0.410D+00 0.558D+00

Coeff: -0.325D-02 0.354D-01 0.410D+00 0.558D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=6.47D-08 MaxDP=3.54D-06 DE=-1.95D-09 OVMax= 8.69D-06

Cycle 5 Pass 1 IDiag 1:

RMSU= 5.36D-08 CP: 1.00D+00 1.07D+00 9.69D-01 7.76D-01

E= -1359.06304555212 Delta-E= -0.000000001228 Rises=F Damp=F

DIIS: error= 5.93D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.06304555212 IErMin= 5 ErrMin= 5.93D-07

ErrMax= 5.93D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D-10 BMatP= 1.68D-09

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

Coeff-Com: 0.612D-03-0.202D-01 0.547D-01 0.236D+00 0.729D+00

Coeff: 0.612D-03-0.202D-01 0.547D-01 0.236D+00 0.729D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 203839 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.28D-08 MaxDP=5.76D-07 DE=-1.23D-09 OVMax= 3.05D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.93D-09 CP: 1.00D+00 1.07D+00 9.95D-01 8.01D-01 7.01D-01

E= -1359.06304555208 Delta-E= 0.000000000044 Rises=F Damp=F

DIIS: error= 2.27D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 5 EnMin= -1359.06304555212 IErMin= 6 ErrMin= 2.27D-07

ErrMax= 2.27D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.29D-11 BMatP= 1.13D-10

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

Coeff-Com: 0.448D-03-0.125D-01 0.177D-01 0.115D+00 0.414D+00 0.466D+00

Coeff: 0.448D-03-0.125D-01 0.177D-01 0.115D+00 0.414D+00 0.466D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=5.30D-09 MaxDP=1.87D-07 DE= 4.37D-11 OVMax= 8.78D-07

Error on total polarization charges = 0.06212

SCF Done: E(RB3LYP) = -1359.06304555 A.U. after 6 cycles

NFock= 6 Conv=0.53D-08 -V/T= 1.9682

KE= 1.403728043742D+03 PE=-9.362986242703D+03 EE= 3.539744083859D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.27

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:23:47 2019, MaxMem= 1342177280 cpu: 330.5

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44808.

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 = 260

Leave Link 701 at Fri Jul 26 14:23:50 2019, MaxMem= 1342177280 cpu: 43.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

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

Leave Link 702 at Fri Jul 26 14:23:50 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Fri Jul 26 14:23:54 2019, MaxMem= 1342177280 cpu: 43.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 4.97379915D-14 6.11066753D-13 3.27113287D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000009376 0.000001415 -0.000002235

2 6 -0.000019307 -0.000002804 0.000030085

3 7 0.000000000 -0.000023753 -0.000027748

4 6 0.000019307 -0.000002804 0.000030085

5 6 0.000009376 0.000001415 -0.000002235

6 6 -0.000002839 0.000002839 -0.000021339

7 6 0.000002804 -0.000019307 0.000030085

8 7 0.000023753 0.000000000 -0.000027748

9 6 0.000002804 0.000019307 0.000030085

10 6 -0.000001415 0.000009376 -0.000002235

11 6 -0.000001415 -0.000009376 -0.000002235

12 6 0.000002839 0.000002839 -0.000021339

13 6 -0.000002804 -0.000019307 0.000030085

14 6 0.000001415 -0.000009376 -0.000002235

15 6 0.000001415 0.000009376 -0.000002235

16 6 -0.000002804 0.000019307 0.000030085

17 7 -0.000023753 0.000000000 -0.000027748

18 6 0.000002839 -0.000002839 -0.000021339

19 6 -0.000019307 0.000002804 0.000030085

20 6 -0.000009376 -0.000001415 -0.000002235

21 6 0.000009376 -0.000001415 -0.000002235

22 6 0.000019307 0.000002804 0.000030085

23 7 0.000000000 0.000023753 -0.000027748

24 1 -0.000001021 0.000004277 0.000005554

25 1 0.000001021 0.000004277 0.000005554

26 1 -0.000004277 0.000001021 0.000005554

27 1 -0.000004277 -0.000001021 0.000005554

28 1 0.000004277 -0.000001021 0.000005554

29 1 0.000004277 0.000001021 0.000005554

30 1 -0.000001021 -0.000004277 0.000005554

31 1 0.000001021 -0.000004277 0.000005554

32 30 0.000000000 0.000000000 -0.000006992

33 6 -0.000002839 -0.000002839 -0.000021339

34 6 0.000020796 0.000020796 -0.000012936

35 6 -0.000020796 -0.000020796 -0.000012936

36 6 -0.000005453 -0.000005453 -0.000007401

37 6 0.000005453 0.000005453 -0.000007401

38 6 0.000020796 -0.000020796 -0.000012936

39 6 -0.000005453 0.000005453 -0.000007401

40 6 -0.000020796 0.000020796 -0.000012936

41 6 0.000005453 -0.000005453 -0.000007401

42 1 -0.000001901 0.000001901 0.000004364

43 1 0.000001901 0.000001901 0.000004364

44 1 0.000001901 -0.000001901 0.000004364

45 1 -0.000001901 -0.000001901 0.000004364

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

Cartesian Forces: Max 0.000030085 RMS 0.000013168

Leave Link 716 at Fri Jul 26 14:23:54 2019, MaxMem= 1342177280 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000025808 RMS 0.000007730

Search for a local minimum.

Step number 15 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .77302D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 2 3 4 5 7

9 8 10 11 12

13 14 15

DE= -8.85D-07 DEPred=-6.44D-07 R= 1.37D+00

Trust test= 1.37D+00 RLast= 9.59D-03 DXMaxT set to 8.41D-02

ITU= 0 1 1 -1 1 0 -1 0 0 -1 1 0 -1 -1 0

Eigenvalues --- 0.00534 0.00534 0.00534 0.00534 0.00534

Eigenvalues --- 0.00534 0.00535 0.00585 0.01129 0.01158

Eigenvalues --- 0.01158 0.01167 0.01384 0.01384 0.01617

Eigenvalues --- 0.01646 0.01674 0.01726 0.01726 0.01805

Eigenvalues --- 0.01805 0.01825 0.01831 0.01859 0.01859

Eigenvalues --- 0.01868 0.01868 0.01868 0.01908 0.01920

Eigenvalues --- 0.01927 0.01927 0.01933 0.01960 0.01961

Eigenvalues --- 0.01961 0.02178 0.02180 0.02184 0.02184

Eigenvalues --- 0.02265 0.02707 0.03317 0.03724 0.04654

Eigenvalues --- 0.04654 0.04654 0.04654 0.04654 0.04654

Eigenvalues --- 0.04654 0.08774 0.13847 0.14999 0.14999

Eigenvalues --- 0.15329 0.15999 0.15999 0.15999 0.15999

Eigenvalues --- 0.16000 0.16000 0.16000 0.18717 0.22832

Eigenvalues --- 0.22868 0.22872 0.22872 0.24759 0.24774

Eigenvalues --- 0.24774 0.24836 0.24865 0.24979 0.24979

Eigenvalues --- 0.24998 0.24998 0.24998 0.24998 0.24999

Eigenvalues --- 0.27079 0.35035 0.35035 0.35468 0.35499

Eigenvalues --- 0.35762 0.36034 0.36034 0.36034 0.36034

Eigenvalues --- 0.36034 0.36034 0.36034 0.36079 0.36780

Eigenvalues --- 0.36864 0.36864 0.37312 0.37563 0.37563

Eigenvalues --- 0.37563 0.37779 0.38967 0.38967 0.39538

Eigenvalues --- 0.41397 0.41397 0.41397 0.41439 0.41516

Eigenvalues --- 0.41516 0.41789 0.42522 0.43514 0.43778

Eigenvalues --- 0.43778 0.45556 0.47912 0.49087 0.49087

Eigenvalues --- 0.50131 0.51399 0.51901 0.51901 0.52914

Eigenvalues --- 1.01831 1.01831 1.01831 1.01977

En-DIIS/RFO-DIIS IScMMF= 0 using points: 15 14 13 12 11

RFO step: Lambda=-5.81069056D-08.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= -1.77D-06 SmlDif= 1.00D-05

RMS Error= 0.3837834392D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.74725 -0.84237 0.08710 -0.00295 0.01097

Iteration 1 RMS(Cart)= 0.00096648 RMS(Int)= 0.00000025

Iteration 2 RMS(Cart)= 0.00000036 RMS(Int)= 0.00000019

ITry= 1 IFail=0 DXMaxC= 4.67D-03 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 4.36D-05 for atom 45.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73459 0.00000 0.00006 -0.00005 0.00001 2.73461

R2 2.57446 -0.00002 -0.00004 0.00001 -0.00003 2.57442

R3 2.04038 0.00000 0.00000 0.00000 0.00001 2.04039

R4 2.58208 -0.00002 -0.00001 -0.00001 -0.00003 2.58205

R5 2.67452 -0.00001 0.00000 -0.00002 -0.00002 2.67450

R6 2.58208 -0.00002 -0.00001 -0.00001 -0.00003 2.58205

R7 3.94743 -0.00003 0.00000 -0.00011 -0.00011 3.94732

R8 2.73459 0.00000 0.00006 -0.00005 0.00001 2.73461

R9 2.67452 -0.00001 0.00000 -0.00002 -0.00002 2.67450

R10 2.04038 0.00000 0.00000 0.00000 0.00001 2.04039

R11 2.67452 -0.00001 0.00000 -0.00002 -0.00002 2.67450

R12 2.69675 -0.00002 -0.00012 0.00007 -0.00005 2.69670

R13 2.58208 -0.00002 -0.00001 -0.00001 -0.00003 2.58205

R14 2.73459 0.00000 0.00006 -0.00005 0.00001 2.73461

R15 2.58208 -0.00002 -0.00001 -0.00001 -0.00003 2.58205

R16 3.94743 -0.00003 0.00000 -0.00011 -0.00011 3.94732

R17 2.73459 0.00000 0.00006 -0.00005 0.00001 2.73461

R18 2.67452 -0.00001 0.00000 -0.00002 -0.00002 2.67450

R19 2.57446 -0.00002 -0.00004 0.00001 -0.00003 2.57442

R20 2.04038 0.00000 0.00000 0.00000 0.00001 2.04039

R21 2.04038 0.00000 0.00000 0.00000 0.00001 2.04039

R22 2.67452 -0.00001 0.00000 -0.00002 -0.00002 2.67450

R23 2.69675 -0.00002 -0.00012 0.00007 -0.00005 2.69670

R24 2.73459 0.00000 0.00006 -0.00005 0.00001 2.73461

R25 2.58208 -0.00002 -0.00001 -0.00001 -0.00003 2.58205

R26 2.57446 -0.00002 -0.00004 0.00001 -0.00003 2.57442

R27 2.04038 0.00000 0.00000 0.00000 0.00001 2.04039

R28 2.73459 0.00000 0.00006 -0.00005 0.00001 2.73461

R29 2.04038 0.00000 0.00000 0.00000 0.00001 2.04039

R30 2.58208 -0.00002 -0.00001 -0.00001 -0.00003 2.58205

R31 2.67452 -0.00001 0.00000 -0.00002 -0.00002 2.67450

R32 3.94743 -0.00003 0.00000 -0.00011 -0.00011 3.94732

R33 2.67452 -0.00001 0.00000 -0.00002 -0.00002 2.67450

R34 2.69675 -0.00002 -0.00012 0.00007 -0.00005 2.69670

R35 2.73459 0.00000 0.00006 -0.00005 0.00001 2.73461

R36 2.58208 -0.00002 -0.00001 -0.00001 -0.00003 2.58205

R37 2.57446 -0.00002 -0.00004 0.00001 -0.00003 2.57442

R38 2.04038 0.00000 0.00000 0.00000 0.00001 2.04039

R39 2.73459 0.00000 0.00006 -0.00005 0.00001 2.73461

R40 2.04038 0.00000 0.00000 0.00000 0.00001 2.04039

R41 2.58208 -0.00002 -0.00001 -0.00001 -0.00003 2.58205

R42 2.67452 -0.00001 0.00000 -0.00002 -0.00002 2.67450

R43 3.94743 -0.00003 0.00000 -0.00011 -0.00011 3.94732

R44 2.69675 -0.00002 -0.00012 0.00007 -0.00005 2.69670

R45 2.27863 0.00001 -0.00002 0.00002 0.00001 2.27864

R46 2.27863 0.00001 -0.00002 0.00002 0.00001 2.27864

R47 2.01699 0.00000 0.00000 -0.00001 -0.00001 2.01698

R48 2.01699 0.00000 0.00000 -0.00001 -0.00001 2.01698

R49 2.27863 0.00001 -0.00002 0.00002 0.00001 2.27864

R50 2.01699 0.00000 0.00000 -0.00001 -0.00001 2.01698

R51 2.27863 0.00001 -0.00002 0.00002 0.00001 2.27864

R52 2.01699 0.00000 0.00000 -0.00001 -0.00001 2.01698

A1 1.86588 -0.00001 -0.00001 0.00000 -0.00001 1.86587

A2 2.19054 0.00001 0.00004 -0.00001 0.00003 2.19058

A3 2.22675 0.00000 -0.00003 0.00001 -0.00002 2.22672

A4 1.90825 0.00001 0.00002 0.00000 0.00003 1.90828

A5 2.18404 0.00000 0.00003 -0.00003 0.00000 2.18404

A6 2.19082 -0.00001 -0.00006 0.00003 -0.00003 2.19079

A7 1.87650 -0.00001 -0.00003 0.00000 -0.00003 1.87647

A8 2.20227 0.00000 -0.00001 0.00000 -0.00001 2.20226

A9 2.20227 0.00000 -0.00001 0.00000 -0.00001 2.20226

A10 1.90825 0.00001 0.00002 0.00000 0.00003 1.90828

A11 2.19082 -0.00001 -0.00006 0.00003 -0.00003 2.19079

A12 2.18404 0.00000 0.00003 -0.00003 0.00000 2.18404

A13 1.86588 -0.00001 -0.00001 0.00000 -0.00001 1.86587

A14 2.22675 0.00000 -0.00003 0.00001 -0.00002 2.22672

A15 2.19054 0.00001 0.00004 -0.00001 0.00003 2.19058

A16 2.20755 0.00001 0.00009 -0.00006 0.00002 2.20757

A17 2.03778 0.00000 -0.00004 0.00003 -0.00001 2.03777

A18 2.03778 0.00000 -0.00004 0.00003 -0.00001 2.03777

A19 2.19082 -0.00001 -0.00006 0.00003 -0.00003 2.19079

A20 2.18404 0.00000 0.00003 -0.00003 0.00000 2.18404

A21 1.90825 0.00001 0.00002 0.00000 0.00003 1.90828

A22 1.87650 -0.00001 -0.00003 0.00000 -0.00003 1.87647

A23 2.20227 0.00000 -0.00001 0.00000 -0.00001 2.20226

A24 2.20227 0.00000 -0.00001 0.00000 -0.00001 2.20226

A25 1.90825 0.00001 0.00002 0.00000 0.00003 1.90828

A26 2.19082 -0.00001 -0.00006 0.00003 -0.00003 2.19079

A27 2.18404 0.00000 0.00003 -0.00003 0.00000 2.18404

A28 1.86588 -0.00001 -0.00001 0.00000 -0.00001 1.86587

A29 2.19054 0.00001 0.00004 -0.00001 0.00003 2.19058

A30 2.22675 0.00000 -0.00003 0.00001 -0.00002 2.22672

A31 1.86588 -0.00001 -0.00001 0.00000 -0.00001 1.86587

A32 2.19054 0.00001 0.00004 -0.00001 0.00003 2.19058

A33 2.22675 0.00000 -0.00003 0.00001 -0.00002 2.22672

A34 2.20755 0.00001 0.00009 -0.00006 0.00002 2.20757

A35 2.03778 0.00000 -0.00004 0.00003 -0.00001 2.03777

A36 2.03778 0.00000 -0.00004 0.00003 -0.00001 2.03777

A37 2.18404 0.00000 0.00003 -0.00003 0.00000 2.18404

A38 2.19082 -0.00001 -0.00006 0.00003 -0.00003 2.19079

A39 1.90825 0.00001 0.00002 0.00000 0.00003 1.90828

A40 1.86588 -0.00001 -0.00001 0.00000 -0.00001 1.86587

A41 2.19054 0.00001 0.00004 -0.00001 0.00003 2.19058

A42 2.22675 0.00000 -0.00003 0.00001 -0.00002 2.22672

A43 1.86588 -0.00001 -0.00001 0.00000 -0.00001 1.86587

A44 2.22675 0.00000 -0.00003 0.00001 -0.00002 2.22672

A45 2.19054 0.00001 0.00004 -0.00001 0.00003 2.19058

A46 1.90825 0.00001 0.00002 0.00000 0.00003 1.90828

A47 2.18404 0.00000 0.00003 -0.00003 0.00000 2.18404

A48 2.19082 -0.00001 -0.00006 0.00003 -0.00003 2.19079

A49 1.87650 -0.00001 -0.00003 0.00000 -0.00003 1.87647

A50 2.20227 0.00000 -0.00001 0.00000 -0.00001 2.20226

A51 2.20227 0.00000 -0.00001 0.00000 -0.00001 2.20226

A52 2.20755 0.00001 0.00009 -0.00006 0.00002 2.20757

A53 2.03778 0.00000 -0.00004 0.00003 -0.00001 2.03777

A54 2.03778 0.00000 -0.00004 0.00003 -0.00001 2.03777

A55 2.18404 0.00000 0.00003 -0.00003 0.00000 2.18404

A56 2.19082 -0.00001 -0.00006 0.00003 -0.00003 2.19079

A57 1.90825 0.00001 0.00002 0.00000 0.00003 1.90828

A58 1.86588 -0.00001 -0.00001 0.00000 -0.00001 1.86587

A59 2.19054 0.00001 0.00004 -0.00001 0.00003 2.19058

A60 2.22675 0.00000 -0.00003 0.00001 -0.00002 2.22672

A61 1.86588 -0.00001 -0.00001 0.00000 -0.00001 1.86587

A62 2.22675 0.00000 -0.00003 0.00001 -0.00002 2.22672

A63 2.19054 0.00001 0.00004 -0.00001 0.00003 2.19058

A64 1.90825 0.00001 0.00002 0.00000 0.00003 1.90828

A65 2.18404 0.00000 0.00003 -0.00003 0.00000 2.18404

A66 2.19082 -0.00001 -0.00006 0.00003 -0.00003 2.19079

A67 1.87650 -0.00001 -0.00003 0.00000 -0.00003 1.87647

A68 2.20227 0.00000 -0.00001 0.00000 -0.00001 2.20226

A69 2.20227 0.00000 -0.00001 0.00000 -0.00001 2.20226

A70 1.56396 0.00000 0.00000 0.00001 0.00001 1.56397

A71 1.56396 0.00000 0.00000 0.00001 0.00001 1.56397

A72 2.97607 0.00001 0.00002 0.00010 0.00012 2.97619

A73 2.97607 0.00001 0.00002 0.00010 0.00012 2.97619

A74 1.56396 0.00000 0.00000 0.00001 0.00001 1.56397

A75 1.56396 0.00000 0.00000 0.00001 0.00001 1.56397

A76 2.20755 0.00001 0.00009 -0.00006 0.00002 2.20757

A77 2.03778 0.00000 -0.00004 0.00003 -0.00001 2.03777

A78 2.03778 0.00000 -0.00004 0.00003 -0.00001 2.03777

A79 3.14155 0.00000 0.00000 0.00000 0.00000 3.14154

A80 3.14155 0.00000 0.00000 0.00000 0.00000 3.14154

A81 3.14162 0.00000 0.00000 0.00002 0.00000 3.14162

A82 3.14162 0.00000 0.00000 0.00002 0.00000 3.14162

A83 3.14155 0.00000 0.00000 0.00000 0.00000 3.14154

A84 3.14162 0.00000 0.00000 0.00002 0.00000 3.14162

A85 3.14155 0.00000 0.00000 0.00000 0.00000 3.14154

A86 3.14162 0.00000 0.00000 0.00002 0.00000 3.14162

A87 3.13805 0.00000 -0.00023 -0.00007 -0.00030 3.13776

A88 3.14513 0.00000 0.00023 0.00007 0.00030 3.14543

A89 3.14406 0.00001 0.00015 0.00019 0.00034 3.14440

A90 3.13912 -0.00001 -0.00015 -0.00019 -0.00034 3.13878

A91 3.13805 0.00000 -0.00023 -0.00007 -0.00030 3.13776

A92 3.14406 0.00001 0.00015 0.00019 0.00034 3.14440

A93 3.14513 0.00000 0.00023 0.00007 0.00030 3.14543

A94 3.13912 -0.00001 -0.00015 -0.00019 -0.00034 3.13878

D1 -0.00173 0.00000 0.00007 -0.00004 0.00003 -0.00170

D2 3.12752 0.00000 -0.00016 0.00007 -0.00009 3.12742

D3 -3.13791 0.00000 0.00009 -0.00029 -0.00020 -3.13812

D4 -0.00866 0.00000 -0.00015 -0.00019 -0.00033 -0.00899

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13603 0.00000 0.00002 -0.00026 -0.00024 -3.13628

D7 3.13603 0.00000 -0.00002 0.00026 0.00024 3.13628

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00280 0.00000 -0.00011 0.00006 -0.00006 0.00275

D10 -3.07157 0.00000 0.00046 0.00018 0.00063 -3.07094

D11 -3.12639 0.00000 0.00012 -0.00005 0.00007 -3.12632

D12 0.08242 0.00000 0.00069 0.00007 0.00076 0.08319

D13 -3.11587 -0.00001 -0.00073 -0.00025 -0.00098 -3.11685

D14 0.01209 -0.00001 -0.00063 -0.00032 -0.00095 0.01113

D15 0.01141 -0.00001 -0.00100 -0.00012 -0.00112 0.01028

D16 3.13937 -0.00001 -0.00090 -0.00020 -0.00110 3.13827

D17 -0.00280 0.00000 0.00011 -0.00006 0.00006 -0.00275

D18 3.12639 0.00000 -0.00012 0.00005 -0.00007 3.12632

D19 3.07157 0.00000 -0.00046 -0.00018 -0.00063 3.07094

D20 -0.08242 0.00000 -0.00069 -0.00007 -0.00076 -0.08319

D21 -3.09884 0.00000 -0.00035 -0.00012 -0.00046 -3.09930

D22 -0.12220 0.00000 -0.00033 -0.00002 -0.00035 -0.12255

D23 -1.61052 0.00000 -0.00034 -0.00007 -0.00041 -1.61093

D24 0.12220 0.00000 0.00033 0.00002 0.00035 0.12255

D25 3.09884 0.00000 0.00035 0.00012 0.00046 3.09930

D26 1.61052 0.00000 0.00034 0.00007 0.00041 1.61093

D27 0.00173 0.00000 -0.00007 0.00004 -0.00003 0.00170

D28 3.13791 0.00000 -0.00009 0.00029 0.00020 3.13812

D29 -3.12752 0.00000 0.00016 -0.00007 0.00009 -3.12742

D30 0.00866 0.00000 0.00015 0.00019 0.00033 0.00899

D31 -0.01141 0.00001 0.00100 0.00012 0.00112 -0.01028

D32 -3.13937 0.00001 0.00090 0.00020 0.00110 -3.13827

D33 3.11587 0.00001 0.00073 0.00025 0.00098 3.11685

D34 -0.01209 0.00001 0.00063 0.00032 0.00095 -0.01113

D35 0.01141 -0.00001 -0.00100 -0.00012 -0.00112 0.01028

D36 -3.11587 -0.00001 -0.00073 -0.00025 -0.00098 -3.11685

D37 3.13937 -0.00001 -0.00090 -0.00020 -0.00110 3.13827

D38 0.01209 -0.00001 -0.00063 -0.00032 -0.00095 0.01113

D39 -3.12639 0.00000 0.00012 -0.00005 0.00007 -3.12632

D40 0.08242 0.00000 0.00069 0.00007 0.00076 0.08319

D41 0.00280 0.00000 -0.00011 0.00006 -0.00006 0.00275

D42 -3.07157 0.00000 0.00046 0.00018 0.00063 -3.07094

D43 3.12752 0.00000 -0.00016 0.00007 -0.00009 3.12742

D44 -0.00866 0.00000 -0.00015 -0.00019 -0.00033 -0.00899

D45 -0.00173 0.00000 0.00007 -0.00004 0.00003 -0.00170

D46 -3.13791 0.00000 0.00009 -0.00029 -0.00020 -3.13812

D47 -0.00280 0.00000 0.00011 -0.00006 0.00006 -0.00275

D48 3.12639 0.00000 -0.00012 0.00005 -0.00007 3.12632

D49 3.07157 0.00000 -0.00046 -0.00018 -0.00063 3.07094

D50 -0.08242 0.00000 -0.00069 -0.00007 -0.00076 -0.08319

D51 -0.12220 0.00000 -0.00033 -0.00002 -0.00035 -0.12255

D52 -1.61052 0.00000 -0.00034 -0.00007 -0.00041 -1.61093

D53 -3.09884 0.00000 -0.00035 -0.00012 -0.00046 -3.09930

D54 3.09884 0.00000 0.00035 0.00012 0.00046 3.09930

D55 1.61052 0.00000 0.00034 0.00007 0.00041 1.61093

D56 0.12220 0.00000 0.00033 0.00002 0.00035 0.12255

D57 0.00173 0.00000 -0.00007 0.00004 -0.00003 0.00170

D58 3.13791 0.00000 -0.00009 0.00029 0.00020 3.13812

D59 -3.12752 0.00000 0.00016 -0.00007 0.00009 -3.12742

D60 0.00866 0.00000 0.00015 0.00019 0.00033 0.00899

D61 -0.01141 0.00001 0.00100 0.00012 0.00112 -0.01028

D62 -3.13937 0.00001 0.00090 0.00020 0.00110 -3.13827

D63 3.11587 0.00001 0.00073 0.00025 0.00098 3.11685

D64 -0.01209 0.00001 0.00063 0.00032 0.00095 -0.01113

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13603 0.00000 -0.00002 0.00026 0.00024 3.13628

D67 -3.13603 0.00000 0.00002 -0.00026 -0.00024 -3.13628

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.11587 0.00001 0.00073 0.00025 0.00098 3.11685

D70 -0.01141 0.00001 0.00100 0.00012 0.00112 -0.01028

D71 -0.01209 0.00001 0.00063 0.00032 0.00095 -0.01113

D72 -3.13937 0.00001 0.00090 0.00020 0.00110 -3.13827

D73 -3.12752 0.00000 0.00016 -0.00007 0.00009 -3.12742

D74 0.00866 0.00000 0.00015 0.00019 0.00033 0.00899

D75 0.00173 0.00000 -0.00007 0.00004 -0.00003 0.00170

D76 3.13791 0.00000 -0.00009 0.00029 0.00020 3.13812

D77 3.12639 0.00000 -0.00012 0.00005 -0.00007 3.12632

D78 -0.08242 0.00000 -0.00069 -0.00007 -0.00076 -0.08319

D79 -0.00280 0.00000 0.00011 -0.00006 0.00006 -0.00275

D80 3.07157 0.00000 -0.00046 -0.00018 -0.00063 3.07094

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 3.13603 0.00000 -0.00002 0.00026 0.00024 3.13628

D83 -3.13603 0.00000 0.00002 -0.00026 -0.00024 -3.13628

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 -0.00173 0.00000 0.00007 -0.00004 0.00003 -0.00170

D86 3.12752 0.00000 -0.00016 0.00007 -0.00009 3.12742

D87 -3.13791 0.00000 0.00009 -0.00029 -0.00020 -3.13812

D88 -0.00866 0.00000 -0.00015 -0.00019 -0.00033 -0.00899

D89 0.00280 0.00000 -0.00011 0.00006 -0.00006 0.00275

D90 -3.07157 0.00000 0.00046 0.00018 0.00063 -3.07094

D91 -3.12639 0.00000 0.00012 -0.00005 0.00007 -3.12632

D92 0.08242 0.00000 0.00069 0.00007 0.00076 0.08319

D93 -3.11587 -0.00001 -0.00073 -0.00025 -0.00098 -3.11685

D94 0.01209 -0.00001 -0.00063 -0.00032 -0.00095 0.01113

D95 0.01141 -0.00001 -0.00100 -0.00012 -0.00112 0.01028

D96 3.13937 -0.00001 -0.00090 -0.00020 -0.00110 3.13827

D97 0.12220 0.00000 0.00033 0.00002 0.00035 0.12255

D98 1.61052 0.00000 0.00034 0.00007 0.00041 1.61093

D99 3.09884 0.00000 0.00035 0.00012 0.00046 3.09930

D100 -3.09884 0.00000 -0.00035 -0.00012 -0.00046 -3.09930

D101 -1.61052 0.00000 -0.00034 -0.00007 -0.00041 -1.61093

D102 -0.12220 0.00000 -0.00033 -0.00002 -0.00035 -0.12255

D103 3.11587 0.00001 0.00073 0.00025 0.00098 3.11685

D104 -0.01141 0.00001 0.00100 0.00012 0.00112 -0.01028

D105 -0.01209 0.00001 0.00063 0.00032 0.00095 -0.01113

D106 -3.13937 0.00001 0.00090 0.00020 0.00110 -3.13827

D107 -3.12752 0.00000 0.00016 -0.00007 0.00009 -3.12742

D108 0.00866 0.00000 0.00015 0.00019 0.00033 0.00899

D109 0.00173 0.00000 -0.00007 0.00004 -0.00003 0.00170

D110 3.13791 0.00000 -0.00009 0.00029 0.00020 3.13812

D111 3.12639 0.00000 -0.00012 0.00005 -0.00007 3.12632

D112 -0.08242 0.00000 -0.00069 -0.00007 -0.00076 -0.08319

D113 -0.00280 0.00000 0.00011 -0.00006 0.00006 -0.00275

D114 3.07157 0.00000 -0.00046 -0.00018 -0.00063 3.07094

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.13603 0.00000 -0.00002 0.00026 0.00024 3.13628

D117 -3.13603 0.00000 0.00002 -0.00026 -0.00024 -3.13628

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 -0.00173 0.00000 0.00007 -0.00004 0.00003 -0.00170

D120 3.12752 0.00000 -0.00016 0.00007 -0.00009 3.12742

D121 -3.13791 0.00000 0.00009 -0.00029 -0.00020 -3.13812

D122 -0.00866 0.00000 -0.00015 -0.00019 -0.00033 -0.00899

D123 0.00280 0.00000 -0.00011 0.00006 -0.00006 0.00275

D124 -3.07157 0.00000 0.00046 0.00018 0.00063 -3.07094

D125 -3.12639 0.00000 0.00012 -0.00005 0.00007 -3.12632

D126 0.08242 0.00000 0.00069 0.00007 0.00076 0.08319

D127 -3.11587 -0.00001 -0.00073 -0.00025 -0.00098 -3.11685

D128 0.01209 -0.00001 -0.00063 -0.00032 -0.00095 0.01113

D129 0.01141 -0.00001 -0.00100 -0.00012 -0.00112 0.01028

D130 3.13937 -0.00001 -0.00090 -0.00020 -0.00110 3.13827

D131 1.61052 0.00000 0.00034 0.00007 0.00041 1.61093

D132 3.09884 0.00000 0.00035 0.00012 0.00046 3.09930

D133 0.12220 0.00000 0.00033 0.00002 0.00035 0.12255

D134 -1.61052 0.00000 -0.00034 -0.00007 -0.00041 -1.61093

D135 -0.12220 0.00000 -0.00033 -0.00002 -0.00035 -0.12255

D136 -3.09884 0.00000 -0.00035 -0.00012 -0.00046 -3.09930

Item Value Threshold Converged?

Maximum Force 0.000026 0.000450 YES

RMS Force 0.000008 0.000300 YES

Maximum Displacement 0.004673 0.001800 NO

RMS Displacement 0.000967 0.001200 YES

Predicted change in Energy=-2.044517D-07

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:23:54 2019, MaxMem= 1342177280 cpu: 1.1

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.681163 4.273295 -0.039628

2 6 0 1.101995 2.889186 -0.004749

3 7 0 0.000000 2.081690 0.017787

4 6 0 -1.101995 2.889186 -0.004749

5 6 0 -0.681163 4.273295 -0.039628

6 6 0 -2.446135 2.446135 -0.009987

7 6 0 -2.889186 1.101995 -0.004749

8 7 0 -2.081690 0.000000 0.017787

9 6 0 -2.889186 -1.101995 -0.004749

10 6 0 -4.273295 -0.681163 -0.039628

11 6 0 -4.273295 0.681163 -0.039628

12 6 0 2.446135 2.446135 -0.009987

13 6 0 2.889186 1.101995 -0.004749

14 6 0 4.273295 0.681163 -0.039628

15 6 0 4.273295 -0.681163 -0.039628

16 6 0 2.889186 -1.101995 -0.004749

17 7 0 2.081690 0.000000 0.017787

18 6 0 2.446135 -2.446135 -0.009987

19 6 0 1.101995 -2.889186 -0.004749

20 6 0 0.681163 -4.273295 -0.039628

21 6 0 -0.681163 -4.273295 -0.039628

22 6 0 -1.101995 -2.889186 -0.004749

23 7 0 0.000000 -2.081690 0.017787

24 1 0 1.339682 5.128561 -0.065729

25 1 0 -1.339682 5.128561 -0.065729

26 1 0 -5.128561 -1.339682 -0.065729

27 1 0 -5.128561 1.339682 -0.065729

28 1 0 5.128561 1.339682 -0.065729

29 1 0 5.128561 -1.339682 -0.065729

30 1 0 1.339682 -5.128561 -0.065729

31 1 0 -1.339682 -5.128561 -0.065729

32 30 0 0.000000 0.000000 0.190341

33 6 0 -2.446135 -2.446135 -0.009987

34 6 0 -3.454989 -3.454989 -0.039056

35 6 0 3.454989 3.454989 -0.039056

36 6 0 -4.307371 -4.307371 -0.068214

37 6 0 4.307371 4.307371 -0.068214

38 6 0 -3.454989 3.454989 -0.039056

39 6 0 -4.307371 4.307371 -0.068214

40 6 0 3.454989 -3.454989 -0.039056

41 6 0 4.307371 -4.307371 -0.068214

42 1 0 5.061915 -5.061915 -0.091417

43 1 0 -5.061915 -5.061915 -0.091417

44 1 0 -5.061915 5.061915 -0.091417

45 1 0 5.061915 5.061915 -0.091417

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.447091 0.000000

3 N 2.295737 1.366364 0.000000

4 C 2.257571 2.203990 1.366364 0.000000

5 C 1.362327 2.257571 2.295737 1.447091 0.000000

6 C 3.622069 3.575688 2.473290 1.415286 2.540574

7 C 4.775537 4.373052 3.050854 2.527470 3.864418

8 N 5.088979 4.299274 2.943955 3.050854 4.497313

9 C 6.453089 5.644383 4.299274 4.373052 5.811224

10 C 7.006662 6.453089 5.088979 4.775537 6.119645

11 C 6.119645 5.811224 4.497313 3.864418 5.080041

12 C 2.540574 1.415286 2.473290 3.575688 3.622069

13 C 3.864418 2.527470 3.050854 4.373052 4.775537

14 C 5.080041 3.864418 4.497313 5.811224 6.119645

15 C 6.119645 4.775537 5.088979 6.453089 7.006662

16 C 5.811224 4.373052 4.299274 5.644383 6.453089

17 N 4.497313 3.050854 2.943955 4.299274 5.088979

18 C 6.947426 5.502035 5.146411 6.407410 7.411586

19 C 7.174918 5.778373 5.091613 6.184429 7.381193

20 C 8.546589 7.174918 6.391644 7.381193 8.654486

21 C 8.654486 7.381193 6.391644 7.174918 8.546589

22 C 7.381193 6.184429 5.091613 5.778373 7.174918

23 N 6.391644 5.091613 4.163381 5.091613 6.391644

24 H 1.079726 2.252779 3.329436 3.313654 2.194534

25 H 2.194534 3.313654 3.329436 2.252779 1.079726

26 H 8.078310 7.530397 6.165623 5.839545 7.161392

27 H 6.508430 6.420632 5.182633 4.314848 5.327861

28 H 5.327861 4.314848 5.182633 6.420632 6.508430

29 H 7.161392 5.839545 6.165623 7.530397 8.078310

30 H 9.424925 8.021501 7.334129 8.381514 9.616620

31 H 9.616620 8.381514 7.334129 8.021501 9.424925

32 Zn 4.333349 3.098363 2.088830 3.098363 4.333349

33 C 7.411586 6.407410 5.146411 5.502035 6.947426

34 C 8.765508 7.811264 6.526485 6.766559 8.210997

35 C 2.892012 2.420308 3.718350 4.592104 4.216323

36 C 9.925428 9.003095 7.705904 7.878382 9.315473

37 C 3.626481 3.505669 4.849175 5.592542 4.988733

38 C 4.216323 4.592104 3.718350 2.420308 2.892012

39 C 4.988733 5.592542 4.849175 3.505669 3.626481

40 C 8.210997 6.766559 6.526485 7.811264 8.765508

41 C 9.315473 7.878382 7.705904 9.003095 9.925428

42 H 10.312120 8.883046 8.755913 10.060881 10.960464

43 H 10.960464 10.060881 8.755913 8.883046 10.312120

44 H 5.797203 6.536211 5.875088 4.517658 4.451471

45 H 4.451471 4.517658 5.875088 6.536211 5.797203

6 7 8 9 10

6 C 0.000000

7 C 1.415286 0.000000

8 N 2.473290 1.366364 0.000000

9 C 3.575688 2.203990 1.366364 0.000000

10 C 3.622069 2.257571 2.295737 1.447091 0.000000

11 C 2.540574 1.447091 2.295737 2.257571 1.362327

12 C 4.892269 5.502035 5.146411 6.407410 7.411586

13 C 5.502035 5.778373 5.091613 6.184429 7.381193

14 C 6.947426 7.174918 6.391644 7.381193 8.654486

15 C 7.411586 7.381193 6.391644 7.174918 8.546589

16 C 6.407410 6.184429 5.091613 5.778373 7.174918

17 N 5.146411 5.091613 4.163381 5.091613 6.391644

18 C 6.918714 6.407410 5.146411 5.502035 6.947426

19 C 6.407410 5.644383 4.299274 4.373052 5.811224

20 C 7.411586 6.453089 5.088979 4.775537 6.119645

21 C 6.947426 5.811224 4.497313 3.864418 5.080041

22 C 5.502035 4.373052 3.050854 2.527470 3.864418

23 N 5.146411 4.299274 2.943955 3.050854 4.497313

24 H 4.640143 5.839545 6.165623 7.530397 8.078310

25 H 2.902198 4.314848 5.182633 6.420632 6.508430

26 H 4.640143 3.313654 3.329436 2.252779 1.079726

27 H 2.902198 2.252779 3.329436 3.313654 2.194534

28 H 7.655283 8.021501 7.334129 8.381514 9.616620

29 H 8.468266 8.381514 7.334129 8.021501 9.424925

30 H 8.468266 7.530397 6.165623 5.839545 7.161392

31 H 7.655283 6.420632 5.182633 4.314848 5.327861

32 Zn 3.465152 3.098363 2.088830 3.098363 4.333349

33 C 4.892269 3.575688 2.473290 1.415286 2.540574

34 C 5.986810 4.592104 3.718350 2.420308 2.892012

35 C 5.986810 6.766559 6.526485 7.811264 8.765508

36 C 7.005529 5.592542 4.849175 3.505669 3.626481

37 C 7.005529 7.878382 7.705904 9.003095 9.925428

38 C 1.427032 2.420308 3.718350 4.592104 4.216323

39 C 2.632830 3.505669 4.849175 5.592542 4.988733

40 C 8.345500 7.811264 6.526485 6.766559 8.210997

41 C 9.551077 9.003095 7.705904 7.878382 9.315473

42 H 10.618298 10.060881 8.755913 8.883046 10.312120

43 H 7.951085 6.536211 5.875088 4.517658 4.451471

44 H 3.700169 4.517658 5.875088 6.536211 5.797203

45 H 7.951085 8.883046 8.755913 10.060881 10.960464

11 12 13 14 15

11 C 0.000000

12 C 6.947426 0.000000

13 C 7.174918 1.415286 0.000000

14 C 8.546589 2.540574 1.447091 0.000000

15 C 8.654486 3.622069 2.257571 1.362327 0.000000

16 C 7.381193 3.575688 2.203990 2.257571 1.447091

17 N 6.391644 2.473290 1.366364 2.295737 2.295737

18 C 7.411586 4.892269 3.575688 3.622069 2.540574

19 C 6.453089 5.502035 4.373052 4.775537 3.864418

20 C 7.006662 6.947426 5.811224 6.119645 5.080041

21 C 6.119645 7.411586 6.453089 7.006662 6.119645

22 C 4.775537 6.407410 5.644383 6.453089 5.811224

23 N 5.088979 5.146411 4.299274 5.088979 4.497313

24 H 7.161392 2.902198 4.314848 5.327861 6.508430

25 H 5.327861 4.640143 5.839545 7.161392 8.078310

26 H 2.194534 8.468266 8.381514 9.616620 9.424925

27 H 1.079726 7.655283 8.021501 9.424925 9.616620

28 H 9.424925 2.902198 2.252779 1.079726 2.194534

29 H 9.616620 4.640143 3.313654 2.194534 1.079726

30 H 8.078310 7.655283 6.420632 6.508430 5.327861

31 H 6.508430 8.468266 7.530397 8.078310 7.161392

32 Zn 4.333349 3.465152 3.098363 4.333349 4.333349

33 C 3.622069 6.918714 6.407410 7.411586 6.947426

34 C 4.216323 8.345500 7.811264 8.765508 8.210997

35 C 8.210997 1.427032 2.420308 2.892012 4.216323

36 C 4.988733 9.551077 9.003095 9.925428 9.315473

37 C 9.315473 2.632830 3.505669 3.626481 4.988733

38 C 2.892012 5.986810 6.766559 8.210997 8.765508

39 C 3.626481 7.005529 7.878382 9.315473 9.925428

40 C 8.765508 5.986810 4.592104 4.216323 2.892012

41 C 9.925428 7.005529 5.592542 4.988733 3.626481

42 H 10.960464 7.951085 6.536211 5.797203 4.451471

43 H 5.797203 10.618298 10.060881 10.960464 10.312120

44 H 4.451471 7.951085 8.883046 10.312120 10.960464

45 H 10.312120 3.700169 4.517658 4.451471 5.797203

16 17 18 19 20

16 C 0.000000

17 N 1.366364 0.000000

18 C 1.415286 2.473290 0.000000

19 C 2.527470 3.050854 1.415286 0.000000

20 C 3.864418 4.497313 2.540574 1.447091 0.000000

21 C 4.775537 5.088979 3.622069 2.257571 1.362327

22 C 4.373052 4.299274 3.575688 2.203990 2.257571

23 N 3.050854 2.943955 2.473290 1.366364 2.295737

24 H 6.420632 5.182633 7.655283 8.021501 9.424925

25 H 7.530397 6.165623 8.468266 8.381514 9.616620

26 H 8.021501 7.334129 7.655283 6.420632 6.508430

27 H 8.381514 7.334129 8.468266 7.530397 8.078310

28 H 3.313654 3.329436 4.640143 5.839545 7.161392

29 H 2.252779 3.329436 2.902198 4.314848 5.327861

30 H 4.314848 5.182633 2.902198 2.252779 1.079726

31 H 5.839545 6.165623 4.640143 3.313654 2.194534

32 Zn 3.098363 2.088830 3.465152 3.098363 4.333349

33 C 5.502035 5.146411 4.892269 3.575688 3.622069

34 C 6.766559 6.526485 5.986810 4.592104 4.216323

35 C 4.592104 3.718350 5.986810 6.766559 8.210997

36 C 7.878382 7.705904 7.005529 5.592542 4.988733

37 C 5.592542 4.849175 7.005529 7.878382 9.315473

38 C 7.811264 6.526485 8.345500 7.811264 8.765508

39 C 9.003095 7.705904 9.551077 9.003095 9.925428

40 C 2.420308 3.718350 1.427032 2.420308 2.892012

41 C 3.505669 4.849175 2.632830 3.505669 3.626481

42 H 4.517658 5.875088 3.700169 4.517658 4.451471

43 H 8.883046 8.755913 7.951085 6.536211 5.797203

44 H 10.060881 8.755913 10.618298 10.060881 10.960464

45 H 6.536211 5.875088 7.951085 8.883046 10.312120

21 22 23 24 25

21 C 0.000000

22 C 1.447091 0.000000

23 N 2.295737 1.366364 0.000000

24 H 9.616620 8.381514 7.334129 0.000000

25 H 9.424925 8.021501 7.334129 2.679365 0.000000

26 H 5.327861 4.314848 5.182633 9.147477 7.496250

27 H 7.161392 5.839545 6.165623 7.496250 5.358283

28 H 8.078310 7.530397 6.165623 5.358283 7.496250

29 H 6.508430 6.420632 5.182633 7.496250 9.147477

30 H 2.194534 3.313654 3.329436 10.257122 10.601299

31 H 1.079726 2.252779 3.329436 10.601299 10.257122

32 Zn 4.333349 3.098363 2.088830 5.306831 5.306831

33 C 2.540574 1.415286 2.473290 8.468266 7.655283

34 C 2.892012 2.420308 3.718350 9.831933 8.840394

35 C 8.765508 7.811264 6.526485 2.697420 5.078428

36 C 3.626481 3.505669 4.849175 10.996638 9.891612

37 C 9.925428 9.003095 7.705904 3.079210 5.706450

38 C 8.210997 6.766559 6.526485 5.078428 2.697420

39 C 9.315473 7.878382 7.705904 5.706450 3.079210

40 C 4.216323 4.592104 3.718350 8.840394 9.831933

41 C 4.988733 5.592542 4.849175 9.891612 10.996638

42 H 5.797203 6.536211 5.875088 10.849031 12.034406

43 H 4.451471 4.517658 5.875088 12.034406 10.849031

44 H 10.312120 8.883046 8.755913 6.401996 3.722918

45 H 10.960464 10.060881 8.755913 3.722918 6.401996

26 27 28 29 30

26 H 0.000000

27 H 2.679365 0.000000

28 H 10.601299 10.257122 0.000000

29 H 10.257122 10.601299 2.679365 0.000000

30 H 7.496250 9.147477 7.496250 5.358283 0.000000

31 H 5.358283 7.496250 9.147477 7.496250 2.679365

32 Zn 5.306831 5.306831 5.306831 5.306831 5.306831

33 C 2.902198 4.640143 8.468266 7.655283 4.640143

34 C 2.697420 5.078428 9.831933 8.840394 5.078428

35 C 9.831933 8.840394 2.697420 5.078428 8.840394

36 C 3.079210 5.706450 10.996638 9.891612 5.706450

37 C 10.996638 9.891612 3.079210 5.706450 9.891612

38 C 5.078428 2.697420 8.840394 9.831933 9.831933

39 C 5.706450 3.079210 9.891612 10.996638 10.996638

40 C 8.840394 9.831933 5.078428 2.697420 2.697420

41 C 9.891612 10.996638 5.706450 3.079210 3.079210

42 H 10.849031 12.034406 6.401996 3.722918 3.722918

43 H 3.722918 6.401996 12.034406 10.849031 6.401996

44 H 6.401996 3.722918 10.849031 12.034406 12.034406

45 H 12.034406 10.849031 3.722918 6.401996 10.849031

31 32 33 34 35

31 H 0.000000

32 Zn 5.306831 0.000000

33 C 2.902198 3.465152 0.000000

34 C 2.697420 4.891474 1.427032 0.000000

35 C 9.831933 4.891474 8.345500 9.772185 0.000000

36 C 3.079210 6.097028 2.632830 1.205803 10.977674

37 C 10.996638 6.097028 9.551077 10.977674 1.205803

38 C 8.840394 4.891474 5.986810 6.909978 6.909978

39 C 9.891612 6.097028 7.005529 7.809074 7.809074

40 C 5.078428 4.891474 5.986810 6.909978 6.909978

41 C 5.706450 6.097028 7.005529 7.809074 7.809074

42 H 6.401996 7.164172 7.951085 8.667330 8.667330

43 H 3.722918 7.164172 3.700169 2.273140 12.044836

44 H 10.849031 7.164172 7.951085 8.667330 8.667330

45 H 12.034406 7.164172 10.618298 12.044836 2.273140

36 37 38 39 40

36 C 0.000000

37 C 12.183086 0.000000

38 C 7.809074 7.809074 0.000000

39 C 8.614743 8.614743 1.205803 0.000000

40 C 7.809074 7.809074 9.772185 10.977674 0.000000

41 C 8.614743 8.614743 10.977674 12.183086 1.205803

42 H 9.399649 9.399649 12.044836 13.250193 2.273140

43 H 1.067339 13.250193 8.667330 9.399649 8.667330

44 H 9.399649 9.399649 2.273140 1.067339 12.044836

45 H 13.250193 1.067339 8.667330 9.399649 8.667330

41 42 43 44 45

41 C 0.000000

42 H 1.067339 0.000000

43 H 9.399649 10.123831 0.000000

44 H 13.250193 14.317259 10.123831 0.000000

45 H 9.399649 10.123831 14.317259 10.123831 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

RotChk: IX=3 Diff= 1.02D-20

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681163 -4.273295 -0.041193

2 6 0 -1.101995 -2.889186 -0.006314

3 7 0 0.000000 -2.081690 0.016222

4 6 0 1.101995 -2.889186 -0.006314

5 6 0 0.681163 -4.273295 -0.041193

6 6 0 2.446135 -2.446135 -0.011552

7 6 0 2.889186 -1.101995 -0.006314

8 7 0 2.081690 0.000000 0.016222

9 6 0 2.889186 1.101995 -0.006314

10 6 0 4.273295 0.681163 -0.041193

11 6 0 4.273295 -0.681163 -0.041193

12 6 0 -2.446135 -2.446135 -0.011552

13 6 0 -2.889186 -1.101995 -0.006314

14 6 0 -4.273295 -0.681163 -0.041193

15 6 0 -4.273295 0.681163 -0.041193

16 6 0 -2.889186 1.101995 -0.006314

17 7 0 -2.081690 0.000000 0.016222

18 6 0 -2.446135 2.446135 -0.011552

19 6 0 -1.101995 2.889186 -0.006314

20 6 0 -0.681163 4.273295 -0.041193

21 6 0 0.681163 4.273295 -0.041193

22 6 0 1.101995 2.889186 -0.006314

23 7 0 0.000000 2.081690 0.016222

24 1 0 -1.339682 -5.128561 -0.067294

25 1 0 1.339682 -5.128561 -0.067294

26 1 0 5.128561 1.339682 -0.067294

27 1 0 5.128561 -1.339682 -0.067294

28 1 0 -5.128561 -1.339682 -0.067294

29 1 0 -5.128561 1.339682 -0.067294

30 1 0 -1.339682 5.128561 -0.067294

31 1 0 1.339682 5.128561 -0.067294

32 30 0 0.000000 0.000000 0.188776

33 6 0 2.446135 2.446135 -0.011552

34 6 0 3.454989 3.454989 -0.040621

35 6 0 -3.454989 -3.454989 -0.040621

36 6 0 4.307371 4.307371 -0.069779

37 6 0 -4.307371 -4.307371 -0.069779

38 6 0 3.454989 -3.454989 -0.040621

39 6 0 4.307371 -4.307371 -0.069779

40 6 0 -3.454989 3.454989 -0.040621

41 6 0 -4.307371 4.307371 -0.069779

42 1 0 -5.061915 5.061915 -0.092982

43 1 0 5.061915 5.061915 -0.092982

44 1 0 5.061915 -5.061915 -0.092982

45 1 0 -5.061915 -5.061915 -0.092982

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

Rotational constants (GHZ): 0.1465170 0.1465170 0.0733190

Leave Link 202 at Fri Jul 26 14:23:54 2019, MaxMem= 1342177280 cpu: 0.1

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 184 symmetry adapted cartesian basis functions of A1 symmetry.

There are 155 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3060.6075485470 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= 9 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= -0.1305299093 Hartrees.

Nuclear repulsion after empirical dispersion term = 3060.4770186377 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: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3898

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.63D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 148

GePol: Fraction of low-weight points (<1% of avg) = 3.80%

GePol: Cavity surface area = 415.581 Ang\*\*2

GePol: Cavity volume = 419.954 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0083977814 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3060.4854164192 Hartrees.

Leave Link 301 at Fri Jul 26 14:23:54 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44808.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.40D-05 NBF= 172 148 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 172 148 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:23:55 2019, MaxMem= 1342177280 cpu: 6.6

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:23:55 2019, MaxMem= 1342177280 cpu: 0.8

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

Initial guess from the checkpoint file: "ZnTSPsim0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Occupied (E) (E) (B2) (A1) (E) (E) (B1) (A1) (B2) (E) (E)

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

(E) (E) (A1) (A2) (E) (E) (B1) (B1) (E) (E) (A1)

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

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

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

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

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

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

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

(E) (E) (A2) (A1)

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(E) (E) (E)

The electronic state of the initial guess is 1-A1.

Leave Link 401 at Fri Jul 26 14:23:56 2019, MaxMem= 1342177280 cpu: 10.4

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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.

An orbital has undefined symmetry, so N\*\*3 symmetry is turned off.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 660000000 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= 0 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= 45583212.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.77D-15 for 2261.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.83D-15 for 3081 2941.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.55D-15 for 1287.

Iteration 1 A^-1\*A deviation from orthogonality is 1.32D-14 for 1170 1072.

E= -1359.06304177654

DIIS: error= 9.40D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.06304177654 IErMin= 1 ErrMin= 9.40D-05

ErrMax= 9.40D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.66D-06 BMatP= 2.66D-06

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

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 3.228 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=5.47D-06 MaxDP=1.50D-04 OVMax= 3.40D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.47D-06 CP: 1.00D+00

E= -1359.06304573199 Delta-E= -0.000003955454 Rises=F Damp=F

DIIS: error= 9.30D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.06304573199 IErMin= 2 ErrMin= 9.30D-06

ErrMax= 9.30D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.53D-08 BMatP= 2.66D-06

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

Coeff-Com: -0.525D-01 0.105D+01

Coeff: -0.525D-01 0.105D+01

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=5.95D-07 MaxDP=1.55D-05 DE=-3.96D-06 OVMax= 5.13D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 5.10D-07 CP: 1.00D+00 1.06D+00

E= -1359.06304578133 Delta-E= -0.000000049337 Rises=F Damp=F

DIIS: error= 4.72D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.06304578133 IErMin= 3 ErrMin= 4.72D-06

ErrMax= 4.72D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.76D-09 BMatP= 2.53D-08

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

Coeff-Com: -0.215D-01 0.356D+00 0.665D+00

Coeff: -0.215D-01 0.356D+00 0.665D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=2.09D-07 MaxDP=8.71D-06 DE=-4.93D-08 OVMax= 2.51D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.77D-07 CP: 1.00D+00 1.06D+00 7.99D-01

E= -1359.06304578359 Delta-E= -0.000000002256 Rises=F Damp=F

DIIS: error= 3.52D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.06304578359 IErMin= 4 ErrMin= 3.52D-06

ErrMax= 3.52D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.28D-09 BMatP= 6.76D-09

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

Coeff-Com: -0.635D-02 0.813D-01 0.438D+00 0.487D+00

Coeff: -0.635D-02 0.813D-01 0.438D+00 0.487D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=9.71D-08 MaxDP=4.62D-06 DE=-2.26D-09 OVMax= 1.39D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 6.61D-08 CP: 1.00D+00 1.06D+00 8.45D-01 6.22D-01

E= -1359.06304578752 Delta-E= -0.000000003932 Rises=F Damp=F

DIIS: error= 6.09D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.06304578752 IErMin= 5 ErrMin= 6.09D-07

ErrMax= 6.09D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.25D-10 BMatP= 4.28D-09

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

Coeff-Com: -0.730D-04-0.121D-01 0.947D-01 0.191D+00 0.727D+00

Coeff: -0.730D-04-0.121D-01 0.947D-01 0.191D+00 0.727D+00

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=2.39D-08 MaxDP=8.94D-07 DE=-3.93D-09 OVMax= 2.11D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.50D-08 CP: 1.00D+00 1.06D+00 8.69D-01 6.66D-01 8.27D-01

E= -1359.06304578762 Delta-E= -0.000000000103 Rises=F Damp=F

DIIS: error= 6.36D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.06304578762 IErMin= 5 ErrMin= 6.09D-07

ErrMax= 6.36D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.20D-11 BMatP= 1.25D-10

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

Coeff-Com: 0.549D-03-0.151D-01 0.137D-01 0.651D-01 0.422D+00 0.514D+00

Coeff: 0.549D-03-0.151D-01 0.137D-01 0.651D-01 0.422D+00 0.514D+00

Gap= 0.092 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1273 IAlg= 4 N= 636 NDim= 636 NE2= 2108188 trying DSYEV.

RMSDP=7.98D-09 MaxDP=4.08D-07 DE=-1.03D-10 OVMax= 8.50D-07

Error on total polarization charges = 0.06212

SCF Done: E(RB3LYP) = -1359.06304579 A.U. after 6 cycles

NFock= 6 Conv=0.80D-08 -V/T= 1.9682

KE= 1.403728956777D+03 PE=-9.363055555584D+03 EE= 3.539778136600D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.27

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:24:25 2019, MaxMem= 1342177280 cpu: 320.4

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44808.

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 = 260

Leave Link 701 at Fri Jul 26 14:24:29 2019, MaxMem= 1342177280 cpu: 43.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

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

Leave Link 702 at Fri Jul 26 14:24:29 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Fri Jul 26 14:24:33 2019, MaxMem= 1342177280 cpu: 43.4

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-1.40332190D-13 2.98427949D-13 3.28974529D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000004068 -0.000001563 -0.000001666

2 6 -0.000005244 0.000001677 0.000001921

3 7 0.000000000 -0.000009377 0.000003013

4 6 0.000005244 0.000001677 0.000001921

5 6 -0.000004068 -0.000001563 -0.000001666

6 6 -0.000002129 0.000002129 -0.000004953

7 6 -0.000001677 -0.000005244 0.000001921

8 7 0.000009377 0.000000000 0.000003013

9 6 -0.000001677 0.000005244 0.000001921

10 6 0.000001563 -0.000004068 -0.000001666

11 6 0.000001563 0.000004068 -0.000001666

12 6 0.000002129 0.000002129 -0.000004953

13 6 0.000001677 -0.000005244 0.000001921

14 6 -0.000001563 0.000004068 -0.000001666

15 6 -0.000001563 -0.000004068 -0.000001666

16 6 0.000001677 0.000005244 0.000001921

17 7 -0.000009377 0.000000000 0.000003013

18 6 0.000002129 -0.000002129 -0.000004953

19 6 -0.000005244 -0.000001677 0.000001921

20 6 0.000004068 0.000001563 -0.000001666

21 6 -0.000004068 0.000001563 -0.000001666

22 6 0.000005244 -0.000001677 0.000001921

23 7 0.000000000 0.000009377 0.000003013

24 1 0.000000651 0.000000200 0.000001394

25 1 -0.000000651 0.000000200 0.000001394

26 1 -0.000000200 -0.000000651 0.000001394

27 1 -0.000000200 0.000000651 0.000001394

28 1 0.000000200 0.000000651 0.000001394

29 1 0.000000200 -0.000000651 0.000001394

30 1 0.000000651 -0.000000200 0.000001394

31 1 -0.000000651 -0.000000200 0.000001394

32 30 0.000000000 0.000000000 -0.000004854

33 6 -0.000002129 -0.000002129 -0.000004953

34 6 -0.000000119 -0.000000119 0.000000141

35 6 0.000000119 0.000000119 0.000000141

36 6 0.000001330 0.000001330 -0.000000133

37 6 -0.000001330 -0.000001330 -0.000000133

38 6 -0.000000119 0.000000119 0.000000141

39 6 0.000001330 -0.000001330 -0.000000133

40 6 0.000000119 -0.000000119 0.000000141

41 6 -0.000001330 0.000001330 -0.000000133

42 1 0.000000167 -0.000000167 -0.000000153

43 1 -0.000000167 -0.000000167 -0.000000153

44 1 -0.000000167 0.000000167 -0.000000153

45 1 0.000000167 0.000000167 -0.000000153

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

Cartesian Forces: Max 0.000009377 RMS 0.000002757

Leave Link 716 at Fri Jul 26 14:24:33 2019, MaxMem= 1342177280 cpu: 0.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000006525 RMS 0.000001286

Search for a local minimum.

Step number 16 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .12856D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 2 3 4 5 7

9 8 10 11 12

13 14 15 16

DE= -2.36D-07 DEPred=-2.04D-07 R= 1.15D+00

Trust test= 1.15D+00 RLast= 7.02D-03 DXMaxT set to 8.41D-02

ITU= 0 0 1 1 -1 1 0 -1 0 0 -1 1 0 -1 -1 0

Eigenvalues --- 0.00534 0.00534 0.00534 0.00534 0.00534

Eigenvalues --- 0.00534 0.00535 0.00598 0.01000 0.01157

Eigenvalues --- 0.01157 0.01167 0.01384 0.01384 0.01636

Eigenvalues --- 0.01646 0.01674 0.01726 0.01726 0.01805

Eigenvalues --- 0.01805 0.01825 0.01831 0.01859 0.01859

Eigenvalues --- 0.01868 0.01868 0.01868 0.01908 0.01920

Eigenvalues --- 0.01927 0.01927 0.01933 0.01961 0.01961

Eigenvalues --- 0.01984 0.02178 0.02180 0.02184 0.02184

Eigenvalues --- 0.02281 0.02548 0.03318 0.03723 0.04654

Eigenvalues --- 0.04654 0.04654 0.04654 0.04654 0.04654

Eigenvalues --- 0.04654 0.08737 0.13847 0.14999 0.14999

Eigenvalues --- 0.15209 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.18318 0.22832

Eigenvalues --- 0.22868 0.22872 0.22872 0.24758 0.24773

Eigenvalues --- 0.24773 0.24833 0.24864 0.24979 0.24979

Eigenvalues --- 0.24998 0.24998 0.24998 0.24998 0.24998

Eigenvalues --- 0.26996 0.35035 0.35035 0.35467 0.35498

Eigenvalues --- 0.35809 0.35958 0.36034 0.36034 0.36034

Eigenvalues --- 0.36034 0.36034 0.36034 0.36035 0.36780

Eigenvalues --- 0.36864 0.36864 0.37174 0.37563 0.37563

Eigenvalues --- 0.37563 0.37688 0.38967 0.38967 0.39538

Eigenvalues --- 0.41157 0.41397 0.41397 0.41397 0.41516

Eigenvalues --- 0.41516 0.41789 0.42522 0.43514 0.43778

Eigenvalues --- 0.43778 0.45461 0.47912 0.49087 0.49087

Eigenvalues --- 0.50131 0.51398 0.51901 0.51901 0.52698

Eigenvalues --- 1.01831 1.01831 1.01831 1.02093

En-DIIS/RFO-DIIS IScMMF= 0 using points: 16 15 14 13 12

RFO step: Lambda= 0.00000000D+00.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 7.42D-05 SmlDif= 1.00D-05

RMS Error= 0.4475138927D-05 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.13755 -0.20463 0.06498 0.00190 0.00020

Iteration 1 RMS(Cart)= 0.00011141 RMS(Int)= 0.00000001

Iteration 2 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000001

ITry= 1 IFail=0 DXMaxC= 6.58D-04 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.19D-05 for atom 44.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73461 0.00000 -0.00001 0.00000 -0.00001 2.73460

R2 2.57442 0.00000 0.00000 0.00001 0.00001 2.57443

R3 2.04039 0.00000 0.00000 0.00000 0.00000 2.04039

R4 2.58205 0.00000 0.00000 0.00000 0.00000 2.58206

R5 2.67450 0.00000 0.00000 0.00000 0.00000 2.67451

R6 2.58205 0.00000 0.00000 0.00000 0.00000 2.58206

R7 3.94732 -0.00001 -0.00003 0.00000 -0.00003 3.94728

R8 2.73461 0.00000 -0.00001 0.00000 -0.00001 2.73460

R9 2.67450 0.00000 0.00000 0.00000 0.00000 2.67451

R10 2.04039 0.00000 0.00000 0.00000 0.00000 2.04039

R11 2.67450 0.00000 0.00000 0.00000 0.00000 2.67451

R12 2.69670 0.00000 -0.00001 0.00000 -0.00001 2.69669

R13 2.58205 0.00000 0.00000 0.00000 0.00000 2.58206

R14 2.73461 0.00000 -0.00001 0.00000 -0.00001 2.73460

R15 2.58205 0.00000 0.00000 0.00000 0.00000 2.58206

R16 3.94732 -0.00001 -0.00003 0.00000 -0.00003 3.94728

R17 2.73461 0.00000 -0.00001 0.00000 -0.00001 2.73460

R18 2.67450 0.00000 0.00000 0.00000 0.00000 2.67451

R19 2.57442 0.00000 0.00000 0.00001 0.00001 2.57443

R20 2.04039 0.00000 0.00000 0.00000 0.00000 2.04039

R21 2.04039 0.00000 0.00000 0.00000 0.00000 2.04039

R22 2.67450 0.00000 0.00000 0.00000 0.00000 2.67451

R23 2.69670 0.00000 -0.00001 0.00000 -0.00001 2.69669

R24 2.73461 0.00000 -0.00001 0.00000 -0.00001 2.73460

R25 2.58205 0.00000 0.00000 0.00000 0.00000 2.58206

R26 2.57442 0.00000 0.00000 0.00001 0.00001 2.57443

R27 2.04039 0.00000 0.00000 0.00000 0.00000 2.04039

R28 2.73461 0.00000 -0.00001 0.00000 -0.00001 2.73460

R29 2.04039 0.00000 0.00000 0.00000 0.00000 2.04039

R30 2.58205 0.00000 0.00000 0.00000 0.00000 2.58206

R31 2.67450 0.00000 0.00000 0.00000 0.00000 2.67451

R32 3.94732 -0.00001 -0.00003 0.00000 -0.00003 3.94728

R33 2.67450 0.00000 0.00000 0.00000 0.00000 2.67451

R34 2.69670 0.00000 -0.00001 0.00000 -0.00001 2.69669

R35 2.73461 0.00000 -0.00001 0.00000 -0.00001 2.73460

R36 2.58205 0.00000 0.00000 0.00000 0.00000 2.58206

R37 2.57442 0.00000 0.00000 0.00001 0.00001 2.57443

R38 2.04039 0.00000 0.00000 0.00000 0.00000 2.04039

R39 2.73461 0.00000 -0.00001 0.00000 -0.00001 2.73460

R40 2.04039 0.00000 0.00000 0.00000 0.00000 2.04039

R41 2.58205 0.00000 0.00000 0.00000 0.00000 2.58206

R42 2.67450 0.00000 0.00000 0.00000 0.00000 2.67451

R43 3.94732 -0.00001 -0.00003 0.00000 -0.00003 3.94728

R44 2.69670 0.00000 -0.00001 0.00000 -0.00001 2.69669

R45 2.27864 0.00000 0.00000 0.00000 0.00000 2.27864

R46 2.27864 0.00000 0.00000 0.00000 0.00000 2.27864

R47 2.01698 0.00000 0.00000 0.00000 0.00000 2.01698

R48 2.01698 0.00000 0.00000 0.00000 0.00000 2.01698

R49 2.27864 0.00000 0.00000 0.00000 0.00000 2.27864

R50 2.01698 0.00000 0.00000 0.00000 0.00000 2.01698

R51 2.27864 0.00000 0.00000 0.00000 0.00000 2.27864

R52 2.01698 0.00000 0.00000 0.00000 0.00000 2.01698

A1 1.86587 0.00000 0.00000 0.00000 0.00000 1.86587

A2 2.19058 0.00000 0.00000 0.00000 0.00000 2.19057

A3 2.22672 0.00000 0.00000 0.00000 0.00001 2.22673

A4 1.90828 0.00000 0.00000 0.00001 0.00001 1.90829

A5 2.18404 0.00000 0.00000 -0.00001 -0.00001 2.18403

A6 2.19079 0.00000 0.00000 0.00000 0.00000 2.19079

A7 1.87647 0.00000 -0.00001 -0.00001 -0.00001 1.87646

A8 2.20226 0.00000 0.00000 0.00000 0.00001 2.20227

A9 2.20226 0.00000 0.00000 0.00000 0.00001 2.20227

A10 1.90828 0.00000 0.00000 0.00001 0.00001 1.90829

A11 2.19079 0.00000 0.00000 0.00000 0.00000 2.19079

A12 2.18404 0.00000 0.00000 -0.00001 -0.00001 2.18403

A13 1.86587 0.00000 0.00000 0.00000 0.00000 1.86587

A14 2.22672 0.00000 0.00000 0.00000 0.00001 2.22673

A15 2.19058 0.00000 0.00000 0.00000 0.00000 2.19057

A16 2.20757 0.00000 -0.00001 0.00000 -0.00001 2.20756

A17 2.03777 0.00000 0.00000 0.00000 0.00001 2.03777

A18 2.03777 0.00000 0.00000 0.00000 0.00001 2.03777

A19 2.19079 0.00000 0.00000 0.00000 0.00000 2.19079

A20 2.18404 0.00000 0.00000 -0.00001 -0.00001 2.18403

A21 1.90828 0.00000 0.00000 0.00001 0.00001 1.90829

A22 1.87647 0.00000 -0.00001 -0.00001 -0.00001 1.87646

A23 2.20226 0.00000 0.00000 0.00000 0.00001 2.20227

A24 2.20226 0.00000 0.00000 0.00000 0.00001 2.20227

A25 1.90828 0.00000 0.00000 0.00001 0.00001 1.90829

A26 2.19079 0.00000 0.00000 0.00000 0.00000 2.19079

A27 2.18404 0.00000 0.00000 -0.00001 -0.00001 2.18403

A28 1.86587 0.00000 0.00000 0.00000 0.00000 1.86587

A29 2.19058 0.00000 0.00000 0.00000 0.00000 2.19057

A30 2.22672 0.00000 0.00000 0.00000 0.00001 2.22673

A31 1.86587 0.00000 0.00000 0.00000 0.00000 1.86587

A32 2.19058 0.00000 0.00000 0.00000 0.00000 2.19057

A33 2.22672 0.00000 0.00000 0.00000 0.00001 2.22673

A34 2.20757 0.00000 -0.00001 0.00000 -0.00001 2.20756

A35 2.03777 0.00000 0.00000 0.00000 0.00001 2.03777

A36 2.03777 0.00000 0.00000 0.00000 0.00001 2.03777

A37 2.18404 0.00000 0.00000 -0.00001 -0.00001 2.18403

A38 2.19079 0.00000 0.00000 0.00000 0.00000 2.19079

A39 1.90828 0.00000 0.00000 0.00001 0.00001 1.90829

A40 1.86587 0.00000 0.00000 0.00000 0.00000 1.86587

A41 2.19058 0.00000 0.00000 0.00000 0.00000 2.19057

A42 2.22672 0.00000 0.00000 0.00000 0.00001 2.22673

A43 1.86587 0.00000 0.00000 0.00000 0.00000 1.86587

A44 2.22672 0.00000 0.00000 0.00000 0.00001 2.22673

A45 2.19058 0.00000 0.00000 0.00000 0.00000 2.19057

A46 1.90828 0.00000 0.00000 0.00001 0.00001 1.90829

A47 2.18404 0.00000 0.00000 -0.00001 -0.00001 2.18403

A48 2.19079 0.00000 0.00000 0.00000 0.00000 2.19079

A49 1.87647 0.00000 -0.00001 -0.00001 -0.00001 1.87646

A50 2.20226 0.00000 0.00000 0.00000 0.00001 2.20227

A51 2.20226 0.00000 0.00000 0.00000 0.00001 2.20227

A52 2.20757 0.00000 -0.00001 0.00000 -0.00001 2.20756

A53 2.03777 0.00000 0.00000 0.00000 0.00001 2.03777

A54 2.03777 0.00000 0.00000 0.00000 0.00001 2.03777

A55 2.18404 0.00000 0.00000 -0.00001 -0.00001 2.18403

A56 2.19079 0.00000 0.00000 0.00000 0.00000 2.19079

A57 1.90828 0.00000 0.00000 0.00001 0.00001 1.90829

A58 1.86587 0.00000 0.00000 0.00000 0.00000 1.86587

A59 2.19058 0.00000 0.00000 0.00000 0.00000 2.19057

A60 2.22672 0.00000 0.00000 0.00000 0.00001 2.22673

A61 1.86587 0.00000 0.00000 0.00000 0.00000 1.86587

A62 2.22672 0.00000 0.00000 0.00000 0.00001 2.22673

A63 2.19058 0.00000 0.00000 0.00000 0.00000 2.19057

A64 1.90828 0.00000 0.00000 0.00001 0.00001 1.90829

A65 2.18404 0.00000 0.00000 -0.00001 -0.00001 2.18403

A66 2.19079 0.00000 0.00000 0.00000 0.00000 2.19079

A67 1.87647 0.00000 -0.00001 -0.00001 -0.00001 1.87646

A68 2.20226 0.00000 0.00000 0.00000 0.00001 2.20227

A69 2.20226 0.00000 0.00000 0.00000 0.00001 2.20227

A70 1.56397 0.00000 0.00000 0.00000 0.00000 1.56397

A71 1.56397 0.00000 0.00000 0.00000 0.00000 1.56397

A72 2.97619 0.00000 0.00005 -0.00003 0.00003 2.97622

A73 2.97619 0.00000 0.00005 -0.00003 0.00003 2.97622

A74 1.56397 0.00000 0.00000 0.00000 0.00000 1.56397

A75 1.56397 0.00000 0.00000 0.00000 0.00000 1.56397

A76 2.20757 0.00000 -0.00001 0.00000 -0.00001 2.20756

A77 2.03777 0.00000 0.00000 0.00000 0.00001 2.03777

A78 2.03777 0.00000 0.00000 0.00000 0.00001 2.03777

A79 3.14154 0.00000 0.00000 0.00000 0.00000 3.14154

A80 3.14154 0.00000 0.00000 0.00000 0.00000 3.14154

A81 3.14162 0.00000 0.00000 0.00000 0.00000 3.14162

A82 3.14162 0.00000 0.00000 0.00000 0.00000 3.14162

A83 3.14154 0.00000 0.00000 0.00000 0.00000 3.14154

A84 3.14162 0.00000 0.00000 0.00000 0.00000 3.14162

A85 3.14154 0.00000 0.00000 0.00000 0.00000 3.14154

A86 3.14162 0.00000 0.00000 0.00000 0.00000 3.14162

A87 3.13776 0.00000 0.00000 -0.00003 -0.00003 3.13773

A88 3.14543 0.00000 0.00000 0.00003 0.00003 3.14546

A89 3.14440 0.00000 0.00002 -0.00002 0.00000 3.14440

A90 3.13878 0.00000 -0.00002 0.00002 0.00000 3.13878

A91 3.13776 0.00000 0.00000 -0.00003 -0.00003 3.13773

A92 3.14440 0.00000 0.00002 -0.00002 0.00000 3.14440

A93 3.14543 0.00000 0.00000 0.00003 0.00003 3.14546

A94 3.13878 0.00000 -0.00002 0.00002 0.00000 3.13878

D1 -0.00170 0.00000 -0.00001 -0.00001 -0.00001 -0.00171

D2 3.12742 0.00000 -0.00001 -0.00004 -0.00005 3.12737

D3 -3.13812 0.00000 -0.00005 -0.00001 -0.00006 -3.13817

D4 -0.00899 0.00000 -0.00006 -0.00004 -0.00010 -0.00909

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13628 0.00000 -0.00005 0.00000 -0.00005 -3.13633

D7 3.13628 0.00000 0.00005 0.00000 0.00005 3.13633

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00275 0.00000 0.00001 0.00001 0.00002 0.00277

D10 -3.07094 0.00000 0.00001 -0.00004 -0.00003 -3.07097

D11 -3.12632 0.00000 0.00002 0.00004 0.00006 -3.12626

D12 0.08319 0.00000 0.00002 -0.00001 0.00001 0.08320

D13 -3.11685 0.00000 -0.00007 0.00002 -0.00004 -3.11689

D14 0.01113 0.00000 -0.00004 0.00000 -0.00004 0.01110

D15 0.01028 0.00000 -0.00008 -0.00001 -0.00009 0.01020

D16 3.13827 0.00000 -0.00005 -0.00003 -0.00008 3.13819

D17 -0.00275 0.00000 -0.00001 -0.00001 -0.00002 -0.00277

D18 3.12632 0.00000 -0.00002 -0.00004 -0.00006 3.12626

D19 3.07094 0.00000 -0.00001 0.00004 0.00003 3.07097

D20 -0.08319 0.00000 -0.00002 0.00001 -0.00001 -0.08320

D21 -3.09930 0.00000 -0.00003 0.00004 0.00002 -3.09929

D22 -0.12255 0.00000 0.00003 0.00002 0.00004 -0.12251

D23 -1.61093 0.00000 0.00000 0.00003 0.00003 -1.61090

D24 0.12255 0.00000 -0.00003 -0.00002 -0.00004 0.12251

D25 3.09930 0.00000 0.00003 -0.00004 -0.00002 3.09929

D26 1.61093 0.00000 0.00000 -0.00003 -0.00003 1.61090

D27 0.00170 0.00000 0.00001 0.00001 0.00001 0.00171

D28 3.13812 0.00000 0.00005 0.00001 0.00006 3.13817

D29 -3.12742 0.00000 0.00001 0.00004 0.00005 -3.12737

D30 0.00899 0.00000 0.00006 0.00004 0.00010 0.00909

D31 -0.01028 0.00000 0.00008 0.00001 0.00009 -0.01020

D32 -3.13827 0.00000 0.00005 0.00003 0.00008 -3.13819

D33 3.11685 0.00000 0.00007 -0.00002 0.00004 3.11689

D34 -0.01113 0.00000 0.00004 0.00000 0.00004 -0.01110

D35 0.01028 0.00000 -0.00008 -0.00001 -0.00009 0.01020

D36 -3.11685 0.00000 -0.00007 0.00002 -0.00004 -3.11689

D37 3.13827 0.00000 -0.00005 -0.00003 -0.00008 3.13819

D38 0.01113 0.00000 -0.00004 0.00000 -0.00004 0.01110

D39 -3.12632 0.00000 0.00002 0.00004 0.00006 -3.12626

D40 0.08319 0.00000 0.00002 -0.00001 0.00001 0.08320

D41 0.00275 0.00000 0.00001 0.00001 0.00002 0.00277

D42 -3.07094 0.00000 0.00001 -0.00004 -0.00003 -3.07097

D43 3.12742 0.00000 -0.00001 -0.00004 -0.00005 3.12737

D44 -0.00899 0.00000 -0.00006 -0.00004 -0.00010 -0.00909

D45 -0.00170 0.00000 -0.00001 -0.00001 -0.00001 -0.00171

D46 -3.13812 0.00000 -0.00005 -0.00001 -0.00006 -3.13817

D47 -0.00275 0.00000 -0.00001 -0.00001 -0.00002 -0.00277

D48 3.12632 0.00000 -0.00002 -0.00004 -0.00006 3.12626

D49 3.07094 0.00000 -0.00001 0.00004 0.00003 3.07097

D50 -0.08319 0.00000 -0.00002 0.00001 -0.00001 -0.08320

D51 -0.12255 0.00000 0.00003 0.00002 0.00004 -0.12251

D52 -1.61093 0.00000 0.00000 0.00003 0.00003 -1.61090

D53 -3.09930 0.00000 -0.00003 0.00004 0.00002 -3.09929

D54 3.09930 0.00000 0.00003 -0.00004 -0.00002 3.09929

D55 1.61093 0.00000 0.00000 -0.00003 -0.00003 1.61090

D56 0.12255 0.00000 -0.00003 -0.00002 -0.00004 0.12251

D57 0.00170 0.00000 0.00001 0.00001 0.00001 0.00171

D58 3.13812 0.00000 0.00005 0.00001 0.00006 3.13817

D59 -3.12742 0.00000 0.00001 0.00004 0.00005 -3.12737

D60 0.00899 0.00000 0.00006 0.00004 0.00010 0.00909

D61 -0.01028 0.00000 0.00008 0.00001 0.00009 -0.01020

D62 -3.13827 0.00000 0.00005 0.00003 0.00008 -3.13819

D63 3.11685 0.00000 0.00007 -0.00002 0.00004 3.11689

D64 -0.01113 0.00000 0.00004 0.00000 0.00004 -0.01110

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13628 0.00000 0.00005 0.00000 0.00005 3.13633

D67 -3.13628 0.00000 -0.00005 0.00000 -0.00005 -3.13633

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.11685 0.00000 0.00007 -0.00002 0.00004 3.11689

D70 -0.01028 0.00000 0.00008 0.00001 0.00009 -0.01020

D71 -0.01113 0.00000 0.00004 0.00000 0.00004 -0.01110

D72 -3.13827 0.00000 0.00005 0.00003 0.00008 -3.13819

D73 -3.12742 0.00000 0.00001 0.00004 0.00005 -3.12737

D74 0.00899 0.00000 0.00006 0.00004 0.00010 0.00909

D75 0.00170 0.00000 0.00001 0.00001 0.00001 0.00171

D76 3.13812 0.00000 0.00005 0.00001 0.00006 3.13817

D77 3.12632 0.00000 -0.00002 -0.00004 -0.00006 3.12626

D78 -0.08319 0.00000 -0.00002 0.00001 -0.00001 -0.08320

D79 -0.00275 0.00000 -0.00001 -0.00001 -0.00002 -0.00277

D80 3.07094 0.00000 -0.00001 0.00004 0.00003 3.07097

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 3.13628 0.00000 0.00005 0.00000 0.00005 3.13633

D83 -3.13628 0.00000 -0.00005 0.00000 -0.00005 -3.13633

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 -0.00170 0.00000 -0.00001 -0.00001 -0.00001 -0.00171

D86 3.12742 0.00000 -0.00001 -0.00004 -0.00005 3.12737

D87 -3.13812 0.00000 -0.00005 -0.00001 -0.00006 -3.13817

D88 -0.00899 0.00000 -0.00006 -0.00004 -0.00010 -0.00909

D89 0.00275 0.00000 0.00001 0.00001 0.00002 0.00277

D90 -3.07094 0.00000 0.00001 -0.00004 -0.00003 -3.07097

D91 -3.12632 0.00000 0.00002 0.00004 0.00006 -3.12626

D92 0.08319 0.00000 0.00002 -0.00001 0.00001 0.08320

D93 -3.11685 0.00000 -0.00007 0.00002 -0.00004 -3.11689

D94 0.01113 0.00000 -0.00004 0.00000 -0.00004 0.01110

D95 0.01028 0.00000 -0.00008 -0.00001 -0.00009 0.01020

D96 3.13827 0.00000 -0.00005 -0.00003 -0.00008 3.13819

D97 0.12255 0.00000 -0.00003 -0.00002 -0.00004 0.12251

D98 1.61093 0.00000 0.00000 -0.00003 -0.00003 1.61090

D99 3.09930 0.00000 0.00003 -0.00004 -0.00002 3.09929

D100 -3.09930 0.00000 -0.00003 0.00004 0.00002 -3.09929

D101 -1.61093 0.00000 0.00000 0.00003 0.00003 -1.61090

D102 -0.12255 0.00000 0.00003 0.00002 0.00004 -0.12251

D103 3.11685 0.00000 0.00007 -0.00002 0.00004 3.11689

D104 -0.01028 0.00000 0.00008 0.00001 0.00009 -0.01020

D105 -0.01113 0.00000 0.00004 0.00000 0.00004 -0.01110

D106 -3.13827 0.00000 0.00005 0.00003 0.00008 -3.13819

D107 -3.12742 0.00000 0.00001 0.00004 0.00005 -3.12737

D108 0.00899 0.00000 0.00006 0.00004 0.00010 0.00909

D109 0.00170 0.00000 0.00001 0.00001 0.00001 0.00171

D110 3.13812 0.00000 0.00005 0.00001 0.00006 3.13817

D111 3.12632 0.00000 -0.00002 -0.00004 -0.00006 3.12626

D112 -0.08319 0.00000 -0.00002 0.00001 -0.00001 -0.08320

D113 -0.00275 0.00000 -0.00001 -0.00001 -0.00002 -0.00277

D114 3.07094 0.00000 -0.00001 0.00004 0.00003 3.07097

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.13628 0.00000 0.00005 0.00000 0.00005 3.13633

D117 -3.13628 0.00000 -0.00005 0.00000 -0.00005 -3.13633

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 -0.00170 0.00000 -0.00001 -0.00001 -0.00001 -0.00171

D120 3.12742 0.00000 -0.00001 -0.00004 -0.00005 3.12737

D121 -3.13812 0.00000 -0.00005 -0.00001 -0.00006 -3.13817

D122 -0.00899 0.00000 -0.00006 -0.00004 -0.00010 -0.00909

D123 0.00275 0.00000 0.00001 0.00001 0.00002 0.00277

D124 -3.07094 0.00000 0.00001 -0.00004 -0.00003 -3.07097

D125 -3.12632 0.00000 0.00002 0.00004 0.00006 -3.12626

D126 0.08319 0.00000 0.00002 -0.00001 0.00001 0.08320

D127 -3.11685 0.00000 -0.00007 0.00002 -0.00004 -3.11689

D128 0.01113 0.00000 -0.00004 0.00000 -0.00004 0.01110

D129 0.01028 0.00000 -0.00008 -0.00001 -0.00009 0.01020

D130 3.13827 0.00000 -0.00005 -0.00003 -0.00008 3.13819

D131 1.61093 0.00000 0.00000 -0.00003 -0.00003 1.61090

D132 3.09930 0.00000 0.00003 -0.00004 -0.00002 3.09929

D133 0.12255 0.00000 -0.00003 -0.00002 -0.00004 0.12251

D134 -1.61093 0.00000 0.00000 0.00003 0.00003 -1.61090

D135 -0.12255 0.00000 0.00003 0.00002 0.00004 -0.12251

D136 -3.09930 0.00000 -0.00003 0.00004 0.00002 -3.09929

Item Value Threshold Converged?

Maximum Force 0.000007 0.000450 YES

RMS Force 0.000001 0.000300 YES

Maximum Displacement 0.000657 0.001800 YES

RMS Displacement 0.000111 0.001200 YES

Predicted change in Energy=-2.810216D-09

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) 1.4471 -DE/DX = 0.0 !

! R2 R(1,5) 1.3623 -DE/DX = 0.0 !

! R3 R(1,24) 1.0797 -DE/DX = 0.0 !

! R4 R(2,3) 1.3664 -DE/DX = 0.0 !

! R5 R(2,12) 1.4153 -DE/DX = 0.0 !

! R6 R(3,4) 1.3664 -DE/DX = 0.0 !

! R7 R(3,32) 2.0888 -DE/DX = 0.0 !

! R8 R(4,5) 1.4471 -DE/DX = 0.0 !

! R9 R(4,6) 1.4153 -DE/DX = 0.0 !

! R10 R(5,25) 1.0797 -DE/DX = 0.0 !

! R11 R(6,7) 1.4153 -DE/DX = 0.0 !

! R12 R(6,38) 1.427 -DE/DX = 0.0 !

! R13 R(7,8) 1.3664 -DE/DX = 0.0 !

! R14 R(7,11) 1.4471 -DE/DX = 0.0 !

! R15 R(8,9) 1.3664 -DE/DX = 0.0 !

! R16 R(8,32) 2.0888 -DE/DX = 0.0 !

! R17 R(9,10) 1.4471 -DE/DX = 0.0 !

! R18 R(9,33) 1.4153 -DE/DX = 0.0 !

! R19 R(10,11) 1.3623 -DE/DX = 0.0 !

! R20 R(10,26) 1.0797 -DE/DX = 0.0 !

! R21 R(11,27) 1.0797 -DE/DX = 0.0 !

! R22 R(12,13) 1.4153 -DE/DX = 0.0 !

! R23 R(12,35) 1.427 -DE/DX = 0.0 !

! R24 R(13,14) 1.4471 -DE/DX = 0.0 !

! R25 R(13,17) 1.3664 -DE/DX = 0.0 !

! R26 R(14,15) 1.3623 -DE/DX = 0.0 !

! R27 R(14,28) 1.0797 -DE/DX = 0.0 !

! R28 R(15,16) 1.4471 -DE/DX = 0.0 !

! R29 R(15,29) 1.0797 -DE/DX = 0.0 !

! R30 R(16,17) 1.3664 -DE/DX = 0.0 !

! R31 R(16,18) 1.4153 -DE/DX = 0.0 !

! R32 R(17,32) 2.0888 -DE/DX = 0.0 !

! R33 R(18,19) 1.4153 -DE/DX = 0.0 !

! R34 R(18,40) 1.427 -DE/DX = 0.0 !

! R35 R(19,20) 1.4471 -DE/DX = 0.0 !

! R36 R(19,23) 1.3664 -DE/DX = 0.0 !

! R37 R(20,21) 1.3623 -DE/DX = 0.0 !

! R38 R(20,30) 1.0797 -DE/DX = 0.0 !

! R39 R(21,22) 1.4471 -DE/DX = 0.0 !

! R40 R(21,31) 1.0797 -DE/DX = 0.0 !

! R41 R(22,23) 1.3664 -DE/DX = 0.0 !

! R42 R(22,33) 1.4153 -DE/DX = 0.0 !

! R43 R(23,32) 2.0888 -DE/DX = 0.0 !

! R44 R(33,34) 1.427 -DE/DX = 0.0 !

! R45 R(34,36) 1.2058 -DE/DX = 0.0 !

! R46 R(35,37) 1.2058 -DE/DX = 0.0 !

! R47 R(36,43) 1.0673 -DE/DX = 0.0 !

! R48 R(37,45) 1.0673 -DE/DX = 0.0 !

! R49 R(38,39) 1.2058 -DE/DX = 0.0 !

! R50 R(39,44) 1.0673 -DE/DX = 0.0 !

! R51 R(40,41) 1.2058 -DE/DX = 0.0 !

! R52 R(41,42) 1.0673 -DE/DX = 0.0 !

! A1 A(2,1,5) 106.9066 -DE/DX = 0.0 !

! A2 A(2,1,24) 125.5108 -DE/DX = 0.0 !

! A3 A(5,1,24) 127.5819 -DE/DX = 0.0 !

! A4 A(1,2,3) 109.3363 -DE/DX = 0.0 !

! A5 A(1,2,12) 125.1365 -DE/DX = 0.0 !

! A6 A(3,2,12) 125.5229 -DE/DX = 0.0 !

! A7 A(2,3,4) 107.5139 -DE/DX = 0.0 !

! A8 A(2,3,32) 126.18 -DE/DX = 0.0 !

! A9 A(4,3,32) 126.18 -DE/DX = 0.0 !

! A10 A(3,4,5) 109.3363 -DE/DX = 0.0 !

! A11 A(3,4,6) 125.5229 -DE/DX = 0.0 !

! A12 A(5,4,6) 125.1365 -DE/DX = 0.0 !

! A13 A(1,5,4) 106.9066 -DE/DX = 0.0 !

! A14 A(1,5,25) 127.5819 -DE/DX = 0.0 !

! A15 A(4,5,25) 125.5108 -DE/DX = 0.0 !

! A16 A(4,6,7) 126.4847 -DE/DX = 0.0 !

! A17 A(4,6,38) 116.7555 -DE/DX = 0.0 !

! A18 A(7,6,38) 116.7555 -DE/DX = 0.0 !

! A19 A(6,7,8) 125.5229 -DE/DX = 0.0 !

! A20 A(6,7,11) 125.1365 -DE/DX = 0.0 !

! A21 A(8,7,11) 109.3363 -DE/DX = 0.0 !

! A22 A(7,8,9) 107.5139 -DE/DX = 0.0 !

! A23 A(7,8,32) 126.18 -DE/DX = 0.0 !

! A24 A(9,8,32) 126.18 -DE/DX = 0.0 !

! A25 A(8,9,10) 109.3363 -DE/DX = 0.0 !

! A26 A(8,9,33) 125.5229 -DE/DX = 0.0 !

! A27 A(10,9,33) 125.1365 -DE/DX = 0.0 !

! A28 A(9,10,11) 106.9066 -DE/DX = 0.0 !

! A29 A(9,10,26) 125.5108 -DE/DX = 0.0 !

! A30 A(11,10,26) 127.5819 -DE/DX = 0.0 !

! A31 A(7,11,10) 106.9066 -DE/DX = 0.0 !

! A32 A(7,11,27) 125.5108 -DE/DX = 0.0 !

! A33 A(10,11,27) 127.5819 -DE/DX = 0.0 !

! A34 A(2,12,13) 126.4847 -DE/DX = 0.0 !

! A35 A(2,12,35) 116.7555 -DE/DX = 0.0 !

! A36 A(13,12,35) 116.7555 -DE/DX = 0.0 !

! A37 A(12,13,14) 125.1365 -DE/DX = 0.0 !

! A38 A(12,13,17) 125.5229 -DE/DX = 0.0 !

! A39 A(14,13,17) 109.3363 -DE/DX = 0.0 !

! A40 A(13,14,15) 106.9066 -DE/DX = 0.0 !

! A41 A(13,14,28) 125.5108 -DE/DX = 0.0 !

! A42 A(15,14,28) 127.5819 -DE/DX = 0.0 !

! A43 A(14,15,16) 106.9066 -DE/DX = 0.0 !

! A44 A(14,15,29) 127.5819 -DE/DX = 0.0 !

! A45 A(16,15,29) 125.5108 -DE/DX = 0.0 !

! A46 A(15,16,17) 109.3363 -DE/DX = 0.0 !

! A47 A(15,16,18) 125.1365 -DE/DX = 0.0 !

! A48 A(17,16,18) 125.5229 -DE/DX = 0.0 !

! A49 A(13,17,16) 107.5139 -DE/DX = 0.0 !

! A50 A(13,17,32) 126.18 -DE/DX = 0.0 !

! A51 A(16,17,32) 126.18 -DE/DX = 0.0 !

! A52 A(16,18,19) 126.4847 -DE/DX = 0.0 !

! A53 A(16,18,40) 116.7555 -DE/DX = 0.0 !

! A54 A(19,18,40) 116.7555 -DE/DX = 0.0 !

! A55 A(18,19,20) 125.1365 -DE/DX = 0.0 !

! A56 A(18,19,23) 125.5229 -DE/DX = 0.0 !

! A57 A(20,19,23) 109.3363 -DE/DX = 0.0 !

! A58 A(19,20,21) 106.9066 -DE/DX = 0.0 !

! A59 A(19,20,30) 125.5108 -DE/DX = 0.0 !

! A60 A(21,20,30) 127.5819 -DE/DX = 0.0 !

! A61 A(20,21,22) 106.9066 -DE/DX = 0.0 !

! A62 A(20,21,31) 127.5819 -DE/DX = 0.0 !

! A63 A(22,21,31) 125.5108 -DE/DX = 0.0 !

! A64 A(21,22,23) 109.3363 -DE/DX = 0.0 !

! A65 A(21,22,33) 125.1365 -DE/DX = 0.0 !

! A66 A(23,22,33) 125.5229 -DE/DX = 0.0 !

! A67 A(19,23,22) 107.5139 -DE/DX = 0.0 !

! A68 A(19,23,32) 126.18 -DE/DX = 0.0 !

! A69 A(22,23,32) 126.18 -DE/DX = 0.0 !

! A70 A(3,32,8) 89.609 -DE/DX = 0.0 !

! A71 A(3,32,17) 89.609 -DE/DX = 0.0 !

! A72 A(3,32,23) 170.5231 -DE/DX = 0.0 !

! A73 A(8,32,17) 170.5231 -DE/DX = 0.0 !

! A74 A(8,32,23) 89.609 -DE/DX = 0.0 !

! A75 A(17,32,23) 89.609 -DE/DX = 0.0 !

! A76 A(9,33,22) 126.4847 -DE/DX = 0.0 !

! A77 A(9,33,34) 116.7555 -DE/DX = 0.0 !

! A78 A(22,33,34) 116.7555 -DE/DX = 0.0 !

! A79 L(33,34,36,26,-1) 179.9973 -DE/DX = 0.0 !

! A80 L(12,35,37,24,-1) 179.9973 -DE/DX = 0.0 !

! A81 L(34,36,43,26,-1) 180.0017 -DE/DX = 0.0 !

! A82 L(35,37,45,24,-1) 180.0017 -DE/DX = 0.0 !

! A83 L(6,38,39,25,-1) 179.9973 -DE/DX = 0.0 !

! A84 L(38,39,44,25,-1) 180.0017 -DE/DX = 0.0 !

! A85 L(18,40,41,29,-1) 179.9973 -DE/DX = 0.0 !

! A86 L(40,41,42,29,-1) 180.0017 -DE/DX = 0.0 !

! A87 L(33,34,36,26,-2) 179.7801 -DE/DX = 0.0 !

! A88 L(12,35,37,24,-2) 180.2199 -DE/DX = 0.0 !

! A89 L(34,36,43,26,-2) 180.1609 -DE/DX = 0.0 !

! A90 L(35,37,45,24,-2) 179.8391 -DE/DX = 0.0 !

! A91 L(6,38,39,25,-2) 179.7801 -DE/DX = 0.0 !

! A92 L(38,39,44,25,-2) 180.1609 -DE/DX = 0.0 !

! A93 L(18,40,41,29,-2) 180.2199 -DE/DX = 0.0 !

! A94 L(40,41,42,29,-2) 179.8391 -DE/DX = 0.0 !

! D1 D(5,1,2,3) -0.0972 -DE/DX = 0.0 !

! D2 D(5,1,2,12) 179.1882 -DE/DX = 0.0 !

! D3 D(24,1,2,3) -179.8008 -DE/DX = 0.0 !

! D4 D(24,1,2,12) -0.5153 -DE/DX = 0.0 !

! D5 D(2,1,5,4) 0.0 -DE/DX = 0.0 !

! D6 D(2,1,5,25) -179.6955 -DE/DX = 0.0 !

! D7 D(24,1,5,4) 179.6955 -DE/DX = 0.0 !

! D8 D(24,1,5,25) 0.0 -DE/DX = 0.0 !

! D9 D(1,2,3,4) 0.1573 -DE/DX = 0.0 !

! D10 D(1,2,3,32) -175.9517 -DE/DX = 0.0 !

! D11 D(12,2,3,4) -179.1247 -DE/DX = 0.0 !

! D12 D(12,2,3,32) 4.7663 -DE/DX = 0.0 !

! D13 D(1,2,12,13) -178.5823 -DE/DX = 0.0 !

! D14 D(1,2,12,35) 0.638 -DE/DX = 0.0 !

! D15 D(3,2,12,13) 0.5893 -DE/DX = 0.0 !

! D16 D(3,2,12,35) 179.8095 -DE/DX = 0.0 !

! D17 D(2,3,4,5) -0.1573 -DE/DX = 0.0 !

! D18 D(2,3,4,6) 179.1247 -DE/DX = 0.0 !

! D19 D(32,3,4,5) 175.9517 -DE/DX = 0.0 !

! D20 D(32,3,4,6) -4.7663 -DE/DX = 0.0 !

! D21 D(2,3,32,8) -177.5769 -DE/DX = 0.0 !

! D22 D(2,3,32,17) -7.0216 -DE/DX = 0.0 !

! D23 D(2,3,32,23) -92.2992 -DE/DX = 0.0 !

! D24 D(4,3,32,8) 7.0216 -DE/DX = 0.0 !

! D25 D(4,3,32,17) 177.5769 -DE/DX = 0.0 !

! D26 D(4,3,32,23) 92.2992 -DE/DX = 0.0 !

! D27 D(3,4,5,1) 0.0972 -DE/DX = 0.0 !

! D28 D(3,4,5,25) 179.8008 -DE/DX = 0.0 !

! D29 D(6,4,5,1) -179.1882 -DE/DX = 0.0 !

! D30 D(6,4,5,25) 0.5153 -DE/DX = 0.0 !

! D31 D(3,4,6,7) -0.5893 -DE/DX = 0.0 !

! D32 D(3,4,6,38) -179.8095 -DE/DX = 0.0 !

! D33 D(5,4,6,7) 178.5823 -DE/DX = 0.0 !

! D34 D(5,4,6,38) -0.638 -DE/DX = 0.0 !

! D35 D(4,6,7,8) 0.5893 -DE/DX = 0.0 !

! D36 D(4,6,7,11) -178.5823 -DE/DX = 0.0 !

! D37 D(38,6,7,8) 179.8095 -DE/DX = 0.0 !

! D38 D(38,6,7,11) 0.638 -DE/DX = 0.0 !

! D39 D(6,7,8,9) -179.1247 -DE/DX = 0.0 !

! D40 D(6,7,8,32) 4.7663 -DE/DX = 0.0 !

! D41 D(11,7,8,9) 0.1573 -DE/DX = 0.0 !

! D42 D(11,7,8,32) -175.9517 -DE/DX = 0.0 !

! D43 D(6,7,11,10) 179.1882 -DE/DX = 0.0 !

! D44 D(6,7,11,27) -0.5153 -DE/DX = 0.0 !

! D45 D(8,7,11,10) -0.0972 -DE/DX = 0.0 !

! D46 D(8,7,11,27) -179.8008 -DE/DX = 0.0 !

! D47 D(7,8,9,10) -0.1573 -DE/DX = 0.0 !

! D48 D(7,8,9,33) 179.1247 -DE/DX = 0.0 !

! D49 D(32,8,9,10) 175.9517 -DE/DX = 0.0 !

! D50 D(32,8,9,33) -4.7663 -DE/DX = 0.0 !

! D51 D(7,8,32,3) -7.0216 -DE/DX = 0.0 !

! D52 D(7,8,32,17) -92.2992 -DE/DX = 0.0 !

! D53 D(7,8,32,23) -177.5769 -DE/DX = 0.0 !

! D54 D(9,8,32,3) 177.5769 -DE/DX = 0.0 !

! D55 D(9,8,32,17) 92.2992 -DE/DX = 0.0 !

! D56 D(9,8,32,23) 7.0216 -DE/DX = 0.0 !

! D57 D(8,9,10,11) 0.0972 -DE/DX = 0.0 !

! D58 D(8,9,10,26) 179.8008 -DE/DX = 0.0 !

! D59 D(33,9,10,11) -179.1882 -DE/DX = 0.0 !

! D60 D(33,9,10,26) 0.5153 -DE/DX = 0.0 !

! D61 D(8,9,33,22) -0.5893 -DE/DX = 0.0 !

! D62 D(8,9,33,34) -179.8095 -DE/DX = 0.0 !

! D63 D(10,9,33,22) 178.5823 -DE/DX = 0.0 !

! D64 D(10,9,33,34) -0.638 -DE/DX = 0.0 !

! D65 D(9,10,11,7) 0.0 -DE/DX = 0.0 !

! D66 D(9,10,11,27) 179.6955 -DE/DX = 0.0 !

! D67 D(26,10,11,7) -179.6955 -DE/DX = 0.0 !

! D68 D(26,10,11,27) 0.0 -DE/DX = 0.0 !

! D69 D(2,12,13,14) 178.5823 -DE/DX = 0.0 !

! D70 D(2,12,13,17) -0.5893 -DE/DX = 0.0 !

! D71 D(35,12,13,14) -0.638 -DE/DX = 0.0 !

! D72 D(35,12,13,17) -179.8095 -DE/DX = 0.0 !

! D73 D(12,13,14,15) -179.1882 -DE/DX = 0.0 !

! D74 D(12,13,14,28) 0.5153 -DE/DX = 0.0 !

! D75 D(17,13,14,15) 0.0972 -DE/DX = 0.0 !

! D76 D(17,13,14,28) 179.8008 -DE/DX = 0.0 !

! D77 D(12,13,17,16) 179.1247 -DE/DX = 0.0 !

! D78 D(12,13,17,32) -4.7663 -DE/DX = 0.0 !

! D79 D(14,13,17,16) -0.1573 -DE/DX = 0.0 !

! D80 D(14,13,17,32) 175.9517 -DE/DX = 0.0 !

! D81 D(13,14,15,16) 0.0 -DE/DX = 0.0 !

! D82 D(13,14,15,29) 179.6955 -DE/DX = 0.0 !

! D83 D(28,14,15,16) -179.6955 -DE/DX = 0.0 !

! D84 D(28,14,15,29) 0.0 -DE/DX = 0.0 !

! D85 D(14,15,16,17) -0.0972 -DE/DX = 0.0 !

! D86 D(14,15,16,18) 179.1882 -DE/DX = 0.0 !

! D87 D(29,15,16,17) -179.8008 -DE/DX = 0.0 !

! D88 D(29,15,16,18) -0.5153 -DE/DX = 0.0 !

! D89 D(15,16,17,13) 0.1573 -DE/DX = 0.0 !

! D90 D(15,16,17,32) -175.9517 -DE/DX = 0.0 !

! D91 D(18,16,17,13) -179.1247 -DE/DX = 0.0 !

! D92 D(18,16,17,32) 4.7663 -DE/DX = 0.0 !

! D93 D(15,16,18,19) -178.5823 -DE/DX = 0.0 !

! D94 D(15,16,18,40) 0.638 -DE/DX = 0.0 !

! D95 D(17,16,18,19) 0.5893 -DE/DX = 0.0 !

! D96 D(17,16,18,40) 179.8095 -DE/DX = 0.0 !

! D97 D(13,17,32,3) 7.0216 -DE/DX = 0.0 !

! D98 D(13,17,32,8) 92.2992 -DE/DX = 0.0 !

! D99 D(13,17,32,23) 177.5769 -DE/DX = 0.0 !

! D100 D(16,17,32,3) -177.5769 -DE/DX = 0.0 !

! D101 D(16,17,32,8) -92.2992 -DE/DX = 0.0 !

! D102 D(16,17,32,23) -7.0216 -DE/DX = 0.0 !

! D103 D(16,18,19,20) 178.5823 -DE/DX = 0.0 !

! D104 D(16,18,19,23) -0.5893 -DE/DX = 0.0 !

! D105 D(40,18,19,20) -0.638 -DE/DX = 0.0 !

! D106 D(40,18,19,23) -179.8095 -DE/DX = 0.0 !

! D107 D(18,19,20,21) -179.1882 -DE/DX = 0.0 !

! D108 D(18,19,20,30) 0.5153 -DE/DX = 0.0 !

! D109 D(23,19,20,21) 0.0972 -DE/DX = 0.0 !

! D110 D(23,19,20,30) 179.8008 -DE/DX = 0.0 !

! D111 D(18,19,23,22) 179.1247 -DE/DX = 0.0 !

! D112 D(18,19,23,32) -4.7663 -DE/DX = 0.0 !

! D113 D(20,19,23,22) -0.1573 -DE/DX = 0.0 !

! D114 D(20,19,23,32) 175.9517 -DE/DX = 0.0 !

! D115 D(19,20,21,22) 0.0 -DE/DX = 0.0 !

! D116 D(19,20,21,31) 179.6955 -DE/DX = 0.0 !

! D117 D(30,20,21,22) -179.6955 -DE/DX = 0.0 !

! D118 D(30,20,21,31) 0.0 -DE/DX = 0.0 !

! D119 D(20,21,22,23) -0.0972 -DE/DX = 0.0 !

! D120 D(20,21,22,33) 179.1882 -DE/DX = 0.0 !

! D121 D(31,21,22,23) -179.8008 -DE/DX = 0.0 !

! D122 D(31,21,22,33) -0.5153 -DE/DX = 0.0 !

! D123 D(21,22,23,19) 0.1573 -DE/DX = 0.0 !

! D124 D(21,22,23,32) -175.9517 -DE/DX = 0.0 !

! D125 D(33,22,23,19) -179.1247 -DE/DX = 0.0 !

! D126 D(33,22,23,32) 4.7663 -DE/DX = 0.0 !

! D127 D(21,22,33,9) -178.5823 -DE/DX = 0.0 !

! D128 D(21,22,33,34) 0.638 -DE/DX = 0.0 !

! D129 D(23,22,33,9) 0.5893 -DE/DX = 0.0 !

! D130 D(23,22,33,34) 179.8095 -DE/DX = 0.0 !

! D131 D(19,23,32,3) 92.2992 -DE/DX = 0.0 !

! D132 D(19,23,32,8) 177.5769 -DE/DX = 0.0 !

! D133 D(19,23,32,17) 7.0216 -DE/DX = 0.0 !

! D134 D(22,23,32,3) -92.2992 -DE/DX = 0.0 !

! D135 D(22,23,32,8) -7.0216 -DE/DX = 0.0 !

! D136 D(22,23,32,17) -177.5769 -DE/DX = 0.0 !

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

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Largest change from initial coordinates is atom 44 5.481 Angstoms.

Leave Link 103 at Fri Jul 26 14:24:33 2019, MaxMem= 1342177280 cpu: 1.1

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.681163 4.273295 -0.039628

2 6 0 1.101995 2.889186 -0.004749

3 7 0 0.000000 2.081690 0.017787

4 6 0 -1.101995 2.889186 -0.004749

5 6 0 -0.681163 4.273295 -0.039628

6 6 0 -2.446135 2.446135 -0.009987

7 6 0 -2.889186 1.101995 -0.004749

8 7 0 -2.081690 0.000000 0.017787

9 6 0 -2.889186 -1.101995 -0.004749

10 6 0 -4.273295 -0.681163 -0.039628

11 6 0 -4.273295 0.681163 -0.039628

12 6 0 2.446135 2.446135 -0.009987

13 6 0 2.889186 1.101995 -0.004749

14 6 0 4.273295 0.681163 -0.039628

15 6 0 4.273295 -0.681163 -0.039628

16 6 0 2.889186 -1.101995 -0.004749

17 7 0 2.081690 0.000000 0.017787

18 6 0 2.446135 -2.446135 -0.009987

19 6 0 1.101995 -2.889186 -0.004749

20 6 0 0.681163 -4.273295 -0.039628

21 6 0 -0.681163 -4.273295 -0.039628

22 6 0 -1.101995 -2.889186 -0.004749

23 7 0 0.000000 -2.081690 0.017787

24 1 0 1.339682 5.128561 -0.065729

25 1 0 -1.339682 5.128561 -0.065729

26 1 0 -5.128561 -1.339682 -0.065729

27 1 0 -5.128561 1.339682 -0.065729

28 1 0 5.128561 1.339682 -0.065729

29 1 0 5.128561 -1.339682 -0.065729

30 1 0 1.339682 -5.128561 -0.065729

31 1 0 -1.339682 -5.128561 -0.065729

32 30 0 0.000000 0.000000 0.190341

33 6 0 -2.446135 -2.446135 -0.009987

34 6 0 -3.454989 -3.454989 -0.039056

35 6 0 3.454989 3.454989 -0.039056

36 6 0 -4.307371 -4.307371 -0.068214

37 6 0 4.307371 4.307371 -0.068214

38 6 0 -3.454989 3.454989 -0.039056

39 6 0 -4.307371 4.307371 -0.068214

40 6 0 3.454989 -3.454989 -0.039056

41 6 0 4.307371 -4.307371 -0.068214

42 1 0 5.061915 -5.061915 -0.091417

43 1 0 -5.061915 -5.061915 -0.091417

44 1 0 -5.061915 5.061915 -0.091417

45 1 0 5.061915 5.061915 -0.091417

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.447091 0.000000

3 N 2.295737 1.366364 0.000000

4 C 2.257571 2.203990 1.366364 0.000000

5 C 1.362327 2.257571 2.295737 1.447091 0.000000

6 C 3.622069 3.575688 2.473290 1.415286 2.540574

7 C 4.775537 4.373052 3.050854 2.527470 3.864418

8 N 5.088979 4.299274 2.943955 3.050854 4.497313

9 C 6.453089 5.644383 4.299274 4.373052 5.811224

10 C 7.006662 6.453089 5.088979 4.775537 6.119645

11 C 6.119645 5.811224 4.497313 3.864418 5.080041

12 C 2.540574 1.415286 2.473290 3.575688 3.622069

13 C 3.864418 2.527470 3.050854 4.373052 4.775537

14 C 5.080041 3.864418 4.497313 5.811224 6.119645

15 C 6.119645 4.775537 5.088979 6.453089 7.006662

16 C 5.811224 4.373052 4.299274 5.644383 6.453089

17 N 4.497313 3.050854 2.943955 4.299274 5.088979

18 C 6.947426 5.502035 5.146411 6.407410 7.411586

19 C 7.174918 5.778373 5.091613 6.184429 7.381193

20 C 8.546589 7.174918 6.391644 7.381193 8.654486

21 C 8.654486 7.381193 6.391644 7.174918 8.546589

22 C 7.381193 6.184429 5.091613 5.778373 7.174918

23 N 6.391644 5.091613 4.163381 5.091613 6.391644

24 H 1.079726 2.252779 3.329436 3.313654 2.194534

25 H 2.194534 3.313654 3.329436 2.252779 1.079726

26 H 8.078310 7.530397 6.165623 5.839545 7.161392

27 H 6.508430 6.420632 5.182633 4.314848 5.327861

28 H 5.327861 4.314848 5.182633 6.420632 6.508430

29 H 7.161392 5.839545 6.165623 7.530397 8.078310

30 H 9.424925 8.021501 7.334129 8.381514 9.616620

31 H 9.616620 8.381514 7.334129 8.021501 9.424925

32 Zn 4.333349 3.098363 2.088830 3.098363 4.333349

33 C 7.411586 6.407410 5.146411 5.502035 6.947426

34 C 8.765508 7.811264 6.526485 6.766559 8.210997

35 C 2.892012 2.420308 3.718350 4.592104 4.216323

36 C 9.925428 9.003095 7.705904 7.878382 9.315473

37 C 3.626481 3.505669 4.849175 5.592542 4.988733

38 C 4.216323 4.592104 3.718350 2.420308 2.892012

39 C 4.988733 5.592542 4.849175 3.505669 3.626481

40 C 8.210997 6.766559 6.526485 7.811264 8.765508

41 C 9.315473 7.878382 7.705904 9.003095 9.925428

42 H 10.312120 8.883046 8.755913 10.060881 10.960464

43 H 10.960464 10.060881 8.755913 8.883046 10.312120

44 H 5.797203 6.536211 5.875088 4.517658 4.451471

45 H 4.451471 4.517658 5.875088 6.536211 5.797203

6 7 8 9 10

6 C 0.000000

7 C 1.415286 0.000000

8 N 2.473290 1.366364 0.000000

9 C 3.575688 2.203990 1.366364 0.000000

10 C 3.622069 2.257571 2.295737 1.447091 0.000000

11 C 2.540574 1.447091 2.295737 2.257571 1.362327

12 C 4.892269 5.502035 5.146411 6.407410 7.411586

13 C 5.502035 5.778373 5.091613 6.184429 7.381193

14 C 6.947426 7.174918 6.391644 7.381193 8.654486

15 C 7.411586 7.381193 6.391644 7.174918 8.546589

16 C 6.407410 6.184429 5.091613 5.778373 7.174918

17 N 5.146411 5.091613 4.163381 5.091613 6.391644

18 C 6.918714 6.407410 5.146411 5.502035 6.947426

19 C 6.407410 5.644383 4.299274 4.373052 5.811224

20 C 7.411586 6.453089 5.088979 4.775537 6.119645

21 C 6.947426 5.811224 4.497313 3.864418 5.080041

22 C 5.502035 4.373052 3.050854 2.527470 3.864418

23 N 5.146411 4.299274 2.943955 3.050854 4.497313

24 H 4.640143 5.839545 6.165623 7.530397 8.078310

25 H 2.902198 4.314848 5.182633 6.420632 6.508430

26 H 4.640143 3.313654 3.329436 2.252779 1.079726

27 H 2.902198 2.252779 3.329436 3.313654 2.194534

28 H 7.655283 8.021501 7.334129 8.381514 9.616620

29 H 8.468266 8.381514 7.334129 8.021501 9.424925

30 H 8.468266 7.530397 6.165623 5.839545 7.161392

31 H 7.655283 6.420632 5.182633 4.314848 5.327861

32 Zn 3.465152 3.098363 2.088830 3.098363 4.333349

33 C 4.892269 3.575688 2.473290 1.415286 2.540574

34 C 5.986810 4.592104 3.718350 2.420308 2.892012

35 C 5.986810 6.766559 6.526485 7.811264 8.765508

36 C 7.005529 5.592542 4.849175 3.505669 3.626481

37 C 7.005529 7.878382 7.705904 9.003095 9.925428

38 C 1.427032 2.420308 3.718350 4.592104 4.216323

39 C 2.632830 3.505669 4.849175 5.592542 4.988733

40 C 8.345500 7.811264 6.526485 6.766559 8.210997

41 C 9.551077 9.003095 7.705904 7.878382 9.315473

42 H 10.618298 10.060881 8.755913 8.883046 10.312120

43 H 7.951085 6.536211 5.875088 4.517658 4.451471

44 H 3.700169 4.517658 5.875088 6.536211 5.797203

45 H 7.951085 8.883046 8.755913 10.060881 10.960464

11 12 13 14 15

11 C 0.000000

12 C 6.947426 0.000000

13 C 7.174918 1.415286 0.000000

14 C 8.546589 2.540574 1.447091 0.000000

15 C 8.654486 3.622069 2.257571 1.362327 0.000000

16 C 7.381193 3.575688 2.203990 2.257571 1.447091

17 N 6.391644 2.473290 1.366364 2.295737 2.295737

18 C 7.411586 4.892269 3.575688 3.622069 2.540574

19 C 6.453089 5.502035 4.373052 4.775537 3.864418

20 C 7.006662 6.947426 5.811224 6.119645 5.080041

21 C 6.119645 7.411586 6.453089 7.006662 6.119645

22 C 4.775537 6.407410 5.644383 6.453089 5.811224

23 N 5.088979 5.146411 4.299274 5.088979 4.497313

24 H 7.161392 2.902198 4.314848 5.327861 6.508430

25 H 5.327861 4.640143 5.839545 7.161392 8.078310

26 H 2.194534 8.468266 8.381514 9.616620 9.424925

27 H 1.079726 7.655283 8.021501 9.424925 9.616620

28 H 9.424925 2.902198 2.252779 1.079726 2.194534

29 H 9.616620 4.640143 3.313654 2.194534 1.079726

30 H 8.078310 7.655283 6.420632 6.508430 5.327861

31 H 6.508430 8.468266 7.530397 8.078310 7.161392

32 Zn 4.333349 3.465152 3.098363 4.333349 4.333349

33 C 3.622069 6.918714 6.407410 7.411586 6.947426

34 C 4.216323 8.345500 7.811264 8.765508 8.210997

35 C 8.210997 1.427032 2.420308 2.892012 4.216323

36 C 4.988733 9.551077 9.003095 9.925428 9.315473

37 C 9.315473 2.632830 3.505669 3.626481 4.988733

38 C 2.892012 5.986810 6.766559 8.210997 8.765508

39 C 3.626481 7.005529 7.878382 9.315473 9.925428

40 C 8.765508 5.986810 4.592104 4.216323 2.892012

41 C 9.925428 7.005529 5.592542 4.988733 3.626481

42 H 10.960464 7.951085 6.536211 5.797203 4.451471

43 H 5.797203 10.618298 10.060881 10.960464 10.312120

44 H 4.451471 7.951085 8.883046 10.312120 10.960464

45 H 10.312120 3.700169 4.517658 4.451471 5.797203

16 17 18 19 20

16 C 0.000000

17 N 1.366364 0.000000

18 C 1.415286 2.473290 0.000000

19 C 2.527470 3.050854 1.415286 0.000000

20 C 3.864418 4.497313 2.540574 1.447091 0.000000

21 C 4.775537 5.088979 3.622069 2.257571 1.362327

22 C 4.373052 4.299274 3.575688 2.203990 2.257571

23 N 3.050854 2.943955 2.473290 1.366364 2.295737

24 H 6.420632 5.182633 7.655283 8.021501 9.424925

25 H 7.530397 6.165623 8.468266 8.381514 9.616620

26 H 8.021501 7.334129 7.655283 6.420632 6.508430

27 H 8.381514 7.334129 8.468266 7.530397 8.078310

28 H 3.313654 3.329436 4.640143 5.839545 7.161392

29 H 2.252779 3.329436 2.902198 4.314848 5.327861

30 H 4.314848 5.182633 2.902198 2.252779 1.079726

31 H 5.839545 6.165623 4.640143 3.313654 2.194534

32 Zn 3.098363 2.088830 3.465152 3.098363 4.333349

33 C 5.502035 5.146411 4.892269 3.575688 3.622069

34 C 6.766559 6.526485 5.986810 4.592104 4.216323

35 C 4.592104 3.718350 5.986810 6.766559 8.210997

36 C 7.878382 7.705904 7.005529 5.592542 4.988733

37 C 5.592542 4.849175 7.005529 7.878382 9.315473

38 C 7.811264 6.526485 8.345500 7.811264 8.765508

39 C 9.003095 7.705904 9.551077 9.003095 9.925428

40 C 2.420308 3.718350 1.427032 2.420308 2.892012

41 C 3.505669 4.849175 2.632830 3.505669 3.626481

42 H 4.517658 5.875088 3.700169 4.517658 4.451471

43 H 8.883046 8.755913 7.951085 6.536211 5.797203

44 H 10.060881 8.755913 10.618298 10.060881 10.960464

45 H 6.536211 5.875088 7.951085 8.883046 10.312120

21 22 23 24 25

21 C 0.000000

22 C 1.447091 0.000000

23 N 2.295737 1.366364 0.000000

24 H 9.616620 8.381514 7.334129 0.000000

25 H 9.424925 8.021501 7.334129 2.679365 0.000000

26 H 5.327861 4.314848 5.182633 9.147477 7.496250

27 H 7.161392 5.839545 6.165623 7.496250 5.358283

28 H 8.078310 7.530397 6.165623 5.358283 7.496250

29 H 6.508430 6.420632 5.182633 7.496250 9.147477

30 H 2.194534 3.313654 3.329436 10.257122 10.601299

31 H 1.079726 2.252779 3.329436 10.601299 10.257122

32 Zn 4.333349 3.098363 2.088830 5.306831 5.306831

33 C 2.540574 1.415286 2.473290 8.468266 7.655283

34 C 2.892012 2.420308 3.718350 9.831933 8.840394

35 C 8.765508 7.811264 6.526485 2.697420 5.078428

36 C 3.626481 3.505669 4.849175 10.996638 9.891612

37 C 9.925428 9.003095 7.705904 3.079210 5.706450

38 C 8.210997 6.766559 6.526485 5.078428 2.697420

39 C 9.315473 7.878382 7.705904 5.706450 3.079210

40 C 4.216323 4.592104 3.718350 8.840394 9.831933

41 C 4.988733 5.592542 4.849175 9.891612 10.996638

42 H 5.797203 6.536211 5.875088 10.849031 12.034406

43 H 4.451471 4.517658 5.875088 12.034406 10.849031

44 H 10.312120 8.883046 8.755913 6.401996 3.722918

45 H 10.960464 10.060881 8.755913 3.722918 6.401996

26 27 28 29 30

26 H 0.000000

27 H 2.679365 0.000000

28 H 10.601299 10.257122 0.000000

29 H 10.257122 10.601299 2.679365 0.000000

30 H 7.496250 9.147477 7.496250 5.358283 0.000000

31 H 5.358283 7.496250 9.147477 7.496250 2.679365

32 Zn 5.306831 5.306831 5.306831 5.306831 5.306831

33 C 2.902198 4.640143 8.468266 7.655283 4.640143

34 C 2.697420 5.078428 9.831933 8.840394 5.078428

35 C 9.831933 8.840394 2.697420 5.078428 8.840394

36 C 3.079210 5.706450 10.996638 9.891612 5.706450

37 C 10.996638 9.891612 3.079210 5.706450 9.891612

38 C 5.078428 2.697420 8.840394 9.831933 9.831933

39 C 5.706450 3.079210 9.891612 10.996638 10.996638

40 C 8.840394 9.831933 5.078428 2.697420 2.697420

41 C 9.891612 10.996638 5.706450 3.079210 3.079210

42 H 10.849031 12.034406 6.401996 3.722918 3.722918

43 H 3.722918 6.401996 12.034406 10.849031 6.401996

44 H 6.401996 3.722918 10.849031 12.034406 12.034406

45 H 12.034406 10.849031 3.722918 6.401996 10.849031

31 32 33 34 35

31 H 0.000000

32 Zn 5.306831 0.000000

33 C 2.902198 3.465152 0.000000

34 C 2.697420 4.891474 1.427032 0.000000

35 C 9.831933 4.891474 8.345500 9.772185 0.000000

36 C 3.079210 6.097028 2.632830 1.205803 10.977674

37 C 10.996638 6.097028 9.551077 10.977674 1.205803

38 C 8.840394 4.891474 5.986810 6.909978 6.909978

39 C 9.891612 6.097028 7.005529 7.809074 7.809074

40 C 5.078428 4.891474 5.986810 6.909978 6.909978

41 C 5.706450 6.097028 7.005529 7.809074 7.809074

42 H 6.401996 7.164172 7.951085 8.667330 8.667330

43 H 3.722918 7.164172 3.700169 2.273140 12.044836

44 H 10.849031 7.164172 7.951085 8.667330 8.667330

45 H 12.034406 7.164172 10.618298 12.044836 2.273140

36 37 38 39 40

36 C 0.000000

37 C 12.183086 0.000000

38 C 7.809074 7.809074 0.000000

39 C 8.614743 8.614743 1.205803 0.000000

40 C 7.809074 7.809074 9.772185 10.977674 0.000000

41 C 8.614743 8.614743 10.977674 12.183086 1.205803

42 H 9.399649 9.399649 12.044836 13.250193 2.273140

43 H 1.067339 13.250193 8.667330 9.399649 8.667330

44 H 9.399649 9.399649 2.273140 1.067339 12.044836

45 H 13.250193 1.067339 8.667330 9.399649 8.667330

41 42 43 44 45

41 C 0.000000

42 H 1.067339 0.000000

43 H 9.399649 10.123831 0.000000

44 H 13.250193 14.317259 10.123831 0.000000

45 H 9.399649 10.123831 14.317259 10.123831 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

RotChk: IX=3 Diff= 0.00D+00

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681163 -4.273295 -0.041193

2 6 0 -1.101995 -2.889186 -0.006314

3 7 0 0.000000 -2.081690 0.016222

4 6 0 1.101995 -2.889186 -0.006314

5 6 0 0.681163 -4.273295 -0.041193

6 6 0 2.446135 -2.446135 -0.011552

7 6 0 2.889186 -1.101995 -0.006314

8 7 0 2.081690 0.000000 0.016222

9 6 0 2.889186 1.101995 -0.006314

10 6 0 4.273295 0.681163 -0.041193

11 6 0 4.273295 -0.681163 -0.041193

12 6 0 -2.446135 -2.446135 -0.011552

13 6 0 -2.889186 -1.101995 -0.006314

14 6 0 -4.273295 -0.681163 -0.041193

15 6 0 -4.273295 0.681163 -0.041193

16 6 0 -2.889186 1.101995 -0.006314

17 7 0 -2.081690 0.000000 0.016222

18 6 0 -2.446135 2.446135 -0.011552

19 6 0 -1.101995 2.889186 -0.006314

20 6 0 -0.681163 4.273295 -0.041193

21 6 0 0.681163 4.273295 -0.041193

22 6 0 1.101995 2.889186 -0.006314

23 7 0 0.000000 2.081690 0.016222

24 1 0 -1.339682 -5.128561 -0.067294

25 1 0 1.339682 -5.128561 -0.067294

26 1 0 5.128561 1.339682 -0.067294

27 1 0 5.128561 -1.339682 -0.067294

28 1 0 -5.128561 -1.339682 -0.067294

29 1 0 -5.128561 1.339682 -0.067294

30 1 0 -1.339682 5.128561 -0.067294

31 1 0 1.339682 5.128561 -0.067294

32 30 0 0.000000 0.000000 0.188776

33 6 0 2.446135 2.446135 -0.011552

34 6 0 3.454989 3.454989 -0.040621

35 6 0 -3.454989 -3.454989 -0.040621

36 6 0 4.307371 4.307371 -0.069779

37 6 0 -4.307371 -4.307371 -0.069779

38 6 0 3.454989 -3.454989 -0.040621

39 6 0 4.307371 -4.307371 -0.069779

40 6 0 -3.454989 3.454989 -0.040621

41 6 0 -4.307371 4.307371 -0.069779

42 1 0 -5.061915 5.061915 -0.092982

43 1 0 5.061915 5.061915 -0.092982

44 1 0 5.061915 -5.061915 -0.092982

45 1 0 -5.061915 -5.061915 -0.092982

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

Rotational constants (GHZ): 0.1465170 0.1465170 0.0733190

Leave Link 202 at Fri Jul 26 14:24:33 2019, MaxMem= 1342177280 cpu: 0.1

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

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

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

Population analysis using the SCF density.

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

Orbital symmetries:

Occupied (E) (E) (B2) (A1) (E) (E) (B1) (A1) (B2) (E) (E)

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

(E) (E) (A1) (A2) (E) (E) (B1) (B1) (E) (E) (A1)

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

(B2) (B1) (E) (E) (A2) (A1) (E) (E) (B1) (B1)

(B2) (E) (E) (B2) (A1) (E) (E) (B1) (A2) (A1)

(E) (E) (A1) (E) (E) (B1) (E) (E) (B2) (A1) (A2)

(E) (E) (A1) (B1) (A1) (E) (E) (E) (E) (B2) (B1)

(B2) (E) (E) (A2) (A1) (B1) (E) (E) (E) (E) (A1)

(B2) (E) (E) (A2) (B1) (E) (E) (B2) (A1) (B2)

(E) (E) (A2) (A1)

Virtual (E) (E) (B1) (A1) (B2) (E) (E) (B2) (B1) (A2)

(E) (E) (A1) (E) (E) (A1) (E) (E) (A2) (A1) (E)

(E) (B1) (B2) (A1) (E) (E) (B1) (E) (E) (A2) (A1)

(A1) (B1) (E) (E) (E) (E) (A1) (B1) (A1) (E) (E)

(B2) (A1) (B1) (E) (E) (E) (E) (B2) (A1) (B1)

(A2) (E) (E) (A1) (B1) (B2) (E) (E) (A1) (E) (E)

(B1) (E) (E) (E) (E) (B2) (B1) (A1) (A1) (A2)

(A2) (B2) (E) (E) (B1) (E) (E) (A1) (E) (E) (B1)

(E) (E) (B2) (A1) (A2) (B1) (E) (E) (E) (E) (A2)

(A1) (E) (E) (E) (E) (A2) (B1) (B2) (B2) (A1)

(E) (E) (B1) (A1) (E) (E) (E) (E) (E) (E) (A2)

(A1) (B1) (E) (E) (B1) (A1) (B2) (A1) (E) (E)

(B2) (E) (E) (B1) (A1) (A2) (E) (E) (A2) (E) (E)

(B2) (A2) (A1) (B1) (E) (E) (E) (E) (A1) (E) (E)

(B1) (E) (E) (B2) (A2) (E) (E) (B1) (B2) (B1)

(E) (E) (A1) (B1) (B2) (E) (E) (E) (E) (A1) (A2)

(A1) (A2) (B1) (A1) (E) (E) (B1) (E) (E) (B2)

(E) (E) (A2) (E) (E) (B1) (A1) (B2) (E) (E) (B2)

(A1) (E) (E) (B1) (A2) (B1) (E) (E) (B2) (E) (E)

(A1) (B1) (E) (E) (A1) (B2) (A1) (E) (E) (E) (E)

(A2) (B2) (A2) (E) (E) (B1) (A1) (E) (E) (A1)

(B1) (A2) (B2) (E) (E) (B1) (E) (E) (E) (E) (A2)

(B2) (A1) (B1) (E) (E) (A1) (A2) (B2) (E) (E)

(A1) (A1) (E) (E) (B1) (E) (E) (B2) (E) (E) (B2)

(E) (E) (A2) (A1) (B2) (B2) (E) (E) (E) (E) (A1)

(A2) (E) (E) (E) (E) (B1) (A1) (B1) (A2) (A1)

(E) (E) (E) (E) (B1) (A1) (B2) (B2) (B1) (E) (E)

(E) (E) (A1) (E) (E) (A2) (A2) (B1) (E) (E) (B2)

(A2) (E) (E) (B2) (B1) (E) (E) (A1) (A1) (A1)

(B1) (B1) (A2) (E) (E) (B2) (E) (E) (E) (E) (A1)

(A2) (B1) (E) (E) (E) (E) (B1) (E) (E) (B2) (A2)

(B2) (A2) (B1) (A1) (A1) (E) (E) (B1) (E) (E)

(E) (E) (A2) (A1) (B1) (E) (E) (B2) (E) (E) (E)

(E) (A1) (B1) (A2) (B1) (E) (E) (A1) (B1) (B2)

(A2) (E) (E) (E) (E) (A1) (B1) (B2) (E) (E) (A2)

(B2) (B2) (E) (E) (E) (E) (B1) (A1) (A1) (E) (E)

(A1) (A2) (E) (E) (A1) (B1) (E) (E) (A2) (B2)

(E) (E) (B1) (E) (E) (A1) (B2) (B1) (E) (E) (E)

(E) (A1) (B2) (E) (E) (A2) (A2) (A1) (A2) (E)

(E) (B2) (B1) (E) (E) (A1) (B1) (E) (E) (B1) (A1)

(B1) (B2) (E) (E) (B1) (E) (E) (A2) (E) (E) (B2)

(A1) (B1) (A1) (E) (E) (E) (E) (A2) (B2) (E) (E)

(A2) (A1) (E) (E) (B1) (E) (E) (A1) (A2) (B1)

(B1) (E) (E) (E) (E) (B2) (A1) (E) (E) (B2) (A1)

(E) (E) (B1) (A2) (A1) (E) (E) (B1) (B2) (A1)

(E) (E) (B2) (E) (E) (A2) (B1) (E) (E) (A2) (E)

(E) (A1) (B1) (B2) (A1) (A1) (E) (E) (B1) (A1)

(E) (E) (B2) (B1) (E) (E) (A1) (A2) (E) (E) (B2)

(B1) (E) (E) (A1) (B1) (E) (E) (A2) (B1) (A1)

(E) (E) (B2) (A1) (E) (E)

The electronic state is 1-A1.

Alpha occ. eigenvalues -- -14.31369 -14.31369 -14.31369 -14.31369 -10.22115

Alpha occ. eigenvalues -- -10.22115 -10.22115 -10.22115 -10.22110 -10.22110

Alpha occ. eigenvalues -- -10.22110 -10.22109 -10.21962 -10.21962 -10.21962

Alpha occ. eigenvalues -- -10.21962 -10.18473 -10.18473 -10.18473 -10.18473

Alpha occ. eigenvalues -- -10.17612 -10.17612 -10.17612 -10.17611 -10.17545

Alpha occ. eigenvalues -- -10.17545 -10.17545 -10.17545 -10.17333 -10.17333

Alpha occ. eigenvalues -- -10.17333 -10.17333 -0.97589 -0.96735 -0.96735

Alpha occ. eigenvalues -- -0.95831 -0.85157 -0.83124 -0.83124 -0.81112

Alpha occ. eigenvalues -- -0.77599 -0.77562 -0.77562 -0.77049 -0.75439

Alpha occ. eigenvalues -- -0.74799 -0.74799 -0.73048 -0.73025 -0.67757

Alpha occ. eigenvalues -- -0.67757 -0.62755 -0.60281 -0.60008 -0.59177

Alpha occ. eigenvalues -- -0.59177 -0.58232 -0.57363 -0.56212 -0.56212

Alpha occ. eigenvalues -- -0.55931 -0.55762 -0.55260 -0.55062 -0.55062

Alpha occ. eigenvalues -- -0.53251 -0.52447 -0.52447 -0.52236 -0.51480

Alpha occ. eigenvalues -- -0.51480 -0.50602 -0.49353 -0.46080 -0.45053

Alpha occ. eigenvalues -- -0.45053 -0.44349 -0.43325 -0.43009 -0.42835

Alpha occ. eigenvalues -- -0.42835 -0.41487 -0.41487 -0.40238 -0.40043

Alpha occ. eigenvalues -- -0.39143 -0.38491 -0.38491 -0.38157 -0.37979

Alpha occ. eigenvalues -- -0.37512 -0.34121 -0.34121 -0.32569 -0.32569

Alpha occ. eigenvalues -- -0.32438 -0.29690 -0.29375 -0.29375 -0.29046

Alpha occ. eigenvalues -- -0.27628 -0.26959 -0.26959 -0.26951 -0.26852

Alpha occ. eigenvalues -- -0.25593 -0.25264 -0.25264 -0.21127 -0.19948

Alpha virt. eigenvalues -- -0.10772 -0.10772 -0.05723 0.02329 0.02815

Alpha virt. eigenvalues -- 0.03136 0.03136 0.03186 0.03560 0.03713

Alpha virt. eigenvalues -- 0.04156 0.04156 0.04667 0.05001 0.05001

Alpha virt. eigenvalues -- 0.05435 0.05692 0.05692 0.06456 0.07825

Alpha virt. eigenvalues -- 0.08474 0.08474 0.08531 0.09705 0.09866

Alpha virt. eigenvalues -- 0.09871 0.09871 0.11480 0.12501 0.12501

Alpha virt. eigenvalues -- 0.13632 0.14222 0.15241 0.16423 0.16440

Alpha virt. eigenvalues -- 0.16440 0.17328 0.17328 0.19266 0.19859

Alpha virt. eigenvalues -- 0.22271 0.23139 0.23139 0.23594 0.24239

Alpha virt. eigenvalues -- 0.24325 0.24978 0.24978 0.25752 0.25752

Alpha virt. eigenvalues -- 0.26476 0.26631 0.26839 0.27939 0.29888

Alpha virt. eigenvalues -- 0.29888 0.30995 0.31128 0.32419 0.32471

Alpha virt. eigenvalues -- 0.32471 0.35157 0.35212 0.35212 0.35222

Alpha virt. eigenvalues -- 0.35666 0.35666 0.36252 0.36252 0.36464

Alpha virt. eigenvalues -- 0.36598 0.36980 0.37934 0.38490 0.39516

Alpha virt. eigenvalues -- 0.40000 0.40456 0.40456 0.40468 0.41370

Alpha virt. eigenvalues -- 0.41370 0.41511 0.42069 0.42069 0.43234

Alpha virt. eigenvalues -- 0.43587 0.43587 0.43666 0.44406 0.44572

Alpha virt. eigenvalues -- 0.45228 0.45651 0.45651 0.47278 0.47278

Alpha virt. eigenvalues -- 0.47752 0.48205 0.48965 0.48965 0.49457

Alpha virt. eigenvalues -- 0.49457 0.50757 0.51108 0.51274 0.51342

Alpha virt. eigenvalues -- 0.51740 0.51995 0.51995 0.52017 0.55011

Alpha virt. eigenvalues -- 0.56221 0.56221 0.57142 0.57142 0.57621

Alpha virt. eigenvalues -- 0.57621 0.57654 0.57724 0.58181 0.58795

Alpha virt. eigenvalues -- 0.58795 0.61353 0.62061 0.62106 0.62334

Alpha virt. eigenvalues -- 0.62351 0.62351 0.63163 0.63383 0.63383

Alpha virt. eigenvalues -- 0.63936 0.64321 0.64882 0.65267 0.65267

Alpha virt. eigenvalues -- 0.65349 0.68252 0.68252 0.68940 0.69020

Alpha virt. eigenvalues -- 0.69898 0.70189 0.70488 0.70488 0.71741

Alpha virt. eigenvalues -- 0.71741 0.73651 0.73721 0.73721 0.74453

Alpha virt. eigenvalues -- 0.74547 0.74547 0.74702 0.74883 0.75272

Alpha virt. eigenvalues -- 0.75272 0.77057 0.77762 0.79147 0.81252

Alpha virt. eigenvalues -- 0.81252 0.81780 0.82354 0.83203 0.84288

Alpha virt. eigenvalues -- 0.84288 0.85799 0.85799 0.85831 0.88301

Alpha virt. eigenvalues -- 0.89968 0.90758 0.91080 0.91320 0.92713

Alpha virt. eigenvalues -- 0.92713 0.94800 0.95712 0.95712 0.95988

Alpha virt. eigenvalues -- 0.97562 0.97562 0.99754 1.00368 1.00368

Alpha virt. eigenvalues -- 1.00855 1.01435 1.01506 1.02202 1.02202

Alpha virt. eigenvalues -- 1.04674 1.05361 1.05555 1.05555 1.06079

Alpha virt. eigenvalues -- 1.07063 1.07160 1.08818 1.08818 1.11556

Alpha virt. eigenvalues -- 1.12268 1.12268 1.12448 1.12486 1.13384

Alpha virt. eigenvalues -- 1.13384 1.13737 1.13900 1.14208 1.15299

Alpha virt. eigenvalues -- 1.15299 1.16299 1.16299 1.16772 1.17345

Alpha virt. eigenvalues -- 1.18291 1.18757 1.18757 1.19175 1.19321

Alpha virt. eigenvalues -- 1.20995 1.20995 1.21156 1.21171 1.22270

Alpha virt. eigenvalues -- 1.23621 1.24722 1.24722 1.25221 1.25864

Alpha virt. eigenvalues -- 1.25864 1.28049 1.28049 1.28443 1.29010

Alpha virt. eigenvalues -- 1.31357 1.32191 1.34067 1.34067 1.34239

Alpha virt. eigenvalues -- 1.37469 1.42229 1.42690 1.42690 1.47389

Alpha virt. eigenvalues -- 1.47634 1.48556 1.48556 1.49560 1.51757

Alpha virt. eigenvalues -- 1.51757 1.52788 1.55154 1.55154 1.55336

Alpha virt. eigenvalues -- 1.55386 1.55386 1.55419 1.56945 1.57633

Alpha virt. eigenvalues -- 1.58167 1.58482 1.58482 1.58932 1.58932

Alpha virt. eigenvalues -- 1.59450 1.61056 1.61544 1.61544 1.62882

Alpha virt. eigenvalues -- 1.62882 1.63251 1.64325 1.65036 1.65594

Alpha virt. eigenvalues -- 1.66246 1.66583 1.66583 1.70017 1.70017

Alpha virt. eigenvalues -- 1.72123 1.72662 1.73685 1.75128 1.76873

Alpha virt. eigenvalues -- 1.76982 1.76982 1.78961 1.78961 1.79362

Alpha virt. eigenvalues -- 1.80018 1.80018 1.80079 1.80733 1.81194

Alpha virt. eigenvalues -- 1.84079 1.84079 1.85428 1.86277 1.87712

Alpha virt. eigenvalues -- 1.87712 1.88534 1.88641 1.89401 1.89401

Alpha virt. eigenvalues -- 1.89526 1.90049 1.90700 1.93421 1.94385

Alpha virt. eigenvalues -- 1.94504 1.94682 1.94682 1.94750 1.95757

Alpha virt. eigenvalues -- 1.95757 1.97368 1.97368 1.99099 1.99859

Alpha virt. eigenvalues -- 2.00617 2.03248 2.03248 2.04267 2.04267

Alpha virt. eigenvalues -- 2.04275 2.09215 2.09215 2.11643 2.11703

Alpha virt. eigenvalues -- 2.13725 2.18046 2.19806 2.25706 2.26961

Alpha virt. eigenvalues -- 2.27870 2.27870 2.28395 2.31370 2.31370

Alpha virt. eigenvalues -- 2.33508 2.33508 2.34669 2.35954 2.36261

Alpha virt. eigenvalues -- 2.36527 2.36527 2.37540 2.40594 2.40594

Alpha virt. eigenvalues -- 2.40748 2.40748 2.41097 2.41410 2.43138

Alpha virt. eigenvalues -- 2.45429 2.48456 2.48456 2.49408 2.49994

Alpha virt. eigenvalues -- 2.52320 2.53379 2.53964 2.53964 2.56228

Alpha virt. eigenvalues -- 2.56228 2.57032 2.57451 2.57739 2.57991

Alpha virt. eigenvalues -- 2.57991 2.60077 2.60560 2.61986 2.62502

Alpha virt. eigenvalues -- 2.62502 2.64689 2.64689 2.64719 2.66654

Alpha virt. eigenvalues -- 2.67614 2.71221 2.71221 2.73413 2.76570

Alpha virt. eigenvalues -- 2.78003 2.78003 2.79920 2.80961 2.82610

Alpha virt. eigenvalues -- 2.82610 2.83369 2.83883 2.87108 2.87108

Alpha virt. eigenvalues -- 2.88554 2.88580 2.88580 2.88617 2.92033

Alpha virt. eigenvalues -- 2.95166 2.95547 2.95547 2.96203 2.96203

Alpha virt. eigenvalues -- 2.97019 2.97823 2.98870 2.98870 2.99784

Alpha virt. eigenvalues -- 3.00241 3.01364 3.03009 3.03843 3.03843

Alpha virt. eigenvalues -- 3.04134 3.04463 3.05477 3.05477 3.06919

Alpha virt. eigenvalues -- 3.07898 3.08318 3.08318 3.09022 3.16978

Alpha virt. eigenvalues -- 3.17708 3.17929 3.18347 3.18347 3.21095

Alpha virt. eigenvalues -- 3.21681 3.21681 3.24246 3.25878 3.25878

Alpha virt. eigenvalues -- 3.28645 3.29945 3.30869 3.31621 3.32327

Alpha virt. eigenvalues -- 3.32327 3.33135 3.33135 3.35494 3.35724

Alpha virt. eigenvalues -- 3.37578 3.37578 3.44351 3.48402 3.52178

Alpha virt. eigenvalues -- 3.52178 3.52998 3.56926 3.56926 3.57171

Alpha virt. eigenvalues -- 3.57507 3.58659 3.62925 3.65470 3.65470

Alpha virt. eigenvalues -- 3.81935 3.81935 3.82132 3.84306 3.85904

Alpha virt. eigenvalues -- 3.85904 3.85979 3.89712 3.93137 3.93137

Alpha virt. eigenvalues -- 3.96707 3.99847 4.11459 4.20185 4.20185

Alpha virt. eigenvalues -- 4.32222 4.33336 4.46988 4.51348 4.51348

Alpha virt. eigenvalues -- 4.61463 4.65301 4.65301 4.65588 5.14284

Alpha virt. eigenvalues -- 5.19431 5.19431 5.32016 7.78665 7.78665

Alpha virt. eigenvalues -- 7.86755 7.92613 8.12981 11.11649 23.26999

Alpha virt. eigenvalues -- 23.32268 23.32268 23.35159 23.51644 23.54832

Alpha virt. eigenvalues -- 23.54832 23.56922 23.74598 23.76313 23.76313

Alpha virt. eigenvalues -- 23.78165 23.90765 23.93314 23.93314 23.95996

Alpha virt. eigenvalues -- 24.00276 24.01839 24.01839 24.02864 24.12630

Alpha virt. eigenvalues -- 24.13089 24.13089 24.13768 24.94111 24.94170

Alpha virt. eigenvalues -- 24.94485 24.94485 35.62586 35.64057 35.65236

Alpha virt. eigenvalues -- 35.65236

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 5.149059 0.403874 -0.077456 -0.062245 0.532933 0.014010

2 C 0.403874 4.873703 0.434511 -0.146366 -0.062245 -0.001304

3 N -0.077456 0.434511 6.953408 0.434511 -0.077456 -0.017626

4 C -0.062245 -0.146366 0.434511 4.873703 0.403874 0.406627

5 C 0.532933 -0.062245 -0.077456 0.403874 5.149059 -0.074407

6 C 0.014010 -0.001304 -0.017626 0.406627 -0.074407 5.211687

7 C -0.001244 -0.000385 -0.020679 -0.104649 0.012920 0.406627

8 N 0.000056 0.000450 -0.013160 -0.020679 -0.000357 -0.017626

9 C -0.000005 0.000001 0.000450 -0.000385 0.000046 -0.001304

10 C 0.000001 -0.000005 0.000056 -0.001244 -0.000006 0.014010

11 C -0.000006 0.000046 -0.000357 0.012920 -0.000158 -0.074407

12 C -0.074407 0.406627 -0.017626 -0.001304 0.014010 -0.002348

13 C 0.012920 -0.104649 -0.020679 -0.000385 -0.001244 0.000218

14 C -0.000158 0.012920 -0.000357 0.000046 -0.000006 0.000001

15 C -0.000006 -0.001244 0.000056 -0.000005 0.000001 0.000000

16 C 0.000046 -0.000385 0.000450 0.000001 -0.000005 0.000001

17 N -0.000357 -0.020679 -0.013160 0.000450 0.000056 -0.000176

18 C 0.000001 0.000218 -0.000176 0.000001 0.000000 0.000003

19 C 0.000000 -0.000065 0.000168 -0.000004 0.000000 0.000001

20 C 0.000000 0.000000 0.000002 0.000000 0.000000 0.000000

21 C 0.000000 0.000000 0.000002 0.000000 0.000000 0.000001

22 C 0.000000 -0.000004 0.000168 -0.000065 0.000000 0.000218

23 N 0.000002 0.000168 -0.001708 0.000168 0.000002 -0.000176

24 H 0.388265 -0.038191 0.005131 0.005560 -0.032996 -0.000165

25 H -0.032996 0.005560 0.005131 -0.038191 0.388265 -0.005200

26 H 0.000000 0.000000 0.000002 0.000010 0.000000 -0.000165

27 H 0.000000 0.000001 -0.000003 0.000009 0.000006 -0.005200

28 H 0.000006 0.000009 -0.000003 0.000001 0.000000 0.000000

29 H 0.000000 0.000010 0.000002 0.000000 0.000000 0.000000

30 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

31 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

32 Zn 0.002023 -0.014094 0.128946 -0.014094 0.002023 -0.011292

33 C 0.000000 0.000001 -0.000176 0.000218 0.000001 -0.002348

34 C 0.000000 0.000000 0.000000 0.000003 0.000000 -0.000056

35 C -0.014881 -0.075725 0.004290 -0.000520 0.002633 -0.000056

36 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

37 C -0.000558 -0.005172 -0.000051 -0.000051 0.000359 -0.000002

38 C 0.002633 -0.000520 0.004290 -0.075725 -0.014881 0.541474

39 C 0.000359 -0.000051 -0.000051 -0.005172 -0.000558 -0.105008

40 C 0.000000 0.000003 0.000000 0.000000 0.000000 0.000000

41 C 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 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000002 0.000000 0.000001 -0.000035 0.000096 0.001819

45 H 0.000096 -0.000035 0.000001 0.000000 0.000002 0.000000

7 8 9 10 11 12

1 C -0.001244 0.000056 -0.000005 0.000001 -0.000006 -0.074407

2 C -0.000385 0.000450 0.000001 -0.000005 0.000046 0.406627

3 N -0.020679 -0.013160 0.000450 0.000056 -0.000357 -0.017626

4 C -0.104649 -0.020679 -0.000385 -0.001244 0.012920 -0.001304

5 C 0.012920 -0.000357 0.000046 -0.000006 -0.000158 0.014010

6 C 0.406627 -0.017626 -0.001304 0.014010 -0.074407 -0.002348

7 C 4.873703 0.434511 -0.146366 -0.062245 0.403874 0.000218

8 N 0.434511 6.953408 0.434511 -0.077456 -0.077456 -0.000176

9 C -0.146366 0.434511 4.873703 0.403874 -0.062245 0.000001

10 C -0.062245 -0.077456 0.403874 5.149059 0.532933 0.000000

11 C 0.403874 -0.077456 -0.062245 0.532933 5.149059 0.000001

12 C 0.000218 -0.000176 0.000001 0.000000 0.000001 5.211687

13 C -0.000065 0.000168 -0.000004 0.000000 0.000000 0.406627

14 C 0.000000 0.000002 0.000000 0.000000 0.000000 -0.074407

15 C 0.000000 0.000002 0.000000 0.000000 0.000000 0.014010

16 C -0.000004 0.000168 -0.000065 0.000000 0.000000 -0.001304

17 N 0.000168 -0.001708 0.000168 0.000002 0.000002 -0.017626

18 C 0.000001 -0.000176 0.000218 0.000001 0.000000 -0.002348

19 C 0.000001 0.000450 -0.000385 0.000046 -0.000005 0.000218

20 C -0.000005 0.000056 -0.001244 -0.000006 0.000001 0.000001

21 C 0.000046 -0.000357 0.012920 -0.000158 -0.000006 0.000000

22 C -0.000385 -0.020679 -0.104649 0.012920 -0.001244 0.000001

23 N 0.000450 -0.013160 -0.020679 -0.000357 0.000056 -0.000176

24 H 0.000010 0.000002 0.000000 0.000000 0.000000 -0.005200

25 H 0.000009 -0.000003 0.000001 0.000000 0.000006 -0.000165

26 H 0.005560 0.005131 -0.038191 0.388265 -0.032996 0.000000

27 H -0.038191 0.005131 0.005560 -0.032996 0.388265 0.000000

28 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.005200

29 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000165

30 H 0.000000 0.000002 0.000010 0.000000 0.000000 0.000000

31 H 0.000001 -0.000003 0.000009 0.000006 0.000000 0.000000

32 Zn -0.014094 0.128946 -0.014094 0.002023 0.002023 -0.011292

33 C -0.001304 -0.017626 0.406627 -0.074407 0.014010 0.000003

34 C -0.000520 0.004290 -0.075725 -0.014881 0.002633 0.000000

35 C 0.000003 0.000000 0.000000 0.000000 0.000000 0.541474

36 C -0.000051 -0.000051 -0.005172 -0.000558 0.000359 0.000000

37 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.105008

38 C -0.075725 0.004290 -0.000520 0.002633 -0.014881 -0.000056

39 C -0.005172 -0.000051 -0.000051 0.000359 -0.000558 -0.000002

40 C 0.000000 0.000000 0.000003 0.000000 0.000000 -0.000056

41 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

43 H 0.000000 0.000001 -0.000035 0.000096 0.000002 0.000000

44 H -0.000035 0.000001 0.000000 0.000002 0.000096 0.000000

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.001819

13 14 15 16 17 18

1 C 0.012920 -0.000158 -0.000006 0.000046 -0.000357 0.000001

2 C -0.104649 0.012920 -0.001244 -0.000385 -0.020679 0.000218

3 N -0.020679 -0.000357 0.000056 0.000450 -0.013160 -0.000176

4 C -0.000385 0.000046 -0.000005 0.000001 0.000450 0.000001

5 C -0.001244 -0.000006 0.000001 -0.000005 0.000056 0.000000

6 C 0.000218 0.000001 0.000000 0.000001 -0.000176 0.000003

7 C -0.000065 0.000000 0.000000 -0.000004 0.000168 0.000001

8 N 0.000168 0.000002 0.000002 0.000168 -0.001708 -0.000176

9 C -0.000004 0.000000 0.000000 -0.000065 0.000168 0.000218

10 C 0.000000 0.000000 0.000000 0.000000 0.000002 0.000001

11 C 0.000000 0.000000 0.000000 0.000000 0.000002 0.000000

12 C 0.406627 -0.074407 0.014010 -0.001304 -0.017626 -0.002348

13 C 4.873703 0.403874 -0.062245 -0.146366 0.434511 -0.001304

14 C 0.403874 5.149059 0.532933 -0.062245 -0.077456 0.014010

15 C -0.062245 0.532933 5.149059 0.403874 -0.077456 -0.074407

16 C -0.146366 -0.062245 0.403874 4.873703 0.434511 0.406627

17 N 0.434511 -0.077456 -0.077456 0.434511 6.953408 -0.017626

18 C -0.001304 0.014010 -0.074407 0.406627 -0.017626 5.211687

19 C -0.000385 -0.001244 0.012920 -0.104649 -0.020679 0.406627

20 C 0.000046 -0.000006 -0.000158 0.012920 -0.000357 -0.074407

21 C -0.000005 0.000001 -0.000006 -0.001244 0.000056 0.014010

22 C 0.000001 -0.000005 0.000046 -0.000385 0.000450 -0.001304

23 N 0.000450 0.000056 -0.000357 -0.020679 -0.013160 -0.017626

24 H 0.000009 0.000006 0.000000 0.000001 -0.000003 0.000000

25 H 0.000010 0.000000 0.000000 0.000000 0.000002 0.000000

26 H 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 H -0.038191 0.388265 -0.032996 0.005560 0.005131 -0.000165

29 H 0.005560 -0.032996 0.388265 -0.038191 0.005131 -0.005200

30 H 0.000001 0.000000 0.000006 0.000009 -0.000003 -0.005200

31 H 0.000000 0.000000 0.000000 0.000010 0.000002 -0.000165

32 Zn -0.014094 0.002023 0.002023 -0.014094 0.128946 -0.011292

33 C 0.000001 0.000000 0.000001 0.000218 -0.000176 -0.002348

34 C 0.000000 0.000000 0.000000 0.000003 0.000000 -0.000056

35 C -0.075725 -0.014881 0.002633 -0.000520 0.004290 -0.000056

36 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

37 C -0.005172 -0.000558 0.000359 -0.000051 -0.000051 -0.000002

38 C 0.000003 0.000000 0.000000 0.000000 0.000000 0.000000

39 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

40 C -0.000520 0.002633 -0.014881 -0.075725 0.004290 0.541474

41 C -0.000051 0.000359 -0.000558 -0.005172 -0.000051 -0.105008

42 H 0.000000 0.000002 0.000096 -0.000035 0.000001 0.001819

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 -0.000035 0.000096 0.000002 0.000000 0.000001 0.000000

19 20 21 22 23 24

1 C 0.000000 0.000000 0.000000 0.000000 0.000002 0.388265

2 C -0.000065 0.000000 0.000000 -0.000004 0.000168 -0.038191

3 N 0.000168 0.000002 0.000002 0.000168 -0.001708 0.005131

4 C -0.000004 0.000000 0.000000 -0.000065 0.000168 0.005560

5 C 0.000000 0.000000 0.000000 0.000000 0.000002 -0.032996

6 C 0.000001 0.000000 0.000001 0.000218 -0.000176 -0.000165

7 C 0.000001 -0.000005 0.000046 -0.000385 0.000450 0.000010

8 N 0.000450 0.000056 -0.000357 -0.020679 -0.013160 0.000002

9 C -0.000385 -0.001244 0.012920 -0.104649 -0.020679 0.000000

10 C 0.000046 -0.000006 -0.000158 0.012920 -0.000357 0.000000

11 C -0.000005 0.000001 -0.000006 -0.001244 0.000056 0.000000

12 C 0.000218 0.000001 0.000000 0.000001 -0.000176 -0.005200

13 C -0.000385 0.000046 -0.000005 0.000001 0.000450 0.000009

14 C -0.001244 -0.000006 0.000001 -0.000005 0.000056 0.000006

15 C 0.012920 -0.000158 -0.000006 0.000046 -0.000357 0.000000

16 C -0.104649 0.012920 -0.001244 -0.000385 -0.020679 0.000001

17 N -0.020679 -0.000357 0.000056 0.000450 -0.013160 -0.000003

18 C 0.406627 -0.074407 0.014010 -0.001304 -0.017626 0.000000

19 C 4.873703 0.403874 -0.062245 -0.146366 0.434511 0.000000

20 C 0.403874 5.149059 0.532933 -0.062245 -0.077456 0.000000

21 C -0.062245 0.532933 5.149059 0.403874 -0.077456 0.000000

22 C -0.146366 -0.062245 0.403874 4.873703 0.434511 0.000000

23 N 0.434511 -0.077456 -0.077456 0.434511 6.953408 0.000000

24 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.427518

25 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.002192

26 H 0.000001 0.000000 0.000006 0.000009 -0.000003 0.000000

27 H 0.000000 0.000000 0.000000 0.000010 0.000002 0.000000

28 H 0.000010 0.000000 0.000000 0.000000 0.000002 -0.000006

29 H 0.000009 0.000006 0.000000 0.000001 -0.000003 0.000000

30 H -0.038191 0.388265 -0.032996 0.005560 0.005131 0.000000

31 H 0.005560 -0.032996 0.388265 -0.038191 0.005131 0.000000

32 Zn -0.014094 0.002023 0.002023 -0.014094 0.128946 -0.000363

33 C -0.001304 0.014010 -0.074407 0.406627 -0.017626 0.000000

34 C -0.000520 0.002633 -0.014881 -0.075725 0.004290 0.000000

35 C 0.000003 0.000000 0.000000 0.000000 0.000000 0.006422

36 C -0.000051 0.000359 -0.000558 -0.005172 -0.000051 0.000000

37 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.003287

38 C 0.000000 0.000000 0.000000 0.000003 0.000000 -0.000084

39 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000009

40 C -0.075725 -0.014881 0.002633 -0.000520 0.004290 0.000000

41 C -0.005172 -0.000558 0.000359 -0.000051 -0.000051 0.000000

42 H -0.000035 0.000096 0.000002 0.000000 0.000001 0.000000

43 H 0.000000 0.000002 0.000096 -0.000035 0.000001 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 0.000054

25 26 27 28 29 30

1 C -0.032996 0.000000 0.000000 0.000006 0.000000 0.000000

2 C 0.005560 0.000000 0.000001 0.000009 0.000010 0.000000

3 N 0.005131 0.000002 -0.000003 -0.000003 0.000002 0.000000

4 C -0.038191 0.000010 0.000009 0.000001 0.000000 0.000000

5 C 0.388265 0.000000 0.000006 0.000000 0.000000 0.000000

6 C -0.005200 -0.000165 -0.005200 0.000000 0.000000 0.000000

7 C 0.000009 0.005560 -0.038191 0.000000 0.000000 0.000000

8 N -0.000003 0.005131 0.005131 0.000000 0.000000 0.000002

9 C 0.000001 -0.038191 0.005560 0.000000 0.000000 0.000010

10 C 0.000000 0.388265 -0.032996 0.000000 0.000000 0.000000

11 C 0.000006 -0.032996 0.388265 0.000000 0.000000 0.000000

12 C -0.000165 0.000000 0.000000 -0.005200 -0.000165 0.000000

13 C 0.000010 0.000000 0.000000 -0.038191 0.005560 0.000001

14 C 0.000000 0.000000 0.000000 0.388265 -0.032996 0.000000

15 C 0.000000 0.000000 0.000000 -0.032996 0.388265 0.000006

16 C 0.000000 0.000000 0.000000 0.005560 -0.038191 0.000009

17 N 0.000002 0.000000 0.000000 0.005131 0.005131 -0.000003

18 C 0.000000 0.000000 0.000000 -0.000165 -0.005200 -0.005200

19 C 0.000000 0.000001 0.000000 0.000010 0.000009 -0.038191

20 C 0.000000 0.000000 0.000000 0.000000 0.000006 0.388265

21 C 0.000000 0.000006 0.000000 0.000000 0.000000 -0.032996

22 C 0.000000 0.000009 0.000010 0.000000 0.000001 0.005560

23 N 0.000000 -0.000003 0.000002 0.000002 -0.000003 0.005131

24 H -0.002192 0.000000 0.000000 -0.000006 0.000000 0.000000

25 H 0.427518 0.000000 -0.000006 0.000000 0.000000 0.000000

26 H 0.000000 0.427518 -0.002192 0.000000 0.000000 0.000000

27 H -0.000006 -0.002192 0.427518 0.000000 0.000000 0.000000

28 H 0.000000 0.000000 0.000000 0.427518 -0.002192 0.000000

29 H 0.000000 0.000000 0.000000 -0.002192 0.427518 -0.000006

30 H 0.000000 0.000000 0.000000 0.000000 -0.000006 0.427518

31 H 0.000000 -0.000006 0.000000 0.000000 0.000000 -0.002192

32 Zn -0.000363 -0.000363 -0.000363 -0.000363 -0.000363 -0.000363

33 C 0.000000 -0.005200 -0.000165 0.000000 0.000000 -0.000165

34 C 0.000000 0.006422 -0.000084 0.000000 0.000000 -0.000084

35 C -0.000084 0.000000 0.000000 0.006422 -0.000084 0.000000

36 C 0.000000 0.003287 -0.000009 0.000000 0.000000 -0.000009

37 C -0.000009 0.000000 0.000000 0.003287 -0.000009 0.000000

38 C 0.006422 -0.000084 0.006422 0.000000 0.000000 0.000000

39 C 0.003287 -0.000009 0.003287 0.000000 0.000000 0.000000

40 C 0.000000 0.000000 0.000000 -0.000084 0.006422 0.006422

41 C 0.000000 0.000000 0.000000 -0.000009 0.003287 0.003287

42 H 0.000000 0.000000 0.000000 0.000000 0.000054 0.000054

43 H 0.000000 0.000054 0.000000 0.000000 0.000000 0.000000

44 H 0.000054 0.000000 0.000054 0.000000 0.000000 0.000000

45 H 0.000000 0.000000 0.000000 0.000054 0.000000 0.000000

31 32 33 34 35 36

1 C 0.000000 0.002023 0.000000 0.000000 -0.014881 0.000000

2 C 0.000000 -0.014094 0.000001 0.000000 -0.075725 0.000000

3 N 0.000000 0.128946 -0.000176 0.000000 0.004290 0.000000

4 C 0.000000 -0.014094 0.000218 0.000003 -0.000520 0.000000

5 C 0.000000 0.002023 0.000001 0.000000 0.002633 0.000000

6 C 0.000000 -0.011292 -0.002348 -0.000056 -0.000056 -0.000002

7 C 0.000001 -0.014094 -0.001304 -0.000520 0.000003 -0.000051

8 N -0.000003 0.128946 -0.017626 0.004290 0.000000 -0.000051

9 C 0.000009 -0.014094 0.406627 -0.075725 0.000000 -0.005172

10 C 0.000006 0.002023 -0.074407 -0.014881 0.000000 -0.000558

11 C 0.000000 0.002023 0.014010 0.002633 0.000000 0.000359

12 C 0.000000 -0.011292 0.000003 0.000000 0.541474 0.000000

13 C 0.000000 -0.014094 0.000001 0.000000 -0.075725 0.000000

14 C 0.000000 0.002023 0.000000 0.000000 -0.014881 0.000000

15 C 0.000000 0.002023 0.000001 0.000000 0.002633 0.000000

16 C 0.000010 -0.014094 0.000218 0.000003 -0.000520 0.000000

17 N 0.000002 0.128946 -0.000176 0.000000 0.004290 0.000000

18 C -0.000165 -0.011292 -0.002348 -0.000056 -0.000056 -0.000002

19 C 0.005560 -0.014094 -0.001304 -0.000520 0.000003 -0.000051

20 C -0.032996 0.002023 0.014010 0.002633 0.000000 0.000359

21 C 0.388265 0.002023 -0.074407 -0.014881 0.000000 -0.000558

22 C -0.038191 -0.014094 0.406627 -0.075725 0.000000 -0.005172

23 N 0.005131 0.128946 -0.017626 0.004290 0.000000 -0.000051

24 H 0.000000 -0.000363 0.000000 0.000000 0.006422 0.000000

25 H 0.000000 -0.000363 0.000000 0.000000 -0.000084 0.000000

26 H -0.000006 -0.000363 -0.005200 0.006422 0.000000 0.003287

27 H 0.000000 -0.000363 -0.000165 -0.000084 0.000000 -0.000009

28 H 0.000000 -0.000363 0.000000 0.000000 0.006422 0.000000

29 H 0.000000 -0.000363 0.000000 0.000000 -0.000084 0.000000

30 H -0.002192 -0.000363 -0.000165 -0.000084 0.000000 -0.000009

31 H 0.427518 -0.000363 -0.005200 0.006422 0.000000 0.003287

32 Zn -0.000363 10.222398 -0.011292 -0.000589 -0.000589 -0.000042

33 C -0.005200 -0.011292 5.211687 0.541474 0.000000 -0.105008

34 C 0.006422 -0.000589 0.541474 4.813297 0.000000 0.856211

35 C 0.000000 -0.000589 0.000000 0.000000 4.813297 0.000000

36 C 0.003287 -0.000042 -0.105008 0.856211 0.000000 5.177595

37 C 0.000000 -0.000042 0.000000 0.000000 0.856211 0.000000

38 C 0.000000 -0.000589 -0.000056 -0.000001 -0.000001 0.000000

39 C 0.000000 -0.000042 -0.000002 0.000000 0.000000 0.000000

40 C -0.000084 -0.000589 -0.000056 -0.000001 -0.000001 0.000000

41 C -0.000009 -0.000042 -0.000002 0.000000 0.000000 0.000000

42 H 0.000000 -0.000003 0.000000 0.000000 0.000000 0.000000

43 H 0.000054 -0.000003 0.001819 -0.019607 0.000000 0.370702

44 H 0.000000 -0.000003 0.000000 0.000000 0.000000 0.000000

45 H 0.000000 -0.000003 0.000000 0.000000 -0.019607 0.000000

37 38 39 40 41 42

1 C -0.000558 0.002633 0.000359 0.000000 0.000000 0.000000

2 C -0.005172 -0.000520 -0.000051 0.000003 0.000000 0.000000

3 N -0.000051 0.004290 -0.000051 0.000000 0.000000 0.000000

4 C -0.000051 -0.075725 -0.005172 0.000000 0.000000 0.000000

5 C 0.000359 -0.014881 -0.000558 0.000000 0.000000 0.000000

6 C -0.000002 0.541474 -0.105008 0.000000 0.000000 0.000000

7 C 0.000000 -0.075725 -0.005172 0.000000 0.000000 0.000000

8 N 0.000000 0.004290 -0.000051 0.000000 0.000000 0.000000

9 C 0.000000 -0.000520 -0.000051 0.000003 0.000000 0.000000

10 C 0.000000 0.002633 0.000359 0.000000 0.000000 0.000000

11 C 0.000000 -0.014881 -0.000558 0.000000 0.000000 0.000000

12 C -0.105008 -0.000056 -0.000002 -0.000056 -0.000002 0.000000

13 C -0.005172 0.000003 0.000000 -0.000520 -0.000051 0.000000

14 C -0.000558 0.000000 0.000000 0.002633 0.000359 0.000002

15 C 0.000359 0.000000 0.000000 -0.014881 -0.000558 0.000096

16 C -0.000051 0.000000 0.000000 -0.075725 -0.005172 -0.000035

17 N -0.000051 0.000000 0.000000 0.004290 -0.000051 0.000001

18 C -0.000002 0.000000 0.000000 0.541474 -0.105008 0.001819

19 C 0.000000 0.000000 0.000000 -0.075725 -0.005172 -0.000035

20 C 0.000000 0.000000 0.000000 -0.014881 -0.000558 0.000096

21 C 0.000000 0.000000 0.000000 0.002633 0.000359 0.000002

22 C 0.000000 0.000003 0.000000 -0.000520 -0.000051 0.000000

23 N 0.000000 0.000000 0.000000 0.004290 -0.000051 0.000001

24 H 0.003287 -0.000084 -0.000009 0.000000 0.000000 0.000000

25 H -0.000009 0.006422 0.003287 0.000000 0.000000 0.000000

26 H 0.000000 -0.000084 -0.000009 0.000000 0.000000 0.000000

27 H 0.000000 0.006422 0.003287 0.000000 0.000000 0.000000

28 H 0.003287 0.000000 0.000000 -0.000084 -0.000009 0.000000

29 H -0.000009 0.000000 0.000000 0.006422 0.003287 0.000054

30 H 0.000000 0.000000 0.000000 0.006422 0.003287 0.000054

31 H 0.000000 0.000000 0.000000 -0.000084 -0.000009 0.000000

32 Zn -0.000042 -0.000589 -0.000042 -0.000589 -0.000042 -0.000003

33 C 0.000000 -0.000056 -0.000002 -0.000056 -0.000002 0.000000

34 C 0.000000 -0.000001 0.000000 -0.000001 0.000000 0.000000

35 C 0.856211 -0.000001 0.000000 -0.000001 0.000000 0.000000

36 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 C 5.177595 0.000000 0.000000 0.000000 0.000000 0.000000

38 C 0.000000 4.813297 0.856211 0.000000 0.000000 0.000000

39 C 0.000000 0.856211 5.177595 0.000000 0.000000 0.000000

40 C 0.000000 0.000000 0.000000 4.813297 0.856211 -0.019607

41 C 0.000000 0.000000 0.000000 0.856211 5.177595 0.370702

42 H 0.000000 0.000000 0.000000 -0.019607 0.370702 0.348410

43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 -0.019607 0.370702 0.000000 0.000000 0.000000

45 H 0.370702 0.000000 0.000000 0.000000 0.000000 0.000000

43 44 45

1 C 0.000000 0.000002 0.000096

2 C 0.000000 0.000000 -0.000035

3 N 0.000000 0.000001 0.000001

4 C 0.000000 -0.000035 0.000000

5 C 0.000000 0.000096 0.000002

6 C 0.000000 0.001819 0.000000

7 C 0.000000 -0.000035 0.000000

8 N 0.000001 0.000001 0.000000

9 C -0.000035 0.000000 0.000000

10 C 0.000096 0.000002 0.000000

11 C 0.000002 0.000096 0.000000

12 C 0.000000 0.000000 0.001819

13 C 0.000000 0.000000 -0.000035

14 C 0.000000 0.000000 0.000096

15 C 0.000000 0.000000 0.000002

16 C 0.000000 0.000000 0.000000

17 N 0.000000 0.000000 0.000001

18 C 0.000000 0.000000 0.000000

19 C 0.000000 0.000000 0.000000

20 C 0.000002 0.000000 0.000000

21 C 0.000096 0.000000 0.000000

22 C -0.000035 0.000000 0.000000

23 N 0.000001 0.000000 0.000000

24 H 0.000000 0.000000 0.000054

25 H 0.000000 0.000054 0.000000

26 H 0.000054 0.000000 0.000000

27 H 0.000000 0.000054 0.000000

28 H 0.000000 0.000000 0.000054

29 H 0.000000 0.000000 0.000000

30 H 0.000000 0.000000 0.000000

31 H 0.000054 0.000000 0.000000

32 Zn -0.000003 -0.000003 -0.000003

33 C 0.001819 0.000000 0.000000

34 C -0.019607 0.000000 0.000000

35 C 0.000000 0.000000 -0.019607

36 C 0.370702 0.000000 0.000000

37 C 0.000000 0.000000 0.370702

38 C 0.000000 -0.019607 0.000000

39 C 0.000000 0.370702 0.000000

40 C 0.000000 0.000000 0.000000

41 C 0.000000 0.000000 0.000000

42 H 0.000000 0.000000 0.000000

43 H 0.348410 0.000000 0.000000

44 H 0.000000 0.348410 0.000000

45 H 0.000000 0.000000 0.348410

Mulliken charges:

1

1 C -0.241966

2 C 0.333019

3 N -0.710850

4 C 0.333019

5 C -0.241966

6 C -0.277830

7 C 0.333019

8 N -0.710850

9 C 0.333019

10 C -0.241966

11 C -0.241966

12 C -0.277830

13 C 0.333019

14 C -0.241966

15 C -0.241966

16 C 0.333019

17 N -0.710850

18 C -0.277830

19 C 0.333019

20 C -0.241966

21 C -0.241966

22 C 0.333019

23 N -0.710850

24 H 0.242944

25 H 0.242944

26 H 0.242944

27 H 0.242944

28 H 0.242944

29 H 0.242944

30 H 0.242944

31 H 0.242944

32 Zn 1.408997

33 C -0.277830

34 C -0.034945

35 C -0.034945

36 C -0.295064

37 C -0.295064

38 C -0.034945

39 C -0.295064

40 C -0.034945

41 C -0.295064

42 H 0.298445

43 H 0.298445

44 H 0.298445

45 H 0.298445

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 C 0.000979

2 C 0.333019

3 N -0.710850

4 C 0.333019

5 C 0.000979

6 C -0.277830

7 C 0.333019

8 N -0.710850

9 C 0.333019

10 C 0.000979

11 C 0.000979

12 C -0.277830

13 C 0.333019

14 C 0.000979

15 C 0.000979

16 C 0.333019

17 N -0.710850

18 C -0.277830

19 C 0.333019

20 C 0.000979

21 C 0.000979

22 C 0.333019

23 N -0.710850

32 Zn 1.408997

33 C -0.277830

34 C -0.034945

35 C -0.034945

36 C 0.003382

37 C 0.003382

38 C -0.034945

39 C 0.003382

40 C -0.034945

41 C 0.003382

Electronic spatial extent (au): <R\*\*2>= 13455.4995

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0000 Y= 0.0000 Z= 0.8362 Tot= 0.8362

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -158.2495 YY= -158.2495 ZZ= -200.1408

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 13.9638 YY= 13.9638 ZZ= -27.9276

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

Octapole moment (field-independent basis, Debye-Ang\*\*2):

XXX= 0.0000 YYY= 0.0000 ZZZ= 12.6982 XYY= 0.0000

XXY= 0.0000 XXZ= -5.0743 XZZ= 0.0000 YZZ= 0.0000

YYZ= -5.0743 XYZ= 0.0000

Hexadecapole moment (field-independent basis, Debye-Ang\*\*3):

XXXX= -7924.4002 YYYY= -7924.4002 ZZZZ= -226.2434 XXXY= 0.0000

XXXZ= 0.0000 YYYX= 0.0000 YYYZ= 0.0000 ZZZX= 0.0000

ZZZY= 0.0000 XXYY= -1844.2759 XXZZ= -1800.2717 YYZZ= -1800.2717

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 3.060485416419D+03 E-N=-9.363055476440D+03 KE= 1.403728956777D+03

Symmetry A1 KE= 4.235679847861D+02

Symmetry A2 KE= 2.911453199211D+02

Symmetry B1 KE= 3.445078260349D+02

Symmetry B2 KE= 3.445078260349D+02

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Fri Jul 26 14:24:34 2019, MaxMem= 1342177280 cpu: 12.9

(Enter /apps/gaussian/g09d01/g09/l9999.exe)

1\1\GINC-K009\FOpt\RB3LYP\GenECP\C28H12N4Zn1\Z5105842\26-Jul-2019\0\\#

p opt freq b3lyp/genecp scrf=(solvent=dmso,smd) empiricaldispersion=gd

3bj\\ZnTSPsim0\\0,1\C,0.6811632879,4.2732946298,-0.0396282291\C,1.1019

95218,2.8891864292,-0.0047490578\N,0.,2.0816904415,0.0177872219\C,-1.1

01995218,2.8891864292,-0.0047490578\C,-0.6811632879,4.2732946298,-0.03

96282291\C,-2.4461346812,2.4461346812,-0.0099866712\C,-2.8891864292,1.

101995218,-0.0047490578\N,-2.0816904415,0.,0.0177872219\C,-2.889186429

2,-1.101995218,-0.0047490578\C,-4.2732946298,-0.6811632879,-0.03962822

91\C,-4.2732946298,0.6811632879,-0.0396282291\C,2.4461346812,2.4461346

812,-0.0099866712\C,2.8891864292,1.101995218,-0.0047490578\C,4.2732946

298,0.6811632879,-0.0396282291\C,4.2732946298,-0.6811632879,-0.0396282

291\C,2.8891864292,-1.101995218,-0.0047490578\N,2.0816904415,0.,0.0177

872219\C,2.4461346812,-2.4461346812,-0.0099866712\C,1.101995218,-2.889

1864292,-0.0047490578\C,0.6811632879,-4.2732946298,-0.0396282291\C,-0.

6811632879,-4.2732946298,-0.0396282291\C,-1.101995218,-2.8891864292,-0

.0047490578\N,0.,-2.0816904415,0.0177872219\H,1.3396824442,5.128560793

1,-0.065729077\H,-1.3396824442,5.1285607931,-0.065729077\H,-5.12856079

31,-1.3396824442,-0.065729077\H,-5.1285607931,1.3396824442,-0.06572907

7\H,5.1285607931,1.3396824442,-0.065729077\H,5.1285607931,-1.339682444

2,-0.065729077\H,1.3396824442,-5.1285607931,-0.065729077\H,-1.33968244

42,-5.1285607931,-0.065729077\Zn,0.,0.,0.190340611\C,-2.4461346812,-2.

4461346812,-0.0099866712\C,-3.4549890716,-3.4549890716,-0.0390558973\C

,3.4549890716,3.4549890716,-0.0390558973\C,-4.3073712967,-4.3073712967

,-0.0682142485\C,4.3073712967,4.3073712967,-0.0682142485\C,-3.45498907

16,3.4549890716,-0.0390558973\C,-4.3073712967,4.3073712967,-0.06821424

85\C,3.4549890716,-3.4549890716,-0.0390558973\C,4.3073712967,-4.307371

2967,-0.0682142485\H,5.061915379,-5.061915379,-0.0914169713\H,-5.06191

5379,-5.061915379,-0.0914169713\H,-5.061915379,5.061915379,-0.09141697

13\H,5.061915379,5.061915379,-0.0914169713\\Version=ES64L-G09RevD.01\S

tate=1-A1\HF=-1359.0630458\RMSD=7.981e-09\RMSF=2.757e-06\Dipole=0.,0.,

0.3289745\Quadrupole=10.3817304,10.3817304,-20.7634608,0.,0.,0.\PG=C04

V [C4(Zn1),2SGV(N2),2SGD(C6H2),X(C16H8)]\\@

THE ONLY DIFFERENCE BETWEEN ECCENTRICS AND JOGGERS

IS THAT JOGGERS WEAR SWEATBANDS WHEN THEY RUN IN THE RAIN.

Leave Link 9999 at Fri Jul 26 14:24:34 2019, MaxMem= 1342177280 cpu: 0.6

Job cpu time: 0 days 2 hours 20 minutes 45.6 seconds.

File lengths (MBytes): RWF= 789 Int= 0 D2E= 0 Chk= 43 Scr= 2

Normal termination of Gaussian 09 at Fri Jul 26 14:24:34 2019.

(Enter /apps/gaussian/g09d01/g09/l1.exe)

Link1: Proceeding to internal job step number 2.

------------------------------------------------------------------

#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/GenECP Freq

------------------------------------------------------------------

1/10=4,29=7,30=1,38=1,40=1/1,3;

2/12=2,40=1/2;

3/5=7,6=2,11=2,14=-4,16=1,17=8,25=1,30=1,70=2,71=2,72=21,74=-5,82=7,116=1,124=41,140=1/1,2,3;

4/5=101/1;

5/5=2,53=21,98=1/2;

8/6=4,10=90,11=11/1;

11/6=1,8=1,9=11,15=111,16=1/1,2,10;

10/6=1/2;

6/7=2,8=2,9=2,10=2,18=1,28=1/1;

7/8=1,10=1,25=1/1,2,3,16;

1/10=4,30=1/3;

99//99;

Leave Link 1 at Fri Jul 26 14:24:34 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l101.exe)

Structure from the checkpoint file: "ZnTSPsim0.chk"

---------

ZnTSPsim0

---------

Charge = 0 Multiplicity = 1

Redundant internal coordinates found in file.

C,0,0.6811632879,4.2732946298,-0.0396282291

C,0,1.101995218,2.8891864292,-0.0047490578

N,0,0.,2.0816904415,0.0177872219

C,0,-1.101995218,2.8891864292,-0.0047490578

C,0,-0.6811632879,4.2732946298,-0.0396282291

C,0,-2.4461346812,2.4461346812,-0.0099866712

C,0,-2.8891864292,1.101995218,-0.0047490578

N,0,-2.0816904415,0.,0.0177872219

C,0,-2.8891864292,-1.101995218,-0.0047490578

C,0,-4.2732946298,-0.6811632879,-0.0396282291

C,0,-4.2732946298,0.6811632879,-0.0396282291

C,0,2.4461346812,2.4461346812,-0.0099866712

C,0,2.8891864292,1.101995218,-0.0047490578

C,0,4.2732946298,0.6811632879,-0.0396282291

C,0,4.2732946298,-0.6811632879,-0.0396282291

C,0,2.8891864292,-1.101995218,-0.0047490578

N,0,2.0816904415,0.,0.0177872219

C,0,2.4461346812,-2.4461346812,-0.0099866712

C,0,1.101995218,-2.8891864292,-0.0047490578

C,0,0.6811632879,-4.2732946298,-0.0396282291

C,0,-0.6811632879,-4.2732946298,-0.0396282291

C,0,-1.101995218,-2.8891864292,-0.0047490578

N,0,0.,-2.0816904415,0.0177872219

H,0,1.3396824442,5.1285607931,-0.065729077

H,0,-1.3396824442,5.1285607931,-0.065729077

H,0,-5.1285607931,-1.3396824442,-0.065729077

H,0,-5.1285607931,1.3396824442,-0.065729077

H,0,5.1285607931,1.3396824442,-0.065729077

H,0,5.1285607931,-1.3396824442,-0.065729077

H,0,1.3396824442,-5.1285607931,-0.065729077

H,0,-1.3396824442,-5.1285607931,-0.065729077

Zn,0,0.,0.,0.190340611

C,0,-2.4461346812,-2.4461346812,-0.0099866712

C,0,-3.4549890716,-3.4549890716,-0.0390558973

C,0,3.4549890716,3.4549890716,-0.0390558973

C,0,-4.3073712967,-4.3073712967,-0.0682142485

C,0,4.3073712967,4.3073712967,-0.0682142485

C,0,-3.4549890716,3.4549890716,-0.0390558973

C,0,-4.3073712967,4.3073712967,-0.0682142485

C,0,3.4549890716,-3.4549890716,-0.0390558973

C,0,4.3073712967,-4.3073712967,-0.0682142485

H,0,5.061915379,-5.061915379,-0.0914169713

H,0,-5.061915379,-5.061915379,-0.0914169713

H,0,-5.061915379,5.061915379,-0.0914169713

H,0,5.061915379,5.061915379,-0.0914169713

Recover connectivity data from disk.

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 12 14 12 12 12 12 14 12 12

AtmWgt= 12.0000000 12.0000000 14.0030740 12.0000000 12.0000000 12.0000000 12.0000000 14.0030740 12.0000000 12.0000000

NucSpn= 0 0 2 0 0 0 0 2 0 0

AtZEff= -3.6000000 -3.6000000 -4.5500000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -4.5500000 -3.6000000 -3.6000000

NQMom= 0.0000000 0.0000000 2.0440000 0.0000000 0.0000000 0.0000000 0.0000000 2.0440000 0.0000000 0.0000000

NMagM= 0.0000000 0.0000000 0.4037610 0.0000000 0.0000000 0.0000000 0.0000000 0.4037610 0.0000000 0.0000000

AtZNuc= 6.0000000 6.0000000 7.0000000 6.0000000 6.0000000 6.0000000 6.0000000 7.0000000 6.0000000 6.0000000

Atom 11 12 13 14 15 16 17 18 19 20

IAtWgt= 12 12 12 12 12 12 14 12 12 12

AtmWgt= 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 14.0030740 12.0000000 12.0000000 12.0000000

NucSpn= 0 0 0 0 0 0 2 0 0 0

AtZEff= -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -4.5500000 -3.6000000 -3.6000000 -3.6000000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 2.0440000 0.0000000 0.0000000 0.0000000

NMagM= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.4037610 0.0000000 0.0000000 0.0000000

AtZNuc= 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 7.0000000 6.0000000 6.0000000 6.0000000

Atom 21 22 23 24 25 26 27 28 29 30

IAtWgt= 12 12 14 1 1 1 1 1 1 1

AtmWgt= 12.0000000 12.0000000 14.0030740 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 0 0 2 1 1 1 1 1 1 1

AtZEff= -3.6000000 -3.6000000 -4.5500000 -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000

NQMom= 0.0000000 0.0000000 2.0440000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 0.0000000 0.0000000 0.4037610 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 6.0000000 6.0000000 7.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Atom 31 32 33 34 35 36 37 38 39 40

IAtWgt= 1 64 12 12 12 12 12 12 12 12

AtmWgt= 1.0078250 63.9291454 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000

NucSpn= 1 0 0 0 0 0 0 0 0 0

AtZEff= -1.0000000 -19.0500000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000

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 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

AtZNuc= 1.0000000 30.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000

Atom 41 42 43 44 45

IAtWgt= 12 1 1 1 1

AtmWgt= 12.0000000 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 0 1 1 1 1

AtZEff= -3.6000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 0.0000000 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 6.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Leave Link 101 at Fri Jul 26 14:24:35 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Initialization pass.

----------------------------

! Initial Parameters !

! (Angstroms and Degrees) !

-------------------------- --------------------------

! Name Definition Value Derivative Info. !

--------------------------------------------------------------------------------

! R1 R(1,2) 1.4471 calculate D2E/DX2 analytically !

! R2 R(1,5) 1.3623 calculate D2E/DX2 analytically !

! R3 R(1,24) 1.0797 calculate D2E/DX2 analytically !

! R4 R(2,3) 1.3664 calculate D2E/DX2 analytically !

! R5 R(2,12) 1.4153 calculate D2E/DX2 analytically !

! R6 R(3,4) 1.3664 calculate D2E/DX2 analytically !

! R7 R(3,32) 2.0888 calculate D2E/DX2 analytically !

! R8 R(4,5) 1.4471 calculate D2E/DX2 analytically !

! R9 R(4,6) 1.4153 calculate D2E/DX2 analytically !

! R10 R(5,25) 1.0797 calculate D2E/DX2 analytically !

! R11 R(6,7) 1.4153 calculate D2E/DX2 analytically !

! R12 R(6,38) 1.427 calculate D2E/DX2 analytically !

! R13 R(7,8) 1.3664 calculate D2E/DX2 analytically !

! R14 R(7,11) 1.4471 calculate D2E/DX2 analytically !

! R15 R(8,9) 1.3664 calculate D2E/DX2 analytically !

! R16 R(8,32) 2.0888 calculate D2E/DX2 analytically !

! R17 R(9,10) 1.4471 calculate D2E/DX2 analytically !

! R18 R(9,33) 1.4153 calculate D2E/DX2 analytically !

! R19 R(10,11) 1.3623 calculate D2E/DX2 analytically !

! R20 R(10,26) 1.0797 calculate D2E/DX2 analytically !

! R21 R(11,27) 1.0797 calculate D2E/DX2 analytically !

! R22 R(12,13) 1.4153 calculate D2E/DX2 analytically !

! R23 R(12,35) 1.427 calculate D2E/DX2 analytically !

! R24 R(13,14) 1.4471 calculate D2E/DX2 analytically !

! R25 R(13,17) 1.3664 calculate D2E/DX2 analytically !

! R26 R(14,15) 1.3623 calculate D2E/DX2 analytically !

! R27 R(14,28) 1.0797 calculate D2E/DX2 analytically !

! R28 R(15,16) 1.4471 calculate D2E/DX2 analytically !

! R29 R(15,29) 1.0797 calculate D2E/DX2 analytically !

! R30 R(16,17) 1.3664 calculate D2E/DX2 analytically !

! R31 R(16,18) 1.4153 calculate D2E/DX2 analytically !

! R32 R(17,32) 2.0888 calculate D2E/DX2 analytically !

! R33 R(18,19) 1.4153 calculate D2E/DX2 analytically !

! R34 R(18,40) 1.427 calculate D2E/DX2 analytically !

! R35 R(19,20) 1.4471 calculate D2E/DX2 analytically !

! R36 R(19,23) 1.3664 calculate D2E/DX2 analytically !

! R37 R(20,21) 1.3623 calculate D2E/DX2 analytically !

! R38 R(20,30) 1.0797 calculate D2E/DX2 analytically !

! R39 R(21,22) 1.4471 calculate D2E/DX2 analytically !

! R40 R(21,31) 1.0797 calculate D2E/DX2 analytically !

! R41 R(22,23) 1.3664 calculate D2E/DX2 analytically !

! R42 R(22,33) 1.4153 calculate D2E/DX2 analytically !

! R43 R(23,32) 2.0888 calculate D2E/DX2 analytically !

! R44 R(33,34) 1.427 calculate D2E/DX2 analytically !

! R45 R(34,36) 1.2058 calculate D2E/DX2 analytically !

! R46 R(35,37) 1.2058 calculate D2E/DX2 analytically !

! R47 R(36,43) 1.0673 calculate D2E/DX2 analytically !

! R48 R(37,45) 1.0673 calculate D2E/DX2 analytically !

! R49 R(38,39) 1.2058 calculate D2E/DX2 analytically !

! R50 R(39,44) 1.0673 calculate D2E/DX2 analytically !

! R51 R(40,41) 1.2058 calculate D2E/DX2 analytically !

! R52 R(41,42) 1.0673 calculate D2E/DX2 analytically !

! A1 A(2,1,5) 106.9066 calculate D2E/DX2 analytically !

! A2 A(2,1,24) 125.5108 calculate D2E/DX2 analytically !

! A3 A(5,1,24) 127.5819 calculate D2E/DX2 analytically !

! A4 A(1,2,3) 109.3363 calculate D2E/DX2 analytically !

! A5 A(1,2,12) 125.1365 calculate D2E/DX2 analytically !

! A6 A(3,2,12) 125.5229 calculate D2E/DX2 analytically !

! A7 A(2,3,4) 107.5139 calculate D2E/DX2 analytically !

! A8 A(2,3,32) 126.18 calculate D2E/DX2 analytically !

! A9 A(4,3,32) 126.18 calculate D2E/DX2 analytically !

! A10 A(3,4,5) 109.3363 calculate D2E/DX2 analytically !

! A11 A(3,4,6) 125.5229 calculate D2E/DX2 analytically !

! A12 A(5,4,6) 125.1365 calculate D2E/DX2 analytically !

! A13 A(1,5,4) 106.9066 calculate D2E/DX2 analytically !

! A14 A(1,5,25) 127.5819 calculate D2E/DX2 analytically !

! A15 A(4,5,25) 125.5108 calculate D2E/DX2 analytically !

! A16 A(4,6,7) 126.4847 calculate D2E/DX2 analytically !

! A17 A(4,6,38) 116.7555 calculate D2E/DX2 analytically !

! A18 A(7,6,38) 116.7555 calculate D2E/DX2 analytically !

! A19 A(6,7,8) 125.5229 calculate D2E/DX2 analytically !

! A20 A(6,7,11) 125.1365 calculate D2E/DX2 analytically !

! A21 A(8,7,11) 109.3363 calculate D2E/DX2 analytically !

! A22 A(7,8,9) 107.5139 calculate D2E/DX2 analytically !

! A23 A(7,8,32) 126.18 calculate D2E/DX2 analytically !

! A24 A(9,8,32) 126.18 calculate D2E/DX2 analytically !

! A25 A(8,9,10) 109.3363 calculate D2E/DX2 analytically !

! A26 A(8,9,33) 125.5229 calculate D2E/DX2 analytically !

! A27 A(10,9,33) 125.1365 calculate D2E/DX2 analytically !

! A28 A(9,10,11) 106.9066 calculate D2E/DX2 analytically !

! A29 A(9,10,26) 125.5108 calculate D2E/DX2 analytically !

! A30 A(11,10,26) 127.5819 calculate D2E/DX2 analytically !

! A31 A(7,11,10) 106.9066 calculate D2E/DX2 analytically !

! A32 A(7,11,27) 125.5108 calculate D2E/DX2 analytically !

! A33 A(10,11,27) 127.5819 calculate D2E/DX2 analytically !

! A34 A(2,12,13) 126.4847 calculate D2E/DX2 analytically !

! A35 A(2,12,35) 116.7555 calculate D2E/DX2 analytically !

! A36 A(13,12,35) 116.7555 calculate D2E/DX2 analytically !

! A37 A(12,13,14) 125.1365 calculate D2E/DX2 analytically !

! A38 A(12,13,17) 125.5229 calculate D2E/DX2 analytically !

! A39 A(14,13,17) 109.3363 calculate D2E/DX2 analytically !

! A40 A(13,14,15) 106.9066 calculate D2E/DX2 analytically !

! A41 A(13,14,28) 125.5108 calculate D2E/DX2 analytically !

! A42 A(15,14,28) 127.5819 calculate D2E/DX2 analytically !

! A43 A(14,15,16) 106.9066 calculate D2E/DX2 analytically !

! A44 A(14,15,29) 127.5819 calculate D2E/DX2 analytically !

! A45 A(16,15,29) 125.5108 calculate D2E/DX2 analytically !

! A46 A(15,16,17) 109.3363 calculate D2E/DX2 analytically !

! A47 A(15,16,18) 125.1365 calculate D2E/DX2 analytically !

! A48 A(17,16,18) 125.5229 calculate D2E/DX2 analytically !

! A49 A(13,17,16) 107.5139 calculate D2E/DX2 analytically !

! A50 A(13,17,32) 126.18 calculate D2E/DX2 analytically !

! A51 A(16,17,32) 126.18 calculate D2E/DX2 analytically !

! A52 A(16,18,19) 126.4847 calculate D2E/DX2 analytically !

! A53 A(16,18,40) 116.7555 calculate D2E/DX2 analytically !

! A54 A(19,18,40) 116.7555 calculate D2E/DX2 analytically !

! A55 A(18,19,20) 125.1365 calculate D2E/DX2 analytically !

! A56 A(18,19,23) 125.5229 calculate D2E/DX2 analytically !

! A57 A(20,19,23) 109.3363 calculate D2E/DX2 analytically !

! A58 A(19,20,21) 106.9066 calculate D2E/DX2 analytically !

! A59 A(19,20,30) 125.5108 calculate D2E/DX2 analytically !

! A60 A(21,20,30) 127.5819 calculate D2E/DX2 analytically !

! A61 A(20,21,22) 106.9066 calculate D2E/DX2 analytically !

! A62 A(20,21,31) 127.5819 calculate D2E/DX2 analytically !

! A63 A(22,21,31) 125.5108 calculate D2E/DX2 analytically !

! A64 A(21,22,23) 109.3363 calculate D2E/DX2 analytically !

! A65 A(21,22,33) 125.1365 calculate D2E/DX2 analytically !

! A66 A(23,22,33) 125.5229 calculate D2E/DX2 analytically !

! A67 A(19,23,22) 107.5139 calculate D2E/DX2 analytically !

! A68 A(19,23,32) 126.18 calculate D2E/DX2 analytically !

! A69 A(22,23,32) 126.18 calculate D2E/DX2 analytically !

! A70 A(3,32,8) 89.609 calculate D2E/DX2 analytically !

! A71 A(3,32,17) 89.609 calculate D2E/DX2 analytically !

! A72 A(3,32,23) 170.5231 calculate D2E/DX2 analytically !

! A73 A(8,32,17) 170.5231 calculate D2E/DX2 analytically !

! A74 A(8,32,23) 89.609 calculate D2E/DX2 analytically !

! A75 A(17,32,23) 89.609 calculate D2E/DX2 analytically !

! A76 A(9,33,22) 126.4847 calculate D2E/DX2 analytically !

! A77 A(9,33,34) 116.7555 calculate D2E/DX2 analytically !

! A78 A(22,33,34) 116.7555 calculate D2E/DX2 analytically !

! A79 L(33,34,36,26,-1) 179.9973 calculate D2E/DX2 analytically !

! A80 L(12,35,37,24,-1) 179.9973 calculate D2E/DX2 analytically !

! A81 L(34,36,43,26,-1) 180.0017 calculate D2E/DX2 analytically !

! A82 L(35,37,45,24,-1) 180.0017 calculate D2E/DX2 analytically !

! A83 L(6,38,39,25,-1) 179.9973 calculate D2E/DX2 analytically !

! A84 L(38,39,44,25,-1) 180.0017 calculate D2E/DX2 analytically !

! A85 L(18,40,41,29,-1) 179.9973 calculate D2E/DX2 analytically !

! A86 L(40,41,42,29,-1) 180.0017 calculate D2E/DX2 analytically !

! A87 L(33,34,36,26,-2) 179.7801 calculate D2E/DX2 analytically !

! A88 L(12,35,37,24,-2) 180.2199 calculate D2E/DX2 analytically !

! A89 L(34,36,43,26,-2) 180.1609 calculate D2E/DX2 analytically !

! A90 L(35,37,45,24,-2) 179.8391 calculate D2E/DX2 analytically !

! A91 L(6,38,39,25,-2) 179.7801 calculate D2E/DX2 analytically !

! A92 L(38,39,44,25,-2) 180.1609 calculate D2E/DX2 analytically !

! A93 L(18,40,41,29,-2) 180.2199 calculate D2E/DX2 analytically !

! A94 L(40,41,42,29,-2) 179.8391 calculate D2E/DX2 analytically !

! D1 D(5,1,2,3) -0.0972 calculate D2E/DX2 analytically !

! D2 D(5,1,2,12) 179.1882 calculate D2E/DX2 analytically !

! D3 D(24,1,2,3) -179.8008 calculate D2E/DX2 analytically !

! D4 D(24,1,2,12) -0.5153 calculate D2E/DX2 analytically !

! D5 D(2,1,5,4) 0.0 calculate D2E/DX2 analytically !

! D6 D(2,1,5,25) -179.6955 calculate D2E/DX2 analytically !

! D7 D(24,1,5,4) 179.6955 calculate D2E/DX2 analytically !

! D8 D(24,1,5,25) 0.0 calculate D2E/DX2 analytically !

! D9 D(1,2,3,4) 0.1573 calculate D2E/DX2 analytically !

! D10 D(1,2,3,32) -175.9517 calculate D2E/DX2 analytically !

! D11 D(12,2,3,4) -179.1247 calculate D2E/DX2 analytically !

! D12 D(12,2,3,32) 4.7663 calculate D2E/DX2 analytically !

! D13 D(1,2,12,13) -178.5823 calculate D2E/DX2 analytically !

! D14 D(1,2,12,35) 0.638 calculate D2E/DX2 analytically !

! D15 D(3,2,12,13) 0.5893 calculate D2E/DX2 analytically !

! D16 D(3,2,12,35) 179.8095 calculate D2E/DX2 analytically !

! D17 D(2,3,4,5) -0.1573 calculate D2E/DX2 analytically !

! D18 D(2,3,4,6) 179.1247 calculate D2E/DX2 analytically !

! D19 D(32,3,4,5) 175.9517 calculate D2E/DX2 analytically !

! D20 D(32,3,4,6) -4.7663 calculate D2E/DX2 analytically !

! D21 D(2,3,32,8) -177.5769 calculate D2E/DX2 analytically !

! D22 D(2,3,32,17) -7.0216 calculate D2E/DX2 analytically !

! D23 D(2,3,32,23) -92.2992 calculate D2E/DX2 analytically !

! D24 D(4,3,32,8) 7.0216 calculate D2E/DX2 analytically !

! D25 D(4,3,32,17) 177.5769 calculate D2E/DX2 analytically !

! D26 D(4,3,32,23) 92.2992 calculate D2E/DX2 analytically !

! D27 D(3,4,5,1) 0.0972 calculate D2E/DX2 analytically !

! D28 D(3,4,5,25) 179.8008 calculate D2E/DX2 analytically !

! D29 D(6,4,5,1) -179.1882 calculate D2E/DX2 analytically !

! D30 D(6,4,5,25) 0.5153 calculate D2E/DX2 analytically !

! D31 D(3,4,6,7) -0.5893 calculate D2E/DX2 analytically !

! D32 D(3,4,6,38) -179.8095 calculate D2E/DX2 analytically !

! D33 D(5,4,6,7) 178.5823 calculate D2E/DX2 analytically !

! D34 D(5,4,6,38) -0.638 calculate D2E/DX2 analytically !

! D35 D(4,6,7,8) 0.5893 calculate D2E/DX2 analytically !

! D36 D(4,6,7,11) -178.5823 calculate D2E/DX2 analytically !

! D37 D(38,6,7,8) 179.8095 calculate D2E/DX2 analytically !

! D38 D(38,6,7,11) 0.638 calculate D2E/DX2 analytically !

! D39 D(6,7,8,9) -179.1247 calculate D2E/DX2 analytically !

! D40 D(6,7,8,32) 4.7663 calculate D2E/DX2 analytically !

! D41 D(11,7,8,9) 0.1573 calculate D2E/DX2 analytically !

! D42 D(11,7,8,32) -175.9517 calculate D2E/DX2 analytically !

! D43 D(6,7,11,10) 179.1882 calculate D2E/DX2 analytically !

! D44 D(6,7,11,27) -0.5153 calculate D2E/DX2 analytically !

! D45 D(8,7,11,10) -0.0972 calculate D2E/DX2 analytically !

! D46 D(8,7,11,27) -179.8008 calculate D2E/DX2 analytically !

! D47 D(7,8,9,10) -0.1573 calculate D2E/DX2 analytically !

! D48 D(7,8,9,33) 179.1247 calculate D2E/DX2 analytically !

! D49 D(32,8,9,10) 175.9517 calculate D2E/DX2 analytically !

! D50 D(32,8,9,33) -4.7663 calculate D2E/DX2 analytically !

! D51 D(7,8,32,3) -7.0216 calculate D2E/DX2 analytically !

! D52 D(7,8,32,17) -92.2992 calculate D2E/DX2 analytically !

! D53 D(7,8,32,23) -177.5769 calculate D2E/DX2 analytically !

! D54 D(9,8,32,3) 177.5769 calculate D2E/DX2 analytically !

! D55 D(9,8,32,17) 92.2992 calculate D2E/DX2 analytically !

! D56 D(9,8,32,23) 7.0216 calculate D2E/DX2 analytically !

! D57 D(8,9,10,11) 0.0972 calculate D2E/DX2 analytically !

! D58 D(8,9,10,26) 179.8008 calculate D2E/DX2 analytically !

! D59 D(33,9,10,11) -179.1882 calculate D2E/DX2 analytically !

! D60 D(33,9,10,26) 0.5153 calculate D2E/DX2 analytically !

! D61 D(8,9,33,22) -0.5893 calculate D2E/DX2 analytically !

! D62 D(8,9,33,34) -179.8095 calculate D2E/DX2 analytically !

! D63 D(10,9,33,22) 178.5823 calculate D2E/DX2 analytically !

! D64 D(10,9,33,34) -0.638 calculate D2E/DX2 analytically !

! D65 D(9,10,11,7) 0.0 calculate D2E/DX2 analytically !

! D66 D(9,10,11,27) 179.6955 calculate D2E/DX2 analytically !

! D67 D(26,10,11,7) -179.6955 calculate D2E/DX2 analytically !

! D68 D(26,10,11,27) 0.0 calculate D2E/DX2 analytically !

! D69 D(2,12,13,14) 178.5823 calculate D2E/DX2 analytically !

! D70 D(2,12,13,17) -0.5893 calculate D2E/DX2 analytically !

! D71 D(35,12,13,14) -0.638 calculate D2E/DX2 analytically !

! D72 D(35,12,13,17) -179.8095 calculate D2E/DX2 analytically !

! D73 D(12,13,14,15) -179.1882 calculate D2E/DX2 analytically !

! D74 D(12,13,14,28) 0.5153 calculate D2E/DX2 analytically !

! D75 D(17,13,14,15) 0.0972 calculate D2E/DX2 analytically !

! D76 D(17,13,14,28) 179.8008 calculate D2E/DX2 analytically !

! D77 D(12,13,17,16) 179.1247 calculate D2E/DX2 analytically !

! D78 D(12,13,17,32) -4.7663 calculate D2E/DX2 analytically !

! D79 D(14,13,17,16) -0.1573 calculate D2E/DX2 analytically !

! D80 D(14,13,17,32) 175.9517 calculate D2E/DX2 analytically !

! D81 D(13,14,15,16) 0.0 calculate D2E/DX2 analytically !

! D82 D(13,14,15,29) 179.6955 calculate D2E/DX2 analytically !

! D83 D(28,14,15,16) -179.6955 calculate D2E/DX2 analytically !

! D84 D(28,14,15,29) 0.0 calculate D2E/DX2 analytically !

! D85 D(14,15,16,17) -0.0972 calculate D2E/DX2 analytically !

! D86 D(14,15,16,18) 179.1882 calculate D2E/DX2 analytically !

! D87 D(29,15,16,17) -179.8008 calculate D2E/DX2 analytically !

! D88 D(29,15,16,18) -0.5153 calculate D2E/DX2 analytically !

! D89 D(15,16,17,13) 0.1573 calculate D2E/DX2 analytically !

! D90 D(15,16,17,32) -175.9517 calculate D2E/DX2 analytically !

! D91 D(18,16,17,13) -179.1247 calculate D2E/DX2 analytically !

! D92 D(18,16,17,32) 4.7663 calculate D2E/DX2 analytically !

! D93 D(15,16,18,19) -178.5823 calculate D2E/DX2 analytically !

! D94 D(15,16,18,40) 0.638 calculate D2E/DX2 analytically !

! D95 D(17,16,18,19) 0.5893 calculate D2E/DX2 analytically !

! D96 D(17,16,18,40) 179.8095 calculate D2E/DX2 analytically !

! D97 D(13,17,32,3) 7.0216 calculate D2E/DX2 analytically !

! D98 D(13,17,32,8) 92.2992 calculate D2E/DX2 analytically !

! D99 D(13,17,32,23) 177.5769 calculate D2E/DX2 analytically !

! D100 D(16,17,32,3) -177.5769 calculate D2E/DX2 analytically !

! D101 D(16,17,32,8) -92.2992 calculate D2E/DX2 analytically !

! D102 D(16,17,32,23) -7.0216 calculate D2E/DX2 analytically !

! D103 D(16,18,19,20) 178.5823 calculate D2E/DX2 analytically !

! D104 D(16,18,19,23) -0.5893 calculate D2E/DX2 analytically !

! D105 D(40,18,19,20) -0.638 calculate D2E/DX2 analytically !

! D106 D(40,18,19,23) -179.8095 calculate D2E/DX2 analytically !

! D107 D(18,19,20,21) -179.1882 calculate D2E/DX2 analytically !

! D108 D(18,19,20,30) 0.5153 calculate D2E/DX2 analytically !

! D109 D(23,19,20,21) 0.0972 calculate D2E/DX2 analytically !

! D110 D(23,19,20,30) 179.8008 calculate D2E/DX2 analytically !

! D111 D(18,19,23,22) 179.1247 calculate D2E/DX2 analytically !

! D112 D(18,19,23,32) -4.7663 calculate D2E/DX2 analytically !

! D113 D(20,19,23,22) -0.1573 calculate D2E/DX2 analytically !

! D114 D(20,19,23,32) 175.9517 calculate D2E/DX2 analytically !

! D115 D(19,20,21,22) 0.0 calculate D2E/DX2 analytically !

! D116 D(19,20,21,31) 179.6955 calculate D2E/DX2 analytically !

! D117 D(30,20,21,22) -179.6955 calculate D2E/DX2 analytically !

! D118 D(30,20,21,31) 0.0 calculate D2E/DX2 analytically !

! D119 D(20,21,22,23) -0.0972 calculate D2E/DX2 analytically !

! D120 D(20,21,22,33) 179.1882 calculate D2E/DX2 analytically !

! D121 D(31,21,22,23) -179.8008 calculate D2E/DX2 analytically !

! D122 D(31,21,22,33) -0.5153 calculate D2E/DX2 analytically !

! D123 D(21,22,23,19) 0.1573 calculate D2E/DX2 analytically !

! D124 D(21,22,23,32) -175.9517 calculate D2E/DX2 analytically !

! D125 D(33,22,23,19) -179.1247 calculate D2E/DX2 analytically !

! D126 D(33,22,23,32) 4.7663 calculate D2E/DX2 analytically !

! D127 D(21,22,33,9) -178.5823 calculate D2E/DX2 analytically !

! D128 D(21,22,33,34) 0.638 calculate D2E/DX2 analytically !

! D129 D(23,22,33,9) 0.5893 calculate D2E/DX2 analytically !

! D130 D(23,22,33,34) 179.8095 calculate D2E/DX2 analytically !

! D131 D(19,23,32,3) 92.2992 calculate D2E/DX2 analytically !

! D132 D(19,23,32,8) 177.5769 calculate D2E/DX2 analytically !

! D133 D(19,23,32,17) 7.0216 calculate D2E/DX2 analytically !

! D134 D(22,23,32,3) -92.2992 calculate D2E/DX2 analytically !

! D135 D(22,23,32,8) -7.0216 calculate D2E/DX2 analytically !

! D136 D(22,23,32,17) -177.5769 calculate D2E/DX2 analytically !

--------------------------------------------------------------------------------

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07

Number of steps in this run= 2 maximum allowed number of steps= 2.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:24:35 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 0.681163 4.273295 -0.039628

2 6 0 1.101995 2.889186 -0.004749

3 7 0 0.000000 2.081690 0.017787

4 6 0 -1.101995 2.889186 -0.004749

5 6 0 -0.681163 4.273295 -0.039628

6 6 0 -2.446135 2.446135 -0.009987

7 6 0 -2.889186 1.101995 -0.004749

8 7 0 -2.081690 0.000000 0.017787

9 6 0 -2.889186 -1.101995 -0.004749

10 6 0 -4.273295 -0.681163 -0.039628

11 6 0 -4.273295 0.681163 -0.039628

12 6 0 2.446135 2.446135 -0.009987

13 6 0 2.889186 1.101995 -0.004749

14 6 0 4.273295 0.681163 -0.039628

15 6 0 4.273295 -0.681163 -0.039628

16 6 0 2.889186 -1.101995 -0.004749

17 7 0 2.081690 0.000000 0.017787

18 6 0 2.446135 -2.446135 -0.009987

19 6 0 1.101995 -2.889186 -0.004749

20 6 0 0.681163 -4.273295 -0.039628

21 6 0 -0.681163 -4.273295 -0.039628

22 6 0 -1.101995 -2.889186 -0.004749

23 7 0 0.000000 -2.081690 0.017787

24 1 0 1.339682 5.128561 -0.065729

25 1 0 -1.339682 5.128561 -0.065729

26 1 0 -5.128561 -1.339682 -0.065729

27 1 0 -5.128561 1.339682 -0.065729

28 1 0 5.128561 1.339682 -0.065729

29 1 0 5.128561 -1.339682 -0.065729

30 1 0 1.339682 -5.128561 -0.065729

31 1 0 -1.339682 -5.128561 -0.065729

32 30 0 0.000000 0.000000 0.190341

33 6 0 -2.446135 -2.446135 -0.009987

34 6 0 -3.454989 -3.454989 -0.039056

35 6 0 3.454989 3.454989 -0.039056

36 6 0 -4.307371 -4.307371 -0.068214

37 6 0 4.307371 4.307371 -0.068214

38 6 0 -3.454989 3.454989 -0.039056

39 6 0 -4.307371 4.307371 -0.068214

40 6 0 3.454989 -3.454989 -0.039056

41 6 0 4.307371 -4.307371 -0.068214

42 1 0 5.061915 -5.061915 -0.091417

43 1 0 -5.061915 -5.061915 -0.091417

44 1 0 -5.061915 5.061915 -0.091417

45 1 0 5.061915 5.061915 -0.091417

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.447091 0.000000

3 N 2.295737 1.366364 0.000000

4 C 2.257571 2.203990 1.366364 0.000000

5 C 1.362327 2.257571 2.295737 1.447091 0.000000

6 C 3.622069 3.575688 2.473290 1.415286 2.540574

7 C 4.775537 4.373052 3.050854 2.527470 3.864418

8 N 5.088979 4.299274 2.943955 3.050854 4.497313

9 C 6.453089 5.644383 4.299274 4.373052 5.811224

10 C 7.006662 6.453089 5.088979 4.775537 6.119645

11 C 6.119645 5.811224 4.497313 3.864418 5.080041

12 C 2.540574 1.415286 2.473290 3.575688 3.622069

13 C 3.864418 2.527470 3.050854 4.373052 4.775537

14 C 5.080041 3.864418 4.497313 5.811224 6.119645

15 C 6.119645 4.775537 5.088979 6.453089 7.006662

16 C 5.811224 4.373052 4.299274 5.644383 6.453089

17 N 4.497313 3.050854 2.943955 4.299274 5.088979

18 C 6.947426 5.502035 5.146411 6.407410 7.411586

19 C 7.174918 5.778373 5.091613 6.184429 7.381193

20 C 8.546589 7.174918 6.391644 7.381193 8.654486

21 C 8.654486 7.381193 6.391644 7.174918 8.546589

22 C 7.381193 6.184429 5.091613 5.778373 7.174918

23 N 6.391644 5.091613 4.163381 5.091613 6.391644

24 H 1.079726 2.252779 3.329436 3.313654 2.194534

25 H 2.194534 3.313654 3.329436 2.252779 1.079726

26 H 8.078310 7.530397 6.165623 5.839545 7.161392

27 H 6.508430 6.420632 5.182633 4.314848 5.327861

28 H 5.327861 4.314848 5.182633 6.420632 6.508430

29 H 7.161392 5.839545 6.165623 7.530397 8.078310

30 H 9.424925 8.021501 7.334129 8.381514 9.616620

31 H 9.616620 8.381514 7.334129 8.021501 9.424925

32 Zn 4.333349 3.098363 2.088830 3.098363 4.333349

33 C 7.411586 6.407410 5.146411 5.502035 6.947426

34 C 8.765508 7.811264 6.526485 6.766559 8.210997

35 C 2.892012 2.420308 3.718350 4.592104 4.216323

36 C 9.925428 9.003095 7.705904 7.878382 9.315473

37 C 3.626481 3.505669 4.849175 5.592542 4.988733

38 C 4.216323 4.592104 3.718350 2.420308 2.892012

39 C 4.988733 5.592542 4.849175 3.505669 3.626481

40 C 8.210997 6.766559 6.526485 7.811264 8.765508

41 C 9.315473 7.878382 7.705904 9.003095 9.925428

42 H 10.312120 8.883046 8.755913 10.060881 10.960464

43 H 10.960464 10.060881 8.755913 8.883046 10.312120

44 H 5.797203 6.536211 5.875088 4.517658 4.451471

45 H 4.451471 4.517658 5.875088 6.536211 5.797203

6 7 8 9 10

6 C 0.000000

7 C 1.415286 0.000000

8 N 2.473290 1.366364 0.000000

9 C 3.575688 2.203990 1.366364 0.000000

10 C 3.622069 2.257571 2.295737 1.447091 0.000000

11 C 2.540574 1.447091 2.295737 2.257571 1.362327

12 C 4.892269 5.502035 5.146411 6.407410 7.411586

13 C 5.502035 5.778373 5.091613 6.184429 7.381193

14 C 6.947426 7.174918 6.391644 7.381193 8.654486

15 C 7.411586 7.381193 6.391644 7.174918 8.546589

16 C 6.407410 6.184429 5.091613 5.778373 7.174918

17 N 5.146411 5.091613 4.163381 5.091613 6.391644

18 C 6.918714 6.407410 5.146411 5.502035 6.947426

19 C 6.407410 5.644383 4.299274 4.373052 5.811224

20 C 7.411586 6.453089 5.088979 4.775537 6.119645

21 C 6.947426 5.811224 4.497313 3.864418 5.080041

22 C 5.502035 4.373052 3.050854 2.527470 3.864418

23 N 5.146411 4.299274 2.943955 3.050854 4.497313

24 H 4.640143 5.839545 6.165623 7.530397 8.078310

25 H 2.902198 4.314848 5.182633 6.420632 6.508430

26 H 4.640143 3.313654 3.329436 2.252779 1.079726

27 H 2.902198 2.252779 3.329436 3.313654 2.194534

28 H 7.655283 8.021501 7.334129 8.381514 9.616620

29 H 8.468266 8.381514 7.334129 8.021501 9.424925

30 H 8.468266 7.530397 6.165623 5.839545 7.161392

31 H 7.655283 6.420632 5.182633 4.314848 5.327861

32 Zn 3.465152 3.098363 2.088830 3.098363 4.333349

33 C 4.892269 3.575688 2.473290 1.415286 2.540574

34 C 5.986810 4.592104 3.718350 2.420308 2.892012

35 C 5.986810 6.766559 6.526485 7.811264 8.765508

36 C 7.005529 5.592542 4.849175 3.505669 3.626481

37 C 7.005529 7.878382 7.705904 9.003095 9.925428

38 C 1.427032 2.420308 3.718350 4.592104 4.216323

39 C 2.632830 3.505669 4.849175 5.592542 4.988733

40 C 8.345500 7.811264 6.526485 6.766559 8.210997

41 C 9.551077 9.003095 7.705904 7.878382 9.315473

42 H 10.618298 10.060881 8.755913 8.883046 10.312120

43 H 7.951085 6.536211 5.875088 4.517658 4.451471

44 H 3.700169 4.517658 5.875088 6.536211 5.797203

45 H 7.951085 8.883046 8.755913 10.060881 10.960464

11 12 13 14 15

11 C 0.000000

12 C 6.947426 0.000000

13 C 7.174918 1.415286 0.000000

14 C 8.546589 2.540574 1.447091 0.000000

15 C 8.654486 3.622069 2.257571 1.362327 0.000000

16 C 7.381193 3.575688 2.203990 2.257571 1.447091

17 N 6.391644 2.473290 1.366364 2.295737 2.295737

18 C 7.411586 4.892269 3.575688 3.622069 2.540574

19 C 6.453089 5.502035 4.373052 4.775537 3.864418

20 C 7.006662 6.947426 5.811224 6.119645 5.080041

21 C 6.119645 7.411586 6.453089 7.006662 6.119645

22 C 4.775537 6.407410 5.644383 6.453089 5.811224

23 N 5.088979 5.146411 4.299274 5.088979 4.497313

24 H 7.161392 2.902198 4.314848 5.327861 6.508430

25 H 5.327861 4.640143 5.839545 7.161392 8.078310

26 H 2.194534 8.468266 8.381514 9.616620 9.424925

27 H 1.079726 7.655283 8.021501 9.424925 9.616620

28 H 9.424925 2.902198 2.252779 1.079726 2.194534

29 H 9.616620 4.640143 3.313654 2.194534 1.079726

30 H 8.078310 7.655283 6.420632 6.508430 5.327861

31 H 6.508430 8.468266 7.530397 8.078310 7.161392

32 Zn 4.333349 3.465152 3.098363 4.333349 4.333349

33 C 3.622069 6.918714 6.407410 7.411586 6.947426

34 C 4.216323 8.345500 7.811264 8.765508 8.210997

35 C 8.210997 1.427032 2.420308 2.892012 4.216323

36 C 4.988733 9.551077 9.003095 9.925428 9.315473

37 C 9.315473 2.632830 3.505669 3.626481 4.988733

38 C 2.892012 5.986810 6.766559 8.210997 8.765508

39 C 3.626481 7.005529 7.878382 9.315473 9.925428

40 C 8.765508 5.986810 4.592104 4.216323 2.892012

41 C 9.925428 7.005529 5.592542 4.988733 3.626481

42 H 10.960464 7.951085 6.536211 5.797203 4.451471

43 H 5.797203 10.618298 10.060881 10.960464 10.312120

44 H 4.451471 7.951085 8.883046 10.312120 10.960464

45 H 10.312120 3.700169 4.517658 4.451471 5.797203

16 17 18 19 20

16 C 0.000000

17 N 1.366364 0.000000

18 C 1.415286 2.473290 0.000000

19 C 2.527470 3.050854 1.415286 0.000000

20 C 3.864418 4.497313 2.540574 1.447091 0.000000

21 C 4.775537 5.088979 3.622069 2.257571 1.362327

22 C 4.373052 4.299274 3.575688 2.203990 2.257571

23 N 3.050854 2.943955 2.473290 1.366364 2.295737

24 H 6.420632 5.182633 7.655283 8.021501 9.424925

25 H 7.530397 6.165623 8.468266 8.381514 9.616620

26 H 8.021501 7.334129 7.655283 6.420632 6.508430

27 H 8.381514 7.334129 8.468266 7.530397 8.078310

28 H 3.313654 3.329436 4.640143 5.839545 7.161392

29 H 2.252779 3.329436 2.902198 4.314848 5.327861

30 H 4.314848 5.182633 2.902198 2.252779 1.079726

31 H 5.839545 6.165623 4.640143 3.313654 2.194534

32 Zn 3.098363 2.088830 3.465152 3.098363 4.333349

33 C 5.502035 5.146411 4.892269 3.575688 3.622069

34 C 6.766559 6.526485 5.986810 4.592104 4.216323

35 C 4.592104 3.718350 5.986810 6.766559 8.210997

36 C 7.878382 7.705904 7.005529 5.592542 4.988733

37 C 5.592542 4.849175 7.005529 7.878382 9.315473

38 C 7.811264 6.526485 8.345500 7.811264 8.765508

39 C 9.003095 7.705904 9.551077 9.003095 9.925428

40 C 2.420308 3.718350 1.427032 2.420308 2.892012

41 C 3.505669 4.849175 2.632830 3.505669 3.626481

42 H 4.517658 5.875088 3.700169 4.517658 4.451471

43 H 8.883046 8.755913 7.951085 6.536211 5.797203

44 H 10.060881 8.755913 10.618298 10.060881 10.960464

45 H 6.536211 5.875088 7.951085 8.883046 10.312120

21 22 23 24 25

21 C 0.000000

22 C 1.447091 0.000000

23 N 2.295737 1.366364 0.000000

24 H 9.616620 8.381514 7.334129 0.000000

25 H 9.424925 8.021501 7.334129 2.679365 0.000000

26 H 5.327861 4.314848 5.182633 9.147477 7.496250

27 H 7.161392 5.839545 6.165623 7.496250 5.358283

28 H 8.078310 7.530397 6.165623 5.358283 7.496250

29 H 6.508430 6.420632 5.182633 7.496250 9.147477

30 H 2.194534 3.313654 3.329436 10.257122 10.601299

31 H 1.079726 2.252779 3.329436 10.601299 10.257122

32 Zn 4.333349 3.098363 2.088830 5.306831 5.306831

33 C 2.540574 1.415286 2.473290 8.468266 7.655283

34 C 2.892012 2.420308 3.718350 9.831933 8.840394

35 C 8.765508 7.811264 6.526485 2.697420 5.078428

36 C 3.626481 3.505669 4.849175 10.996638 9.891612

37 C 9.925428 9.003095 7.705904 3.079210 5.706450

38 C 8.210997 6.766559 6.526485 5.078428 2.697420

39 C 9.315473 7.878382 7.705904 5.706450 3.079210

40 C 4.216323 4.592104 3.718350 8.840394 9.831933

41 C 4.988733 5.592542 4.849175 9.891612 10.996638

42 H 5.797203 6.536211 5.875088 10.849031 12.034406

43 H 4.451471 4.517658 5.875088 12.034406 10.849031

44 H 10.312120 8.883046 8.755913 6.401996 3.722918

45 H 10.960464 10.060881 8.755913 3.722918 6.401996

26 27 28 29 30

26 H 0.000000

27 H 2.679365 0.000000

28 H 10.601299 10.257122 0.000000

29 H 10.257122 10.601299 2.679365 0.000000

30 H 7.496250 9.147477 7.496250 5.358283 0.000000

31 H 5.358283 7.496250 9.147477 7.496250 2.679365

32 Zn 5.306831 5.306831 5.306831 5.306831 5.306831

33 C 2.902198 4.640143 8.468266 7.655283 4.640143

34 C 2.697420 5.078428 9.831933 8.840394 5.078428

35 C 9.831933 8.840394 2.697420 5.078428 8.840394

36 C 3.079210 5.706450 10.996638 9.891612 5.706450

37 C 10.996638 9.891612 3.079210 5.706450 9.891612

38 C 5.078428 2.697420 8.840394 9.831933 9.831933

39 C 5.706450 3.079210 9.891612 10.996638 10.996638

40 C 8.840394 9.831933 5.078428 2.697420 2.697420

41 C 9.891612 10.996638 5.706450 3.079210 3.079210

42 H 10.849031 12.034406 6.401996 3.722918 3.722918

43 H 3.722918 6.401996 12.034406 10.849031 6.401996

44 H 6.401996 3.722918 10.849031 12.034406 12.034406

45 H 12.034406 10.849031 3.722918 6.401996 10.849031

31 32 33 34 35

31 H 0.000000

32 Zn 5.306831 0.000000

33 C 2.902198 3.465152 0.000000

34 C 2.697420 4.891474 1.427032 0.000000

35 C 9.831933 4.891474 8.345500 9.772185 0.000000

36 C 3.079210 6.097028 2.632830 1.205803 10.977674

37 C 10.996638 6.097028 9.551077 10.977674 1.205803

38 C 8.840394 4.891474 5.986810 6.909978 6.909978

39 C 9.891612 6.097028 7.005529 7.809074 7.809074

40 C 5.078428 4.891474 5.986810 6.909978 6.909978

41 C 5.706450 6.097028 7.005529 7.809074 7.809074

42 H 6.401996 7.164172 7.951085 8.667330 8.667330

43 H 3.722918 7.164172 3.700169 2.273140 12.044836

44 H 10.849031 7.164172 7.951085 8.667330 8.667330

45 H 12.034406 7.164172 10.618298 12.044836 2.273140

36 37 38 39 40

36 C 0.000000

37 C 12.183086 0.000000

38 C 7.809074 7.809074 0.000000

39 C 8.614743 8.614743 1.205803 0.000000

40 C 7.809074 7.809074 9.772185 10.977674 0.000000

41 C 8.614743 8.614743 10.977674 12.183086 1.205803

42 H 9.399649 9.399649 12.044836 13.250193 2.273140

43 H 1.067339 13.250193 8.667330 9.399649 8.667330

44 H 9.399649 9.399649 2.273140 1.067339 12.044836

45 H 13.250193 1.067339 8.667330 9.399649 8.667330

41 42 43 44 45

41 C 0.000000

42 H 1.067339 0.000000

43 H 9.399649 10.123831 0.000000

44 H 13.250193 14.317259 10.123831 0.000000

45 H 9.399649 10.123831 14.317259 10.123831 0.000000

Stoichiometry C28H12N4Zn

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

RotChk: IX=3 Diff= 0.00D+00

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -0.681163 -4.273295 -0.041193

2 6 0 -1.101995 -2.889186 -0.006314

3 7 0 0.000000 -2.081690 0.016222

4 6 0 1.101995 -2.889186 -0.006314

5 6 0 0.681163 -4.273295 -0.041193

6 6 0 2.446135 -2.446135 -0.011552

7 6 0 2.889186 -1.101995 -0.006314

8 7 0 2.081690 0.000000 0.016222

9 6 0 2.889186 1.101995 -0.006314

10 6 0 4.273295 0.681163 -0.041193

11 6 0 4.273295 -0.681163 -0.041193

12 6 0 -2.446135 -2.446135 -0.011552

13 6 0 -2.889186 -1.101995 -0.006314

14 6 0 -4.273295 -0.681163 -0.041193

15 6 0 -4.273295 0.681163 -0.041193

16 6 0 -2.889186 1.101995 -0.006314

17 7 0 -2.081690 0.000000 0.016222

18 6 0 -2.446135 2.446135 -0.011552

19 6 0 -1.101995 2.889186 -0.006314

20 6 0 -0.681163 4.273295 -0.041193

21 6 0 0.681163 4.273295 -0.041193

22 6 0 1.101995 2.889186 -0.006314

23 7 0 0.000000 2.081690 0.016222

24 1 0 -1.339682 -5.128561 -0.067294

25 1 0 1.339682 -5.128561 -0.067294

26 1 0 5.128561 1.339682 -0.067294

27 1 0 5.128561 -1.339682 -0.067294

28 1 0 -5.128561 -1.339682 -0.067294

29 1 0 -5.128561 1.339682 -0.067294

30 1 0 -1.339682 5.128561 -0.067294

31 1 0 1.339682 5.128561 -0.067294

32 30 0 0.000000 0.000000 0.188776

33 6 0 2.446135 2.446135 -0.011552

34 6 0 3.454989 3.454989 -0.040621

35 6 0 -3.454989 -3.454989 -0.040621

36 6 0 4.307371 4.307371 -0.069779

37 6 0 -4.307371 -4.307371 -0.069779

38 6 0 3.454989 -3.454989 -0.040621

39 6 0 4.307371 -4.307371 -0.069779

40 6 0 -3.454989 3.454989 -0.040621

41 6 0 -4.307371 4.307371 -0.069779

42 1 0 -5.061915 5.061915 -0.092982

43 1 0 5.061915 5.061915 -0.092982

44 1 0 5.061915 -5.061915 -0.092982

45 1 0 -5.061915 -5.061915 -0.092982

---------------------------------------------------------------------

Rotational constants (GHZ): 0.1465170 0.1465170 0.0733190

Leave Link 202 at Fri Jul 26 14:24:35 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from chk: "ZnTSPsim0.chk" (5D, 7F)

Pseudo-potential data read from chk file.

There are 184 symmetry adapted cartesian basis functions of A1 symmetry.

There are 155 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

110 alpha electrons 110 beta electrons

nuclear repulsion energy 3060.6075485470 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= 9 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= -0.1305299093 Hartrees.

Nuclear repulsion after empirical dispersion term = 3060.4770186377 Hartrees.

No density basis found on file 20724.

Force inversion solution in PCM.

------------------------------------------------------------------------------

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 : Matrix inversion.

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: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

2nd derivatives : Analytical E(r).r(xy)/FMM algorithm (CHGder, D2EAlg=3).

Cavity 2nd 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 = 3898

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.63D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 148

GePol: Fraction of low-weight points (<1% of avg) = 3.80%

GePol: Cavity surface area = 415.581 Ang\*\*2

GePol: Cavity volume = 419.954 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = 0.0083977814 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3060.4854164192 Hartrees.

Leave Link 301 at Fri Jul 26 14:24:35 2019, MaxMem= 1342177280 cpu: 1.3

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44808.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.40D-05 NBF= 172 148 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 172 148 158 158

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= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Fri Jul 26 14:24:35 2019, MaxMem= 1342177280 cpu: 6.5

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 26 14:24:36 2019, MaxMem= 1342177280 cpu: 0.8

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "ZnTSPsim0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Occupied (E) (E) (B2) (A1) (E) (E) (B1) (A1) (B2) (E) (E)

(A2) (B1) (E) (E) (A1) (B1) (E) (E) (A1) (B2)

(E) (E) (A1) (A2) (E) (E) (B1) (B1) (E) (E) (A1)

(A1) (E) (E) (B2) (B1) (E) (E) (A1) (A1) (E) (E)

(B2) (B1) (E) (E) (A2) (A1) (E) (E) (B1) (B1)

(B2) (E) (E) (B2) (A1) (E) (E) (B1) (A2) (A1)

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(B2) (E) (E) (A2) (A1) (B1) (E) (E) (E) (E) (A1)

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(E) (E) (A2) (A1)

Virtual (E) (E) (B1) (A1) (B2) (E) (E) (B2) (B1) (A2)

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(E) (B2) (B1) (E) (E) (A1) (B1) (E) (E) (B1) (A1)

(B1) (B2) (E) (E) (B1) (E) (E) (A2) (E) (E) (B2)

(A1) (B1) (A1) (E) (E) (E) (E) (A2) (B2) (E) (E)

(A2) (A1) (E) (E) (B1) (E) (E) (A1) (A2) (B1)

(B1) (E) (E) (E) (E) (B2) (A1) (E) (E) (B2) (A1)

(E) (E) (B1) (A2) (A1) (E) (E) (B1) (B2) (A1)

(E) (E) (B2) (E) (E) (A2) (B1) (E) (E) (A2) (E)

(E) (A1) (B1) (B2) (A1) (A1) (E) (E) (B1) (A1)

(E) (E) (B2) (B1) (E) (E) (A1) (A2) (E) (E) (B2)

(B1) (E) (E) (A1) (B1) (E) (E) (A2) (B1) (A1)

(E) (E) (B2) (A1) (E) (E)

The electronic state of the initial guess is 1-A1.

Leave Link 401 at Fri Jul 26 14:24:37 2019, MaxMem= 1342177280 cpu: 12.3

(Enter /apps/gaussian/g09d01/g09/l502.exe)

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1385629 IEndB= 1385629 NGot= 1342177280 MDV= 1341259204

LenX= 1341259204 LenY= 1340808292

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.

An orbital has undefined symmetry, so N\*\*3 symmetry is turned off.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 660000000 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= 0 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= 45583212.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.21D-15 for 2261.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.01D-15 for 2192 2004.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.77D-15 for 970.

Iteration 1 A^-1\*A deviation from orthogonality is 1.49D-14 for 1170 1072.

E= -1359.06304578730

DIIS: error= 6.58D-08 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.06304578730 IErMin= 1 ErrMin= 6.58D-08

ErrMax= 6.58D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.18D-12 BMatP= 1.18D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.092 Goal= None Shift= 0.000

RMSDP=3.61D-09 MaxDP=2.11D-07 OVMax= 6.04D-07

Error on total polarization charges = 0.06212

SCF Done: E(RB3LYP) = -1359.06304579 A.U. after 1 cycles

NFock= 1 Conv=0.36D-08 -V/T= 1.9682

KE= 1.403728960756D+03 PE=-9.363055480419D+03 EE= 3.539778057456D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.27

(included in total energy above)

Leave Link 502 at Fri Jul 26 14:24:52 2019, MaxMem= 1342177280 cpu: 150.7

(Enter /apps/gaussian/g09d01/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 636

NBasis= 636 NAE= 110 NBE= 110 NFC= 0 NFV= 0

NROrb= 636 NOA= 110 NOB= 110 NVA= 526 NVB= 526

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.17146699D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.91764214D-01

Leave Link 801 at Fri Jul 26 14:24:52 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l1101.exe)

Using compressed storage, NAtomX= 45.

Will process 46 centers per pass.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44808.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 6 by ecpmxn.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Fri Jul 26 14:24:54 2019, MaxMem= 1342177280 cpu: 22.0

(Enter /apps/gaussian/g09d01/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Fri Jul 26 14:24:54 2019, MaxMem= 1342177280 cpu: 0.8

(Enter /apps/gaussian/g09d01/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 45.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 1342176816.

G2DrvN: will do 46 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFJK: IHMeth= 1 ICntrl= 3107 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= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 0 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

G2PCM: DoFxE=T DoFxN=T DoGrad=T DoDP/DQ/DG/TGxP=FFFF NFrqRd= 0 IEInf=0 SqF1=F DoCFld=F IF1Alg=4.

GePol: Maximum number of non-zero 1st derivatives = 260

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Fri Jul 26 14:25:54 2019, MaxMem= 1342177280 cpu: 707.3

(Enter /apps/gaussian/g09d01/g09/l1002.exe)

Minotr: Closed shell wavefunction.

IDoAtm=111111111111111111111111111111111111111111111

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Using symmetry in CPHF.

Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.

Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.

NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 1342176190 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 0.

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 660000000 NMat= 30 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

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= 0 I1Cent= 0 NGrid= 0

NMat0= 30 NMatS0= 30 NMatT0= 0 NMatD0= 30 NMtDS0= 0 NMtDT0= 0

Integrals replicated using symmetry in FoFCou.

There are 30 degrees of freedom in the 1st order CPHF. IDoFFX=4 NUNeed= 30.

30 vectors produced by pass 0 Test12= 1.93D-13 3.33D-09 XBig12= 2.83D+03 3.63D+01.

AX will form 30 AO Fock derivatives at one time.

30 vectors produced by pass 1 Test12= 1.93D-13 3.33D-09 XBig12= 3.47D+02 3.29D+00.

30 vectors produced by pass 2 Test12= 1.93D-13 3.33D-09 XBig12= 3.73D+01 1.04D+00.

30 vectors produced by pass 3 Test12= 1.93D-13 3.33D-09 XBig12= 9.68D+00 4.75D-01.

30 vectors produced by pass 4 Test12= 1.93D-13 3.33D-09 XBig12= 4.86D-01 9.15D-02.

30 vectors produced by pass 5 Test12= 1.93D-13 3.33D-09 XBig12= 1.43D-02 1.60D-02.

30 vectors produced by pass 6 Test12= 1.93D-13 3.33D-09 XBig12= 3.19D-04 1.93D-03.

30 vectors produced by pass 7 Test12= 1.93D-13 3.33D-09 XBig12= 4.46D-06 1.93D-04.

25 vectors produced by pass 8 Test12= 1.93D-13 3.33D-09 XBig12= 7.38D-08 2.83D-05.

12 vectors produced by pass 9 Test12= 1.93D-13 3.33D-09 XBig12= 5.24D-10 1.95D-06.

3 vectors produced by pass 10 Test12= 1.93D-13 3.33D-09 XBig12= 3.80D-12 1.75D-07.

2 vectors produced by pass 11 Test12= 1.93D-13 3.33D-09 XBig12= 3.44D-14 1.11D-08.

1 vectors produced by pass 12 Test12= 1.93D-13 3.33D-09 XBig12= 9.54D-16 3.58D-09.

InvSVY: IOpt=1 It= 1 EMax= 4.97D-14

Solved reduced A of dimension 283 with 30 vectors.

FullF1: Do perturbations 1 to 30.

Isotropic polarizability for W= 0.000000 904.43 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Fri Jul 26 14:35:16 2019, MaxMem= 1342177280 cpu: 6723.9

(Enter /apps/gaussian/g09d01/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Population analysis using the SCF density.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Orbital symmetries:

Occupied (E) (E) (B2) (A1) (E) (E) (B1) (A1) (B2) (E) (E)

(A2) (B1) (E) (E) (A1) (B1) (E) (E) (A1) (B2)

(E) (E) (A1) (A2) (E) (E) (B1) (B1) (E) (E) (A1)

(A1) (E) (E) (B2) (B1) (E) (E) (A1) (A1) (E) (E)

(B2) (B1) (E) (E) (A2) (A1) (E) (E) (B1) (B1)

(B2) (E) (E) (B2) (A1) (E) (E) (B1) (A2) (A1)

(E) (E) (A1) (E) (E) (B1) (E) (E) (B2) (A1) (A2)

(E) (E) (A1) (B1) (A1) (E) (E) (E) (E) (B2) (B1)

(B2) (E) (E) (A2) (A1) (B1) (E) (E) (E) (E) (A1)

(B2) (E) (E) (A2) (B1) (E) (E) (B2) (A1) (B2)

(E) (E) (A2) (A1)

Virtual (E) (E) (B1) (A1) (B2) (E) (E) (B2) (B1) (A2)

(E) (E) (A1) (E) (E) (A1) (E) (E) (A2) (A1) (E)

(E) (B1) (B2) (A1) (E) (E) (B1) (E) (E) (A2) (A1)

(A1) (B1) (E) (E) (E) (E) (A1) (B1) (A1) (E) (E)

(B2) (A1) (B1) (E) (E) (E) (E) (B2) (A1) (B1)

(A2) (E) (E) (A1) (B1) (B2) (E) (E) (A1) (E) (E)

(B1) (E) (E) (E) (E) (B2) (B1) (A1) (A1) (A2)

(A2) (B2) (E) (E) (B1) (E) (E) (A1) (E) (E) (B1)

(E) (E) (B2) (A1) (A2) (B1) (E) (E) (E) (E) (A2)

(A1) (E) (E) (E) (E) (A2) (B1) (B2) (B2) (A1)

(E) (E) (B1) (A1) (E) (E) (E) (E) (E) (E) (A2)

(A1) (B1) (E) (E) (B1) (A1) (B2) (A1) (E) (E)

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(E) (E) (A1) (E) (E) (A2) (A2) (B1) (E) (E) (B2)

(A2) (E) (E) (B2) (B1) (E) (E) (A1) (A1) (A1)

(B1) (B1) (A2) (E) (E) (B2) (E) (E) (E) (E) (A1)

(A2) (B1) (E) (E) (E) (E) (B1) (E) (E) (B2) (A2)

(B2) (A2) (B1) (A1) (A1) (E) (E) (B1) (E) (E)

(E) (E) (A2) (A1) (B1) (E) (E) (B2) (E) (E) (E)

(E) (A1) (B1) (A2) (B1) (E) (E) (A1) (B1) (B2)

(A2) (E) (E) (E) (E) (A1) (B1) (B2) (E) (E) (A2)

(B2) (B2) (E) (E) (E) (E) (B1) (A1) (A1) (E) (E)

(A1) (A2) (E) (E) (A1) (B1) (E) (E) (A2) (B2)

(E) (E) (B1) (E) (E) (A1) (B2) (B1) (E) (E) (E)

(E) (A1) (B2) (E) (E) (A2) (A2) (A1) (A2) (E)

(E) (B2) (B1) (E) (E) (A1) (B1) (E) (E) (B1) (A1)

(B1) (B2) (E) (E) (B1) (E) (E) (A2) (E) (E) (B2)

(A1) (B1) (A1) (E) (E) (E) (E) (A2) (B2) (E) (E)

(A2) (A1) (E) (E) (B1) (E) (E) (A1) (A2) (B1)

(B1) (E) (E) (E) (E) (B2) (A1) (E) (E) (B2) (A1)

(E) (E) (B1) (A2) (A1) (E) (E) (B1) (B2) (A1)

(E) (E) (B2) (E) (E) (A2) (B1) (E) (E) (A2) (E)

(E) (A1) (B1) (B2) (A1) (A1) (E) (E) (B1) (A1)

(E) (E) (B2) (B1) (E) (E) (A1) (A2) (E) (E) (B2)

(B1) (E) (E) (A1) (B1) (E) (E) (A2) (B1) (A1)

(E) (E) (B2) (A1) (E) (E)

The electronic state is 1-A1.

Alpha occ. eigenvalues -- -14.31369 -14.31369 -14.31369 -14.31369 -10.22115

Alpha occ. eigenvalues -- -10.22115 -10.22115 -10.22115 -10.22110 -10.22110

Alpha occ. eigenvalues -- -10.22110 -10.22109 -10.21962 -10.21962 -10.21962

Alpha occ. eigenvalues -- -10.21962 -10.18473 -10.18473 -10.18473 -10.18473

Alpha occ. eigenvalues -- -10.17612 -10.17612 -10.17612 -10.17612 -10.17545

Alpha occ. eigenvalues -- -10.17545 -10.17545 -10.17545 -10.17333 -10.17333

Alpha occ. eigenvalues -- -10.17333 -10.17333 -0.97589 -0.96735 -0.96735

Alpha occ. eigenvalues -- -0.95831 -0.85157 -0.83124 -0.83124 -0.81112

Alpha occ. eigenvalues -- -0.77599 -0.77562 -0.77562 -0.77049 -0.75439

Alpha occ. eigenvalues -- -0.74799 -0.74799 -0.73048 -0.73025 -0.67757

Alpha occ. eigenvalues -- -0.67757 -0.62755 -0.60281 -0.60008 -0.59177

Alpha occ. eigenvalues -- -0.59177 -0.58232 -0.57363 -0.56212 -0.56212

Alpha occ. eigenvalues -- -0.55931 -0.55762 -0.55260 -0.55062 -0.55062

Alpha occ. eigenvalues -- -0.53251 -0.52447 -0.52447 -0.52236 -0.51480

Alpha occ. eigenvalues -- -0.51480 -0.50602 -0.49353 -0.46080 -0.45053

Alpha occ. eigenvalues -- -0.45053 -0.44349 -0.43325 -0.43009 -0.42836

Alpha occ. eigenvalues -- -0.42836 -0.41487 -0.41487 -0.40238 -0.40043

Alpha occ. eigenvalues -- -0.39143 -0.38491 -0.38491 -0.38157 -0.37979

Alpha occ. eigenvalues -- -0.37512 -0.34121 -0.34121 -0.32569 -0.32569

Alpha occ. eigenvalues -- -0.32438 -0.29690 -0.29375 -0.29375 -0.29046

Alpha occ. eigenvalues -- -0.27628 -0.26959 -0.26959 -0.26951 -0.26852

Alpha occ. eigenvalues -- -0.25593 -0.25264 -0.25264 -0.21127 -0.19948

Alpha virt. eigenvalues -- -0.10772 -0.10772 -0.05723 0.02329 0.02815

Alpha virt. eigenvalues -- 0.03136 0.03136 0.03186 0.03560 0.03713

Alpha virt. eigenvalues -- 0.04156 0.04156 0.04667 0.05001 0.05001

Alpha virt. eigenvalues -- 0.05435 0.05692 0.05692 0.06456 0.07825

Alpha virt. eigenvalues -- 0.08474 0.08474 0.08531 0.09705 0.09866

Alpha virt. eigenvalues -- 0.09871 0.09871 0.11480 0.12501 0.12501

Alpha virt. eigenvalues -- 0.13632 0.14222 0.15241 0.16423 0.16440

Alpha virt. eigenvalues -- 0.16440 0.17328 0.17328 0.19266 0.19859

Alpha virt. eigenvalues -- 0.22271 0.23139 0.23139 0.23594 0.24239

Alpha virt. eigenvalues -- 0.24325 0.24978 0.24978 0.25752 0.25752

Alpha virt. eigenvalues -- 0.26476 0.26631 0.26839 0.27939 0.29888

Alpha virt. eigenvalues -- 0.29888 0.30995 0.31128 0.32419 0.32471

Alpha virt. eigenvalues -- 0.32471 0.35157 0.35212 0.35212 0.35222

Alpha virt. eigenvalues -- 0.35666 0.35666 0.36252 0.36252 0.36464

Alpha virt. eigenvalues -- 0.36598 0.36980 0.37934 0.38490 0.39516

Alpha virt. eigenvalues -- 0.40000 0.40456 0.40456 0.40468 0.41370

Alpha virt. eigenvalues -- 0.41370 0.41511 0.42069 0.42069 0.43234

Alpha virt. eigenvalues -- 0.43587 0.43587 0.43666 0.44406 0.44572

Alpha virt. eigenvalues -- 0.45228 0.45651 0.45651 0.47278 0.47278

Alpha virt. eigenvalues -- 0.47752 0.48205 0.48965 0.48965 0.49457

Alpha virt. eigenvalues -- 0.49457 0.50757 0.51108 0.51274 0.51342

Alpha virt. eigenvalues -- 0.51740 0.51995 0.51995 0.52017 0.55011

Alpha virt. eigenvalues -- 0.56221 0.56221 0.57142 0.57142 0.57621

Alpha virt. eigenvalues -- 0.57621 0.57654 0.57724 0.58181 0.58795

Alpha virt. eigenvalues -- 0.58795 0.61353 0.62061 0.62106 0.62334

Alpha virt. eigenvalues -- 0.62351 0.62351 0.63163 0.63383 0.63383

Alpha virt. eigenvalues -- 0.63936 0.64321 0.64882 0.65267 0.65267

Alpha virt. eigenvalues -- 0.65349 0.68252 0.68252 0.68940 0.69020

Alpha virt. eigenvalues -- 0.69898 0.70189 0.70488 0.70488 0.71741

Alpha virt. eigenvalues -- 0.71741 0.73651 0.73721 0.73721 0.74453

Alpha virt. eigenvalues -- 0.74547 0.74547 0.74702 0.74883 0.75272

Alpha virt. eigenvalues -- 0.75272 0.77057 0.77762 0.79147 0.81252

Alpha virt. eigenvalues -- 0.81252 0.81780 0.82354 0.83203 0.84288

Alpha virt. eigenvalues -- 0.84288 0.85799 0.85799 0.85831 0.88301

Alpha virt. eigenvalues -- 0.89968 0.90758 0.91080 0.91320 0.92713

Alpha virt. eigenvalues -- 0.92713 0.94800 0.95712 0.95712 0.95988

Alpha virt. eigenvalues -- 0.97562 0.97562 0.99754 1.00368 1.00368

Alpha virt. eigenvalues -- 1.00855 1.01435 1.01506 1.02202 1.02202

Alpha virt. eigenvalues -- 1.04674 1.05361 1.05555 1.05555 1.06079

Alpha virt. eigenvalues -- 1.07063 1.07160 1.08818 1.08818 1.11556

Alpha virt. eigenvalues -- 1.12268 1.12268 1.12448 1.12486 1.13384

Alpha virt. eigenvalues -- 1.13384 1.13737 1.13900 1.14208 1.15299

Alpha virt. eigenvalues -- 1.15299 1.16299 1.16299 1.16772 1.17345

Alpha virt. eigenvalues -- 1.18291 1.18757 1.18757 1.19175 1.19321

Alpha virt. eigenvalues -- 1.20995 1.20995 1.21156 1.21171 1.22270

Alpha virt. eigenvalues -- 1.23621 1.24722 1.24722 1.25221 1.25864

Alpha virt. eigenvalues -- 1.25864 1.28049 1.28049 1.28443 1.29010

Alpha virt. eigenvalues -- 1.31357 1.32191 1.34067 1.34067 1.34239

Alpha virt. eigenvalues -- 1.37469 1.42229 1.42690 1.42690 1.47389

Alpha virt. eigenvalues -- 1.47634 1.48556 1.48556 1.49560 1.51757

Alpha virt. eigenvalues -- 1.51757 1.52788 1.55154 1.55154 1.55336

Alpha virt. eigenvalues -- 1.55386 1.55386 1.55419 1.56945 1.57633

Alpha virt. eigenvalues -- 1.58167 1.58482 1.58482 1.58932 1.58932

Alpha virt. eigenvalues -- 1.59450 1.61056 1.61544 1.61544 1.62882

Alpha virt. eigenvalues -- 1.62882 1.63251 1.64325 1.65036 1.65594

Alpha virt. eigenvalues -- 1.66246 1.66583 1.66583 1.70017 1.70017

Alpha virt. eigenvalues -- 1.72123 1.72662 1.73685 1.75128 1.76873

Alpha virt. eigenvalues -- 1.76982 1.76982 1.78961 1.78961 1.79362

Alpha virt. eigenvalues -- 1.80018 1.80018 1.80079 1.80733 1.81194

Alpha virt. eigenvalues -- 1.84079 1.84079 1.85428 1.86277 1.87712

Alpha virt. eigenvalues -- 1.87712 1.88534 1.88641 1.89401 1.89401

Alpha virt. eigenvalues -- 1.89526 1.90049 1.90700 1.93421 1.94385

Alpha virt. eigenvalues -- 1.94504 1.94682 1.94682 1.94750 1.95757

Alpha virt. eigenvalues -- 1.95757 1.97368 1.97368 1.99099 1.99859

Alpha virt. eigenvalues -- 2.00617 2.03248 2.03248 2.04267 2.04267

Alpha virt. eigenvalues -- 2.04275 2.09215 2.09215 2.11643 2.11703

Alpha virt. eigenvalues -- 2.13725 2.18046 2.19806 2.25706 2.26961

Alpha virt. eigenvalues -- 2.27870 2.27870 2.28395 2.31370 2.31370

Alpha virt. eigenvalues -- 2.33508 2.33508 2.34669 2.35954 2.36261

Alpha virt. eigenvalues -- 2.36527 2.36527 2.37540 2.40594 2.40594

Alpha virt. eigenvalues -- 2.40748 2.40748 2.41097 2.41410 2.43138

Alpha virt. eigenvalues -- 2.45429 2.48456 2.48456 2.49408 2.49994

Alpha virt. eigenvalues -- 2.52320 2.53379 2.53964 2.53964 2.56228

Alpha virt. eigenvalues -- 2.56228 2.57032 2.57451 2.57739 2.57991

Alpha virt. eigenvalues -- 2.57991 2.60077 2.60560 2.61986 2.62502

Alpha virt. eigenvalues -- 2.62502 2.64689 2.64689 2.64719 2.66654

Alpha virt. eigenvalues -- 2.67614 2.71221 2.71221 2.73413 2.76570

Alpha virt. eigenvalues -- 2.78003 2.78003 2.79920 2.80961 2.82610

Alpha virt. eigenvalues -- 2.82610 2.83369 2.83883 2.87108 2.87108

Alpha virt. eigenvalues -- 2.88554 2.88580 2.88580 2.88617 2.92033

Alpha virt. eigenvalues -- 2.95166 2.95547 2.95547 2.96203 2.96203

Alpha virt. eigenvalues -- 2.97019 2.97823 2.98870 2.98870 2.99784

Alpha virt. eigenvalues -- 3.00241 3.01364 3.03009 3.03843 3.03843

Alpha virt. eigenvalues -- 3.04134 3.04463 3.05477 3.05477 3.06919

Alpha virt. eigenvalues -- 3.07898 3.08318 3.08318 3.09022 3.16978

Alpha virt. eigenvalues -- 3.17708 3.17929 3.18347 3.18347 3.21095

Alpha virt. eigenvalues -- 3.21681 3.21681 3.24246 3.25878 3.25878

Alpha virt. eigenvalues -- 3.28645 3.29945 3.30869 3.31621 3.32327

Alpha virt. eigenvalues -- 3.32327 3.33135 3.33135 3.35494 3.35724

Alpha virt. eigenvalues -- 3.37578 3.37578 3.44351 3.48402 3.52178

Alpha virt. eigenvalues -- 3.52178 3.52998 3.56926 3.56926 3.57171

Alpha virt. eigenvalues -- 3.57507 3.58659 3.62925 3.65470 3.65470

Alpha virt. eigenvalues -- 3.81935 3.81935 3.82132 3.84306 3.85904

Alpha virt. eigenvalues -- 3.85904 3.85979 3.89712 3.93137 3.93137

Alpha virt. eigenvalues -- 3.96707 3.99847 4.11459 4.20185 4.20185

Alpha virt. eigenvalues -- 4.32222 4.33336 4.46988 4.51348 4.51348

Alpha virt. eigenvalues -- 4.61463 4.65301 4.65301 4.65588 5.14284

Alpha virt. eigenvalues -- 5.19431 5.19431 5.32016 7.78665 7.78665

Alpha virt. eigenvalues -- 7.86755 7.92613 8.12981 11.11649 23.26999

Alpha virt. eigenvalues -- 23.32268 23.32268 23.35159 23.51644 23.54832

Alpha virt. eigenvalues -- 23.54832 23.56922 23.74598 23.76313 23.76313

Alpha virt. eigenvalues -- 23.78165 23.90765 23.93313 23.93313 23.95996

Alpha virt. eigenvalues -- 24.00276 24.01839 24.01839 24.02864 24.12630

Alpha virt. eigenvalues -- 24.13089 24.13089 24.13768 24.94111 24.94170

Alpha virt. eigenvalues -- 24.94485 24.94485 35.62586 35.64057 35.65236

Alpha virt. eigenvalues -- 35.65236

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 5.149060 0.403874 -0.077456 -0.062245 0.532933 0.014010

2 C 0.403874 4.873704 0.434511 -0.146366 -0.062245 -0.001304

3 N -0.077456 0.434511 6.953406 0.434511 -0.077456 -0.017626

4 C -0.062245 -0.146366 0.434511 4.873704 0.403874 0.406627

5 C 0.532933 -0.062245 -0.077456 0.403874 5.149060 -0.074407

6 C 0.014010 -0.001304 -0.017626 0.406627 -0.074407 5.211688

7 C -0.001244 -0.000385 -0.020679 -0.104649 0.012920 0.406627

8 N 0.000056 0.000450 -0.013160 -0.020679 -0.000357 -0.017626

9 C -0.000005 0.000001 0.000450 -0.000385 0.000046 -0.001304

10 C 0.000001 -0.000005 0.000056 -0.001244 -0.000006 0.014010

11 C -0.000006 0.000046 -0.000357 0.012920 -0.000158 -0.074407

12 C -0.074407 0.406627 -0.017626 -0.001304 0.014010 -0.002349

13 C 0.012920 -0.104649 -0.020679 -0.000385 -0.001244 0.000218

14 C -0.000158 0.012920 -0.000357 0.000046 -0.000006 0.000001

15 C -0.000006 -0.001244 0.000056 -0.000005 0.000001 0.000000

16 C 0.000046 -0.000385 0.000450 0.000001 -0.000005 0.000001

17 N -0.000357 -0.020679 -0.013160 0.000450 0.000056 -0.000176

18 C 0.000001 0.000218 -0.000176 0.000001 0.000000 0.000003

19 C 0.000000 -0.000065 0.000168 -0.000004 0.000000 0.000001

20 C 0.000000 0.000000 0.000002 0.000000 0.000000 0.000000

21 C 0.000000 0.000000 0.000002 0.000000 0.000000 0.000001

22 C 0.000000 -0.000004 0.000168 -0.000065 0.000000 0.000218

23 N 0.000002 0.000168 -0.001708 0.000168 0.000002 -0.000176

24 H 0.388265 -0.038191 0.005131 0.005560 -0.032996 -0.000165

25 H -0.032996 0.005560 0.005131 -0.038191 0.388265 -0.005200

26 H 0.000000 0.000000 0.000002 0.000010 0.000000 -0.000165

27 H 0.000000 0.000001 -0.000003 0.000009 0.000006 -0.005200

28 H 0.000006 0.000009 -0.000003 0.000001 0.000000 0.000000

29 H 0.000000 0.000010 0.000002 0.000000 0.000000 0.000000

30 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

31 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

32 Zn 0.002023 -0.014094 0.128946 -0.014094 0.002023 -0.011292

33 C 0.000000 0.000001 -0.000176 0.000218 0.000001 -0.002349

34 C 0.000000 0.000000 0.000000 0.000003 0.000000 -0.000056

35 C -0.014881 -0.075725 0.004290 -0.000520 0.002633 -0.000056

36 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

37 C -0.000558 -0.005172 -0.000051 -0.000051 0.000359 -0.000002

38 C 0.002633 -0.000520 0.004290 -0.075725 -0.014881 0.541474

39 C 0.000359 -0.000051 -0.000051 -0.005172 -0.000558 -0.105008

40 C 0.000000 0.000003 0.000000 0.000000 0.000000 0.000000

41 C 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 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000002 0.000000 0.000001 -0.000035 0.000096 0.001819

45 H 0.000096 -0.000035 0.000001 0.000000 0.000002 0.000000

7 8 9 10 11 12

1 C -0.001244 0.000056 -0.000005 0.000001 -0.000006 -0.074407

2 C -0.000385 0.000450 0.000001 -0.000005 0.000046 0.406627

3 N -0.020679 -0.013160 0.000450 0.000056 -0.000357 -0.017626

4 C -0.104649 -0.020679 -0.000385 -0.001244 0.012920 -0.001304

5 C 0.012920 -0.000357 0.000046 -0.000006 -0.000158 0.014010

6 C 0.406627 -0.017626 -0.001304 0.014010 -0.074407 -0.002349

7 C 4.873704 0.434511 -0.146366 -0.062245 0.403874 0.000218

8 N 0.434511 6.953406 0.434511 -0.077456 -0.077456 -0.000176

9 C -0.146366 0.434511 4.873704 0.403874 -0.062245 0.000001

10 C -0.062245 -0.077456 0.403874 5.149060 0.532933 0.000000

11 C 0.403874 -0.077456 -0.062245 0.532933 5.149060 0.000001

12 C 0.000218 -0.000176 0.000001 0.000000 0.000001 5.211688

13 C -0.000065 0.000168 -0.000004 0.000000 0.000000 0.406627

14 C 0.000000 0.000002 0.000000 0.000000 0.000000 -0.074407

15 C 0.000000 0.000002 0.000000 0.000000 0.000000 0.014010

16 C -0.000004 0.000168 -0.000065 0.000000 0.000000 -0.001304

17 N 0.000168 -0.001708 0.000168 0.000002 0.000002 -0.017626

18 C 0.000001 -0.000176 0.000218 0.000001 0.000000 -0.002349

19 C 0.000001 0.000450 -0.000385 0.000046 -0.000005 0.000218

20 C -0.000005 0.000056 -0.001244 -0.000006 0.000001 0.000001

21 C 0.000046 -0.000357 0.012920 -0.000158 -0.000006 0.000000

22 C -0.000385 -0.020679 -0.104649 0.012920 -0.001244 0.000001

23 N 0.000450 -0.013160 -0.020679 -0.000357 0.000056 -0.000176

24 H 0.000010 0.000002 0.000000 0.000000 0.000000 -0.005200

25 H 0.000009 -0.000003 0.000001 0.000000 0.000006 -0.000165

26 H 0.005560 0.005131 -0.038191 0.388265 -0.032996 0.000000

27 H -0.038191 0.005131 0.005560 -0.032996 0.388265 0.000000

28 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.005200

29 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000165

30 H 0.000000 0.000002 0.000010 0.000000 0.000000 0.000000

31 H 0.000001 -0.000003 0.000009 0.000006 0.000000 0.000000

32 Zn -0.014094 0.128946 -0.014094 0.002023 0.002023 -0.011292

33 C -0.001304 -0.017626 0.406627 -0.074407 0.014010 0.000003

34 C -0.000520 0.004290 -0.075725 -0.014881 0.002633 0.000000

35 C 0.000003 0.000000 0.000000 0.000000 0.000000 0.541474

36 C -0.000051 -0.000051 -0.005172 -0.000558 0.000359 0.000000

37 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.105008

38 C -0.075725 0.004290 -0.000520 0.002633 -0.014881 -0.000056

39 C -0.005172 -0.000051 -0.000051 0.000359 -0.000558 -0.000002

40 C 0.000000 0.000000 0.000003 0.000000 0.000000 -0.000056

41 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

43 H 0.000000 0.000001 -0.000035 0.000096 0.000002 0.000000

44 H -0.000035 0.000001 0.000000 0.000002 0.000096 0.000000

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.001819

13 14 15 16 17 18

1 C 0.012920 -0.000158 -0.000006 0.000046 -0.000357 0.000001

2 C -0.104649 0.012920 -0.001244 -0.000385 -0.020679 0.000218

3 N -0.020679 -0.000357 0.000056 0.000450 -0.013160 -0.000176

4 C -0.000385 0.000046 -0.000005 0.000001 0.000450 0.000001

5 C -0.001244 -0.000006 0.000001 -0.000005 0.000056 0.000000

6 C 0.000218 0.000001 0.000000 0.000001 -0.000176 0.000003

7 C -0.000065 0.000000 0.000000 -0.000004 0.000168 0.000001

8 N 0.000168 0.000002 0.000002 0.000168 -0.001708 -0.000176

9 C -0.000004 0.000000 0.000000 -0.000065 0.000168 0.000218

10 C 0.000000 0.000000 0.000000 0.000000 0.000002 0.000001

11 C 0.000000 0.000000 0.000000 0.000000 0.000002 0.000000

12 C 0.406627 -0.074407 0.014010 -0.001304 -0.017626 -0.002349

13 C 4.873704 0.403874 -0.062245 -0.146366 0.434511 -0.001304

14 C 0.403874 5.149060 0.532933 -0.062245 -0.077456 0.014010

15 C -0.062245 0.532933 5.149060 0.403874 -0.077456 -0.074407

16 C -0.146366 -0.062245 0.403874 4.873704 0.434511 0.406627

17 N 0.434511 -0.077456 -0.077456 0.434511 6.953406 -0.017626

18 C -0.001304 0.014010 -0.074407 0.406627 -0.017626 5.211688

19 C -0.000385 -0.001244 0.012920 -0.104649 -0.020679 0.406627

20 C 0.000046 -0.000006 -0.000158 0.012920 -0.000357 -0.074407

21 C -0.000005 0.000001 -0.000006 -0.001244 0.000056 0.014010

22 C 0.000001 -0.000005 0.000046 -0.000385 0.000450 -0.001304

23 N 0.000450 0.000056 -0.000357 -0.020679 -0.013160 -0.017626

24 H 0.000009 0.000006 0.000000 0.000001 -0.000003 0.000000

25 H 0.000010 0.000000 0.000000 0.000000 0.000002 0.000000

26 H 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 H -0.038191 0.388265 -0.032996 0.005560 0.005131 -0.000165

29 H 0.005560 -0.032996 0.388265 -0.038191 0.005131 -0.005200

30 H 0.000001 0.000000 0.000006 0.000009 -0.000003 -0.005200

31 H 0.000000 0.000000 0.000000 0.000010 0.000002 -0.000165

32 Zn -0.014094 0.002023 0.002023 -0.014094 0.128946 -0.011292

33 C 0.000001 0.000000 0.000001 0.000218 -0.000176 -0.002349

34 C 0.000000 0.000000 0.000000 0.000003 0.000000 -0.000056

35 C -0.075725 -0.014881 0.002633 -0.000520 0.004290 -0.000056

36 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

37 C -0.005172 -0.000558 0.000359 -0.000051 -0.000051 -0.000002

38 C 0.000003 0.000000 0.000000 0.000000 0.000000 0.000000

39 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

40 C -0.000520 0.002633 -0.014881 -0.075725 0.004290 0.541474

41 C -0.000051 0.000359 -0.000558 -0.005172 -0.000051 -0.105008

42 H 0.000000 0.000002 0.000096 -0.000035 0.000001 0.001819

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 -0.000035 0.000096 0.000002 0.000000 0.000001 0.000000

19 20 21 22 23 24

1 C 0.000000 0.000000 0.000000 0.000000 0.000002 0.388265

2 C -0.000065 0.000000 0.000000 -0.000004 0.000168 -0.038191

3 N 0.000168 0.000002 0.000002 0.000168 -0.001708 0.005131

4 C -0.000004 0.000000 0.000000 -0.000065 0.000168 0.005560

5 C 0.000000 0.000000 0.000000 0.000000 0.000002 -0.032996

6 C 0.000001 0.000000 0.000001 0.000218 -0.000176 -0.000165

7 C 0.000001 -0.000005 0.000046 -0.000385 0.000450 0.000010

8 N 0.000450 0.000056 -0.000357 -0.020679 -0.013160 0.000002

9 C -0.000385 -0.001244 0.012920 -0.104649 -0.020679 0.000000

10 C 0.000046 -0.000006 -0.000158 0.012920 -0.000357 0.000000

11 C -0.000005 0.000001 -0.000006 -0.001244 0.000056 0.000000

12 C 0.000218 0.000001 0.000000 0.000001 -0.000176 -0.005200

13 C -0.000385 0.000046 -0.000005 0.000001 0.000450 0.000009

14 C -0.001244 -0.000006 0.000001 -0.000005 0.000056 0.000006

15 C 0.012920 -0.000158 -0.000006 0.000046 -0.000357 0.000000

16 C -0.104649 0.012920 -0.001244 -0.000385 -0.020679 0.000001

17 N -0.020679 -0.000357 0.000056 0.000450 -0.013160 -0.000003

18 C 0.406627 -0.074407 0.014010 -0.001304 -0.017626 0.000000

19 C 4.873704 0.403874 -0.062245 -0.146366 0.434511 0.000000

20 C 0.403874 5.149060 0.532933 -0.062245 -0.077456 0.000000

21 C -0.062245 0.532933 5.149060 0.403874 -0.077456 0.000000

22 C -0.146366 -0.062245 0.403874 4.873704 0.434511 0.000000

23 N 0.434511 -0.077456 -0.077456 0.434511 6.953406 0.000000

24 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.427518

25 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.002192

26 H 0.000001 0.000000 0.000006 0.000009 -0.000003 0.000000

27 H 0.000000 0.000000 0.000000 0.000010 0.000002 0.000000

28 H 0.000010 0.000000 0.000000 0.000000 0.000002 -0.000006

29 H 0.000009 0.000006 0.000000 0.000001 -0.000003 0.000000

30 H -0.038191 0.388265 -0.032996 0.005560 0.005131 0.000000

31 H 0.005560 -0.032996 0.388265 -0.038191 0.005131 0.000000

32 Zn -0.014094 0.002023 0.002023 -0.014094 0.128946 -0.000363

33 C -0.001304 0.014010 -0.074407 0.406627 -0.017626 0.000000

34 C -0.000520 0.002633 -0.014881 -0.075725 0.004290 0.000000

35 C 0.000003 0.000000 0.000000 0.000000 0.000000 0.006422

36 C -0.000051 0.000359 -0.000558 -0.005172 -0.000051 0.000000

37 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.003287

38 C 0.000000 0.000000 0.000000 0.000003 0.000000 -0.000084

39 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000009

40 C -0.075725 -0.014881 0.002633 -0.000520 0.004290 0.000000

41 C -0.005172 -0.000558 0.000359 -0.000051 -0.000051 0.000000

42 H -0.000035 0.000096 0.000002 0.000000 0.000001 0.000000

43 H 0.000000 0.000002 0.000096 -0.000035 0.000001 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 0.000054

25 26 27 28 29 30

1 C -0.032996 0.000000 0.000000 0.000006 0.000000 0.000000

2 C 0.005560 0.000000 0.000001 0.000009 0.000010 0.000000

3 N 0.005131 0.000002 -0.000003 -0.000003 0.000002 0.000000

4 C -0.038191 0.000010 0.000009 0.000001 0.000000 0.000000

5 C 0.388265 0.000000 0.000006 0.000000 0.000000 0.000000

6 C -0.005200 -0.000165 -0.005200 0.000000 0.000000 0.000000

7 C 0.000009 0.005560 -0.038191 0.000000 0.000000 0.000000

8 N -0.000003 0.005131 0.005131 0.000000 0.000000 0.000002

9 C 0.000001 -0.038191 0.005560 0.000000 0.000000 0.000010

10 C 0.000000 0.388265 -0.032996 0.000000 0.000000 0.000000

11 C 0.000006 -0.032996 0.388265 0.000000 0.000000 0.000000

12 C -0.000165 0.000000 0.000000 -0.005200 -0.000165 0.000000

13 C 0.000010 0.000000 0.000000 -0.038191 0.005560 0.000001

14 C 0.000000 0.000000 0.000000 0.388265 -0.032996 0.000000

15 C 0.000000 0.000000 0.000000 -0.032996 0.388265 0.000006

16 C 0.000000 0.000000 0.000000 0.005560 -0.038191 0.000009

17 N 0.000002 0.000000 0.000000 0.005131 0.005131 -0.000003

18 C 0.000000 0.000000 0.000000 -0.000165 -0.005200 -0.005200

19 C 0.000000 0.000001 0.000000 0.000010 0.000009 -0.038191

20 C 0.000000 0.000000 0.000000 0.000000 0.000006 0.388265

21 C 0.000000 0.000006 0.000000 0.000000 0.000000 -0.032996

22 C 0.000000 0.000009 0.000010 0.000000 0.000001 0.005560

23 N 0.000000 -0.000003 0.000002 0.000002 -0.000003 0.005131

24 H -0.002192 0.000000 0.000000 -0.000006 0.000000 0.000000

25 H 0.427518 0.000000 -0.000006 0.000000 0.000000 0.000000

26 H 0.000000 0.427518 -0.002192 0.000000 0.000000 0.000000

27 H -0.000006 -0.002192 0.427518 0.000000 0.000000 0.000000

28 H 0.000000 0.000000 0.000000 0.427518 -0.002192 0.000000

29 H 0.000000 0.000000 0.000000 -0.002192 0.427518 -0.000006

30 H 0.000000 0.000000 0.000000 0.000000 -0.000006 0.427518

31 H 0.000000 -0.000006 0.000000 0.000000 0.000000 -0.002192

32 Zn -0.000363 -0.000363 -0.000363 -0.000363 -0.000363 -0.000363

33 C 0.000000 -0.005200 -0.000165 0.000000 0.000000 -0.000165

34 C 0.000000 0.006422 -0.000084 0.000000 0.000000 -0.000084

35 C -0.000084 0.000000 0.000000 0.006422 -0.000084 0.000000

36 C 0.000000 0.003287 -0.000009 0.000000 0.000000 -0.000009

37 C -0.000009 0.000000 0.000000 0.003287 -0.000009 0.000000

38 C 0.006422 -0.000084 0.006422 0.000000 0.000000 0.000000

39 C 0.003287 -0.000009 0.003287 0.000000 0.000000 0.000000

40 C 0.000000 0.000000 0.000000 -0.000084 0.006422 0.006422

41 C 0.000000 0.000000 0.000000 -0.000009 0.003287 0.003287

42 H 0.000000 0.000000 0.000000 0.000000 0.000054 0.000054

43 H 0.000000 0.000054 0.000000 0.000000 0.000000 0.000000

44 H 0.000054 0.000000 0.000054 0.000000 0.000000 0.000000

45 H 0.000000 0.000000 0.000000 0.000054 0.000000 0.000000

31 32 33 34 35 36

1 C 0.000000 0.002023 0.000000 0.000000 -0.014881 0.000000

2 C 0.000000 -0.014094 0.000001 0.000000 -0.075725 0.000000

3 N 0.000000 0.128946 -0.000176 0.000000 0.004290 0.000000

4 C 0.000000 -0.014094 0.000218 0.000003 -0.000520 0.000000

5 C 0.000000 0.002023 0.000001 0.000000 0.002633 0.000000

6 C 0.000000 -0.011292 -0.002349 -0.000056 -0.000056 -0.000002

7 C 0.000001 -0.014094 -0.001304 -0.000520 0.000003 -0.000051

8 N -0.000003 0.128946 -0.017626 0.004290 0.000000 -0.000051

9 C 0.000009 -0.014094 0.406627 -0.075725 0.000000 -0.005172

10 C 0.000006 0.002023 -0.074407 -0.014881 0.000000 -0.000558

11 C 0.000000 0.002023 0.014010 0.002633 0.000000 0.000359

12 C 0.000000 -0.011292 0.000003 0.000000 0.541474 0.000000

13 C 0.000000 -0.014094 0.000001 0.000000 -0.075725 0.000000

14 C 0.000000 0.002023 0.000000 0.000000 -0.014881 0.000000

15 C 0.000000 0.002023 0.000001 0.000000 0.002633 0.000000

16 C 0.000010 -0.014094 0.000218 0.000003 -0.000520 0.000000

17 N 0.000002 0.128946 -0.000176 0.000000 0.004290 0.000000

18 C -0.000165 -0.011292 -0.002349 -0.000056 -0.000056 -0.000002

19 C 0.005560 -0.014094 -0.001304 -0.000520 0.000003 -0.000051

20 C -0.032996 0.002023 0.014010 0.002633 0.000000 0.000359

21 C 0.388265 0.002023 -0.074407 -0.014881 0.000000 -0.000558

22 C -0.038191 -0.014094 0.406627 -0.075725 0.000000 -0.005172

23 N 0.005131 0.128946 -0.017626 0.004290 0.000000 -0.000051

24 H 0.000000 -0.000363 0.000000 0.000000 0.006422 0.000000

25 H 0.000000 -0.000363 0.000000 0.000000 -0.000084 0.000000

26 H -0.000006 -0.000363 -0.005200 0.006422 0.000000 0.003287

27 H 0.000000 -0.000363 -0.000165 -0.000084 0.000000 -0.000009

28 H 0.000000 -0.000363 0.000000 0.000000 0.006422 0.000000

29 H 0.000000 -0.000363 0.000000 0.000000 -0.000084 0.000000

30 H -0.002192 -0.000363 -0.000165 -0.000084 0.000000 -0.000009

31 H 0.427518 -0.000363 -0.005200 0.006422 0.000000 0.003287

32 Zn -0.000363 10.222399 -0.011292 -0.000589 -0.000589 -0.000042

33 C -0.005200 -0.011292 5.211688 0.541474 0.000000 -0.105008

34 C 0.006422 -0.000589 0.541474 4.813300 0.000000 0.856211

35 C 0.000000 -0.000589 0.000000 0.000000 4.813300 0.000000

36 C 0.003287 -0.000042 -0.105008 0.856211 0.000000 5.177592

37 C 0.000000 -0.000042 0.000000 0.000000 0.856211 0.000000

38 C 0.000000 -0.000589 -0.000056 -0.000001 -0.000001 0.000000

39 C 0.000000 -0.000042 -0.000002 0.000000 0.000000 0.000000

40 C -0.000084 -0.000589 -0.000056 -0.000001 -0.000001 0.000000

41 C -0.000009 -0.000042 -0.000002 0.000000 0.000000 0.000000

42 H 0.000000 -0.000003 0.000000 0.000000 0.000000 0.000000

43 H 0.000054 -0.000003 0.001819 -0.019607 0.000000 0.370702

44 H 0.000000 -0.000003 0.000000 0.000000 0.000000 0.000000

45 H 0.000000 -0.000003 0.000000 0.000000 -0.019607 0.000000

37 38 39 40 41 42

1 C -0.000558 0.002633 0.000359 0.000000 0.000000 0.000000

2 C -0.005172 -0.000520 -0.000051 0.000003 0.000000 0.000000

3 N -0.000051 0.004290 -0.000051 0.000000 0.000000 0.000000

4 C -0.000051 -0.075725 -0.005172 0.000000 0.000000 0.000000

5 C 0.000359 -0.014881 -0.000558 0.000000 0.000000 0.000000

6 C -0.000002 0.541474 -0.105008 0.000000 0.000000 0.000000

7 C 0.000000 -0.075725 -0.005172 0.000000 0.000000 0.000000

8 N 0.000000 0.004290 -0.000051 0.000000 0.000000 0.000000

9 C 0.000000 -0.000520 -0.000051 0.000003 0.000000 0.000000

10 C 0.000000 0.002633 0.000359 0.000000 0.000000 0.000000

11 C 0.000000 -0.014881 -0.000558 0.000000 0.000000 0.000000

12 C -0.105008 -0.000056 -0.000002 -0.000056 -0.000002 0.000000

13 C -0.005172 0.000003 0.000000 -0.000520 -0.000051 0.000000

14 C -0.000558 0.000000 0.000000 0.002633 0.000359 0.000002

15 C 0.000359 0.000000 0.000000 -0.014881 -0.000558 0.000096

16 C -0.000051 0.000000 0.000000 -0.075725 -0.005172 -0.000035

17 N -0.000051 0.000000 0.000000 0.004290 -0.000051 0.000001

18 C -0.000002 0.000000 0.000000 0.541474 -0.105008 0.001819

19 C 0.000000 0.000000 0.000000 -0.075725 -0.005172 -0.000035

20 C 0.000000 0.000000 0.000000 -0.014881 -0.000558 0.000096

21 C 0.000000 0.000000 0.000000 0.002633 0.000359 0.000002

22 C 0.000000 0.000003 0.000000 -0.000520 -0.000051 0.000000

23 N 0.000000 0.000000 0.000000 0.004290 -0.000051 0.000001

24 H 0.003287 -0.000084 -0.000009 0.000000 0.000000 0.000000

25 H -0.000009 0.006422 0.003287 0.000000 0.000000 0.000000

26 H 0.000000 -0.000084 -0.000009 0.000000 0.000000 0.000000

27 H 0.000000 0.006422 0.003287 0.000000 0.000000 0.000000

28 H 0.003287 0.000000 0.000000 -0.000084 -0.000009 0.000000

29 H -0.000009 0.000000 0.000000 0.006422 0.003287 0.000054

30 H 0.000000 0.000000 0.000000 0.006422 0.003287 0.000054

31 H 0.000000 0.000000 0.000000 -0.000084 -0.000009 0.000000

32 Zn -0.000042 -0.000589 -0.000042 -0.000589 -0.000042 -0.000003

33 C 0.000000 -0.000056 -0.000002 -0.000056 -0.000002 0.000000

34 C 0.000000 -0.000001 0.000000 -0.000001 0.000000 0.000000

35 C 0.856211 -0.000001 0.000000 -0.000001 0.000000 0.000000

36 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 C 5.177592 0.000000 0.000000 0.000000 0.000000 0.000000

38 C 0.000000 4.813300 0.856211 0.000000 0.000000 0.000000

39 C 0.000000 0.856211 5.177592 0.000000 0.000000 0.000000

40 C 0.000000 0.000000 0.000000 4.813300 0.856211 -0.019607

41 C 0.000000 0.000000 0.000000 0.856211 5.177592 0.370702

42 H 0.000000 0.000000 0.000000 -0.019607 0.370702 0.348410

43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 -0.019607 0.370702 0.000000 0.000000 0.000000

45 H 0.370702 0.000000 0.000000 0.000000 0.000000 0.000000

43 44 45

1 C 0.000000 0.000002 0.000096

2 C 0.000000 0.000000 -0.000035

3 N 0.000000 0.000001 0.000001

4 C 0.000000 -0.000035 0.000000

5 C 0.000000 0.000096 0.000002

6 C 0.000000 0.001819 0.000000

7 C 0.000000 -0.000035 0.000000

8 N 0.000001 0.000001 0.000000

9 C -0.000035 0.000000 0.000000

10 C 0.000096 0.000002 0.000000

11 C 0.000002 0.000096 0.000000

12 C 0.000000 0.000000 0.001819

13 C 0.000000 0.000000 -0.000035

14 C 0.000000 0.000000 0.000096

15 C 0.000000 0.000000 0.000002

16 C 0.000000 0.000000 0.000000

17 N 0.000000 0.000000 0.000001

18 C 0.000000 0.000000 0.000000

19 C 0.000000 0.000000 0.000000

20 C 0.000002 0.000000 0.000000

21 C 0.000096 0.000000 0.000000

22 C -0.000035 0.000000 0.000000

23 N 0.000001 0.000000 0.000000

24 H 0.000000 0.000000 0.000054

25 H 0.000000 0.000054 0.000000

26 H 0.000054 0.000000 0.000000

27 H 0.000000 0.000054 0.000000

28 H 0.000000 0.000000 0.000054

29 H 0.000000 0.000000 0.000000

30 H 0.000000 0.000000 0.000000

31 H 0.000054 0.000000 0.000000

32 Zn -0.000003 -0.000003 -0.000003

33 C 0.001819 0.000000 0.000000

34 C -0.019607 0.000000 0.000000

35 C 0.000000 0.000000 -0.019607

36 C 0.370702 0.000000 0.000000

37 C 0.000000 0.000000 0.370702

38 C 0.000000 -0.019607 0.000000

39 C 0.000000 0.370702 0.000000

40 C 0.000000 0.000000 0.000000

41 C 0.000000 0.000000 0.000000

42 H 0.000000 0.000000 0.000000

43 H 0.348410 0.000000 0.000000

44 H 0.000000 0.348410 0.000000

45 H 0.000000 0.000000 0.348410

Mulliken charges:

1

1 C -0.241966

2 C 0.333019

3 N -0.710849

4 C 0.333019

5 C -0.241966

6 C -0.277831

7 C 0.333019

8 N -0.710849

9 C 0.333019

10 C -0.241966

11 C -0.241966

12 C -0.277831

13 C 0.333019

14 C -0.241966

15 C -0.241966

16 C 0.333019

17 N -0.710849

18 C -0.277831

19 C 0.333019

20 C -0.241966

21 C -0.241966

22 C 0.333019

23 N -0.710849

24 H 0.242944

25 H 0.242944

26 H 0.242944

27 H 0.242944

28 H 0.242944

29 H 0.242944

30 H 0.242944

31 H 0.242944

32 Zn 1.408997

33 C -0.277831

34 C -0.034948

35 C -0.034948

36 C -0.295061

37 C -0.295061

38 C -0.034948

39 C -0.295061

40 C -0.034948

41 C -0.295061

42 H 0.298445

43 H 0.298445

44 H 0.298445

45 H 0.298445

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 C 0.000978

2 C 0.333019

3 N -0.710849

4 C 0.333019

5 C 0.000978

6 C -0.277831

7 C 0.333019

8 N -0.710849

9 C 0.333019

10 C 0.000978

11 C 0.000978

12 C -0.277831

13 C 0.333019

14 C 0.000978

15 C 0.000978

16 C 0.333019

17 N -0.710849

18 C -0.277831

19 C 0.333019

20 C 0.000978

21 C 0.000978

22 C 0.333019

23 N -0.710849

32 Zn 1.408997

33 C -0.277831

34 C -0.034948

35 C -0.034948

36 C 0.003384

37 C 0.003384

38 C -0.034948

39 C 0.003384

40 C -0.034948

41 C 0.003384

APT charges:

1

1 C 0.124110

2 C 0.029799

3 N -0.803609

4 C 0.029799

5 C 0.124110

6 C 0.124467

7 C 0.029799

8 N -0.803609

9 C 0.029799

10 C 0.124110

11 C 0.124110

12 C 0.124467

13 C 0.029799

14 C 0.124110

15 C 0.124110

16 C 0.029799

17 N -0.803609

18 C 0.124467

19 C 0.029799

20 C 0.124110

21 C 0.124110

22 C 0.029799

23 N -0.803609

24 H 0.093871

25 H 0.093871

26 H 0.093871

27 H 0.093871

28 H 0.093871

29 H 0.093871

30 H 0.093871

31 H 0.093871

32 Zn 1.357411

33 C 0.124467

34 C 0.208696

35 C 0.208696

36 C -0.688312

37 C -0.688312

38 C 0.208696

39 C -0.688312

40 C 0.208696

41 C -0.688312

42 H 0.323847

43 H 0.323847

44 H 0.323847

45 H 0.323847

Sum of APT charges = 0.00000

APT charges with hydrogens summed into heavy atoms:

1

1 C 0.217981

2 C 0.029799

3 N -0.803609

4 C 0.029799

5 C 0.217981

6 C 0.124467

7 C 0.029799

8 N -0.803609

9 C 0.029799

10 C 0.217981

11 C 0.217981

12 C 0.124467

13 C 0.029799

14 C 0.217981

15 C 0.217981

16 C 0.029799

17 N -0.803609

18 C 0.124467

19 C 0.029799

20 C 0.217981

21 C 0.217981

22 C 0.029799

23 N -0.803609

32 Zn 1.357411

33 C 0.124467

34 C 0.208696

35 C 0.208696

36 C -0.364465

37 C -0.364465

38 C 0.208696

39 C -0.364465

40 C 0.208696

41 C -0.364465

Electronic spatial extent (au): <R\*\*2>= 13455.4990

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0000 Y= 0.0000 Z= 0.8362 Tot= 0.8362

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -158.2491 YY= -158.2491 ZZ= -200.1408

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 13.9639 YY= 13.9639 ZZ= -27.9278

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

Octapole moment (field-independent basis, Debye-Ang\*\*2):

XXX= 0.0000 YYY= 0.0000 ZZZ= 12.6982 XYY= 0.0000

XXY= 0.0000 XXZ= -5.0744 XZZ= 0.0000 YZZ= 0.0000

YYZ= -5.0744 XYZ= 0.0000

Hexadecapole moment (field-independent basis, Debye-Ang\*\*3):

XXXX= -7924.3895 YYYY= -7924.3895 ZZZZ= -226.2434 XXXY= 0.0000

XXXZ= 0.0000 YYYX= 0.0000 YYYZ= 0.0000 ZZZX= 0.0000

ZZZY= 0.0000 XXYY= -1844.2655 XXZZ= -1800.2715 YYZZ= -1800.2715

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 3.060485416419D+03 E-N=-9.363055529628D+03 KE= 1.403728960756D+03

Symmetry A1 KE= 4.235679858195D+02

Symmetry A2 KE= 2.911453213532D+02

Symmetry B1 KE= 3.445078267917D+02

Symmetry B2 KE= 3.445078267917D+02

Exact polarizability:1266.219 0.0001266.219 0.000 0.000 180.848

Approx polarizability:1453.144 0.0001453.144 0.000 0.000 214.286

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Fri Jul 26 14:35:18 2019, MaxMem= 1342177280 cpu: 23.6

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44808.

LDataN: DoStor=T MaxTD1= 7 Len= 274

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 260

Leave Link 701 at Fri Jul 26 14:35:40 2019, MaxMem= 1342177280 cpu: 259.0

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Fri Jul 26 14:35:40 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral second derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 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= 100127 IOpCl= 0 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 Fri Jul 26 14:36:19 2019, MaxMem= 1342177280 cpu: 473.9

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-8.65370275D-13 2.65155953D-13 3.28972572D-01

Polarizability= 1.26621908D+03 3.36622937D-07 1.26621908D+03

2.17074098D-07 2.87571919D-07 1.80847690D+02

Full mass-weighted force constant matrix:

Low frequencies --- -21.7062 -13.7576 -13.7576 -0.0007 0.0003 0.0006

Low frequencies --- 8.1222 39.4313 50.9368

Diagonal vibrational polarizability:

53.0841201 53.0841181 129.0806399

Harmonic frequencies (cm\*\*-1), IR intensities (KM/Mole), Raman scattering

activities (A\*\*4/AMU), depolarization ratios for plane and unpolarized

incident light, reduced masses (AMU), force constants (mDyne/A),

and normal coordinates:

1 2 3

B1 A1 B2

Frequencies -- 8.1222 39.4313 50.9368

Red. masses -- 6.3005 6.2534 5.5181

Frc consts -- 0.0002 0.0057 0.0084

IR Inten -- 0.0000 1.6661 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.03 0.00 0.00 0.00 0.00 -0.01 0.21

2 6 0.00 0.00 0.05 0.00 0.00 0.05 0.00 -0.01 0.09

3 7 0.00 0.00 0.00 0.00 0.00 0.10 0.00 -0.01 0.04

4 6 0.00 0.00 -0.05 0.00 0.00 0.05 0.00 -0.01 0.09

5 6 0.00 0.00 -0.03 0.00 0.00 0.00 0.00 -0.01 0.21

6 6 0.00 0.00 -0.09 0.00 0.00 0.02 0.00 0.00 0.00

7 6 0.00 0.00 -0.05 0.00 0.00 0.05 -0.01 0.00 -0.09

8 7 0.00 0.00 0.00 0.00 0.00 0.10 -0.01 0.00 -0.04

9 6 0.00 0.00 0.05 0.00 0.00 0.05 -0.01 0.00 -0.09

10 6 0.00 0.00 0.03 0.00 0.00 0.00 -0.01 0.00 -0.21

11 6 0.00 0.00 -0.03 0.00 0.00 0.00 -0.01 0.00 -0.21

12 6 0.00 0.00 0.09 0.00 0.00 0.02 0.00 0.00 0.00

13 6 0.00 0.00 0.05 0.00 0.00 0.05 0.01 0.00 -0.09

14 6 0.00 0.00 0.03 0.00 0.00 0.00 0.01 0.00 -0.21

15 6 0.00 0.00 -0.03 0.00 0.00 0.00 0.01 0.00 -0.21

16 6 0.00 0.00 -0.05 0.00 0.00 0.05 0.01 0.00 -0.09

17 7 0.00 0.00 0.00 0.00 0.00 0.10 0.01 0.00 -0.04

18 6 0.00 0.00 -0.09 0.00 0.00 0.02 0.00 0.00 0.00

19 6 0.00 0.00 -0.05 0.00 0.00 0.05 0.00 0.01 0.09

20 6 0.00 0.00 -0.03 0.00 0.00 0.00 0.00 0.01 0.21

21 6 0.00 0.00 0.03 0.00 0.00 0.00 0.00 0.01 0.21

22 6 0.00 0.00 0.05 0.00 0.00 0.05 0.00 0.01 0.09

23 7 0.00 0.00 0.00 0.00 0.00 0.10 0.00 0.01 0.04

24 1 0.00 0.00 0.06 0.00 0.00 -0.03 0.00 -0.01 0.27

25 1 0.00 0.00 -0.06 0.00 0.00 -0.03 0.00 -0.01 0.27

26 1 0.00 0.00 0.06 0.00 0.00 -0.03 -0.01 0.00 -0.27

27 1 0.00 0.00 -0.06 0.00 0.00 -0.03 -0.01 0.00 -0.27

28 1 0.00 0.00 0.06 0.00 0.00 -0.03 0.01 0.00 -0.27

29 1 0.00 0.00 -0.06 0.00 0.00 -0.03 0.01 0.00 -0.27

30 1 0.00 0.00 -0.06 0.00 0.00 -0.03 0.00 0.01 0.27

31 1 0.00 0.00 0.06 0.00 0.00 -0.03 0.00 0.01 0.27

32 30 0.00 0.00 0.00 0.00 0.00 0.12 0.00 0.00 0.00

33 6 0.00 0.00 0.09 0.00 0.00 0.02 0.00 0.00 0.00

34 6 0.00 0.00 0.18 0.00 0.00 -0.11 0.00 0.00 0.00

35 6 0.00 0.00 0.18 0.00 0.00 -0.11 0.00 0.00 0.00

36 6 0.00 0.00 0.27 -0.01 -0.01 -0.26 0.00 0.00 0.00

37 6 0.00 0.00 0.27 0.01 0.01 -0.26 0.00 0.00 0.00

38 6 0.00 0.00 -0.18 0.00 0.00 -0.11 0.00 0.00 0.00

39 6 0.00 0.00 -0.27 -0.01 0.01 -0.26 0.00 0.00 0.00

40 6 0.00 0.00 -0.18 0.00 0.00 -0.11 0.00 0.00 0.00

41 6 0.00 0.00 -0.27 0.01 -0.01 -0.26 0.00 0.00 0.00

42 1 0.01 -0.01 -0.35 0.01 -0.01 -0.38 0.00 0.00 0.00

43 1 0.01 0.01 0.35 -0.01 -0.01 -0.38 0.00 0.00 0.00

44 1 -0.01 0.01 -0.35 -0.01 0.01 -0.38 0.00 0.00 0.00

45 1 -0.01 -0.01 0.35 0.01 0.01 -0.38 0.00 0.00 0.00

4 5 6

E E A1

Frequencies -- 59.2108 59.2108 88.6449

Red. masses -- 5.3276 5.3276 5.8306

Frc consts -- 0.0110 0.0110 0.0270

IR Inten -- 0.1179 0.1179 0.1955

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 -0.17 0.00 0.00 0.01 0.00 -0.01 0.17

2 6 0.00 0.00 -0.10 0.00 0.00 0.00 0.00 0.00 0.02

3 7 0.00 0.00 -0.08 0.00 0.00 0.00 0.00 0.00 -0.07

4 6 0.00 0.00 -0.10 0.00 0.00 0.01 0.00 0.00 0.02

5 6 0.00 0.01 -0.17 0.00 0.00 0.00 0.00 -0.01 0.17

6 6 0.00 0.00 -0.03 0.00 0.00 0.03 0.00 0.00 0.01

7 6 0.00 0.00 0.00 0.00 0.00 0.10 0.00 0.00 0.02

8 7 0.00 0.00 0.00 0.00 0.00 0.08 0.00 0.00 -0.07

9 6 0.00 0.00 0.01 0.00 0.00 0.10 0.00 0.00 0.02

10 6 0.00 0.00 0.00 0.01 0.00 0.17 0.01 0.00 0.17

11 6 0.00 0.00 0.01 0.00 0.00 0.17 0.01 0.00 0.17

12 6 0.00 0.00 -0.03 0.00 0.00 -0.03 0.00 0.00 0.01

13 6 0.00 0.00 -0.01 0.00 0.00 -0.10 0.00 0.00 0.02

14 6 0.00 0.00 0.00 0.01 0.00 -0.17 -0.01 0.00 0.17

15 6 0.00 0.00 -0.01 0.00 0.00 -0.17 -0.01 0.00 0.17

16 6 0.00 0.00 0.00 0.00 0.00 -0.10 0.00 0.00 0.02

17 7 0.00 0.00 0.00 0.00 0.00 -0.08 0.00 0.00 -0.07

18 6 0.00 0.00 0.03 0.00 0.00 -0.03 0.00 0.00 0.01

19 6 0.00 0.00 0.10 0.00 0.00 -0.01 0.00 0.00 0.02

20 6 0.00 0.01 0.17 0.00 0.00 0.00 0.00 0.01 0.17

21 6 0.00 0.00 0.17 0.00 0.00 -0.01 0.00 0.01 0.17

22 6 0.00 0.00 0.10 0.00 0.00 0.00 0.00 0.00 0.02

23 7 0.00 0.00 0.08 0.00 0.00 0.00 0.00 0.00 -0.07

24 1 0.00 0.01 -0.22 0.00 0.00 0.01 0.00 -0.01 0.27

25 1 0.00 0.01 -0.22 0.00 0.00 0.01 0.00 -0.01 0.27

26 1 0.00 0.00 0.01 0.01 0.00 0.22 0.01 0.00 0.27

27 1 0.00 0.00 0.01 0.01 0.00 0.22 0.01 0.00 0.27

28 1 0.00 0.00 -0.01 0.01 0.00 -0.22 -0.01 0.00 0.27

29 1 0.00 0.00 -0.01 0.01 0.00 -0.22 -0.01 0.00 0.27

30 1 0.00 0.01 0.22 0.00 0.00 -0.01 0.00 0.01 0.27

31 1 0.00 0.01 0.22 0.00 0.00 -0.01 0.00 0.01 0.27

32 30 0.00 -0.02 0.00 -0.02 0.00 0.00 0.00 0.00 -0.16

33 6 0.00 0.00 0.03 0.00 0.00 0.03 0.00 0.00 0.01

34 6 0.00 0.00 -0.07 0.00 0.00 -0.07 0.00 0.00 -0.02

35 6 0.00 0.00 0.07 0.00 0.00 0.07 0.00 0.00 -0.02

36 6 -0.01 0.00 -0.23 0.00 -0.01 -0.21 0.00 0.00 -0.10

37 6 -0.01 0.00 0.23 0.00 -0.01 0.21 0.00 0.00 -0.10

38 6 0.00 0.00 0.07 0.00 0.00 -0.07 0.00 0.00 -0.02

39 6 0.01 0.00 0.21 0.00 0.01 -0.23 0.00 0.00 -0.10

40 6 0.00 0.00 -0.07 0.00 0.00 0.07 0.00 0.00 -0.02

41 6 0.01 0.00 -0.21 0.00 0.01 0.23 0.00 0.00 -0.10

42 1 0.01 0.00 -0.31 0.00 0.01 0.34 0.00 0.00 -0.15

43 1 -0.01 0.00 -0.34 0.00 -0.01 -0.31 0.00 0.00 -0.15

44 1 0.01 0.00 0.31 0.00 0.01 -0.34 0.00 0.00 -0.15

45 1 -0.01 0.00 0.34 0.00 -0.01 0.31 0.00 0.00 -0.15

7 8 9

B2 E E

Frequencies -- 108.5358 111.7966 111.7966

Red. masses -- 4.3624 4.4978 4.4978

Frc consts -- 0.0303 0.0331 0.0331

IR Inten -- 0.0000 2.0013 2.0013

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.02 0.00 0.01 0.00 0.00 0.00 0.03 -0.02

2 6 0.00 -0.02 0.00 0.02 0.00 0.01 0.00 0.03 0.01

3 7 0.00 -0.02 0.01 0.02 0.00 0.00 0.00 0.04 0.02

4 6 0.00 -0.02 0.00 0.02 0.00 -0.01 0.00 0.03 0.00

5 6 0.00 -0.02 0.00 0.01 0.00 0.00 0.00 0.03 -0.02

6 6 0.00 0.00 0.00 0.02 0.00 -0.01 0.00 0.02 0.01

7 6 -0.02 0.00 0.00 0.03 0.00 -0.01 0.00 0.02 0.01

8 7 -0.02 0.00 -0.01 0.04 0.00 -0.02 0.00 0.02 0.00

9 6 -0.02 0.00 0.00 0.03 0.00 0.00 0.00 0.02 -0.01

10 6 -0.02 0.00 0.00 0.03 0.00 0.02 0.00 0.01 0.00

11 6 -0.02 0.00 0.00 0.03 0.00 0.02 0.00 0.01 0.00

12 6 0.00 0.00 0.00 0.02 0.00 0.01 0.00 0.02 0.01

13 6 0.02 0.00 0.00 0.03 0.00 0.00 0.00 0.02 0.01

14 6 0.02 0.00 0.00 0.03 0.00 -0.02 0.00 0.01 0.00

15 6 0.02 0.00 0.00 0.03 0.00 -0.02 0.00 0.01 0.00

16 6 0.02 0.00 0.00 0.03 0.00 0.01 0.00 0.02 -0.01

17 7 0.02 0.00 -0.01 0.04 0.00 0.02 0.00 0.02 0.00

18 6 0.00 0.00 0.00 0.02 0.00 0.01 0.00 0.02 -0.01

19 6 0.00 0.02 0.00 0.02 0.00 0.01 0.00 0.03 0.00

20 6 0.00 0.02 0.00 0.01 0.00 0.00 0.00 0.03 0.02

21 6 0.00 0.02 0.00 0.01 0.00 0.00 0.00 0.03 0.02

22 6 0.00 0.02 0.00 0.02 0.00 -0.01 0.00 0.03 -0.01

23 7 0.00 0.02 0.01 0.02 0.00 0.00 0.00 0.04 -0.02

24 1 0.00 -0.02 -0.01 0.01 0.00 0.01 0.00 0.04 -0.04

25 1 0.00 -0.02 -0.01 0.01 0.00 -0.01 0.00 0.04 -0.04

26 1 -0.02 0.00 0.01 0.04 0.00 0.04 0.00 0.01 -0.01

27 1 -0.02 0.00 0.01 0.04 0.00 0.04 0.00 0.01 0.01

28 1 0.02 0.00 0.01 0.04 0.00 -0.04 0.00 0.01 0.01

29 1 0.02 0.00 0.01 0.04 0.00 -0.04 0.00 0.01 -0.01

30 1 0.00 0.02 -0.01 0.01 0.00 0.01 0.00 0.04 0.04

31 1 0.00 0.02 -0.01 0.01 0.00 -0.01 0.00 0.04 0.04

32 30 0.00 0.00 0.00 0.05 0.00 0.00 0.00 0.05 0.00

33 6 0.00 0.00 0.00 0.02 0.00 -0.01 0.00 0.02 -0.01

34 6 0.04 -0.04 0.00 -0.03 0.05 0.00 0.05 -0.02 0.00

35 6 -0.04 0.04 0.00 -0.03 0.05 0.00 0.05 -0.02 0.00

36 6 0.19 -0.19 0.00 -0.18 0.20 0.00 0.19 -0.17 0.00

37 6 -0.19 0.19 0.00 -0.18 0.20 0.00 0.19 -0.17 0.00

38 6 0.04 0.04 0.00 -0.02 -0.05 0.00 -0.05 -0.03 0.00

39 6 0.19 0.19 0.00 -0.17 -0.19 0.00 -0.20 -0.18 0.00

40 6 -0.04 -0.04 0.00 -0.02 -0.05 0.00 -0.05 -0.03 0.00

41 6 -0.19 -0.19 0.00 -0.17 -0.19 0.00 -0.20 -0.18 0.00

42 1 -0.29 -0.29 0.00 -0.27 -0.30 0.00 -0.31 -0.29 0.00

43 1 0.29 -0.29 0.00 -0.29 0.31 0.00 0.30 -0.27 0.00

44 1 0.29 0.29 0.00 -0.27 -0.30 0.00 -0.31 -0.29 0.00

45 1 -0.29 0.29 0.00 -0.29 0.31 0.00 0.30 -0.27 0.00

10 11 12

E E A2

Frequencies -- 128.5321 128.5321 139.2673

Red. masses -- 5.5931 5.5931 4.2893

Frc consts -- 0.0544 0.0544 0.0490

IR Inten -- 1.8436 1.8436 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.02 0.00 -0.08 0.00 -0.01 -0.16 0.08 -0.02 0.00

2 6 0.01 0.00 -0.07 0.00 -0.01 0.10 0.05 -0.03 0.00

3 7 0.01 0.00 0.03 0.00 -0.02 0.24 0.03 0.00 0.00

4 6 0.01 0.00 0.09 0.00 -0.01 0.08 0.05 0.03 0.00

5 6 0.02 0.00 0.04 0.00 -0.01 -0.18 0.08 0.02 0.00

6 6 0.01 0.00 0.12 0.00 -0.01 0.09 0.05 0.05 0.00

7 6 0.01 0.00 0.10 0.00 -0.01 0.07 0.03 0.05 0.00

8 7 0.02 0.00 0.24 0.00 -0.01 -0.03 0.00 0.03 0.00

9 6 0.01 0.00 0.08 0.00 -0.01 -0.09 -0.03 0.05 0.00

10 6 0.01 0.00 -0.18 0.00 -0.02 -0.04 -0.02 0.08 0.00

11 6 0.01 0.00 -0.16 0.00 -0.02 0.08 0.02 0.08 0.00

12 6 0.01 0.00 -0.09 0.00 -0.01 0.12 0.05 -0.05 0.00

13 6 0.01 0.00 -0.08 0.00 -0.01 0.09 0.03 -0.05 0.00

14 6 0.01 0.00 0.18 0.00 -0.02 0.04 0.02 -0.08 0.00

15 6 0.01 0.00 0.16 0.00 -0.02 -0.08 -0.02 -0.08 0.00

16 6 0.01 0.00 -0.10 0.00 -0.01 -0.07 -0.03 -0.05 0.00

17 7 0.02 0.00 -0.24 0.00 -0.01 0.03 0.00 -0.03 0.00

18 6 0.01 0.00 -0.12 0.00 -0.01 -0.09 -0.05 -0.05 0.00

19 6 0.01 0.00 -0.09 0.00 -0.01 -0.08 -0.05 -0.03 0.00

20 6 0.02 0.00 -0.04 0.00 -0.01 0.18 -0.08 -0.02 0.00

21 6 0.02 0.00 0.08 0.00 -0.01 0.16 -0.08 0.02 0.00

22 6 0.01 0.00 0.07 0.00 -0.01 -0.10 -0.05 0.03 0.00

23 7 0.01 0.00 -0.03 0.00 -0.02 -0.24 -0.03 0.00 0.00

24 1 0.02 0.00 -0.15 0.00 0.00 -0.34 0.10 -0.03 0.00

25 1 0.02 0.00 0.07 0.00 0.00 -0.37 0.10 0.03 0.00

26 1 0.00 0.00 -0.37 0.00 -0.02 -0.07 -0.03 0.10 0.00

27 1 0.00 0.00 -0.34 0.00 -0.02 0.15 0.03 0.10 0.00

28 1 0.00 0.00 0.37 0.00 -0.02 0.07 0.03 -0.10 0.00

29 1 0.00 0.00 0.34 0.00 -0.02 -0.15 -0.03 -0.10 0.00

30 1 0.02 0.00 -0.07 0.00 0.00 0.37 -0.10 -0.03 0.00

31 1 0.02 0.00 0.15 0.00 0.00 0.34 -0.10 0.03 0.00

32 30 -0.05 0.01 0.00 0.01 0.05 0.00 0.00 0.00 0.00

33 6 0.01 0.00 0.09 0.00 -0.01 -0.12 -0.05 0.05 0.00

34 6 0.01 0.00 0.04 -0.01 -0.01 -0.05 -0.01 0.01 0.00

35 6 0.01 0.00 -0.04 -0.01 -0.01 0.05 0.01 -0.01 0.00

36 6 -0.02 0.03 -0.04 -0.03 0.02 0.05 0.16 -0.16 0.00

37 6 -0.02 0.03 0.04 -0.03 0.02 -0.05 -0.16 0.16 0.00

38 6 0.01 -0.01 0.05 0.00 -0.01 0.04 0.01 0.01 0.00

39 6 -0.02 -0.03 -0.05 0.03 0.02 -0.04 -0.16 -0.16 0.00

40 6 0.01 -0.01 -0.05 0.00 -0.01 -0.04 -0.01 -0.01 0.00

41 6 -0.02 -0.03 0.05 0.03 0.02 0.04 0.16 0.16 0.00

42 1 -0.03 -0.04 0.12 0.05 0.04 0.10 0.28 0.28 0.00

43 1 -0.04 0.05 -0.10 -0.04 0.03 0.12 0.28 -0.28 0.00

44 1 -0.03 -0.04 -0.12 0.05 0.04 -0.10 -0.28 -0.28 0.00

45 1 -0.04 0.05 0.10 -0.04 0.03 -0.12 -0.28 0.28 0.00

13 14 15

B1 B1 B2

Frequencies -- 144.8185 164.8920 168.6379

Red. masses -- 5.4711 9.6199 7.9119

Frc consts -- 0.0676 0.1541 0.1326

IR Inten -- 0.0000 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 0.00 -0.08 0.03 0.04 0.01 0.00 -0.08 -0.06

2 6 0.01 0.01 -0.12 0.12 0.07 0.01 0.01 -0.08 0.11

3 7 0.01 0.00 0.00 0.16 0.00 0.00 0.00 -0.09 0.27

4 6 0.01 -0.01 0.12 0.12 -0.07 -0.01 -0.01 -0.08 0.11

5 6 0.01 0.00 0.08 0.03 -0.04 -0.01 0.00 -0.08 -0.06

6 6 0.01 -0.01 0.17 0.14 -0.14 -0.02 -0.03 -0.03 0.00

7 6 0.01 -0.01 0.12 0.07 -0.12 -0.01 -0.08 -0.01 -0.11

8 7 0.00 -0.01 0.00 0.00 -0.16 0.00 -0.09 0.00 -0.27

9 6 -0.01 -0.01 -0.12 -0.07 -0.12 0.01 -0.08 0.01 -0.11

10 6 0.00 -0.01 -0.08 -0.04 -0.03 0.01 -0.08 0.00 0.06

11 6 0.00 -0.01 0.08 0.04 -0.03 -0.01 -0.08 0.00 0.06

12 6 0.01 0.01 -0.17 0.14 0.14 0.02 0.03 -0.03 0.00

13 6 0.01 0.01 -0.12 0.07 0.12 0.01 0.08 -0.01 -0.11

14 6 0.00 0.01 -0.08 0.04 0.03 0.01 0.08 0.00 0.06

15 6 0.00 0.01 0.08 -0.04 0.03 -0.01 0.08 0.00 0.06

16 6 -0.01 0.01 0.12 -0.07 0.12 -0.01 0.08 0.01 -0.11

17 7 0.00 0.01 0.00 0.00 0.16 0.00 0.09 0.00 -0.27

18 6 -0.01 0.01 0.17 -0.14 0.14 -0.02 0.03 0.03 0.00

19 6 -0.01 0.01 0.12 -0.12 0.07 -0.01 0.01 0.08 0.11

20 6 -0.01 0.00 0.08 -0.03 0.04 -0.01 0.00 0.08 -0.06

21 6 -0.01 0.00 -0.08 -0.03 -0.04 0.01 0.00 0.08 -0.06

22 6 -0.01 -0.01 -0.12 -0.12 -0.07 0.01 -0.01 0.08 0.11

23 7 -0.01 0.00 0.00 -0.16 0.00 0.00 0.00 0.09 0.27

24 1 0.00 0.01 -0.16 -0.02 0.09 0.02 0.00 -0.08 -0.21

25 1 0.00 -0.01 0.16 -0.02 -0.09 -0.02 0.00 -0.08 -0.21

26 1 -0.01 0.00 -0.16 -0.09 0.02 0.02 -0.08 0.00 0.21

27 1 0.01 0.00 0.16 0.09 0.02 -0.02 -0.08 0.00 0.21

28 1 0.01 0.00 -0.16 0.09 -0.02 0.02 0.08 0.00 0.21

29 1 -0.01 0.00 0.16 -0.09 -0.02 -0.02 0.08 0.00 0.21

30 1 0.00 0.01 0.16 0.02 0.09 -0.02 0.00 0.08 -0.21

31 1 0.00 -0.01 -0.16 0.02 -0.09 0.02 0.00 0.08 -0.21

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 -0.01 -0.01 -0.17 -0.14 -0.14 0.02 -0.03 0.03 0.00

34 6 -0.01 -0.01 -0.09 -0.14 -0.14 0.02 0.00 0.00 0.00

35 6 0.01 0.01 -0.09 0.14 0.14 0.02 0.00 0.00 0.00

36 6 -0.01 -0.01 0.15 -0.14 -0.14 -0.01 -0.03 0.03 0.00

37 6 0.01 0.01 0.15 0.14 0.14 -0.01 0.03 -0.03 0.00

38 6 0.01 -0.01 0.09 0.14 -0.14 -0.02 0.00 0.00 0.00

39 6 0.01 -0.01 -0.15 0.14 -0.14 0.01 -0.03 -0.03 0.00

40 6 -0.01 0.01 0.09 -0.14 0.14 -0.02 0.00 0.00 0.00

41 6 -0.01 0.01 -0.15 -0.14 0.14 0.01 0.03 0.03 0.00

42 1 0.00 0.00 -0.31 -0.14 0.14 0.03 0.04 0.04 0.00

43 1 0.00 0.00 0.31 -0.14 -0.14 -0.03 -0.04 0.04 0.00

44 1 0.00 0.00 -0.31 0.14 -0.14 0.03 -0.04 -0.04 0.00

45 1 0.00 0.00 0.31 0.14 0.14 -0.03 0.04 -0.04 0.00

16 17 18

A1 B2 E

Frequencies -- 191.7498 206.2589 216.6261

Red. masses -- 9.7684 8.6713 9.6105

Frc consts -- 0.2116 0.2173 0.2657

IR Inten -- 82.4517 0.0000 6.5391

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.02 0.11 0.00 0.17 -0.02 0.02 -0.02 0.05

2 6 0.01 0.02 -0.10 -0.01 0.15 0.08 0.03 -0.01 0.08

3 7 0.00 0.04 -0.19 0.00 0.14 0.16 0.01 0.01 0.14

4 6 -0.01 0.02 -0.10 0.01 0.15 0.08 0.00 -0.01 0.02

5 6 0.00 0.02 0.11 0.00 0.17 -0.02 0.01 -0.01 -0.01

6 6 -0.01 0.01 -0.12 0.05 0.05 0.00 0.00 -0.05 -0.14

7 6 -0.02 0.01 -0.10 0.15 0.01 -0.08 -0.01 -0.06 -0.14

8 7 -0.04 0.00 -0.19 0.14 0.00 -0.16 0.00 -0.06 0.03

9 6 -0.02 -0.01 -0.10 0.15 -0.01 -0.08 0.01 -0.06 0.16

10 6 -0.02 0.00 0.11 0.17 0.00 0.02 0.01 -0.07 0.13

11 6 -0.02 0.00 0.11 0.17 0.00 0.02 0.00 -0.07 -0.13

12 6 0.01 0.01 -0.12 -0.05 0.05 0.00 0.02 -0.06 -0.09

13 6 0.02 0.01 -0.10 -0.15 0.01 -0.08 0.01 -0.06 -0.16

14 6 0.02 0.00 0.11 -0.17 0.00 0.02 0.01 -0.07 -0.13

15 6 0.02 0.00 0.11 -0.17 0.00 0.02 0.00 -0.07 0.13

16 6 0.02 -0.01 -0.10 -0.15 -0.01 -0.08 -0.01 -0.06 0.14

17 7 0.04 0.00 -0.19 -0.14 0.00 -0.16 0.00 -0.06 -0.03

18 6 0.01 -0.01 -0.12 -0.05 -0.05 0.00 0.00 -0.05 0.14

19 6 0.01 -0.02 -0.10 -0.01 -0.15 0.08 0.00 -0.01 -0.02

20 6 0.00 -0.02 0.11 0.00 -0.17 -0.02 0.01 -0.01 0.01

21 6 0.00 -0.02 0.11 0.00 -0.17 -0.02 0.02 -0.02 -0.05

22 6 -0.01 -0.02 -0.10 0.01 -0.15 0.08 0.03 -0.01 -0.08

23 7 0.00 -0.04 -0.19 0.00 -0.14 0.16 0.01 0.01 -0.14

24 1 0.00 0.02 0.25 0.01 0.17 -0.11 0.01 -0.01 0.02

25 1 0.00 0.02 0.25 -0.01 0.17 -0.11 0.02 0.00 -0.08

26 1 -0.02 0.00 0.25 0.17 0.01 0.11 0.02 -0.08 0.24

27 1 -0.02 0.00 0.25 0.17 -0.01 0.11 -0.02 -0.08 -0.25

28 1 0.02 0.00 0.25 -0.17 -0.01 0.11 0.02 -0.08 -0.24

29 1 0.02 0.00 0.25 -0.17 0.01 0.11 -0.02 -0.08 0.25

30 1 0.00 -0.02 0.25 0.01 -0.17 -0.11 0.02 0.00 0.08

31 1 0.00 -0.02 0.25 -0.01 -0.17 -0.11 0.01 -0.01 -0.02

32 30 0.00 0.00 0.25 0.00 0.00 0.00 -0.05 0.24 0.00

33 6 -0.01 -0.01 -0.12 0.05 -0.05 0.00 0.02 -0.06 0.09

34 6 -0.01 -0.01 -0.06 0.00 0.00 0.00 0.02 -0.06 0.08

35 6 0.01 0.01 -0.06 0.00 0.00 0.00 0.02 -0.06 -0.08

36 6 -0.01 -0.01 0.02 0.03 -0.03 0.00 -0.05 0.00 -0.07

37 6 0.01 0.01 0.02 -0.03 0.03 0.00 -0.05 0.00 0.07

38 6 -0.01 0.01 -0.06 0.00 0.00 0.00 0.00 -0.06 -0.13

39 6 -0.01 0.01 0.02 0.03 0.03 0.00 0.05 -0.02 0.10

40 6 0.01 -0.01 -0.06 0.00 0.00 0.00 0.00 -0.06 0.13

41 6 0.01 -0.01 0.02 -0.03 -0.03 0.00 0.05 -0.02 -0.10

42 1 0.01 -0.01 0.08 -0.04 -0.04 0.00 0.09 0.01 -0.25

43 1 -0.01 -0.01 0.08 0.04 -0.04 0.00 -0.10 0.05 -0.17

44 1 -0.01 0.01 0.08 0.04 0.04 0.00 0.09 0.01 0.25

45 1 0.01 0.01 0.08 -0.04 0.04 0.00 -0.10 0.05 0.17

19 20 21

E E E

Frequencies -- 216.6261 241.8595 241.8595

Red. masses -- 9.6105 9.4887 9.4887

Frc consts -- 0.2657 0.3270 0.3270

IR Inten -- 6.5391 3.7187 3.7187

Atom AN X Y Z X Y Z X Y Z

1 6 -0.07 0.00 -0.13 -0.08 0.00 0.12 0.00 0.01 0.03

2 6 -0.06 0.01 -0.14 -0.07 0.00 0.14 0.01 0.01 -0.10

3 7 -0.06 0.00 0.03 -0.07 0.00 0.02 -0.01 0.05 -0.25

4 6 -0.06 -0.01 0.16 -0.07 0.00 -0.12 -0.02 0.01 -0.13

5 6 -0.07 -0.01 0.13 -0.08 0.00 -0.12 -0.01 0.01 0.01

6 6 -0.06 -0.02 0.09 -0.06 0.00 -0.07 -0.01 -0.06 0.06

7 6 -0.01 -0.03 -0.08 0.01 -0.01 0.10 0.00 -0.07 0.14

8 7 0.01 -0.01 -0.14 0.05 0.01 0.25 0.00 -0.07 0.02

9 6 -0.01 0.00 -0.02 0.01 0.02 0.13 0.00 -0.07 -0.12

10 6 -0.01 -0.01 0.01 0.01 0.01 -0.01 0.00 -0.08 -0.12

11 6 -0.02 -0.02 -0.05 0.01 0.00 -0.03 0.00 -0.08 0.12

12 6 -0.05 0.00 -0.14 -0.06 0.01 0.06 0.00 -0.06 0.07

13 6 -0.01 0.00 0.02 0.01 0.02 -0.13 0.00 -0.07 0.12

14 6 -0.01 -0.01 -0.01 0.01 0.01 0.01 0.00 -0.08 0.12

15 6 -0.02 -0.02 0.05 0.01 0.00 0.03 0.00 -0.08 -0.12

16 6 -0.01 -0.03 0.08 0.01 -0.01 -0.10 0.00 -0.07 -0.14

17 7 0.01 -0.01 0.14 0.05 0.01 -0.25 0.00 -0.07 -0.02

18 6 -0.06 -0.02 -0.09 -0.06 0.00 0.07 -0.01 -0.06 -0.06

19 6 -0.06 -0.01 -0.16 -0.07 0.00 0.12 -0.02 0.01 0.13

20 6 -0.07 -0.01 -0.13 -0.08 0.00 0.12 -0.01 0.01 -0.01

21 6 -0.07 0.00 0.13 -0.08 0.00 -0.12 0.00 0.01 -0.03

22 6 -0.06 0.01 0.14 -0.07 0.00 -0.14 0.01 0.01 0.10

23 7 -0.06 0.00 -0.03 -0.07 0.00 -0.02 -0.01 0.05 0.25

24 1 -0.08 0.02 -0.25 -0.09 0.00 0.21 -0.01 0.01 0.17

25 1 -0.08 -0.02 0.24 -0.09 0.00 -0.24 0.00 0.01 0.13

26 1 0.00 -0.02 0.08 0.01 0.00 -0.13 0.00 -0.09 -0.24

27 1 -0.01 -0.01 -0.02 0.01 0.01 -0.17 0.00 -0.09 0.21

28 1 0.00 -0.02 -0.08 0.01 0.00 0.13 0.00 -0.09 0.24

29 1 -0.01 -0.01 0.02 0.01 0.01 0.17 0.00 -0.09 -0.21

30 1 -0.08 -0.02 -0.24 -0.09 0.00 0.24 0.00 0.01 -0.13

31 1 -0.08 0.02 0.25 -0.09 0.00 -0.21 -0.01 0.01 -0.17

32 30 0.24 0.05 0.00 0.21 -0.02 0.00 0.02 0.21 0.00

33 6 -0.05 0.00 0.14 -0.06 0.01 -0.06 0.00 -0.06 -0.07

34 6 -0.06 0.00 0.13 -0.08 0.02 -0.09 0.00 -0.07 -0.10

35 6 -0.06 0.00 -0.13 -0.08 0.02 0.09 0.00 -0.07 0.10

36 6 -0.02 -0.05 -0.10 0.00 -0.05 0.05 -0.05 -0.01 0.06

37 6 -0.02 -0.05 0.10 0.00 -0.05 -0.05 -0.05 -0.01 -0.06

38 6 -0.06 -0.02 0.08 -0.07 0.00 -0.10 -0.02 -0.08 0.09

39 6 0.00 0.05 -0.07 -0.01 0.05 0.06 0.05 0.00 -0.05

40 6 -0.06 -0.02 -0.08 -0.07 0.00 0.10 -0.02 -0.08 -0.09

41 6 0.00 0.05 0.07 -0.01 0.05 -0.06 0.05 0.00 0.05

42 1 0.05 0.10 0.17 0.03 0.09 -0.16 0.10 0.04 0.14

43 1 0.01 -0.09 -0.25 0.04 -0.10 0.14 -0.09 0.03 0.16

44 1 0.05 0.10 -0.17 0.03 0.09 0.16 0.10 0.04 -0.14

45 1 0.01 -0.09 0.25 0.04 -0.10 -0.14 -0.09 0.03 -0.16

22 23 24

A2 A1 E

Frequencies -- 288.8683 317.7941 320.8929

Red. masses -- 4.8361 7.3359 6.4371

Frc consts -- 0.2378 0.4365 0.3905

IR Inten -- 0.0000 0.9572 20.3829

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 -0.15 0.00 0.08 -0.04 0.14 -0.09 -0.01

2 6 0.00 0.00 -0.14 0.02 0.07 -0.02 -0.04 -0.13 -0.01

3 7 0.00 0.00 0.00 0.00 0.08 -0.10 -0.12 0.00 0.00

4 6 0.00 0.00 0.14 -0.02 0.07 -0.02 -0.04 0.13 0.00

5 6 0.00 0.00 0.15 0.00 0.08 -0.04 0.14 0.09 0.01

6 6 0.00 0.00 0.00 -0.05 0.05 0.12 -0.04 0.11 0.00

7 6 0.00 0.00 -0.14 -0.07 0.02 -0.02 0.07 0.03 -0.01

8 7 0.00 0.00 0.00 -0.08 0.00 -0.10 0.07 0.00 -0.02

9 6 0.00 0.00 0.14 -0.07 -0.02 -0.02 0.08 -0.03 -0.01

10 6 0.00 0.00 0.15 -0.08 0.00 -0.04 0.10 0.00 0.00

11 6 0.00 0.00 -0.15 -0.08 0.00 -0.04 0.10 0.00 0.00

12 6 0.00 0.00 0.00 0.05 0.05 0.12 -0.04 -0.11 0.00

13 6 0.00 0.00 0.14 0.07 0.02 -0.02 0.08 -0.03 0.01

14 6 0.00 0.00 0.15 0.08 0.00 -0.04 0.10 0.00 0.00

15 6 0.00 0.00 -0.15 0.08 0.00 -0.04 0.10 0.00 0.00

16 6 0.00 0.00 -0.14 0.07 -0.02 -0.02 0.07 0.03 0.01

17 7 0.00 0.00 0.00 0.08 0.00 -0.10 0.07 0.00 0.02

18 6 0.00 0.00 0.00 0.05 -0.05 0.12 -0.04 0.11 0.00

19 6 0.00 0.00 0.14 0.02 -0.07 -0.02 -0.04 0.13 0.00

20 6 0.00 0.00 0.15 0.00 -0.08 -0.04 0.14 0.09 -0.01

21 6 0.00 0.00 -0.15 0.00 -0.08 -0.04 0.14 -0.09 0.01

22 6 0.00 0.00 -0.14 -0.02 -0.07 -0.02 -0.04 -0.13 0.01

23 7 0.00 0.00 0.00 0.00 -0.08 -0.10 -0.12 0.00 0.00

24 1 0.00 0.01 -0.29 -0.01 0.09 -0.03 0.26 -0.19 -0.01

25 1 0.00 -0.01 0.29 0.01 0.09 -0.03 0.26 0.18 0.01

26 1 0.01 0.00 0.29 -0.09 0.01 -0.03 0.09 0.01 0.01

27 1 -0.01 0.00 -0.29 -0.09 -0.01 -0.03 0.08 -0.02 0.01

28 1 -0.01 0.00 0.29 0.09 -0.01 -0.03 0.09 0.01 -0.01

29 1 0.01 0.00 -0.29 0.09 0.01 -0.03 0.08 -0.02 -0.01

30 1 0.00 0.01 0.29 -0.01 -0.09 -0.03 0.26 0.18 -0.01

31 1 0.00 -0.01 -0.29 0.01 -0.09 -0.03 0.26 -0.19 0.01

32 30 0.00 0.00 0.00 0.00 0.00 0.00 -0.03 0.00 0.00

33 6 0.00 0.00 0.00 -0.05 -0.05 0.12 -0.04 -0.11 0.00

34 6 0.00 0.00 0.00 -0.06 -0.06 0.23 -0.10 -0.08 0.01

35 6 0.00 0.00 0.00 0.06 0.06 0.23 -0.10 -0.08 -0.01

36 6 0.00 0.00 0.00 -0.06 -0.06 -0.10 -0.09 -0.10 0.00

37 6 0.00 0.00 0.00 0.06 0.06 -0.10 -0.09 -0.10 0.00

38 6 0.00 0.00 0.00 -0.06 0.06 0.23 -0.10 0.09 0.01

39 6 0.00 0.00 0.00 -0.06 0.06 -0.10 -0.09 0.10 0.00

40 6 0.00 0.00 0.00 0.06 -0.06 0.23 -0.10 0.09 -0.01

41 6 0.00 0.00 0.00 0.06 -0.06 -0.10 -0.09 0.10 0.00

42 1 0.00 0.00 0.00 0.07 -0.07 -0.29 -0.10 0.10 0.00

43 1 0.00 0.00 0.00 -0.07 -0.07 -0.29 -0.09 -0.10 0.00

44 1 0.00 0.00 0.00 -0.07 0.07 -0.29 -0.10 0.10 0.00

45 1 0.00 0.00 0.00 0.07 0.07 -0.29 -0.09 -0.10 0.00

25 26 27

E A1 E

Frequencies -- 320.8929 331.1347 373.3159

Red. masses -- 6.4371 8.1454 5.8834

Frc consts -- 0.3905 0.5262 0.4831

IR Inten -- 20.3829 0.3436 6.1750

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.10 0.00 0.00 -0.11 -0.02 0.01 0.09 -0.02

2 6 -0.03 0.07 0.01 -0.03 -0.10 -0.03 0.02 0.07 0.01

3 7 0.00 0.07 0.02 0.00 -0.10 -0.09 0.00 0.09 -0.03

4 6 0.03 0.08 0.01 0.03 -0.10 -0.03 -0.02 0.07 0.01

5 6 0.00 0.10 0.00 0.00 -0.11 -0.02 0.00 0.09 -0.03

6 6 0.11 -0.04 0.00 0.08 -0.08 0.07 -0.02 -0.01 0.06

7 6 0.13 -0.04 -0.01 0.10 -0.03 -0.03 -0.01 -0.03 -0.10

8 7 0.00 -0.12 0.00 0.10 0.00 -0.09 0.00 -0.03 0.00

9 6 -0.13 -0.04 0.00 0.10 0.03 -0.03 0.01 -0.03 0.10

10 6 -0.09 0.14 0.01 0.11 0.00 -0.02 0.01 -0.08 0.14

11 6 0.09 0.14 -0.01 0.11 0.00 -0.02 -0.02 -0.08 -0.14

12 6 -0.11 -0.04 0.00 -0.08 -0.08 0.07 0.03 -0.01 0.05

13 6 -0.13 -0.04 0.00 -0.10 -0.03 -0.03 0.01 -0.03 -0.10

14 6 -0.09 0.14 -0.01 -0.11 0.00 -0.02 0.01 -0.08 -0.14

15 6 0.09 0.14 0.01 -0.11 0.00 -0.02 -0.02 -0.08 0.14

16 6 0.13 -0.04 0.01 -0.10 0.03 -0.03 -0.01 -0.03 0.10

17 7 0.00 -0.12 0.00 -0.10 0.00 -0.09 0.00 -0.03 0.00

18 6 0.11 -0.04 0.00 -0.08 0.08 0.07 -0.02 -0.01 -0.06

19 6 0.03 0.08 -0.01 -0.03 0.10 -0.03 -0.02 0.07 -0.01

20 6 0.00 0.10 0.00 0.00 0.11 -0.02 0.00 0.09 0.03

21 6 0.00 0.10 0.00 0.00 0.11 -0.02 0.01 0.09 0.02

22 6 -0.03 0.07 -0.01 0.03 0.10 -0.03 0.02 0.07 -0.01

23 7 0.00 0.07 -0.02 0.00 0.10 -0.09 0.00 0.09 0.03

24 1 0.02 0.08 -0.01 0.01 -0.12 0.00 0.00 0.10 -0.06

25 1 -0.01 0.09 -0.01 -0.01 -0.12 0.00 0.01 0.10 -0.08

26 1 -0.18 0.26 0.01 0.12 -0.01 0.00 0.03 -0.10 0.26

27 1 0.19 0.26 -0.01 0.12 0.01 0.00 -0.04 -0.10 -0.27

28 1 -0.18 0.26 -0.01 -0.12 0.01 0.00 0.03 -0.10 -0.26

29 1 0.19 0.26 0.01 -0.12 -0.01 0.00 -0.04 -0.10 0.27

30 1 -0.01 0.09 0.01 0.01 0.12 0.00 0.01 0.10 0.08

31 1 0.02 0.08 0.01 -0.01 0.12 0.00 0.00 0.10 0.06

32 30 0.00 -0.03 0.00 0.00 0.00 0.05 0.00 -0.05 0.00

33 6 -0.11 -0.04 0.00 0.08 0.08 0.07 0.03 -0.01 -0.05

34 6 -0.09 -0.10 0.01 0.10 0.10 0.17 0.08 -0.05 -0.18

35 6 -0.09 -0.10 -0.01 -0.10 -0.10 0.17 0.08 -0.05 0.18

36 6 -0.10 -0.09 0.00 0.10 0.10 -0.07 0.00 0.03 0.06

37 6 -0.10 -0.09 0.00 -0.10 -0.10 -0.07 0.00 0.03 -0.06

38 6 0.08 -0.10 -0.01 0.10 -0.10 0.17 -0.07 -0.05 0.19

39 6 0.10 -0.09 0.00 0.10 -0.10 -0.07 0.00 0.03 -0.07

40 6 0.08 -0.10 0.01 -0.10 0.10 0.17 -0.07 -0.05 -0.19

41 6 0.10 -0.09 0.00 -0.10 0.10 -0.07 0.00 0.03 0.07

42 1 0.10 -0.09 0.00 -0.10 0.10 -0.21 0.04 0.08 0.20

43 1 -0.10 -0.10 0.00 0.10 0.10 -0.21 -0.05 0.08 0.19

44 1 0.10 -0.09 0.00 0.10 -0.10 -0.21 0.04 0.08 -0.20

45 1 -0.10 -0.10 0.00 -0.10 -0.10 -0.21 -0.05 0.08 -0.19

28 29 30

E E E

Frequencies -- 373.3159 376.4185 376.4185

Red. masses -- 5.8834 6.9155 6.9155

Frc consts -- 0.4831 0.5773 0.5773

IR Inten -- 6.1750 13.7308 13.7308

Atom AN X Y Z X Y Z X Y Z

1 6 -0.08 0.02 -0.14 -0.02 -0.13 0.00 0.12 -0.03 -0.10

2 6 -0.03 0.01 -0.10 -0.03 -0.11 -0.01 0.04 -0.02 -0.07

3 7 -0.03 0.00 0.00 0.00 -0.13 -0.05 0.04 -0.02 -0.01

4 6 -0.03 -0.01 0.10 0.02 -0.11 -0.03 0.05 0.00 0.07

5 6 -0.08 -0.01 0.14 -0.01 -0.14 -0.03 0.12 0.00 0.09

6 6 -0.01 -0.03 -0.05 0.04 0.00 0.04 0.01 0.04 -0.03

7 6 0.07 -0.02 -0.01 0.02 0.04 -0.07 -0.11 0.03 0.01

8 7 0.09 0.00 0.03 0.02 0.04 -0.01 -0.13 0.00 0.05

9 6 0.07 0.02 -0.01 0.00 0.05 0.07 -0.11 -0.02 0.03

10 6 0.09 0.00 0.03 0.00 0.12 0.09 -0.14 0.01 0.03

11 6 0.09 -0.01 0.02 0.03 0.12 -0.10 -0.13 0.02 0.00

12 6 -0.01 0.02 0.06 -0.04 0.01 0.03 0.00 -0.04 0.04

13 6 0.07 0.02 0.01 0.00 0.05 -0.07 -0.11 -0.02 -0.03

14 6 0.09 0.00 -0.03 0.00 0.12 -0.09 -0.14 0.01 -0.03

15 6 0.09 -0.01 -0.02 0.03 0.12 0.10 -0.13 0.02 0.00

16 6 0.07 -0.02 0.01 0.02 0.04 0.07 -0.11 0.03 -0.01

17 7 0.09 0.00 -0.03 0.02 0.04 0.01 -0.13 0.00 -0.05

18 6 -0.01 -0.03 0.05 0.04 0.00 -0.04 0.01 0.04 0.03

19 6 -0.03 -0.01 -0.10 0.02 -0.11 0.03 0.05 0.00 -0.07

20 6 -0.08 -0.01 -0.14 -0.01 -0.14 0.03 0.12 0.00 -0.09

21 6 -0.08 0.02 0.14 -0.02 -0.13 0.00 0.12 -0.03 0.10

22 6 -0.03 0.01 0.10 -0.03 -0.11 0.01 0.04 -0.02 0.07

23 7 -0.03 0.00 0.00 0.00 -0.13 0.05 0.04 -0.02 0.01

24 1 -0.10 0.04 -0.27 -0.01 -0.15 0.00 0.16 -0.06 -0.18

25 1 -0.10 -0.03 0.26 -0.03 -0.16 -0.04 0.16 0.02 0.18

26 1 0.10 -0.01 0.08 -0.02 0.16 0.18 -0.16 0.03 0.04

27 1 0.10 0.00 0.06 0.06 0.16 -0.18 -0.15 0.01 0.00

28 1 0.10 -0.01 -0.08 -0.02 0.16 -0.18 -0.16 0.03 -0.04

29 1 0.10 0.00 -0.06 0.06 0.16 0.18 -0.15 0.01 0.00

30 1 -0.10 -0.03 -0.26 -0.03 -0.16 0.04 0.16 0.02 -0.18

31 1 -0.10 0.04 0.27 -0.01 -0.15 0.00 0.16 -0.06 0.18

32 30 -0.05 0.00 0.00 -0.01 0.08 0.00 0.08 0.01 0.00

33 6 -0.01 0.02 -0.06 -0.04 0.01 -0.03 0.00 -0.04 -0.04

34 6 -0.05 0.07 -0.19 -0.13 0.08 -0.13 0.06 -0.11 -0.17

35 6 -0.05 0.07 0.19 -0.13 0.08 0.13 0.06 -0.11 0.17

36 6 0.03 0.00 0.07 0.00 -0.04 0.05 -0.04 -0.01 0.06

37 6 0.03 0.00 -0.07 0.00 -0.04 -0.05 -0.04 -0.01 -0.06

38 6 -0.05 -0.08 -0.18 0.11 0.06 0.17 0.08 0.13 -0.13

39 6 0.03 0.00 0.06 0.01 -0.04 -0.06 -0.04 0.00 0.05

40 6 -0.05 -0.08 0.18 0.11 0.06 -0.17 0.08 0.13 0.13

41 6 0.03 0.00 -0.06 0.01 -0.04 0.06 -0.04 0.00 -0.05

42 1 0.08 0.05 -0.19 -0.06 -0.10 0.17 -0.12 -0.09 -0.14

43 1 0.08 -0.04 0.20 0.09 -0.12 0.14 -0.10 0.06 0.17

44 1 0.08 0.05 0.19 -0.06 -0.10 -0.17 -0.12 -0.09 0.14

45 1 0.08 -0.04 -0.20 0.09 -0.12 -0.14 -0.10 0.06 -0.17

31 32 33

B1 A2 B1

Frequencies -- 401.0333 403.4449 431.4373

Red. masses -- 5.5711 5.6656 4.2789

Frc consts -- 0.5279 0.5433 0.4693

IR Inten -- 0.0000 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 0.00 -0.11 -0.08 0.08 0.00 0.18 -0.05 0.01

2 6 0.00 0.00 -0.08 0.05 0.11 0.00 0.03 -0.05 0.00

3 7 0.00 0.00 0.00 0.12 0.00 0.00 0.00 0.00 0.00

4 6 0.00 0.00 0.08 0.05 -0.11 0.00 0.03 0.05 0.00

5 6 0.01 0.00 0.11 -0.08 -0.08 0.00 0.18 0.05 -0.01

6 6 0.00 0.00 -0.03 0.01 0.01 0.00 0.00 0.00 0.00

7 6 0.00 0.00 0.08 -0.11 0.05 0.00 -0.05 -0.03 0.00

8 7 0.00 0.00 0.00 0.00 0.12 0.00 0.00 0.00 0.00

9 6 0.00 0.00 -0.08 0.11 0.05 0.00 0.05 -0.03 0.00

10 6 0.00 -0.01 -0.11 0.08 -0.08 0.00 0.05 -0.18 0.01

11 6 0.00 -0.01 0.11 -0.08 -0.08 0.00 -0.05 -0.18 -0.01

12 6 0.00 0.00 0.03 0.01 -0.01 0.00 0.00 0.00 0.00

13 6 0.00 0.00 -0.08 -0.11 -0.05 0.00 -0.05 0.03 0.00

14 6 0.00 0.01 -0.11 -0.08 0.08 0.00 -0.05 0.18 0.01

15 6 0.00 0.01 0.11 0.08 0.08 0.00 0.05 0.18 -0.01

16 6 0.00 0.00 0.08 0.11 -0.05 0.00 0.05 0.03 0.00

17 7 0.00 0.00 0.00 0.00 -0.12 0.00 0.00 0.00 0.00

18 6 0.00 0.00 -0.03 -0.01 -0.01 0.00 0.00 0.00 0.00

19 6 0.00 0.00 0.08 -0.05 0.11 0.00 -0.03 -0.05 0.00

20 6 -0.01 0.00 0.11 0.08 0.08 0.00 -0.18 -0.05 -0.01

21 6 -0.01 0.00 -0.11 0.08 -0.08 0.00 -0.18 0.05 0.01

22 6 0.00 0.00 -0.08 -0.05 -0.11 0.00 -0.03 0.05 0.00

23 7 0.00 0.00 0.00 -0.12 0.00 0.00 0.00 0.00 0.00

24 1 0.01 0.00 -0.22 -0.19 0.16 0.00 0.27 -0.12 0.01

25 1 0.01 0.00 0.22 -0.19 -0.16 0.00 0.27 0.12 -0.01

26 1 0.00 -0.01 -0.22 0.16 -0.19 0.00 0.12 -0.27 0.01

27 1 0.00 -0.01 0.22 -0.16 -0.19 0.00 -0.12 -0.27 -0.01

28 1 0.00 0.01 -0.22 -0.16 0.19 0.00 -0.12 0.27 0.01

29 1 0.00 0.01 0.22 0.16 0.19 0.00 0.12 0.27 -0.01

30 1 -0.01 0.00 0.22 0.19 0.16 0.00 -0.27 -0.12 -0.01

31 1 -0.01 0.00 -0.22 0.19 -0.16 0.00 -0.27 0.12 0.01

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.00 0.00 0.03 -0.01 0.01 0.00 0.00 0.00 0.00

34 6 0.00 0.00 0.24 -0.13 0.13 0.00 0.00 0.00 0.00

35 6 0.00 0.00 0.24 0.13 -0.13 0.00 0.00 0.00 0.00

36 6 0.00 0.00 -0.08 0.02 -0.02 0.00 0.01 0.01 0.00

37 6 0.00 0.00 -0.08 -0.02 0.02 0.00 -0.01 -0.01 0.00

38 6 0.00 0.00 -0.24 0.13 0.13 0.00 0.00 0.00 0.00

39 6 0.00 0.00 0.08 -0.02 -0.02 0.00 -0.01 0.01 0.00

40 6 0.00 0.00 -0.24 -0.13 -0.13 0.00 0.00 0.00 0.00

41 6 0.00 0.00 0.08 0.02 0.02 0.00 0.01 -0.01 0.00

42 1 0.00 0.00 0.23 0.11 0.11 0.00 0.01 -0.01 0.00

43 1 0.00 0.00 -0.23 0.11 -0.11 0.00 0.01 0.01 0.00

44 1 0.00 0.00 0.23 -0.11 -0.11 0.00 -0.01 0.01 0.00

45 1 0.00 0.00 -0.23 -0.11 0.11 0.00 -0.01 -0.01 0.00

34 35 36

B2 A1 E

Frequencies -- 453.5965 455.3435 477.8337

Red. masses -- 7.4836 8.3449 6.1386

Frc consts -- 0.9072 1.0194 0.8258

IR Inten -- 0.0000 0.3320 19.7710

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 0.00 0.00 0.00 0.14 0.00 0.14 -0.06 0.00

2 6 0.04 0.01 0.00 -0.02 0.09 0.01 0.00 -0.06 0.00

3 7 0.00 0.02 0.00 0.00 0.12 0.01 -0.04 0.00 0.00

4 6 -0.04 0.01 0.00 0.02 0.09 0.01 0.00 0.06 0.00

5 6 -0.01 0.00 0.00 0.00 0.14 0.00 0.14 0.06 0.00

6 6 -0.06 -0.06 0.00 0.08 -0.08 0.01 0.00 -0.06 0.00

7 6 0.01 -0.04 0.00 -0.09 -0.02 0.01 -0.04 -0.03 0.01

8 7 0.02 0.00 0.00 -0.12 0.00 0.01 -0.06 0.00 0.00

9 6 0.01 0.04 0.00 -0.09 0.02 0.01 -0.04 0.03 0.01

10 6 0.00 0.01 0.00 -0.14 0.00 0.00 -0.08 0.00 0.00

11 6 0.00 -0.01 0.00 -0.14 0.00 0.00 -0.08 0.00 0.00

12 6 0.06 -0.06 0.00 -0.08 -0.08 0.01 0.00 0.06 0.00

13 6 -0.01 -0.04 0.00 0.09 -0.02 0.01 -0.04 0.03 -0.01

14 6 0.00 -0.01 0.00 0.14 0.00 0.00 -0.08 0.00 0.00

15 6 0.00 0.01 0.00 0.14 0.00 0.00 -0.08 0.00 0.00

16 6 -0.01 0.04 0.00 0.09 0.02 0.01 -0.04 -0.03 -0.01

17 7 -0.02 0.00 0.00 0.12 0.00 0.01 -0.06 0.00 0.00

18 6 0.06 0.06 0.00 -0.08 0.08 0.01 0.00 -0.06 0.00

19 6 0.04 -0.01 0.00 -0.02 -0.09 0.01 0.00 0.06 0.00

20 6 0.01 0.00 0.00 0.00 -0.14 0.00 0.14 0.06 0.00

21 6 -0.01 0.00 0.00 0.00 -0.14 0.00 0.14 -0.06 0.00

22 6 -0.04 -0.01 0.00 0.02 -0.09 0.01 0.00 -0.06 0.00

23 7 0.00 -0.02 0.00 0.00 -0.12 0.01 -0.04 0.00 0.00

24 1 -0.01 0.01 0.00 0.01 0.14 -0.01 0.24 -0.14 0.01

25 1 0.01 0.01 0.00 -0.01 0.14 -0.01 0.24 0.14 -0.01

26 1 0.01 -0.01 0.00 -0.14 -0.01 -0.01 -0.08 0.00 -0.01

27 1 0.01 0.01 0.00 -0.14 0.01 -0.01 -0.08 0.00 -0.01

28 1 -0.01 0.01 0.00 0.14 0.01 -0.01 -0.08 0.00 0.01

29 1 -0.01 -0.01 0.00 0.14 -0.01 -0.01 -0.08 0.00 0.01

30 1 -0.01 -0.01 0.00 0.01 -0.14 -0.01 0.24 0.14 0.01

31 1 0.01 -0.01 0.00 -0.01 -0.14 -0.01 0.24 -0.14 -0.01

32 30 0.00 0.00 0.00 0.00 0.00 -0.02 0.02 0.00 0.00

33 6 -0.06 0.06 0.00 0.08 0.08 0.01 0.00 0.06 0.00

34 6 -0.26 0.26 0.00 0.13 0.13 -0.02 -0.11 0.23 -0.01

35 6 0.26 -0.26 0.00 -0.13 -0.13 -0.02 -0.11 0.23 0.01

36 6 0.03 -0.03 0.00 0.15 0.15 0.00 0.08 0.05 0.00

37 6 -0.03 0.03 0.00 -0.15 -0.15 0.00 0.08 0.05 0.00

38 6 -0.26 -0.26 0.00 0.13 -0.13 -0.02 -0.11 -0.23 -0.01

39 6 0.03 0.03 0.00 0.15 -0.15 0.00 0.08 -0.05 0.00

40 6 0.26 0.26 0.00 -0.13 0.13 -0.02 -0.11 -0.23 0.01

41 6 -0.03 -0.03 0.00 -0.15 0.15 0.00 0.08 -0.05 0.00

42 1 -0.23 -0.23 0.00 -0.15 0.15 0.00 0.21 0.07 0.00

43 1 0.23 -0.23 0.00 0.15 0.15 0.00 0.21 -0.07 0.00

44 1 0.23 0.23 0.00 0.15 -0.15 0.00 0.21 0.07 0.00

45 1 -0.23 0.23 0.00 -0.15 -0.15 0.00 0.21 -0.07 0.00

37 38 39

E B1 E

Frequencies -- 477.8337 551.6289 560.6544

Red. masses -- 6.1386 5.8668 7.1247

Frc consts -- 0.8258 1.0518 1.3195

IR Inten -- 19.7710 0.0000 0.0026

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.08 0.00 0.00 0.00 0.13 0.01 0.00 -0.14

2 6 0.03 -0.04 -0.01 0.00 0.00 -0.05 0.00 0.00 0.07

3 7 0.00 -0.06 0.00 0.00 0.00 0.00 0.00 0.00 0.00

4 6 -0.03 -0.04 -0.01 0.00 0.00 0.05 0.00 0.00 -0.07

5 6 0.00 -0.08 0.00 0.00 0.00 -0.13 0.01 0.00 0.14

6 6 -0.06 0.00 0.00 0.00 0.00 0.21 0.00 0.00 -0.24

7 6 0.06 0.00 0.00 0.00 0.00 0.05 -0.01 0.00 -0.04

8 7 0.00 -0.04 0.00 0.00 0.00 0.00 0.00 0.00 0.15

9 6 -0.06 0.00 0.00 0.00 0.00 -0.05 -0.01 0.00 -0.04

10 6 -0.06 0.14 0.00 0.00 0.00 0.13 -0.01 0.00 0.03

11 6 0.06 0.14 0.00 0.00 0.00 -0.13 -0.01 0.00 0.03

12 6 0.06 0.00 0.00 0.00 0.00 -0.21 0.00 0.00 0.24

13 6 -0.06 0.00 0.00 0.00 0.00 -0.05 -0.01 0.00 0.04

14 6 -0.06 0.14 0.00 0.00 0.00 0.13 -0.01 0.00 -0.03

15 6 0.06 0.14 0.00 0.00 0.00 -0.13 -0.01 0.00 -0.03

16 6 0.06 0.00 0.00 0.00 0.00 0.05 -0.01 0.00 0.04

17 7 0.00 -0.04 0.00 0.00 0.00 0.00 0.00 0.00 -0.15

18 6 -0.06 0.00 0.00 0.00 0.00 0.21 0.00 0.00 0.24

19 6 -0.03 -0.04 0.01 0.00 0.00 0.05 0.00 0.00 0.07

20 6 0.00 -0.08 0.00 0.00 0.00 -0.13 0.01 0.00 -0.14

21 6 0.00 -0.08 0.00 0.00 0.00 0.13 0.01 0.00 0.14

22 6 0.03 -0.04 0.01 0.00 0.00 -0.05 0.00 0.00 -0.07

23 7 0.00 -0.06 0.00 0.00 0.00 0.00 0.00 0.00 0.00

24 1 0.00 -0.08 0.01 -0.01 0.00 0.25 0.01 0.00 -0.27

25 1 0.00 -0.08 0.01 -0.01 0.00 -0.25 0.01 0.00 0.27

26 1 -0.14 0.24 -0.01 0.00 0.01 0.25 -0.01 0.00 0.03

27 1 0.14 0.24 0.01 0.00 0.01 -0.25 -0.01 0.00 0.03

28 1 -0.14 0.24 0.01 0.00 -0.01 0.25 -0.01 0.00 -0.03

29 1 0.14 0.24 -0.01 0.00 -0.01 -0.25 -0.01 0.00 -0.03

30 1 0.00 -0.08 -0.01 0.01 0.00 -0.25 0.01 0.00 -0.27

31 1 0.00 -0.08 -0.01 0.01 0.00 0.25 0.01 0.00 0.27

32 30 0.00 0.02 0.00 0.00 0.00 0.00 0.01 0.00 0.00

33 6 0.06 0.00 0.00 0.00 0.00 -0.21 0.00 0.00 -0.24

34 6 0.23 -0.11 -0.01 0.00 0.00 0.15 0.00 0.00 0.18

35 6 0.23 -0.11 0.01 0.00 0.00 0.15 0.00 0.00 -0.18

36 6 0.05 0.08 0.00 0.00 0.00 -0.07 0.00 0.00 -0.08

37 6 0.05 0.08 0.00 0.00 0.00 -0.07 0.00 0.00 0.08

38 6 -0.23 -0.11 0.01 0.00 0.00 -0.15 0.00 0.00 0.18

39 6 -0.05 0.08 0.00 0.00 0.00 0.07 0.00 0.00 -0.08

40 6 -0.23 -0.11 -0.01 0.00 0.00 -0.15 0.00 0.00 -0.18

41 6 -0.05 0.08 0.00 0.00 0.00 0.07 0.00 0.00 0.08

42 1 0.07 0.21 0.00 0.00 0.00 -0.12 0.00 0.00 -0.19

43 1 -0.07 0.21 0.00 0.00 0.00 0.12 0.00 0.00 0.19

44 1 0.07 0.21 0.00 0.00 0.00 -0.12 0.00 0.00 0.19

45 1 -0.07 0.21 0.00 0.00 0.00 0.12 0.00 0.00 -0.19

40 41 42

E A1 A2

Frequencies -- 560.6544 571.8193 579.6336

Red. masses -- 7.1247 7.6556 7.6883

Frc consts -- 1.3195 1.4749 1.5219

IR Inten -- 0.0026 3.2196 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.01 -0.03 0.00 -0.01 -0.03 -0.06 -0.07 0.00

2 6 0.00 -0.01 0.04 0.00 -0.01 0.05 -0.09 -0.07 0.00

3 7 0.00 0.00 -0.15 0.00 0.00 -0.15 -0.16 0.00 0.00

4 6 0.00 -0.01 0.04 0.00 -0.01 0.05 -0.09 0.07 0.00

5 6 0.00 -0.01 -0.03 0.00 -0.01 -0.03 -0.06 0.07 0.00

6 6 0.00 0.00 0.24 0.00 0.00 0.26 -0.01 -0.01 0.00

7 6 0.00 0.00 0.07 0.01 0.00 0.05 0.07 -0.09 0.00

8 7 0.00 0.00 0.00 0.00 0.00 -0.15 0.00 -0.16 0.00

9 6 0.00 0.00 -0.07 0.01 0.00 0.05 -0.07 -0.09 0.00

10 6 0.00 0.01 0.14 0.01 0.00 -0.03 -0.07 -0.06 0.00

11 6 0.00 0.01 -0.14 0.01 0.00 -0.03 0.07 -0.06 0.00

12 6 0.00 0.00 0.24 0.00 0.00 0.26 -0.01 0.01 0.00

13 6 0.00 0.00 0.07 -0.01 0.00 0.05 0.07 0.09 0.00

14 6 0.00 0.01 -0.14 -0.01 0.00 -0.03 0.07 0.06 0.00

15 6 0.00 0.01 0.14 -0.01 0.00 -0.03 -0.07 0.06 0.00

16 6 0.00 0.00 -0.07 -0.01 0.00 0.05 -0.07 0.09 0.00

17 7 0.00 0.00 0.00 0.00 0.00 -0.15 0.00 0.16 0.00

18 6 0.00 0.00 -0.24 0.00 0.00 0.26 0.01 0.01 0.00

19 6 0.00 -0.01 -0.04 0.00 0.01 0.05 0.09 -0.07 0.00

20 6 0.00 -0.01 0.03 0.00 0.01 -0.03 0.06 -0.07 0.00

21 6 0.00 -0.01 0.03 0.00 0.01 -0.03 0.06 0.07 0.00

22 6 0.00 -0.01 -0.04 0.00 0.01 0.05 0.09 0.07 0.00

23 7 0.00 0.00 0.15 0.00 0.00 -0.15 0.16 0.00 0.00

24 1 0.00 -0.01 -0.03 0.00 -0.01 -0.03 0.02 -0.13 -0.01

25 1 0.00 -0.01 -0.03 0.00 -0.01 -0.03 0.02 0.13 0.01

26 1 0.00 0.01 0.27 0.01 0.00 -0.03 -0.13 0.02 0.01

27 1 0.00 0.01 -0.27 0.01 0.00 -0.03 0.13 0.02 -0.01

28 1 0.00 0.01 -0.27 -0.01 0.00 -0.03 0.13 -0.02 0.01

29 1 0.00 0.01 0.27 -0.01 0.00 -0.03 -0.13 -0.02 -0.01

30 1 0.00 -0.01 0.03 0.00 0.01 -0.03 -0.02 -0.13 0.01

31 1 0.00 -0.01 0.03 0.00 0.01 -0.03 -0.02 0.13 -0.01

32 30 0.00 0.01 0.00 0.00 0.00 0.01 0.00 0.00 0.00

33 6 0.00 0.00 -0.24 0.00 0.00 0.26 0.01 -0.01 0.00

34 6 0.00 0.00 0.18 -0.01 -0.01 -0.20 -0.20 0.20 0.00

35 6 0.00 0.00 -0.18 0.01 0.01 -0.20 0.20 -0.20 0.00

36 6 0.00 0.00 -0.08 0.00 0.00 0.10 0.01 -0.01 0.00

37 6 0.00 0.00 0.08 0.00 0.00 0.10 -0.01 0.01 0.00

38 6 0.00 0.00 -0.18 -0.01 0.01 -0.20 0.20 0.20 0.00

39 6 0.00 0.00 0.08 0.00 0.00 0.10 -0.01 -0.01 0.00

40 6 0.00 0.00 0.18 0.01 -0.01 -0.20 -0.20 -0.20 0.00

41 6 0.00 0.00 -0.08 0.00 0.00 0.10 0.01 0.01 0.00

42 1 0.00 0.00 0.19 0.01 -0.01 -0.32 0.18 0.18 0.00

43 1 0.00 0.00 0.19 -0.01 -0.01 -0.32 0.18 -0.18 0.00

44 1 0.00 0.00 -0.19 -0.01 0.01 -0.32 -0.18 -0.18 0.00

45 1 0.00 0.00 -0.19 0.01 0.01 -0.32 -0.18 0.18 0.00

43 44 45

E E B1

Frequencies -- 596.7188 596.7188 610.5347

Red. masses -- 7.6551 7.6551 1.2336

Frc consts -- 1.6060 1.6060 0.2709

IR Inten -- 0.5247 0.5247 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.07 0.12 0.01 0.00 -0.01 0.00 0.00 0.00 0.01

2 6 0.13 0.13 0.00 -0.01 0.00 0.00 0.00 0.00 -0.01

3 7 0.23 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

4 6 0.13 -0.13 0.00 0.01 0.00 0.00 0.00 0.00 0.01

5 6 0.07 -0.12 -0.01 -0.01 0.00 0.00 0.00 0.00 -0.01

6 6 -0.01 0.02 0.00 0.02 -0.01 0.00 0.00 0.00 0.02

7 6 0.00 0.01 0.00 -0.13 0.13 0.00 0.00 0.00 0.01

8 7 0.00 0.00 0.00 0.00 0.23 0.00 0.00 0.00 0.00

9 6 0.00 -0.01 0.00 0.13 0.13 0.00 0.00 0.00 -0.01

10 6 0.00 0.01 0.00 0.12 0.07 -0.01 0.00 0.00 0.01

11 6 -0.01 0.00 0.00 -0.12 0.07 0.01 0.00 0.00 -0.01

12 6 -0.01 -0.02 0.00 -0.02 -0.01 0.00 0.00 0.00 -0.02

13 6 0.00 -0.01 0.00 0.13 0.13 0.00 0.00 0.00 -0.01

14 6 0.00 0.01 0.00 0.12 0.07 0.01 0.00 0.00 0.01

15 6 -0.01 0.00 0.00 -0.12 0.07 -0.01 0.00 0.00 -0.01

16 6 0.00 0.01 0.00 -0.13 0.13 0.00 0.00 0.00 0.01

17 7 0.00 0.00 0.00 0.00 0.23 0.00 0.00 0.00 0.00

18 6 -0.01 0.02 0.00 0.02 -0.01 0.00 0.00 0.00 0.02

19 6 0.13 -0.13 0.00 0.01 0.00 0.00 0.00 0.00 0.01

20 6 0.07 -0.12 0.01 -0.01 0.00 0.00 0.00 0.00 -0.01

21 6 0.07 0.12 -0.01 0.00 -0.01 0.00 0.00 0.00 0.01

22 6 0.13 0.13 0.00 -0.01 0.00 0.00 0.00 0.00 -0.01

23 7 0.23 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

24 1 -0.06 0.22 0.02 0.01 -0.01 -0.01 0.00 0.00 0.03

25 1 -0.06 -0.22 -0.02 -0.01 -0.01 -0.01 0.00 0.00 -0.03

26 1 -0.01 0.01 0.01 0.22 -0.06 -0.02 0.00 0.00 0.03

27 1 -0.01 -0.01 0.01 -0.22 -0.06 0.02 0.00 0.00 -0.03

28 1 -0.01 0.01 -0.01 0.22 -0.06 0.02 0.00 0.00 0.03

29 1 -0.01 -0.01 -0.01 -0.22 -0.06 -0.02 0.00 0.00 -0.03

30 1 -0.06 -0.22 0.02 -0.01 -0.01 0.01 0.00 0.00 -0.03

31 1 -0.06 0.22 -0.02 0.01 -0.01 0.01 0.00 0.00 0.03

32 30 -0.01 0.00 0.00 0.00 -0.01 0.00 0.00 0.00 0.00

33 6 -0.01 -0.02 0.00 -0.02 -0.01 0.00 0.00 0.00 -0.02

34 6 -0.21 0.03 0.00 0.03 -0.21 0.00 0.00 0.00 -0.01

35 6 -0.21 0.03 0.00 0.03 -0.21 0.00 0.00 0.00 -0.01

36 6 -0.10 -0.11 0.00 -0.11 -0.10 0.00 0.00 0.00 0.06

37 6 -0.10 -0.11 0.00 -0.11 -0.10 0.00 0.00 0.00 0.06

38 6 -0.21 -0.03 0.00 -0.03 -0.21 0.00 0.00 0.00 0.01

39 6 -0.10 0.11 0.00 0.11 -0.10 0.00 0.00 0.00 -0.06

40 6 -0.21 -0.03 0.00 -0.03 -0.21 0.00 0.00 0.00 0.01

41 6 -0.10 0.11 0.00 0.11 -0.10 0.00 0.00 0.00 -0.06

42 1 0.01 0.22 -0.02 0.22 0.00 0.02 -0.01 0.01 0.49

43 1 0.00 -0.22 0.02 -0.22 0.01 0.02 -0.01 -0.01 -0.49

44 1 0.01 0.22 0.02 0.22 0.00 -0.02 0.01 -0.01 0.49

45 1 0.00 -0.22 -0.02 -0.22 0.01 -0.02 0.01 0.01 -0.49

46 47 48

E E A1

Frequencies -- 611.7001 611.7001 613.9432

Red. masses -- 1.2495 1.2495 1.3025

Frc consts -- 0.2755 0.2755 0.2893

IR Inten -- 0.0034 0.0034 318.8325

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.02 0.00 0.00 0.00 0.00 0.00 0.00

2 6 0.00 0.00 -0.02 0.00 0.00 -0.01 0.00 0.00 -0.02

3 7 0.00 0.00 0.00 0.00 0.00 0.02 0.00 0.00 0.03

4 6 0.00 0.00 0.02 0.00 0.00 -0.01 0.00 0.00 -0.02

5 6 0.00 0.00 -0.02 0.00 0.00 0.00 0.00 0.00 0.00

6 6 0.00 0.00 0.03 0.00 0.00 -0.03 0.00 0.00 -0.04

7 6 0.00 0.00 0.01 0.00 0.00 -0.02 0.00 0.00 -0.02

8 7 0.00 0.00 -0.02 0.00 0.00 0.00 0.00 0.00 0.03

9 6 0.00 0.00 0.01 0.00 0.00 0.02 0.00 0.00 -0.02

10 6 0.00 0.00 0.00 0.00 0.00 -0.02 0.00 0.00 0.00

11 6 0.00 0.00 0.00 0.00 0.00 0.02 0.00 0.00 0.00

12 6 0.00 0.00 -0.03 0.00 0.00 -0.03 0.00 0.00 -0.04

13 6 0.00 0.00 -0.01 0.00 0.00 -0.02 0.00 0.00 -0.02

14 6 0.00 0.00 0.00 0.00 0.00 0.02 0.00 0.00 0.00

15 6 0.00 0.00 0.00 0.00 0.00 -0.02 0.00 0.00 0.00

16 6 0.00 0.00 -0.01 0.00 0.00 0.02 0.00 0.00 -0.02

17 7 0.00 0.00 0.02 0.00 0.00 0.00 0.00 0.00 0.03

18 6 0.00 0.00 -0.03 0.00 0.00 0.03 0.00 0.00 -0.04

19 6 0.00 0.00 -0.02 0.00 0.00 0.01 0.00 0.00 -0.02

20 6 0.00 0.00 0.02 0.00 0.00 0.00 0.00 0.00 0.00

21 6 0.00 0.00 -0.02 0.00 0.00 0.00 0.00 0.00 0.00

22 6 0.00 0.00 0.02 0.00 0.00 0.01 0.00 0.00 -0.02

23 7 0.00 0.00 0.00 0.00 0.00 -0.02 0.00 0.00 0.03

24 1 0.00 0.00 0.04 0.00 0.00 0.01 0.00 0.00 0.02

25 1 0.00 0.00 -0.04 0.00 0.00 0.01 0.00 0.00 0.02

26 1 0.00 0.00 -0.01 0.00 0.00 -0.04 0.00 0.00 0.02

27 1 0.00 0.00 -0.01 0.00 0.00 0.04 0.00 0.00 0.02

28 1 0.00 0.00 0.01 0.00 0.00 0.04 0.00 0.00 0.02

29 1 0.00 0.00 0.01 0.00 0.00 -0.04 0.00 0.00 0.02

30 1 0.00 0.00 0.04 0.00 0.00 -0.01 0.00 0.00 0.02

31 1 0.00 0.00 -0.04 0.00 0.00 -0.01 0.00 0.00 0.02

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.00 0.00 0.03 0.00 0.00 0.03 0.00 0.00 -0.04

34 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.01

35 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.01

36 6 0.00 0.00 -0.06 0.00 0.00 -0.06 0.00 0.00 0.06

37 6 0.00 0.00 0.06 0.00 0.00 0.06 0.00 0.00 0.06

38 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.01

39 6 0.00 0.00 -0.06 0.00 0.00 0.06 0.00 0.00 0.06

40 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.01

41 6 0.00 0.00 0.06 0.00 0.00 -0.06 0.00 0.00 0.06

42 1 0.01 -0.01 -0.49 -0.01 0.01 0.49 0.01 -0.01 -0.49

43 1 0.01 0.01 0.49 0.01 0.01 0.49 -0.01 -0.01 -0.49

44 1 0.01 -0.01 0.49 -0.01 0.01 -0.49 -0.01 0.01 -0.49

45 1 0.01 0.01 -0.49 0.01 0.01 -0.49 0.01 0.01 -0.49

49 50 51

B1 B2 A2

Frequencies -- 619.2352 673.2285 682.5755

Red. masses -- 7.6235 2.8285 1.2757

Frc consts -- 1.7223 0.7553 0.3502

IR Inten -- 0.0000 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.05 -0.09 0.00 0.00 0.00 0.00 0.00 0.00 0.00

2 6 -0.08 -0.09 0.00 0.00 0.00 0.11 0.00 0.00 0.00

3 7 -0.17 0.00 0.00 0.00 0.01 -0.12 0.00 0.00 0.00

4 6 -0.08 0.09 0.00 0.00 0.00 0.11 0.00 0.00 0.00

5 6 -0.05 0.09 0.00 0.00 0.00 0.00 0.00 0.00 0.00

6 6 0.01 -0.01 0.01 0.00 0.00 0.00 0.00 0.00 0.00

7 6 -0.09 0.08 0.00 0.00 0.00 -0.11 0.00 0.00 0.00

8 7 0.00 0.17 0.00 0.01 0.00 0.12 0.00 0.00 0.00

9 6 0.09 0.08 0.00 0.00 0.00 -0.11 0.00 0.00 0.00

10 6 0.09 0.05 0.00 0.00 0.00 0.00 0.00 0.00 0.00

11 6 -0.09 0.05 0.00 0.00 0.00 0.00 0.00 0.00 0.00

12 6 0.01 0.01 -0.01 0.00 0.00 0.00 0.00 0.00 0.00

13 6 -0.09 -0.08 0.00 0.00 0.00 -0.11 0.00 0.00 0.00

14 6 -0.09 -0.05 0.00 0.00 0.00 0.00 0.00 0.00 0.00

15 6 0.09 -0.05 0.00 0.00 0.00 0.00 0.00 0.00 0.00

16 6 0.09 -0.08 0.00 0.00 0.00 -0.11 0.00 0.00 0.00

17 7 0.00 -0.17 0.00 -0.01 0.00 0.12 0.00 0.00 0.00

18 6 -0.01 0.01 0.01 0.00 0.00 0.00 0.00 0.00 0.00

19 6 0.08 -0.09 0.00 0.00 0.00 0.11 0.00 0.00 0.00

20 6 0.05 -0.09 0.00 0.00 0.00 0.00 0.00 0.00 0.00

21 6 0.05 0.09 0.00 0.00 0.00 0.00 0.00 0.00 0.00

22 6 0.08 0.09 0.00 0.00 0.00 0.11 0.00 0.00 0.00

23 7 0.17 0.00 0.00 0.00 -0.01 -0.12 0.00 0.00 0.00

24 1 0.05 -0.17 0.00 0.00 0.01 -0.32 0.00 0.00 0.00

25 1 0.05 0.17 0.00 0.00 0.01 -0.32 0.00 0.00 0.00

26 1 0.17 -0.05 0.00 0.01 0.00 0.32 0.00 0.00 0.00

27 1 -0.17 -0.05 0.00 0.01 0.00 0.32 0.00 0.00 0.00

28 1 -0.17 0.05 0.00 -0.01 0.00 0.32 0.00 0.00 0.00

29 1 0.17 0.05 0.00 -0.01 0.00 0.32 0.00 0.00 0.00

30 1 -0.05 -0.17 0.00 0.00 -0.01 -0.32 0.00 0.00 0.00

31 1 -0.05 0.17 0.00 0.00 -0.01 -0.32 0.00 0.00 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 -0.01 -0.01 -0.01 0.00 0.00 0.00 0.00 0.00 0.00

34 6 -0.11 -0.11 0.00 0.00 0.00 0.00 0.02 -0.02 0.00

35 6 0.11 0.11 0.00 0.00 0.00 0.00 -0.02 0.02 0.00

36 6 -0.14 -0.14 0.01 0.00 0.00 0.00 -0.05 0.05 0.00

37 6 0.14 0.14 0.01 0.00 0.00 0.00 0.05 -0.05 0.00

38 6 0.11 -0.11 0.00 0.00 0.00 0.00 -0.02 -0.02 0.00

39 6 0.14 -0.14 -0.01 0.00 0.00 0.00 0.05 0.05 0.00

40 6 -0.11 0.11 0.00 0.00 0.00 0.00 0.02 0.02 0.00

41 6 -0.14 0.14 -0.01 0.00 0.00 0.00 -0.05 -0.05 0.00

42 1 -0.14 0.14 0.05 0.00 0.00 0.00 0.35 0.35 0.00

43 1 -0.14 -0.14 -0.05 0.00 0.00 0.00 0.35 -0.35 0.00

44 1 0.14 -0.14 0.05 0.00 0.00 0.00 -0.35 -0.35 0.00

45 1 0.14 0.14 -0.05 0.00 0.00 0.00 -0.35 0.35 0.00

52 53 54

E E B2

Frequencies -- 682.6254 682.6254 682.6407

Red. masses -- 1.2813 1.2813 1.2660

Frc consts -- 0.3518 0.3518 0.3476

IR Inten -- 147.2352 147.2352 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.00 0.00 0.00 -0.01 0.00 0.00 0.00

2 6 0.00 0.00 -0.01 0.00 0.00 0.01 0.00 0.00 0.00

3 7 0.00 0.00 0.01 0.00 0.00 0.00 0.00 0.00 0.00

4 6 0.00 0.00 -0.01 0.00 0.00 -0.01 0.00 0.00 0.00

5 6 0.00 0.00 0.00 0.00 0.00 0.01 0.00 0.00 0.00

6 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

7 6 0.00 0.00 0.01 0.00 0.00 0.01 0.00 0.00 0.00

8 7 0.00 0.00 0.00 0.00 0.00 -0.01 0.00 0.00 0.00

9 6 0.00 0.00 -0.01 0.00 0.00 0.01 0.00 0.00 0.00

10 6 0.00 0.00 0.01 0.00 0.00 0.00 0.00 0.00 0.00

11 6 0.00 0.00 -0.01 0.00 0.00 0.00 0.00 0.00 0.00

12 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

13 6 0.00 0.00 0.01 0.00 0.00 -0.01 0.00 0.00 0.00

14 6 0.00 0.00 -0.01 0.00 0.00 0.00 0.00 0.00 0.00

15 6 0.00 0.00 0.01 0.00 0.00 0.00 0.00 0.00 0.00

16 6 0.00 0.00 -0.01 0.00 0.00 -0.01 0.00 0.00 0.00

17 7 0.00 0.00 0.00 0.00 0.00 0.01 0.00 0.00 0.00

18 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

19 6 0.00 0.00 0.01 0.00 0.00 0.01 0.00 0.00 0.00

20 6 0.00 0.00 0.00 0.00 0.00 -0.01 0.00 0.00 0.00

21 6 0.00 0.00 0.00 0.00 0.00 0.01 0.00 0.00 0.00

22 6 0.00 0.00 0.01 0.00 0.00 -0.01 0.00 0.00 0.00

23 7 0.00 0.00 -0.01 0.00 0.00 0.00 0.00 0.00 0.00

24 1 0.00 0.00 0.03 0.00 0.00 -0.01 0.00 0.00 0.00

25 1 0.00 0.00 0.03 0.00 0.00 0.01 0.00 0.00 0.00

26 1 0.00 0.00 0.01 0.00 0.00 -0.03 0.00 0.00 0.00

27 1 0.00 0.00 -0.01 0.00 0.00 -0.03 0.00 0.00 0.00

28 1 0.00 0.00 -0.01 0.00 0.00 0.03 0.00 0.00 0.00

29 1 0.00 0.00 0.01 0.00 0.00 0.03 0.00 0.00 0.00

30 1 0.00 0.00 -0.03 0.00 0.00 -0.01 0.00 0.00 0.00

31 1 0.00 0.00 -0.03 0.00 0.00 0.01 0.00 0.00 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

34 6 0.02 -0.02 0.00 -0.02 0.02 0.00 -0.02 0.02 0.00

35 6 0.02 -0.02 0.00 -0.02 0.02 0.00 0.02 -0.02 0.00

36 6 -0.05 0.05 0.00 0.05 -0.05 0.00 0.05 -0.05 0.00

37 6 -0.05 0.05 0.00 0.05 -0.05 0.00 -0.05 0.05 0.00

38 6 -0.02 -0.02 0.00 -0.02 -0.02 0.00 -0.02 -0.02 0.00

39 6 0.05 0.05 0.00 0.05 0.05 0.00 0.05 0.05 0.00

40 6 -0.02 -0.02 0.00 -0.02 -0.02 0.00 0.02 0.02 0.00

41 6 0.05 0.05 0.00 0.05 0.05 0.00 -0.05 -0.05 0.00

42 1 -0.35 -0.35 0.00 -0.35 -0.35 0.00 0.35 0.35 0.00

43 1 0.35 -0.35 0.00 -0.35 0.35 0.00 -0.35 0.35 0.00

44 1 -0.35 -0.35 0.00 -0.35 -0.35 0.00 -0.35 -0.35 0.00

45 1 0.35 -0.35 0.00 -0.35 0.35 0.00 0.35 -0.35 0.00

55 56 57

E E A2

Frequencies -- 683.4033 683.4033 688.8548

Red. masses -- 3.1168 3.1168 4.7614

Frc consts -- 0.8577 0.8577 1.3312

IR Inten -- 2.2224 2.2224 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.02 0.00 0.00 0.07 0.00 0.00 0.11

2 6 0.00 0.01 -0.16 0.00 0.00 -0.06 0.00 0.00 -0.17

3 7 0.00 -0.01 0.14 0.00 0.00 -0.04 0.00 0.00 0.00

4 6 0.00 0.00 -0.10 0.00 0.00 0.14 0.00 0.00 0.17

5 6 0.00 0.01 -0.03 0.00 0.00 -0.07 0.00 0.00 -0.11

6 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

7 6 0.00 0.00 0.06 -0.01 0.00 -0.16 0.00 0.00 -0.17

8 7 0.00 0.00 0.04 0.01 0.00 0.14 0.00 0.00 0.00

9 6 0.00 0.00 -0.14 0.00 0.00 -0.10 0.00 0.00 0.17

10 6 0.00 0.00 0.07 -0.01 0.00 -0.03 0.00 0.00 -0.11

11 6 0.00 0.00 -0.07 0.00 0.00 0.02 0.00 0.00 0.11

12 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

13 6 0.00 0.00 0.14 0.00 0.00 0.10 0.00 0.00 0.17

14 6 0.00 0.00 -0.07 -0.01 0.00 0.03 0.00 0.00 -0.11

15 6 0.00 0.00 0.07 0.00 0.00 -0.02 0.00 0.00 0.11

16 6 0.00 0.00 -0.06 -0.01 0.00 0.16 0.00 0.00 -0.17

17 7 0.00 0.00 -0.04 0.01 0.00 -0.14 0.00 0.00 0.00

18 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

19 6 0.00 0.00 0.10 0.00 0.00 -0.14 0.00 0.00 0.17

20 6 0.00 0.01 0.03 0.00 0.00 0.07 0.00 0.00 -0.11

21 6 0.00 0.00 -0.02 0.00 0.00 -0.07 0.00 0.00 0.11

22 6 0.00 0.01 0.16 0.00 0.00 0.06 0.00 0.00 -0.17

23 7 0.00 -0.01 -0.14 0.00 0.00 0.04 0.00 0.00 0.00

24 1 0.00 -0.01 0.44 0.00 -0.01 0.05 0.00 -0.01 0.29

25 1 0.00 -0.01 0.33 0.00 0.01 -0.29 0.00 0.01 -0.29

26 1 0.01 0.00 0.29 0.01 0.00 0.33 -0.01 0.00 -0.29

27 1 -0.01 0.00 -0.05 0.01 0.00 0.44 0.01 0.00 0.29

28 1 0.01 0.00 -0.29 0.01 0.00 -0.33 0.01 0.00 -0.29

29 1 -0.01 0.00 0.05 0.01 0.00 -0.44 -0.01 0.00 0.29

30 1 0.00 -0.01 -0.33 0.00 0.01 0.29 0.00 -0.01 -0.29

31 1 0.00 -0.01 -0.44 0.00 -0.01 -0.05 0.00 0.01 0.29

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

34 6 0.00 0.00 -0.01 0.00 0.00 0.01 0.00 0.00 0.00

35 6 0.00 0.00 0.01 0.00 0.00 -0.01 0.00 0.00 0.00

36 6 0.01 -0.01 0.00 0.01 0.00 0.00 0.00 0.00 0.00

37 6 0.01 -0.01 0.00 0.01 0.00 0.00 0.00 0.00 0.00

38 6 0.00 0.00 0.01 0.00 0.00 0.01 0.00 0.00 0.00

39 6 0.00 -0.01 0.00 0.01 0.01 0.00 0.00 0.00 0.00

40 6 0.00 0.00 -0.01 0.00 0.00 -0.01 0.00 0.00 0.00

41 6 0.00 -0.01 0.00 0.01 0.01 0.00 0.00 0.00 0.00

42 1 0.04 0.04 0.00 -0.08 -0.08 0.00 0.01 0.01 0.00

43 1 -0.08 0.08 0.00 -0.04 0.04 0.00 0.01 -0.01 0.00

44 1 0.04 0.04 0.00 -0.08 -0.08 0.00 -0.01 -0.01 0.00

45 1 -0.08 0.08 0.00 -0.04 0.04 0.00 -0.01 0.01 0.00

58 59 60

A1 E E

Frequencies -- 725.4221 738.5943 738.5943

Red. masses -- 1.9298 3.0741 3.0741

Frc consts -- 0.5983 0.9880 0.9880

IR Inten -- 106.5013 0.0009 0.0009

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 -0.03 0.00 0.00 0.06 0.00 0.00 0.04

2 6 0.00 0.00 -0.07 0.00 0.00 -0.15 0.00 0.00 0.05

3 7 0.00 0.00 0.07 0.00 0.00 0.00 0.00 0.00 -0.05

4 6 0.00 0.00 -0.07 0.00 0.00 0.15 0.00 0.00 0.06

5 6 0.00 0.00 -0.03 0.00 0.00 -0.06 0.00 0.00 0.04

6 6 0.00 0.00 0.07 0.00 0.00 -0.11 0.00 0.00 -0.11

7 6 0.00 0.00 -0.07 0.00 0.00 0.05 0.00 0.00 0.15

8 7 0.00 0.00 0.07 0.00 0.00 -0.05 0.00 0.00 0.00

9 6 0.00 0.00 -0.07 0.00 0.00 0.06 0.00 0.00 -0.15

10 6 0.00 0.00 -0.03 0.00 0.00 0.04 0.00 0.00 0.06

11 6 0.00 0.00 -0.03 0.00 0.00 0.04 0.00 0.00 -0.06

12 6 0.00 0.00 0.07 0.00 0.00 0.11 0.00 0.00 -0.11

13 6 0.00 0.00 -0.07 0.00 0.00 -0.06 0.00 0.00 0.15

14 6 0.00 0.00 -0.03 0.00 0.00 -0.04 0.00 0.00 -0.06

15 6 0.00 0.00 -0.03 0.00 0.00 -0.04 0.00 0.00 0.06

16 6 0.00 0.00 -0.07 0.00 0.00 -0.05 0.00 0.00 -0.15

17 7 0.00 0.00 0.07 0.00 0.00 0.05 0.00 0.00 0.00

18 6 0.00 0.00 0.07 0.00 0.00 0.11 0.00 0.00 0.11

19 6 0.00 0.00 -0.07 0.00 0.00 -0.15 0.00 0.00 -0.06

20 6 0.00 0.00 -0.03 0.00 0.00 0.06 0.00 0.00 -0.04

21 6 0.00 0.00 -0.03 0.00 0.00 -0.06 0.00 0.00 -0.04

22 6 0.00 0.00 -0.07 0.00 0.00 0.15 0.00 0.00 -0.05

23 7 0.00 0.00 0.07 0.00 0.00 0.00 0.00 0.00 0.05

24 1 0.00 -0.01 0.34 0.00 -0.01 0.22 0.00 0.01 -0.39

25 1 0.00 -0.01 0.34 0.00 0.01 -0.21 0.00 0.01 -0.39

26 1 0.01 0.00 0.34 -0.01 0.00 -0.39 0.01 0.00 0.21

27 1 0.01 0.00 0.34 -0.01 0.00 -0.39 -0.01 0.00 -0.22

28 1 -0.01 0.00 0.34 -0.01 0.00 0.39 0.01 0.00 -0.21

29 1 -0.01 0.00 0.34 -0.01 0.00 0.39 -0.01 0.00 0.22

30 1 0.00 0.01 0.34 0.00 0.01 0.21 0.00 0.01 0.39

31 1 0.00 0.01 0.34 0.00 -0.01 -0.22 0.00 0.01 0.39

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.00 0.00 0.07 0.00 0.00 -0.11 0.00 0.00 0.11

34 6 0.00 0.00 -0.01 0.00 0.00 0.03 0.00 0.00 -0.03

35 6 0.00 0.00 -0.01 0.00 0.00 -0.03 0.00 0.00 0.03

36 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

37 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

38 6 0.00 0.00 -0.01 0.00 0.00 0.03 0.00 0.00 0.03

39 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

40 6 0.00 0.00 -0.01 0.00 0.00 -0.03 0.00 0.00 -0.03

41 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

42 1 0.00 0.00 0.05 0.00 0.00 0.07 0.00 0.00 0.08

43 1 0.00 0.00 0.05 0.00 0.00 -0.08 0.00 0.00 0.07

44 1 0.00 0.00 0.05 0.00 0.00 -0.07 0.00 0.00 -0.08

45 1 0.00 0.00 0.05 0.00 0.00 0.08 0.00 0.00 -0.07

61 62 63

B1 B2 E

Frequencies -- 754.8172 799.3769 805.3303

Red. masses -- 6.1884 1.7654 2.1670

Frc consts -- 2.0774 0.6646 0.8280

IR Inten -- 0.0000 0.0000 0.7669

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 -0.07 0.00 0.00 -0.06 0.00 0.00 0.00

2 6 0.00 0.00 0.19 0.00 0.00 0.06 0.00 0.00 0.03

3 7 0.00 0.00 0.00 0.00 0.00 -0.03 0.00 0.00 0.00

4 6 0.00 0.00 -0.19 0.00 0.00 0.06 0.00 0.00 -0.02

5 6 0.00 0.00 0.07 0.00 0.00 -0.06 0.00 0.00 0.00

6 6 0.00 0.00 0.19 0.00 0.00 0.00 0.00 0.00 0.05

7 6 0.00 0.00 -0.19 0.00 0.00 -0.06 0.00 0.00 -0.11

8 7 0.00 0.00 0.00 0.00 0.00 0.03 0.01 0.00 0.06

9 6 0.00 0.00 0.19 0.00 0.00 -0.06 0.00 0.00 -0.11

10 6 0.00 0.00 -0.07 0.00 0.00 0.06 0.00 0.00 0.09

11 6 0.00 0.00 0.07 0.00 0.00 0.06 0.00 0.00 0.09

12 6 0.00 0.00 -0.19 0.00 0.00 0.00 0.00 0.00 -0.05

13 6 0.00 0.00 0.19 0.00 0.00 -0.06 0.00 0.00 0.11

14 6 0.00 0.00 -0.07 0.00 0.00 0.06 0.00 0.00 -0.09

15 6 0.00 0.00 0.07 0.00 0.00 0.06 0.00 0.00 -0.09

16 6 0.00 0.00 -0.19 0.00 0.00 -0.06 0.00 0.00 0.11

17 7 0.00 0.00 0.00 0.00 0.00 0.03 0.01 0.00 -0.06

18 6 0.00 0.00 0.19 0.00 0.00 0.00 0.00 0.00 -0.05

19 6 0.00 0.00 -0.19 0.00 0.00 0.06 0.00 0.00 0.02

20 6 0.00 0.00 0.07 0.00 0.00 -0.06 0.00 0.00 0.00

21 6 0.00 0.00 -0.07 0.00 0.00 -0.06 0.00 0.00 0.00

22 6 0.00 0.00 0.19 0.00 0.00 0.06 0.00 0.00 -0.03

23 7 0.00 0.00 0.00 0.00 0.00 -0.03 0.00 0.00 0.00

24 1 0.00 0.01 -0.24 0.00 -0.01 0.34 0.00 0.00 -0.04

25 1 0.00 -0.01 0.24 0.00 -0.01 0.34 0.00 0.00 0.04

26 1 -0.01 0.00 -0.24 -0.01 0.00 -0.34 -0.01 -0.01 -0.47

27 1 0.01 0.00 0.24 -0.01 0.00 -0.34 -0.01 0.01 -0.47

28 1 0.01 0.00 -0.24 0.01 0.00 -0.34 -0.01 -0.01 0.47

29 1 -0.01 0.00 0.24 0.01 0.00 -0.34 -0.01 0.01 0.47

30 1 0.00 0.01 0.24 0.00 0.01 0.34 0.00 0.00 -0.04

31 1 0.00 -0.01 -0.24 0.00 0.01 0.34 0.00 0.00 0.04

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.00 0.00 -0.19 0.00 0.00 0.00 0.00 0.00 0.05

34 6 0.00 0.00 0.05 0.00 0.00 0.00 0.00 0.00 -0.01

35 6 0.00 0.00 0.05 0.00 0.00 0.00 0.00 0.00 0.01

36 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

37 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

38 6 0.00 0.00 -0.05 0.00 0.00 0.00 0.00 0.00 -0.01

39 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

40 6 0.00 0.00 -0.05 0.00 0.00 0.00 0.00 0.00 0.01

41 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

42 1 0.00 0.00 0.11 0.00 0.00 0.00 0.00 0.00 -0.02

43 1 0.00 0.00 -0.11 0.00 0.00 0.00 0.00 0.00 0.02

44 1 0.00 0.00 0.11 0.00 0.00 0.00 0.00 0.00 0.02

45 1 0.00 0.00 -0.11 0.00 0.00 0.00 0.00 0.00 -0.02

64 65 66

E A1 A2

Frequencies -- 805.3303 810.1096 841.2926

Red. masses -- 2.1670 2.5007 7.9122

Frc consts -- 0.8280 0.9670 3.2994

IR Inten -- 0.7669 252.2851 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.09 0.00 0.00 -0.07 0.16 0.09 0.00

2 6 0.00 0.00 -0.11 0.00 0.00 0.09 -0.09 0.12 0.00

3 7 0.00 -0.01 0.06 0.00 0.00 -0.05 -0.07 0.00 0.00

4 6 0.00 0.00 -0.11 0.00 0.00 0.09 -0.09 -0.12 0.00

5 6 0.00 0.00 0.09 0.00 0.00 -0.07 0.16 -0.09 0.00

6 6 0.00 0.00 0.05 0.00 0.00 -0.07 -0.14 -0.14 0.00

7 6 0.00 0.00 -0.03 0.00 0.00 0.09 -0.12 -0.09 0.00

8 7 0.00 0.00 0.00 0.00 0.00 -0.05 0.00 -0.07 0.00

9 6 0.00 0.00 0.02 0.00 0.00 0.09 0.12 -0.09 0.00

10 6 0.00 0.00 0.00 0.00 0.00 -0.07 0.09 0.16 0.00

11 6 0.00 0.00 0.00 0.00 0.00 -0.07 -0.09 0.16 0.00

12 6 0.00 0.00 0.05 0.00 0.00 -0.07 -0.14 0.14 0.00

13 6 0.00 0.00 -0.02 0.00 0.00 0.09 -0.12 0.09 0.00

14 6 0.00 0.00 0.00 0.00 0.00 -0.07 -0.09 -0.16 0.00

15 6 0.00 0.00 0.00 0.00 0.00 -0.07 0.09 -0.16 0.00

16 6 0.00 0.00 0.03 0.00 0.00 0.09 0.12 0.09 0.00

17 7 0.00 0.00 0.00 0.00 0.00 -0.05 0.00 0.07 0.00

18 6 0.00 0.00 -0.05 0.00 0.00 -0.07 0.14 0.14 0.00

19 6 0.00 0.00 0.11 0.00 0.00 0.09 0.09 0.12 0.00

20 6 0.00 0.00 -0.09 0.00 0.00 -0.07 -0.16 0.09 0.00

21 6 0.00 0.00 -0.09 0.00 0.00 -0.07 -0.16 -0.09 0.00

22 6 0.00 0.00 0.11 0.00 0.00 0.09 0.09 -0.12 0.00

23 7 0.00 -0.01 -0.06 0.00 0.00 -0.05 0.07 0.00 0.00

24 1 0.01 0.01 -0.47 0.00 -0.01 0.33 0.20 0.06 0.00

25 1 -0.01 0.01 -0.47 0.00 -0.01 0.33 0.20 -0.06 0.00

26 1 0.00 0.00 -0.04 0.01 0.00 0.33 0.06 0.20 0.00

27 1 0.00 0.00 0.04 0.01 0.00 0.33 -0.06 0.20 0.00

28 1 0.00 0.00 0.04 -0.01 0.00 0.33 -0.06 -0.20 0.00

29 1 0.00 0.00 -0.04 -0.01 0.00 0.33 0.06 -0.20 0.00

30 1 -0.01 0.01 0.47 0.00 0.01 0.33 -0.20 0.06 0.00

31 1 0.01 0.01 0.47 0.00 0.01 0.33 -0.20 -0.06 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.00 0.00 -0.05 0.00 0.00 -0.07 0.14 -0.14 0.00

34 6 0.00 0.00 0.01 0.00 0.00 0.02 -0.04 0.04 0.00

35 6 0.00 0.00 -0.01 0.00 0.00 0.02 0.04 -0.04 0.00

36 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

37 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

38 6 0.00 0.00 -0.01 0.00 0.00 0.02 0.04 0.04 0.00

39 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

40 6 0.00 0.00 0.01 0.00 0.00 0.02 -0.04 -0.04 0.00

41 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

42 1 0.00 0.00 -0.02 0.00 0.00 -0.03 0.05 0.05 0.00

43 1 0.00 0.00 -0.02 0.00 0.00 -0.03 0.05 -0.05 0.00

44 1 0.00 0.00 0.02 0.00 0.00 -0.03 -0.05 -0.05 0.00

45 1 0.00 0.00 0.02 0.00 0.00 -0.03 -0.05 0.05 0.00

67 68 69

E E B2

Frequencies -- 849.1048 849.1048 874.8357

Red. masses -- 8.3060 8.3060 7.1977

Frc consts -- 3.5283 3.5283 3.2456

IR Inten -- 49.4885 49.4885 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.02 0.02 0.00 0.18 0.12 0.00 -0.01 0.03 0.00

2 6 -0.12 -0.01 0.01 -0.09 0.14 0.00 -0.15 0.01 0.01

3 7 0.00 -0.16 -0.02 -0.11 0.00 0.00 0.00 -0.17 -0.01

4 6 0.12 -0.01 0.01 -0.09 -0.14 0.00 0.15 0.01 0.01

5 6 0.02 0.02 0.00 0.18 -0.12 0.00 0.01 0.03 0.00

6 6 0.15 0.16 0.00 -0.17 -0.15 0.00 0.16 0.16 0.00

7 6 0.14 0.09 0.00 0.01 -0.12 0.01 0.01 0.15 -0.01

8 7 0.00 0.11 0.00 0.16 0.00 -0.02 -0.17 0.00 0.01

9 6 -0.14 0.09 0.00 0.01 0.12 0.01 0.01 -0.15 -0.01

10 6 -0.12 -0.18 0.00 -0.02 0.02 0.00 0.03 -0.01 0.00

11 6 0.12 -0.18 0.00 -0.02 -0.02 0.00 0.03 0.01 0.00

12 6 -0.15 0.17 0.00 -0.16 0.15 0.00 -0.16 0.16 0.00

13 6 -0.14 0.09 0.00 0.01 0.12 -0.01 -0.01 0.15 -0.01

14 6 -0.12 -0.18 0.00 -0.02 0.02 0.00 -0.03 0.01 0.00

15 6 0.12 -0.18 0.00 -0.02 -0.02 0.00 -0.03 -0.01 0.00

16 6 0.14 0.09 0.00 0.01 -0.12 -0.01 -0.01 -0.15 -0.01

17 7 0.00 0.11 0.00 0.16 0.00 0.02 0.17 0.00 0.01

18 6 0.15 0.16 0.00 -0.17 -0.15 0.00 -0.16 -0.16 0.00

19 6 0.12 -0.01 -0.01 -0.09 -0.14 0.00 -0.15 -0.01 0.01

20 6 0.02 0.02 0.00 0.18 -0.12 0.00 -0.01 -0.03 0.00

21 6 -0.02 0.02 0.00 0.18 0.12 0.00 0.01 -0.03 0.00

22 6 -0.12 -0.01 -0.01 -0.09 0.14 0.00 0.15 -0.01 0.01

23 7 0.00 -0.16 0.02 -0.11 0.00 0.00 0.00 0.17 -0.01

24 1 0.13 -0.11 0.02 0.20 0.11 0.01 0.19 -0.13 0.01

25 1 -0.13 -0.11 0.02 0.20 -0.11 -0.01 -0.19 -0.13 0.01

26 1 -0.11 -0.20 0.01 0.11 -0.13 0.02 -0.13 0.19 -0.01

27 1 0.11 -0.20 -0.01 0.11 0.13 0.02 -0.13 -0.19 -0.01

28 1 -0.11 -0.20 -0.01 0.11 -0.13 -0.02 0.13 -0.19 -0.01

29 1 0.11 -0.20 0.01 0.11 0.13 -0.02 0.13 0.19 -0.01

30 1 -0.13 -0.11 -0.02 0.20 -0.11 0.01 0.19 0.13 0.01

31 1 0.13 -0.11 -0.02 0.20 0.11 -0.01 -0.19 0.13 0.01

32 30 0.00 0.02 0.00 -0.02 0.00 0.00 0.00 0.00 0.00

33 6 -0.15 0.17 0.00 -0.16 0.15 0.00 0.16 -0.16 0.00

34 6 0.06 -0.06 0.00 0.06 -0.06 0.00 -0.07 0.07 0.00

35 6 0.06 -0.06 0.00 0.06 -0.06 0.00 0.07 -0.07 0.00

36 6 -0.01 0.00 0.00 0.00 0.01 0.00 0.00 0.00 0.00

37 6 -0.01 0.00 0.00 0.00 0.01 0.00 0.00 0.00 0.00

38 6 -0.06 -0.06 0.00 0.06 0.06 0.00 -0.07 -0.07 0.00

39 6 0.01 0.00 0.00 0.00 -0.01 0.00 0.00 0.00 0.00

40 6 -0.06 -0.06 0.00 0.06 0.06 0.00 0.07 0.07 0.00

41 6 0.01 0.00 0.00 0.00 -0.01 0.00 0.00 0.00 0.00

42 1 0.07 0.06 0.00 -0.06 -0.07 0.00 -0.06 -0.06 0.00

43 1 -0.07 0.06 0.00 -0.06 0.07 0.00 0.06 -0.06 0.00

44 1 0.07 0.06 0.00 -0.06 -0.07 0.00 0.06 0.06 0.00

45 1 -0.07 0.06 0.00 -0.06 0.07 0.00 -0.06 0.06 0.00

70 71 72

A2 E E

Frequencies -- 919.3888 921.2257 921.2257

Red. masses -- 1.3475 1.3553 1.3553

Frc consts -- 0.6711 0.6777 0.6777

IR Inten -- 0.0000 0.0355 0.0355

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.06 0.00 0.00 0.00 0.00 0.00 -0.09

2 6 0.00 0.00 -0.01 0.00 0.00 0.00 0.00 0.00 0.01

3 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

4 6 0.00 0.00 0.01 0.00 0.00 0.00 0.00 0.00 -0.01

5 6 0.00 0.00 -0.06 0.00 0.00 0.00 0.00 0.00 0.09

6 6 0.00 0.00 0.00 0.00 0.00 -0.01 0.00 0.00 0.01

7 6 0.00 0.00 -0.01 0.00 0.00 0.01 0.00 0.00 0.00

8 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

9 6 0.00 0.00 0.01 0.00 0.00 -0.01 0.00 0.00 0.00

10 6 0.00 0.00 -0.06 0.00 0.00 0.09 0.00 0.00 0.00

11 6 0.00 0.00 0.06 0.00 0.00 -0.09 0.00 0.00 0.00

12 6 0.00 0.00 0.00 0.00 0.00 -0.01 0.00 0.00 -0.01

13 6 0.00 0.00 0.01 0.00 0.00 0.01 0.00 0.00 0.00

14 6 0.00 0.00 -0.06 0.00 0.00 -0.09 0.00 0.00 0.00

15 6 0.00 0.00 0.06 0.00 0.00 0.09 0.00 0.00 0.00

16 6 0.00 0.00 -0.01 0.00 0.00 -0.01 0.00 0.00 0.00

17 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

18 6 0.00 0.00 0.00 0.00 0.00 0.01 0.00 0.00 -0.01

19 6 0.00 0.00 0.01 0.00 0.00 0.00 0.00 0.00 0.01

20 6 0.00 0.00 -0.06 0.00 0.00 0.00 0.00 0.00 -0.09

21 6 0.00 0.00 0.06 0.00 0.00 0.00 0.00 0.00 0.09

22 6 0.00 0.00 -0.01 0.00 0.00 0.00 0.00 0.00 -0.01

23 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

24 1 0.00 0.01 -0.35 0.00 0.00 0.00 0.00 -0.01 0.49

25 1 0.00 -0.01 0.35 0.00 0.00 0.00 0.00 0.01 -0.49

26 1 0.01 0.00 0.35 -0.01 0.00 -0.49 0.00 0.00 0.00

27 1 -0.01 0.00 -0.35 0.01 0.00 0.49 0.00 0.00 0.00

28 1 -0.01 0.00 0.35 -0.01 0.00 0.49 0.00 0.00 0.00

29 1 0.01 0.00 -0.35 0.01 0.00 -0.49 0.00 0.00 0.00

30 1 0.00 0.01 0.35 0.00 0.00 0.00 0.00 0.01 0.49

31 1 0.00 -0.01 -0.35 0.00 0.00 0.00 0.00 -0.01 -0.49

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.00 0.00 0.00 0.00 0.00 0.01 0.00 0.00 0.01

34 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

35 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

36 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

37 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

38 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

39 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

40 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

41 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

42 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

43 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

44 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

45 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

73 74 75

B1 B1 E

Frequencies -- 922.8120 934.5564 958.8163

Red. masses -- 1.3595 5.3255 5.0887

Frc consts -- 0.6821 2.7404 2.7563

IR Inten -- 0.0000 0.0000 100.2033

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 -0.06 -0.09 -0.14 -0.01 0.00 -0.12 0.00

2 6 0.00 0.00 0.01 0.06 -0.05 0.00 0.10 0.03 0.00

3 7 0.00 0.00 0.00 0.12 0.00 0.00 0.00 0.16 0.01

4 6 0.00 0.00 -0.01 0.06 0.05 0.00 -0.10 0.03 0.00

5 6 0.00 0.00 0.06 -0.09 0.14 0.01 0.00 -0.12 0.00

6 6 0.00 0.00 0.01 0.06 -0.06 0.00 -0.09 0.02 0.00

7 6 0.00 0.00 -0.01 -0.05 -0.06 0.00 0.02 0.04 0.00

8 7 0.00 0.00 0.00 0.00 -0.12 0.00 0.00 0.12 0.00

9 6 0.00 0.00 0.01 0.05 -0.06 0.00 -0.02 0.04 0.00

10 6 0.00 0.00 -0.06 0.14 0.09 -0.01 -0.14 -0.07 0.00

11 6 0.00 0.00 0.06 -0.14 0.09 0.01 0.14 -0.07 0.00

12 6 0.00 0.00 -0.01 0.06 0.06 0.00 0.09 0.02 0.00

13 6 0.00 0.00 0.01 -0.05 0.06 0.00 -0.02 0.04 0.00

14 6 0.00 0.00 -0.06 -0.14 -0.09 -0.01 -0.14 -0.07 0.00

15 6 0.00 0.00 0.06 0.14 -0.09 0.01 0.14 -0.07 0.00

16 6 0.00 0.00 -0.01 0.05 0.06 0.00 0.02 0.04 0.00

17 7 0.00 0.00 0.00 0.00 0.12 0.00 0.00 0.12 0.00

18 6 0.00 0.00 0.01 -0.06 0.06 0.00 -0.09 0.02 0.00

19 6 0.00 0.00 -0.01 -0.06 -0.05 0.00 -0.10 0.03 0.00

20 6 0.00 0.00 0.06 0.09 -0.14 0.01 0.00 -0.12 0.00

21 6 0.00 0.00 -0.06 0.09 0.14 -0.01 0.00 -0.12 0.00

22 6 0.00 0.00 0.01 -0.06 0.05 0.00 0.10 0.03 0.00

23 7 0.00 0.00 0.00 -0.12 0.00 0.00 0.00 0.16 -0.01

24 1 0.00 -0.01 0.35 0.06 -0.27 0.00 -0.22 0.05 0.00

25 1 0.00 0.01 -0.35 0.06 0.27 0.00 0.21 0.04 0.00

26 1 0.01 0.00 0.35 0.27 -0.06 0.00 -0.30 0.13 0.01

27 1 -0.01 0.00 -0.35 -0.27 -0.06 0.00 0.30 0.13 -0.01

28 1 -0.01 0.00 0.35 -0.27 0.06 0.00 -0.30 0.13 -0.01

29 1 0.01 0.00 -0.35 0.27 0.06 0.00 0.30 0.13 0.01

30 1 0.00 -0.01 -0.35 -0.06 -0.27 0.00 0.21 0.04 0.00

31 1 0.00 0.01 0.35 -0.06 0.27 0.00 -0.22 0.05 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 -0.01 0.00

33 6 0.00 0.00 -0.01 -0.06 -0.06 0.00 0.09 0.02 0.00

34 6 0.00 0.00 0.00 0.03 0.03 0.00 -0.04 -0.01 0.00

35 6 0.00 0.00 0.00 -0.03 -0.03 0.00 -0.04 -0.01 0.00

36 6 0.00 0.00 0.00 0.04 0.04 0.00 -0.04 -0.04 0.00

37 6 0.00 0.00 0.00 -0.04 -0.04 0.00 -0.04 -0.04 0.00

38 6 0.00 0.00 0.00 -0.03 0.03 0.00 0.04 -0.01 0.00

39 6 0.00 0.00 0.00 -0.04 0.04 0.00 0.04 -0.04 0.00

40 6 0.00 0.00 0.00 0.03 -0.03 0.00 0.04 -0.01 0.00

41 6 0.00 0.00 0.00 0.04 -0.04 0.00 0.04 -0.04 0.00

42 1 0.00 0.00 0.00 0.05 -0.05 0.00 0.04 -0.06 0.00

43 1 0.00 0.00 0.00 0.05 0.05 0.00 -0.04 -0.06 0.00

44 1 0.00 0.00 0.00 -0.05 0.05 0.00 0.04 -0.06 0.00

45 1 0.00 0.00 0.00 -0.05 -0.05 0.00 -0.04 -0.06 0.00

76 77 78

E A1 A2

Frequencies -- 958.8163 985.8707 1020.5462

Red. masses -- 5.0887 6.2672 2.5885

Frc consts -- 2.7563 3.5889 1.5884

IR Inten -- 100.2033 0.1398 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.07 -0.14 0.00 0.01 0.15 0.00 -0.02 -0.08 0.00

2 6 0.04 -0.02 0.00 -0.09 -0.04 0.00 -0.02 0.04 0.00

3 7 0.12 0.00 0.00 0.00 -0.18 -0.01 0.10 0.00 0.00

4 6 0.04 0.02 0.00 0.09 -0.04 0.00 -0.02 -0.04 0.00

5 6 -0.07 0.14 0.00 -0.01 0.15 0.00 -0.02 0.08 0.00

6 6 0.02 -0.09 0.00 0.06 -0.06 0.00 -0.05 -0.05 0.00

7 6 0.03 -0.10 0.00 0.04 -0.09 0.00 -0.04 -0.02 0.00

8 7 0.16 0.00 -0.01 0.18 0.00 -0.01 0.00 0.10 0.00

9 6 0.03 0.10 0.00 0.04 0.09 0.00 0.04 -0.02 0.00

10 6 -0.12 0.00 0.00 -0.15 -0.01 0.00 -0.08 -0.02 0.00

11 6 -0.12 0.00 0.00 -0.15 0.01 0.00 0.08 -0.02 0.00

12 6 0.02 0.09 0.00 -0.06 -0.06 0.00 -0.05 0.05 0.00

13 6 0.03 0.10 0.00 -0.04 -0.09 0.00 -0.04 0.02 0.00

14 6 -0.12 0.00 0.00 0.15 0.01 0.00 0.08 0.02 0.00

15 6 -0.12 0.00 0.00 0.15 -0.01 0.00 -0.08 0.02 0.00

16 6 0.03 -0.10 0.00 -0.04 0.09 0.00 0.04 0.02 0.00

17 7 0.16 0.00 0.01 -0.18 0.00 -0.01 0.00 -0.10 0.00

18 6 0.02 -0.09 0.00 -0.06 0.06 0.00 0.05 0.05 0.00

19 6 0.04 0.02 0.00 -0.09 0.04 0.00 0.02 0.04 0.00

20 6 -0.07 0.14 0.00 0.01 -0.15 0.00 0.02 -0.08 0.00

21 6 -0.07 -0.14 0.00 -0.01 -0.15 0.00 0.02 0.08 0.00

22 6 0.04 -0.02 0.00 0.09 0.04 0.00 0.02 -0.04 0.00

23 7 0.12 0.00 0.00 0.00 0.18 -0.01 -0.10 0.00 0.00

24 1 0.13 -0.30 -0.01 0.25 -0.03 0.00 0.20 -0.26 -0.01

25 1 0.13 0.30 0.01 -0.25 -0.03 0.00 0.20 0.26 0.01

26 1 0.04 -0.21 0.00 0.03 -0.25 0.00 -0.26 0.20 0.01

27 1 0.05 0.22 0.00 0.03 0.25 0.00 0.26 0.20 -0.01

28 1 0.04 -0.21 0.00 -0.03 0.25 0.00 0.26 -0.20 0.01

29 1 0.05 0.22 0.00 -0.03 -0.25 0.00 -0.26 -0.20 -0.01

30 1 0.13 0.30 -0.01 0.25 0.03 0.00 -0.20 -0.26 0.01

31 1 0.13 -0.30 0.01 -0.25 0.03 0.00 -0.20 0.26 -0.01

32 30 -0.01 0.00 0.00 0.00 0.00 0.01 0.00 0.00 0.00

33 6 0.02 0.09 0.00 0.06 0.06 0.00 0.05 -0.05 0.00

34 6 -0.01 -0.04 0.00 -0.03 -0.03 0.00 0.00 0.00 0.00

35 6 -0.01 -0.04 0.00 0.03 0.03 0.00 0.00 0.00 0.00

36 6 -0.04 -0.04 0.00 -0.05 -0.05 0.00 0.00 0.00 0.00

37 6 -0.04 -0.04 0.00 0.05 0.05 0.00 0.00 0.00 0.00

38 6 -0.01 0.04 0.00 -0.03 0.03 0.00 0.00 0.00 0.00

39 6 -0.04 0.04 0.00 -0.05 0.05 0.00 0.00 0.00 0.00

40 6 -0.01 0.04 0.00 0.03 -0.03 0.00 0.00 0.00 0.00

41 6 -0.04 0.04 0.00 0.05 -0.05 0.00 0.00 0.00 0.00

42 1 -0.06 0.04 0.00 0.05 -0.05 0.00 0.01 0.01 0.00

43 1 -0.06 -0.04 0.00 -0.05 -0.05 0.00 0.01 -0.01 0.00

44 1 -0.06 0.04 0.00 -0.05 0.05 0.00 -0.01 -0.01 0.00

45 1 -0.06 -0.04 0.00 0.05 0.05 0.00 -0.01 0.01 0.00

79 80 81

E E B2

Frequencies -- 1024.8304 1024.8304 1033.2926

Red. masses -- 4.2724 4.2724 7.0678

Frc consts -- 2.6438 2.6438 4.4461

IR Inten -- 101.8830 101.8830 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 0.07 0.00 0.01 -0.16 0.00 0.01 -0.18 0.00

2 6 0.04 -0.06 0.00 -0.03 0.08 0.00 -0.04 0.08 0.00

3 7 -0.12 0.00 0.00 0.00 0.16 0.01 0.00 0.18 0.01

4 6 0.04 0.06 0.00 0.03 0.08 0.00 0.04 0.08 0.00

5 6 0.01 -0.07 0.00 -0.01 -0.16 0.00 -0.01 -0.18 0.00

6 6 0.05 0.07 0.00 0.07 0.05 0.00 0.09 0.09 0.00

7 6 0.08 0.03 0.00 0.06 0.04 0.00 0.08 0.04 0.00

8 7 0.16 0.00 -0.01 0.00 -0.12 0.00 0.18 0.00 -0.01

9 6 0.08 -0.03 0.00 -0.06 0.04 0.00 0.08 -0.04 0.00

10 6 -0.16 0.01 0.00 0.07 0.01 0.00 -0.18 0.01 0.00

11 6 -0.16 -0.01 0.00 -0.07 0.01 0.00 -0.18 -0.01 0.00

12 6 0.05 -0.07 0.00 -0.07 0.05 0.00 -0.09 0.09 0.00

13 6 0.08 -0.03 0.00 -0.06 0.04 0.00 -0.08 0.04 0.00

14 6 -0.16 0.01 0.00 0.07 0.01 0.00 0.18 -0.01 0.00

15 6 -0.16 -0.01 0.00 -0.07 0.01 0.00 0.18 0.01 0.00

16 6 0.08 0.03 0.00 0.06 0.04 0.00 -0.08 -0.04 0.00

17 7 0.16 0.00 0.01 0.00 -0.12 0.00 -0.18 0.00 -0.01

18 6 0.05 0.07 0.00 0.07 0.05 0.00 -0.09 -0.09 0.00

19 6 0.04 0.06 0.00 0.03 0.08 0.00 -0.04 -0.08 0.00

20 6 0.01 -0.07 0.00 -0.01 -0.16 0.00 0.01 0.18 0.00

21 6 0.01 0.07 0.00 0.01 -0.16 0.00 -0.01 0.18 0.00

22 6 0.04 -0.06 0.00 -0.03 0.08 0.00 0.04 -0.08 0.00

23 7 -0.12 0.00 0.00 0.00 0.16 -0.01 0.00 -0.18 0.01

24 1 -0.25 0.28 0.00 0.04 -0.19 -0.01 0.05 -0.24 -0.01

25 1 -0.25 -0.28 0.00 -0.04 -0.20 -0.01 -0.05 -0.24 -0.01

26 1 -0.20 0.04 0.01 0.28 -0.25 0.00 -0.24 0.05 0.01

27 1 -0.19 -0.04 0.01 -0.28 -0.25 0.00 -0.24 -0.05 0.01

28 1 -0.20 0.04 -0.01 0.28 -0.25 0.00 0.24 -0.05 0.01

29 1 -0.19 -0.04 -0.01 -0.28 -0.25 0.00 0.24 0.05 0.01

30 1 -0.25 -0.28 0.00 -0.04 -0.20 0.01 0.05 0.24 -0.01

31 1 -0.25 0.28 0.00 0.04 -0.19 0.01 -0.05 0.24 -0.01

32 30 -0.01 0.00 0.00 0.00 -0.01 0.00 0.00 0.00 0.00

33 6 0.05 -0.07 0.00 -0.07 0.05 0.00 0.09 -0.09 0.00

34 6 0.00 0.01 0.00 0.01 0.00 0.00 -0.01 0.01 0.00

35 6 0.00 0.01 0.00 0.01 0.00 0.00 0.01 -0.01 0.00

36 6 0.01 0.01 0.00 0.01 0.01 0.00 0.00 0.00 0.00

37 6 0.01 0.01 0.00 0.01 0.01 0.00 0.00 0.00 0.00

38 6 0.00 -0.01 0.00 -0.01 0.00 0.00 -0.01 -0.01 0.00

39 6 0.01 -0.01 0.00 -0.01 0.01 0.00 0.00 0.00 0.00

40 6 0.00 -0.01 0.00 -0.01 0.00 0.00 0.01 0.01 0.00

41 6 0.01 -0.01 0.00 -0.01 0.01 0.00 0.00 0.00 0.00

42 1 0.02 0.00 0.00 0.00 0.02 0.00 -0.02 -0.02 0.00

43 1 0.02 0.00 0.00 0.00 0.02 0.00 0.02 -0.02 0.00

44 1 0.02 0.00 0.00 0.00 0.02 0.00 0.02 0.02 0.00

45 1 0.02 0.00 0.00 0.00 0.02 0.00 -0.02 0.02 0.00

82 83 84

E E A1

Frequencies -- 1080.6017 1080.6017 1086.6341

Red. masses -- 1.1894 1.1894 1.2312

Frc consts -- 0.8183 0.8183 0.8565

IR Inten -- 74.8207 74.8207 0.1428

Atom AN X Y Z X Y Z X Y Z

1 6 -0.01 -0.02 0.00 -0.04 -0.01 0.00 -0.03 0.01 0.00

2 6 0.00 0.02 0.00 0.01 -0.01 0.00 0.01 -0.01 0.00

3 7 0.01 0.00 0.00 0.00 -0.03 0.00 0.00 -0.05 0.00

4 6 0.00 -0.02 0.00 -0.01 -0.01 0.00 -0.01 -0.01 0.00

5 6 -0.01 0.02 0.00 0.04 -0.01 0.00 0.03 0.01 0.00

6 6 -0.02 -0.02 0.00 0.02 0.02 0.00 -0.01 0.01 0.00

7 6 0.01 0.01 0.00 0.02 0.00 0.00 0.01 0.01 0.00

8 7 0.03 0.00 0.00 0.00 -0.01 0.00 0.05 0.00 0.00

9 6 0.01 -0.01 0.00 -0.02 0.00 0.00 0.01 -0.01 0.00

10 6 0.01 0.04 0.00 0.02 0.01 0.00 -0.01 0.03 0.00

11 6 0.01 -0.04 0.00 -0.02 0.01 0.00 -0.01 -0.03 0.00

12 6 -0.02 0.02 0.00 -0.02 0.02 0.00 0.01 0.01 0.00

13 6 0.01 -0.01 0.00 -0.02 0.00 0.00 -0.01 0.01 0.00

14 6 0.01 0.04 0.00 0.02 0.01 0.00 0.01 -0.03 0.00

15 6 0.01 -0.04 0.00 -0.02 0.01 0.00 0.01 0.03 0.00

16 6 0.01 0.01 0.00 0.02 0.00 0.00 -0.01 -0.01 0.00

17 7 0.03 0.00 0.00 0.00 -0.01 0.00 -0.05 0.00 0.00

18 6 -0.02 -0.02 0.00 0.02 0.02 0.00 0.01 -0.01 0.00

19 6 0.00 -0.02 0.00 -0.01 -0.01 0.00 0.01 0.01 0.00

20 6 -0.01 0.02 0.00 0.04 -0.01 0.00 -0.03 -0.01 0.00

21 6 -0.01 -0.02 0.00 -0.04 -0.01 0.00 0.03 -0.01 0.00

22 6 0.00 0.02 0.00 0.01 -0.01 0.00 -0.01 0.01 0.00

23 7 0.01 0.00 0.00 0.00 -0.03 0.00 0.00 0.05 0.00

24 1 0.06 -0.07 0.00 -0.41 0.27 0.01 -0.28 0.21 0.00

25 1 0.06 0.08 0.00 0.41 0.27 0.01 0.28 0.21 0.00

26 1 -0.27 0.41 0.01 0.08 -0.06 0.00 -0.21 0.28 0.00

27 1 -0.27 -0.41 0.01 -0.07 -0.06 0.00 -0.21 -0.28 0.00

28 1 -0.27 0.41 -0.01 0.08 -0.06 0.00 0.21 -0.28 0.00

29 1 -0.27 -0.41 -0.01 -0.07 -0.06 0.00 0.21 0.28 0.00

30 1 0.06 0.08 0.00 0.41 0.27 -0.01 -0.28 -0.21 0.00

31 1 0.06 -0.07 0.00 -0.41 0.27 -0.01 0.28 -0.21 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 -0.02 0.02 0.00 -0.02 0.02 0.00 -0.01 -0.01 0.00

34 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

35 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

36 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

37 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

38 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

39 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

40 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

41 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

42 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

43 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

44 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

45 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

85 86 87

B2 A1 E

Frequencies -- 1090.8457 1138.0969 1163.2043

Red. masses -- 1.2114 7.1875 6.2112

Frc consts -- 0.8493 5.4851 4.9515

IR Inten -- 0.0000 0.3511 68.5165

Atom AN X Y Z X Y Z X Y Z

1 6 0.03 0.02 0.00 0.03 0.04 0.00 -0.03 -0.04 0.00

2 6 0.00 -0.01 0.00 0.08 0.02 0.00 -0.09 -0.04 0.00

3 7 0.00 0.02 0.00 0.00 -0.14 -0.01 -0.01 0.16 0.01

4 6 0.00 -0.01 0.00 -0.08 0.02 0.00 0.10 -0.03 0.00

5 6 -0.03 0.02 0.00 -0.03 0.04 0.00 0.04 -0.04 0.00

6 6 -0.03 -0.03 0.00 -0.20 0.20 0.01 0.20 -0.15 0.00

7 6 -0.01 0.00 0.00 -0.02 0.08 0.00 -0.05 -0.06 0.00

8 7 0.02 0.00 0.00 0.14 0.00 -0.01 -0.01 0.15 0.00

9 6 -0.01 0.00 0.00 -0.02 -0.08 0.00 0.06 -0.05 0.00

10 6 0.02 0.03 0.00 -0.04 -0.03 0.00 -0.01 -0.02 0.00

11 6 0.02 -0.03 0.00 -0.04 0.03 0.00 0.01 -0.02 0.00

12 6 0.03 -0.03 0.00 0.20 0.20 0.01 -0.19 -0.14 0.00

13 6 0.01 0.00 0.00 0.02 0.08 0.00 0.06 -0.05 0.00

14 6 -0.02 -0.03 0.00 0.04 0.03 0.00 -0.01 -0.02 0.00

15 6 -0.02 0.03 0.00 0.04 -0.03 0.00 0.01 -0.02 0.00

16 6 0.01 0.00 0.00 0.02 -0.08 0.00 -0.05 -0.06 0.00

17 7 -0.02 0.00 0.00 -0.14 0.00 -0.01 -0.01 0.15 0.00

18 6 0.03 0.03 0.00 0.20 -0.20 0.01 0.20 -0.15 0.00

19 6 0.00 0.01 0.00 0.08 -0.02 0.00 0.10 -0.03 0.00

20 6 0.03 -0.02 0.00 0.03 -0.04 0.00 0.04 -0.04 0.00

21 6 -0.03 -0.02 0.00 -0.03 -0.04 0.00 -0.03 -0.04 0.00

22 6 0.00 0.01 0.00 -0.08 -0.02 0.00 -0.09 -0.04 0.00

23 7 0.00 -0.02 0.00 0.00 0.14 -0.01 -0.01 0.16 -0.01

24 1 0.30 -0.18 0.00 0.20 -0.08 0.00 -0.15 0.04 0.00

25 1 -0.30 -0.18 0.00 -0.20 -0.08 0.00 0.13 0.02 0.00

26 1 -0.18 0.30 0.00 0.08 -0.20 0.00 -0.21 0.24 0.01

27 1 -0.18 -0.30 0.00 0.08 0.20 0.00 0.21 0.23 -0.01

28 1 0.18 -0.30 0.00 -0.08 0.20 0.00 -0.21 0.24 -0.01

29 1 0.18 0.30 0.00 -0.08 -0.20 0.00 0.21 0.23 0.01

30 1 0.30 0.18 0.00 0.20 0.08 0.00 0.13 0.02 0.00

31 1 -0.30 0.18 0.00 -0.20 0.08 0.00 -0.15 0.04 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 -0.03 0.03 0.00 -0.20 -0.20 0.01 -0.19 -0.14 0.00

34 6 0.01 -0.01 0.00 0.04 0.04 0.00 0.04 0.02 0.00

35 6 -0.01 0.01 0.00 -0.04 -0.04 0.00 0.04 0.02 0.00

36 6 0.00 0.00 0.00 0.09 0.09 0.00 0.07 0.07 0.00

37 6 0.00 0.00 0.00 -0.09 -0.09 0.00 0.07 0.07 0.00

38 6 0.01 0.01 0.00 0.04 -0.04 0.00 -0.04 0.02 0.00

39 6 0.00 0.00 0.00 0.09 -0.09 0.00 -0.08 0.08 0.00

40 6 -0.01 -0.01 0.00 -0.04 0.04 0.00 -0.04 0.02 0.00

41 6 0.00 0.00 0.00 -0.09 0.09 0.00 -0.08 0.08 0.00

42 1 0.01 0.01 0.00 -0.11 0.11 0.00 -0.08 0.10 0.00

43 1 -0.01 0.01 0.00 0.11 0.11 0.00 0.08 0.09 0.00

44 1 -0.01 -0.01 0.00 0.11 -0.11 0.00 -0.08 0.10 0.00

45 1 0.01 -0.01 0.00 -0.11 -0.11 0.00 0.08 0.09 0.00

88 89 90

E B1 B1

Frequencies -- 1163.2043 1181.9751 1235.5509

Red. masses -- 6.2112 2.1256 6.6817

Frc consts -- 4.9515 1.7496 6.0098

IR Inten -- 68.5165 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.02 0.01 0.00 0.02 0.00 0.00 0.00 0.00 0.00

2 6 0.06 -0.05 0.00 0.04 -0.08 0.00 -0.02 -0.11 0.00

3 7 -0.15 -0.01 0.00 -0.04 0.00 0.00 0.19 0.00 0.00

4 6 0.05 0.06 0.00 0.04 0.08 0.00 -0.02 0.11 0.00

5 6 0.02 -0.01 0.00 0.02 0.00 0.00 0.00 0.00 0.00

6 6 0.14 -0.19 0.00 0.05 -0.05 0.00 -0.17 0.17 0.00

7 6 0.04 -0.09 0.00 -0.08 -0.04 0.00 -0.11 0.02 0.00

8 7 -0.16 -0.01 0.01 0.00 0.04 0.00 0.00 -0.19 0.00

9 6 0.03 0.10 0.00 0.08 -0.04 0.00 0.11 0.02 0.00

10 6 0.04 0.04 0.00 0.00 -0.02 0.00 0.00 0.00 0.00

11 6 0.04 -0.03 0.00 0.00 -0.02 0.00 0.00 0.00 0.00

12 6 0.15 0.20 0.00 0.05 0.05 0.00 -0.17 -0.17 0.00

13 6 0.03 0.10 0.00 -0.08 0.04 0.00 -0.11 -0.02 0.00

14 6 0.04 0.04 0.00 0.00 0.02 0.00 0.00 0.00 0.00

15 6 0.04 -0.03 0.00 0.00 0.02 0.00 0.00 0.00 0.00

16 6 0.04 -0.09 0.00 0.08 0.04 0.00 0.11 -0.02 0.00

17 7 -0.16 -0.01 -0.01 0.00 -0.04 0.00 0.00 0.19 0.00

18 6 0.14 -0.19 0.00 -0.05 0.05 0.00 0.17 -0.17 0.00

19 6 0.05 0.06 0.00 -0.04 -0.08 0.00 0.02 -0.11 0.00

20 6 0.02 -0.01 0.00 -0.02 0.00 0.00 0.00 0.00 0.00

21 6 0.02 0.01 0.00 -0.02 0.00 0.00 0.00 0.00 0.00

22 6 0.06 -0.05 0.00 -0.04 0.08 0.00 0.02 0.11 0.00

23 7 -0.15 -0.01 0.00 0.04 0.00 0.00 -0.19 0.00 0.00

24 1 -0.23 0.21 0.01 -0.26 0.21 0.00 -0.19 0.15 0.00

25 1 -0.24 -0.21 -0.01 -0.26 -0.21 0.00 -0.19 -0.15 0.00

26 1 -0.02 0.13 0.00 -0.21 0.26 0.00 -0.15 0.19 0.00

27 1 -0.04 -0.15 0.00 0.21 0.26 0.00 0.15 0.19 0.00

28 1 -0.02 0.13 0.00 0.21 -0.26 0.00 0.15 -0.19 0.00

29 1 -0.04 -0.15 0.00 -0.21 -0.26 0.00 -0.15 -0.19 0.00

30 1 -0.24 -0.21 0.01 0.26 0.21 0.00 0.19 0.15 0.00

31 1 -0.23 0.21 -0.01 0.26 -0.21 0.00 0.19 -0.15 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.15 0.20 0.00 -0.05 -0.05 0.00 0.17 0.17 0.00

34 6 -0.02 -0.04 0.00 0.01 0.01 0.00 -0.02 -0.02 0.00

35 6 -0.02 -0.04 0.00 -0.01 -0.01 0.00 0.02 0.02 0.00

36 6 -0.08 -0.08 0.00 0.02 0.02 0.00 -0.06 -0.06 0.00

37 6 -0.08 -0.08 0.00 -0.02 -0.02 0.00 0.06 0.06 0.00

38 6 -0.02 0.04 0.00 -0.01 0.01 0.00 0.02 -0.02 0.00

39 6 -0.07 0.07 0.00 -0.02 0.02 0.00 0.06 -0.06 0.00

40 6 -0.02 0.04 0.00 0.01 -0.01 0.00 -0.02 0.02 0.00

41 6 -0.07 0.07 0.00 0.02 -0.02 0.00 -0.06 0.06 0.00

42 1 -0.09 0.08 0.00 0.03 -0.03 0.00 -0.08 0.08 0.00

43 1 -0.10 -0.08 0.00 0.03 0.03 0.00 -0.08 -0.08 0.00

44 1 -0.09 0.08 0.00 -0.03 0.03 0.00 0.08 -0.08 0.00

45 1 -0.10 -0.08 0.00 -0.03 -0.03 0.00 0.08 0.08 0.00

91 92 93

E E A2

Frequencies -- 1238.3778 1238.3778 1276.8362

Red. masses -- 3.7798 3.7798 6.0322

Frc consts -- 3.4152 3.4152 5.7943

IR Inten -- 152.1547 152.1547 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.04 0.02 0.00 0.00 0.03 0.00 0.03 0.03 0.00

2 6 -0.07 -0.16 0.00 0.07 -0.08 0.00 -0.12 -0.13 0.00

3 7 0.16 0.00 0.00 0.00 0.06 0.00 0.19 0.00 0.00

4 6 -0.07 0.16 0.00 -0.07 -0.08 0.00 -0.12 0.13 0.00

5 6 0.04 -0.02 0.00 0.00 0.03 0.00 0.03 -0.03 0.00

6 6 -0.04 -0.01 0.00 -0.01 -0.04 0.00 -0.05 -0.05 0.00

7 6 -0.08 -0.07 0.00 0.16 -0.07 0.00 0.13 -0.12 0.00

8 7 0.06 0.00 0.00 0.00 0.16 0.00 0.00 0.19 0.00

9 6 -0.08 0.07 0.00 -0.16 -0.07 0.00 -0.13 -0.12 0.00

10 6 0.03 0.00 0.00 0.02 0.04 0.00 0.03 0.03 0.00

11 6 0.03 0.00 0.00 -0.02 0.04 0.00 -0.03 0.03 0.00

12 6 -0.04 0.01 0.00 0.01 -0.04 0.00 -0.05 0.05 0.00

13 6 -0.08 0.07 0.00 -0.16 -0.07 0.00 0.13 0.12 0.00

14 6 0.03 0.00 0.00 0.02 0.04 0.00 -0.03 -0.03 0.00

15 6 0.03 0.00 0.00 -0.02 0.04 0.00 0.03 -0.03 0.00

16 6 -0.08 -0.07 0.00 0.16 -0.07 0.00 -0.13 0.12 0.00

17 7 0.06 0.00 0.00 0.00 0.16 0.00 0.00 -0.19 0.00

18 6 -0.04 -0.01 0.00 -0.01 -0.04 0.00 0.05 0.05 0.00

19 6 -0.07 0.16 0.00 -0.07 -0.08 0.00 0.12 -0.13 0.00

20 6 0.04 -0.02 0.00 0.00 0.03 0.00 -0.03 0.03 0.00

21 6 0.04 0.02 0.00 0.00 0.03 0.00 -0.03 -0.03 0.00

22 6 -0.07 -0.16 0.00 0.07 -0.08 0.00 0.12 0.13 0.00

23 7 0.16 0.00 0.00 0.00 0.06 0.00 -0.19 0.00 0.00

24 1 -0.30 0.28 0.01 0.13 -0.06 0.00 -0.18 0.19 0.00

25 1 -0.30 -0.28 -0.01 -0.13 -0.06 0.00 -0.18 -0.19 0.00

26 1 -0.06 0.13 0.00 0.28 -0.30 -0.01 0.19 -0.18 0.00

27 1 -0.06 -0.13 0.00 -0.28 -0.30 0.01 -0.19 -0.18 0.00

28 1 -0.06 0.13 0.00 0.28 -0.30 0.01 -0.19 0.18 0.00

29 1 -0.06 -0.13 0.00 -0.28 -0.30 -0.01 0.19 0.18 0.00

30 1 -0.30 -0.28 0.01 -0.13 -0.06 0.00 0.18 0.19 0.00

31 1 -0.30 0.28 -0.01 0.13 -0.06 0.00 0.18 -0.19 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 -0.04 0.01 0.00 0.01 -0.04 0.00 0.05 -0.05 0.00

34 6 0.01 -0.01 0.00 -0.01 0.01 0.00 -0.02 0.02 0.00

35 6 0.01 -0.01 0.00 -0.01 0.01 0.00 0.02 -0.02 0.00

36 6 0.01 0.01 0.00 0.01 0.01 0.00 0.00 0.00 0.00

37 6 0.01 0.01 0.00 0.01 0.01 0.00 0.00 0.00 0.00

38 6 0.01 0.01 0.00 0.01 0.01 0.00 0.02 0.02 0.00

39 6 0.01 -0.01 0.00 -0.01 0.01 0.00 0.00 0.00 0.00

40 6 0.01 0.01 0.00 0.01 0.01 0.00 -0.02 -0.02 0.00

41 6 0.01 -0.01 0.00 -0.01 0.01 0.00 0.00 0.00 0.00

42 1 0.00 -0.01 0.00 -0.01 0.00 0.00 0.01 0.01 0.00

43 1 0.00 0.01 0.00 0.01 0.00 0.00 0.01 -0.01 0.00

44 1 0.00 -0.01 0.00 -0.01 0.00 0.00 -0.01 -0.01 0.00

45 1 0.00 0.01 0.00 0.01 0.00 0.00 -0.01 0.01 0.00

94 95 96

E E B2

Frequencies -- 1309.5249 1309.5249 1323.9242

Red. masses -- 3.4430 3.4430 12.3893

Frc consts -- 3.4787 3.4787 12.7944

IR Inten -- 0.3141 0.3141 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.04 0.03 0.00 0.02 -0.12 0.00 -0.08 0.07 0.00

2 6 -0.02 -0.04 0.00 0.14 0.02 0.00 -0.11 -0.25 -0.01

3 7 0.00 0.01 0.00 -0.06 0.00 0.00 0.00 0.26 0.01

4 6 0.02 -0.04 0.00 0.14 -0.02 0.00 0.11 -0.25 -0.01

5 6 -0.04 0.03 0.00 0.02 0.12 0.00 0.08 0.07 0.00

6 6 -0.01 -0.12 0.00 -0.12 -0.01 0.00 0.04 0.04 0.00

7 6 -0.02 0.14 0.00 -0.04 0.02 0.00 -0.25 0.11 0.01

8 7 0.00 -0.06 0.00 0.01 0.00 0.00 0.26 0.00 -0.01

9 6 0.02 0.14 0.00 -0.04 -0.02 0.00 -0.25 -0.11 0.01

10 6 -0.12 0.02 0.00 0.03 0.04 0.00 0.07 -0.08 0.00

11 6 0.12 0.02 0.00 0.03 -0.04 0.00 0.07 0.08 0.00

12 6 0.01 -0.12 0.00 -0.12 0.01 0.00 -0.04 0.04 0.00

13 6 0.02 0.14 0.00 -0.04 -0.02 0.00 0.25 0.11 0.01

14 6 -0.12 0.02 0.00 0.03 0.04 0.00 -0.07 0.08 0.00

15 6 0.12 0.02 0.00 0.03 -0.04 0.00 -0.07 -0.08 0.00

16 6 -0.02 0.14 0.00 -0.04 0.02 0.00 0.25 -0.11 0.01

17 7 0.00 -0.06 0.00 0.01 0.00 0.00 -0.26 0.00 -0.01

18 6 -0.01 -0.12 0.00 -0.12 -0.01 0.00 -0.04 -0.04 0.00

19 6 0.02 -0.04 0.00 0.14 -0.02 0.00 -0.11 0.25 -0.01

20 6 -0.04 0.03 0.00 0.02 0.12 0.00 -0.08 -0.07 0.00

21 6 0.04 0.03 0.00 0.02 -0.12 0.00 0.08 -0.07 0.00

22 6 -0.02 -0.04 0.00 0.14 0.02 0.00 0.11 0.25 -0.01

23 7 0.00 0.01 0.00 -0.06 0.00 0.00 0.00 -0.26 0.01

24 1 -0.05 0.10 0.00 -0.38 0.18 0.00 -0.03 0.03 0.00

25 1 0.05 0.10 0.00 -0.38 -0.18 0.00 0.03 0.03 0.00

26 1 0.18 -0.38 0.00 0.10 -0.05 0.00 0.03 -0.03 0.00

27 1 -0.18 -0.38 0.00 0.10 0.05 0.00 0.03 0.03 0.00

28 1 0.18 -0.38 0.00 0.10 -0.05 0.00 -0.03 0.03 0.00

29 1 -0.18 -0.38 0.00 0.10 0.05 0.00 -0.03 -0.03 0.00

30 1 0.05 0.10 0.00 -0.38 -0.18 0.00 -0.03 -0.03 0.00

31 1 -0.05 0.10 0.00 -0.38 0.18 0.00 0.03 -0.03 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.01 -0.12 0.00 -0.12 0.01 0.00 0.04 -0.04 0.00

34 6 0.00 0.01 0.00 0.01 0.00 0.00 -0.03 0.03 0.00

35 6 0.00 0.01 0.00 0.01 0.00 0.00 0.03 -0.03 0.00

36 6 0.02 0.01 0.00 0.01 0.02 0.00 0.00 0.00 0.00

37 6 0.02 0.01 0.00 0.01 0.02 0.00 0.00 0.00 0.00

38 6 0.00 0.01 0.00 0.01 0.00 0.00 -0.03 -0.03 0.00

39 6 -0.02 0.01 0.00 0.01 -0.02 0.00 0.00 0.00 0.00

40 6 0.00 0.01 0.00 0.01 0.00 0.00 0.03 0.03 0.00

41 6 -0.02 0.01 0.00 0.01 -0.02 0.00 0.00 0.00 0.00

42 1 -0.02 0.01 0.00 0.01 -0.02 0.00 -0.01 -0.01 0.00

43 1 0.02 0.01 0.00 0.01 0.02 0.00 0.01 -0.01 0.00

44 1 -0.02 0.01 0.00 0.01 -0.02 0.00 0.01 0.01 0.00

45 1 0.02 0.01 0.00 0.01 0.02 0.00 -0.01 0.01 0.00

97 98 99

A2 E E

Frequencies -- 1347.2069 1355.4051 1355.4051

Red. masses -- 2.2345 11.7883 11.7883

Frc consts -- 2.3894 12.7597 12.7597

IR Inten -- 0.0000 93.2196 93.2196

Atom AN X Y Z X Y Z X Y Z

1 6 0.03 -0.09 0.00 0.01 0.00 0.00 0.11 -0.09 0.00

2 6 0.04 0.02 0.00 -0.04 -0.06 0.00 0.04 0.34 0.01

3 7 -0.02 0.00 0.00 0.15 0.00 0.00 0.00 -0.31 -0.01

4 6 0.04 -0.02 0.00 -0.04 0.06 0.00 -0.04 0.34 0.01

5 6 0.03 0.09 0.00 0.01 0.00 0.00 -0.11 -0.09 0.00

6 6 -0.06 -0.06 0.00 -0.18 0.01 0.00 0.01 -0.18 0.00

7 6 -0.02 0.04 0.00 0.34 -0.04 -0.01 0.06 -0.04 0.00

8 7 0.00 -0.02 0.00 -0.31 0.00 0.01 0.00 0.15 0.00

9 6 0.02 0.04 0.00 0.34 0.04 -0.01 -0.06 -0.04 0.00

10 6 -0.09 0.03 0.00 -0.09 0.11 0.00 0.00 0.01 0.00

11 6 0.09 0.03 0.00 -0.09 -0.11 0.00 0.00 0.01 0.00

12 6 -0.06 0.06 0.00 -0.18 -0.01 0.00 -0.01 -0.18 0.00

13 6 -0.02 -0.04 0.00 0.34 0.04 0.01 -0.06 -0.04 0.00

14 6 0.09 -0.03 0.00 -0.09 0.11 0.00 0.00 0.01 0.00

15 6 -0.09 -0.03 0.00 -0.09 -0.11 0.00 0.00 0.01 0.00

16 6 0.02 -0.04 0.00 0.34 -0.04 0.01 0.06 -0.04 0.00

17 7 0.00 0.02 0.00 -0.31 0.00 -0.01 0.00 0.15 0.00

18 6 0.06 0.06 0.00 -0.18 0.01 0.00 0.01 -0.18 0.00

19 6 -0.04 0.02 0.00 -0.04 0.06 0.00 -0.04 0.34 -0.01

20 6 -0.03 -0.09 0.00 0.01 0.00 0.00 -0.11 -0.09 0.00

21 6 -0.03 0.09 0.00 0.01 0.00 0.00 0.11 -0.09 0.00

22 6 -0.04 -0.02 0.00 -0.04 -0.06 0.00 0.04 0.34 -0.01

23 7 0.02 0.00 0.00 0.15 0.00 0.00 0.00 -0.31 0.01

24 1 -0.29 0.16 0.00 -0.07 0.06 0.00 -0.06 0.03 0.00

25 1 -0.29 -0.16 0.00 -0.07 -0.06 0.00 0.06 0.03 0.00

26 1 0.16 -0.29 0.00 0.03 -0.06 0.00 0.06 -0.07 0.00

27 1 -0.16 -0.29 0.00 0.03 0.06 0.00 -0.06 -0.07 0.00

28 1 -0.16 0.29 0.00 0.03 -0.06 0.00 0.06 -0.07 0.00

29 1 0.16 0.29 0.00 0.03 0.06 0.00 -0.06 -0.07 0.00

30 1 0.29 0.16 0.00 -0.07 -0.06 0.00 0.06 0.03 0.00

31 1 0.29 -0.16 0.00 -0.07 0.06 0.00 -0.06 0.03 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.06 -0.06 0.00 -0.18 -0.01 0.00 -0.01 -0.18 0.00

34 6 0.00 0.00 0.00 0.03 -0.02 0.00 -0.02 0.03 0.00

35 6 0.00 0.00 0.00 0.03 -0.02 0.00 -0.02 0.03 0.00

36 6 0.00 0.00 0.00 0.03 0.03 0.00 0.03 0.03 0.00

37 6 0.00 0.00 0.00 0.03 0.03 0.00 0.03 0.03 0.00

38 6 0.00 0.00 0.00 0.03 0.02 0.00 0.02 0.03 0.00

39 6 0.00 0.00 0.00 0.03 -0.03 0.00 -0.03 0.03 0.00

40 6 0.00 0.00 0.00 0.03 0.02 0.00 0.02 0.03 0.00

41 6 0.00 0.00 0.00 0.03 -0.03 0.00 -0.03 0.03 0.00

42 1 0.01 0.01 0.00 0.02 -0.05 0.00 -0.05 0.02 0.00

43 1 0.01 -0.01 0.00 0.02 0.05 0.00 0.05 0.02 0.00

44 1 -0.01 -0.01 0.00 0.02 -0.05 0.00 -0.05 0.02 0.00

45 1 -0.01 0.01 0.00 0.02 0.05 0.00 0.05 0.02 0.00

100 101 102

A1 B1 E

Frequencies -- 1376.1980 1377.9104 1448.3661

Red. masses -- 11.2211 4.5285 4.0635

Frc consts -- 12.5213 5.0657 5.0224

IR Inten -- 0.2823 0.0000 8.9346

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 0.10 0.00 0.02 -0.12 0.00 0.10 0.02 0.00

2 6 0.09 -0.28 -0.01 0.08 0.10 0.00 0.04 -0.05 0.00

3 7 0.00 0.18 0.01 -0.07 0.00 0.00 0.00 0.01 0.00

4 6 -0.09 -0.28 -0.01 0.08 -0.10 0.00 -0.04 -0.05 0.00

5 6 -0.01 0.10 0.00 0.02 0.12 0.00 -0.10 0.02 0.00

6 6 -0.04 0.04 0.00 -0.08 0.08 0.00 0.00 -0.06 0.00

7 6 0.28 0.09 -0.01 0.10 -0.08 0.00 0.11 0.13 0.00

8 7 -0.18 0.00 0.01 0.00 0.07 0.00 0.00 -0.04 0.00

9 6 0.28 -0.09 -0.01 -0.10 -0.08 0.00 -0.11 0.13 0.00

10 6 -0.10 -0.01 0.00 0.12 -0.02 0.00 0.13 -0.07 0.00

11 6 -0.10 0.01 0.00 -0.12 -0.02 0.00 -0.13 -0.07 0.00

12 6 0.04 0.04 0.00 -0.08 -0.08 0.00 0.00 -0.06 0.00

13 6 -0.28 0.09 -0.01 0.10 0.08 0.00 -0.11 0.13 0.00

14 6 0.10 0.01 0.00 -0.12 0.02 0.00 0.13 -0.07 0.00

15 6 0.10 -0.01 0.00 0.12 0.02 0.00 -0.13 -0.07 0.00

16 6 -0.28 -0.09 -0.01 -0.10 0.08 0.00 0.11 0.13 0.00

17 7 0.18 0.00 0.01 0.00 -0.07 0.00 0.00 -0.04 0.00

18 6 0.04 -0.04 0.00 0.08 -0.08 0.00 0.00 -0.06 0.00

19 6 0.09 0.28 -0.01 -0.08 0.10 0.00 -0.04 -0.05 0.00

20 6 0.01 -0.10 0.00 -0.02 -0.12 0.00 -0.10 0.02 0.00

21 6 -0.01 -0.10 0.00 -0.02 0.12 0.00 0.10 0.02 0.00

22 6 -0.09 0.28 -0.01 -0.08 -0.10 0.00 0.04 -0.05 0.00

23 7 0.00 -0.18 0.01 0.07 0.00 0.00 0.00 0.01 0.00

24 1 0.07 0.08 0.00 -0.27 0.10 0.00 -0.02 0.13 0.00

25 1 -0.07 0.08 0.00 -0.27 -0.10 0.00 0.02 0.13 0.00

26 1 -0.08 -0.07 0.00 -0.10 0.27 0.00 -0.19 0.36 0.00

27 1 -0.08 0.07 0.00 0.10 0.27 0.00 0.19 0.36 0.00

28 1 0.08 0.07 0.00 0.10 -0.27 0.00 -0.19 0.36 0.00

29 1 0.08 -0.07 0.00 -0.10 -0.27 0.00 0.19 0.36 0.00

30 1 0.07 -0.08 0.00 0.27 0.10 0.00 0.02 0.13 0.00

31 1 -0.07 -0.08 0.00 0.27 -0.10 0.00 -0.02 0.13 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 -0.04 -0.04 0.00 0.08 0.08 0.00 0.00 -0.06 0.00

34 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.01 0.00

35 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.01 0.00

36 6 0.01 0.01 0.00 -0.02 -0.02 0.00 0.01 0.01 0.00

37 6 -0.01 -0.01 0.00 0.02 0.02 0.00 0.01 0.01 0.00

38 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.01 0.00

39 6 0.01 -0.01 0.00 0.02 -0.02 0.00 -0.01 0.00 0.00

40 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.01 0.00

41 6 -0.01 0.01 0.00 -0.02 0.02 0.00 -0.01 0.00 0.00

42 1 -0.02 0.02 0.00 -0.02 0.02 0.00 -0.01 0.00 0.00

43 1 0.02 0.02 0.00 -0.02 -0.02 0.00 0.01 0.00 0.00

44 1 0.02 -0.02 0.00 0.02 -0.02 0.00 -0.01 0.00 0.00

45 1 -0.02 -0.02 0.00 0.02 0.02 0.00 0.01 0.00 0.00

103 104 105

E B1 A1

Frequencies -- 1448.3661 1476.6071 1477.2429

Red. masses -- 4.0635 5.1958 9.1570

Frc consts -- 5.0224 6.6747 11.7735

IR Inten -- 8.9346 0.0000 0.2651

Atom AN X Y Z X Y Z X Y Z

1 6 -0.07 0.13 0.00 0.06 -0.08 0.00 0.21 0.00 0.00

2 6 0.13 -0.11 0.00 -0.16 0.05 0.00 0.18 0.02 0.00

3 7 -0.04 0.00 0.00 0.08 0.00 0.00 0.00 -0.08 0.00

4 6 0.13 0.11 0.00 -0.16 -0.05 0.00 -0.18 0.02 0.00

5 6 -0.07 -0.13 0.00 0.06 0.08 0.00 -0.21 0.00 0.00

6 6 -0.06 0.00 0.00 0.07 -0.07 0.00 0.11 -0.11 0.00

7 6 -0.05 -0.04 0.00 0.05 0.16 0.00 -0.02 0.18 0.00

8 7 0.01 0.00 0.00 0.00 -0.08 0.00 0.08 0.00 0.00

9 6 -0.05 0.04 0.00 -0.05 0.16 0.00 -0.02 -0.18 0.00

10 6 0.02 0.10 0.00 0.08 -0.06 0.00 0.00 -0.21 0.00

11 6 0.02 -0.10 0.00 -0.08 -0.06 0.00 0.00 0.21 0.00

12 6 -0.06 0.00 0.00 0.07 0.07 0.00 -0.11 -0.11 0.00

13 6 -0.05 0.04 0.00 0.05 -0.16 0.00 0.02 0.18 0.00

14 6 0.02 0.10 0.00 -0.08 0.06 0.00 0.00 0.21 0.00

15 6 0.02 -0.10 0.00 0.08 0.06 0.00 0.00 -0.21 0.00

16 6 -0.05 -0.04 0.00 -0.05 -0.16 0.00 0.02 -0.18 0.00

17 7 0.01 0.00 0.00 0.00 0.08 0.00 -0.08 0.00 0.00

18 6 -0.06 0.00 0.00 -0.07 0.07 0.00 -0.11 0.11 0.00

19 6 0.13 0.11 0.00 0.16 0.05 0.00 0.18 -0.02 0.00

20 6 -0.07 -0.13 0.00 -0.06 -0.08 0.00 0.21 0.00 0.00

21 6 -0.07 0.13 0.00 -0.06 0.08 0.00 -0.21 0.00 0.00

22 6 0.13 -0.11 0.00 0.16 -0.05 0.00 -0.18 -0.02 0.00

23 7 -0.04 0.00 0.00 -0.08 0.00 0.00 0.00 0.08 0.00

24 1 0.36 -0.19 0.00 -0.24 0.14 0.00 0.02 0.18 0.00

25 1 0.36 0.19 0.00 -0.24 -0.14 0.00 -0.02 0.18 0.00

26 1 0.13 -0.02 0.00 -0.14 0.24 0.00 -0.18 -0.02 0.00

27 1 0.13 0.02 0.00 0.14 0.24 0.00 -0.18 0.02 0.00

28 1 0.13 -0.02 0.00 0.14 -0.24 0.00 0.18 0.02 0.00

29 1 0.13 0.02 0.00 -0.14 -0.24 0.00 0.18 -0.02 0.00

30 1 0.36 0.19 0.00 0.24 0.14 0.00 0.02 -0.18 0.00

31 1 0.36 -0.19 0.00 0.24 -0.14 0.00 -0.02 -0.18 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 -0.06 0.00 0.00 -0.07 -0.07 0.00 0.11 0.11 0.00

34 6 0.01 0.00 0.00 0.01 0.01 0.00 0.00 0.00 0.00

35 6 0.01 0.00 0.00 -0.01 -0.01 0.00 0.00 0.00 0.00

36 6 0.00 0.01 0.00 0.01 0.01 0.00 -0.02 -0.02 0.00

37 6 0.00 0.01 0.00 -0.01 -0.01 0.00 0.02 0.02 0.00

38 6 0.01 0.00 0.00 -0.01 0.01 0.00 0.00 0.00 0.00

39 6 0.01 -0.01 0.00 -0.01 0.01 0.00 -0.02 0.02 0.00

40 6 0.01 0.00 0.00 0.01 -0.01 0.00 0.00 0.00 0.00

41 6 0.01 -0.01 0.00 0.01 -0.01 0.00 0.02 -0.02 0.00

42 1 0.00 -0.01 0.00 0.01 -0.01 0.00 0.03 -0.03 0.00

43 1 0.00 0.01 0.00 0.01 0.01 0.00 -0.03 -0.03 0.00

44 1 0.00 -0.01 0.00 -0.01 0.01 0.00 -0.03 0.03 0.00

45 1 0.00 0.01 0.00 -0.01 -0.01 0.00 0.03 0.03 0.00

106 107 108

A2 E E

Frequencies -- 1513.5654 1522.0175 1522.0175

Red. masses -- 8.0021 10.4795 10.4795

Frc consts -- 10.8008 14.3031 14.3031

IR Inten -- 0.0000 168.4355 168.4354

Atom AN X Y Z X Y Z X Y Z

1 6 -0.05 0.08 0.00 0.02 -0.05 0.00 0.19 0.01 0.00

2 6 0.16 -0.12 0.00 -0.03 0.12 0.00 0.30 -0.05 0.00

3 7 -0.02 0.00 0.00 -0.04 0.00 0.00 0.00 -0.04 0.00

4 6 0.16 0.12 0.00 -0.03 -0.12 0.00 -0.30 -0.04 0.00

5 6 -0.05 -0.08 0.00 0.02 0.05 0.00 -0.19 0.01 0.00

6 6 -0.18 -0.18 0.00 0.09 0.24 0.00 0.24 0.09 0.00

7 6 0.12 0.16 0.00 -0.05 -0.30 0.00 -0.12 -0.03 0.00

8 7 0.00 -0.02 0.00 -0.04 0.00 0.00 0.00 -0.04 0.00

9 6 -0.12 0.16 0.00 -0.04 0.30 0.00 0.12 -0.03 0.00

10 6 0.08 -0.05 0.00 0.01 0.19 0.00 -0.05 0.02 0.00

11 6 -0.08 -0.05 0.00 0.01 -0.19 0.00 0.05 0.02 0.00

12 6 -0.18 0.18 0.00 0.09 -0.24 0.00 -0.24 0.09 0.00

13 6 0.12 -0.16 0.00 -0.04 0.30 0.00 0.12 -0.03 0.00

14 6 -0.08 0.05 0.00 0.01 0.19 0.00 -0.05 0.02 0.00

15 6 0.08 0.05 0.00 0.01 -0.19 0.00 0.05 0.02 0.00

16 6 -0.12 -0.16 0.00 -0.05 -0.30 0.00 -0.12 -0.03 0.00

17 7 0.00 0.02 0.00 -0.04 0.00 0.00 0.00 -0.04 0.00

18 6 0.18 0.18 0.00 0.09 0.24 0.00 0.24 0.09 0.00

19 6 -0.16 -0.12 0.00 -0.03 -0.12 0.00 -0.30 -0.04 0.00

20 6 0.05 0.08 0.00 0.02 0.05 0.00 -0.19 0.01 0.00

21 6 0.05 -0.08 0.00 0.02 -0.05 0.00 0.19 0.01 0.00

22 6 -0.16 0.12 0.00 -0.03 0.12 0.00 0.30 -0.05 0.00

23 7 0.02 0.00 0.00 -0.04 0.00 0.00 0.00 -0.04 0.00

24 1 0.19 -0.10 0.00 -0.10 0.02 0.00 0.08 0.13 0.00

25 1 0.19 0.10 0.00 -0.10 -0.02 0.00 -0.08 0.13 0.00

26 1 -0.10 0.19 0.00 0.13 0.08 0.00 0.02 -0.10 0.00

27 1 0.10 0.19 0.00 0.13 -0.08 0.00 -0.02 -0.10 0.00

28 1 0.10 -0.19 0.00 0.13 0.08 0.00 0.02 -0.10 0.00

29 1 -0.10 -0.19 0.00 0.13 -0.08 0.00 -0.02 -0.10 0.00

30 1 -0.19 -0.10 0.00 -0.10 -0.02 0.00 -0.08 0.13 0.00

31 1 -0.19 0.10 0.00 -0.10 0.02 0.00 0.08 0.13 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.18 -0.18 0.00 0.09 -0.24 0.00 -0.24 0.09 0.00

34 6 -0.01 0.01 0.00 -0.01 0.01 0.00 0.01 -0.01 0.00

35 6 0.01 -0.01 0.00 -0.01 0.01 0.00 0.01 -0.01 0.00

36 6 0.00 0.00 0.00 0.02 0.01 0.00 0.01 0.02 0.00

37 6 0.00 0.00 0.00 0.02 0.01 0.00 0.01 0.02 0.00

38 6 0.01 0.01 0.00 -0.01 -0.01 0.00 -0.01 -0.01 0.00

39 6 0.00 0.00 0.00 0.02 -0.01 0.00 -0.01 0.02 0.00

40 6 -0.01 -0.01 0.00 -0.01 -0.01 0.00 -0.01 -0.01 0.00

41 6 0.00 0.00 0.00 0.02 -0.01 0.00 -0.01 0.02 0.00

42 1 0.01 0.01 0.00 0.03 -0.01 0.00 -0.01 0.03 0.00

43 1 0.01 -0.01 0.00 0.03 0.01 0.00 0.01 0.03 0.00

44 1 -0.01 -0.01 0.00 0.03 -0.01 0.00 -0.01 0.03 0.00

45 1 -0.01 0.01 0.00 0.03 0.01 0.00 0.01 0.03 0.00

109 110 111

B2 E E

Frequencies -- 1528.7887 1556.2135 1556.2135

Red. masses -- 5.3888 6.1457 6.1457

Frc consts -- 7.4205 8.7692 8.7692

IR Inten -- 0.0000 42.9999 42.9999

Atom AN X Y Z X Y Z X Y Z

1 6 0.21 -0.01 0.00 0.26 -0.02 0.00 0.02 -0.01 0.00

2 6 -0.06 -0.03 0.00 -0.16 -0.04 0.00 -0.10 0.00 0.00

3 7 0.00 0.02 0.00 0.00 0.05 0.00 0.05 0.00 0.00

4 6 0.06 -0.03 0.00 0.16 -0.04 0.00 -0.10 0.00 0.00

5 6 -0.21 -0.01 0.00 -0.26 -0.02 0.00 0.02 0.01 0.00

6 6 0.00 0.00 0.00 -0.05 0.07 0.00 0.07 -0.05 0.00

7 6 -0.03 0.06 0.00 0.00 -0.10 0.00 -0.04 0.16 0.00

8 7 0.02 0.00 0.00 0.00 0.05 0.00 0.05 0.00 0.00

9 6 -0.03 -0.06 0.00 0.00 -0.10 0.00 -0.04 -0.16 0.00

10 6 -0.01 0.21 0.00 -0.01 0.02 0.00 -0.02 0.26 0.00

11 6 -0.01 -0.21 0.00 0.01 0.02 0.00 -0.02 -0.26 0.00

12 6 0.00 0.00 0.00 0.05 0.07 0.00 0.07 0.05 0.00

13 6 0.03 0.06 0.00 0.00 -0.10 0.00 -0.04 -0.16 0.00

14 6 0.01 -0.21 0.00 -0.01 0.02 0.00 -0.02 0.26 0.00

15 6 0.01 0.21 0.00 0.01 0.02 0.00 -0.02 -0.26 0.00

16 6 0.03 -0.06 0.00 0.00 -0.10 0.00 -0.04 0.16 0.00

17 7 -0.02 0.00 0.00 0.00 0.05 0.00 0.05 0.00 0.00

18 6 0.00 0.00 0.00 -0.05 0.07 0.00 0.07 -0.05 0.00

19 6 -0.06 0.03 0.00 0.16 -0.04 0.00 -0.10 0.00 0.00

20 6 0.21 0.01 0.00 -0.26 -0.02 0.00 0.02 0.01 0.00

21 6 -0.21 0.01 0.00 0.26 -0.02 0.00 0.02 -0.01 0.00

22 6 0.06 0.03 0.00 -0.16 -0.04 0.00 -0.10 0.00 0.00

23 7 0.00 -0.02 0.00 0.00 0.05 0.00 0.05 0.00 0.00

24 1 -0.09 0.26 0.01 -0.15 0.33 0.01 -0.05 0.04 0.00

25 1 0.09 0.26 0.01 0.15 0.33 0.01 -0.06 -0.04 0.00

26 1 0.26 -0.09 -0.01 0.04 -0.06 0.00 0.33 -0.15 -0.01

27 1 0.26 0.09 -0.01 -0.04 -0.05 0.00 0.33 0.15 -0.01

28 1 -0.26 0.09 -0.01 0.04 -0.06 0.00 0.33 -0.15 0.01

29 1 -0.26 -0.09 -0.01 -0.04 -0.05 0.00 0.33 0.15 0.01

30 1 -0.09 -0.26 0.01 0.15 0.33 -0.01 -0.06 -0.04 0.00

31 1 0.09 -0.26 0.01 -0.15 0.33 -0.01 -0.05 0.04 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.00 0.00 0.00 0.05 0.07 0.00 0.07 0.05 0.00

34 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

35 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

36 6 0.00 0.00 0.00 -0.01 -0.01 0.00 -0.01 -0.01 0.00

37 6 0.00 0.00 0.00 -0.01 -0.01 0.00 -0.01 -0.01 0.00

38 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

39 6 0.00 0.00 0.00 0.01 -0.01 0.00 -0.01 0.01 0.00

40 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

41 6 0.00 0.00 0.00 0.01 -0.01 0.00 -0.01 0.01 0.00

42 1 0.00 0.00 0.00 0.01 -0.01 0.00 -0.01 0.01 0.00

43 1 0.00 0.00 0.00 -0.01 -0.01 0.00 -0.01 -0.01 0.00

44 1 0.00 0.00 0.00 0.01 -0.01 0.00 -0.01 0.01 0.00

45 1 0.00 0.00 0.00 -0.01 -0.01 0.00 -0.01 -0.01 0.00

112 113 114

B2 A1 B1

Frequencies -- 1579.0230 1579.8236 2188.6543

Red. masses -- 11.2957 6.5344 6.0089

Frc consts -- 16.5936 9.6089 16.9591

IR Inten -- 0.0000 0.0765 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.06 -0.02 0.00 -0.17 0.02 0.00 0.00 0.00 0.00

2 6 -0.24 0.08 0.00 0.16 0.02 0.00 -0.01 0.00 0.00

3 7 0.00 0.00 0.00 0.00 -0.04 0.00 0.01 0.00 0.00

4 6 0.24 0.08 0.00 -0.16 0.02 0.00 -0.01 0.00 0.00

5 6 0.06 -0.02 0.00 0.17 0.02 0.00 0.00 0.00 0.00

6 6 -0.21 -0.21 0.00 0.07 -0.07 0.00 -0.03 0.03 0.00

7 6 0.08 0.24 0.00 -0.02 0.16 0.00 0.00 0.01 0.00

8 7 0.00 0.00 0.00 0.04 0.00 0.00 0.00 -0.01 0.00

9 6 0.08 -0.24 0.00 -0.02 -0.16 0.00 0.00 0.01 0.00

10 6 -0.02 -0.06 0.00 -0.02 0.17 0.00 0.00 0.00 0.00

11 6 -0.02 0.06 0.00 -0.02 -0.17 0.00 0.00 0.00 0.00

12 6 0.21 -0.21 0.00 -0.07 -0.07 0.00 -0.03 -0.03 0.00

13 6 -0.08 0.24 0.00 0.02 0.16 0.00 0.00 -0.01 0.00

14 6 0.02 0.06 0.00 0.02 -0.17 0.00 0.00 0.00 0.00

15 6 0.02 -0.06 0.00 0.02 0.17 0.00 0.00 0.00 0.00

16 6 -0.08 -0.24 0.00 0.02 -0.16 0.00 0.00 -0.01 0.00

17 7 0.00 0.00 0.00 -0.04 0.00 0.00 0.00 0.01 0.00

18 6 0.21 0.21 0.00 -0.07 0.07 0.00 0.03 -0.03 0.00

19 6 -0.24 -0.08 0.00 0.16 -0.02 0.00 0.01 0.00 0.00

20 6 -0.06 0.02 0.00 -0.17 -0.02 0.00 0.00 0.00 0.00

21 6 0.06 0.02 0.00 0.17 -0.02 0.00 0.00 0.00 0.00

22 6 0.24 -0.08 0.00 -0.16 -0.02 0.00 0.01 0.00 0.00

23 7 0.00 0.00 0.00 0.00 0.04 0.00 -0.01 0.00 0.00

24 1 -0.08 -0.03 0.00 0.11 -0.22 -0.01 0.00 0.00 0.00

25 1 0.08 -0.03 0.00 -0.11 -0.22 -0.01 0.00 0.00 0.00

26 1 -0.03 -0.08 0.00 0.22 -0.11 -0.01 0.00 0.00 0.00

27 1 -0.03 0.08 0.00 0.22 0.11 -0.01 0.00 0.00 0.00

28 1 0.03 0.08 0.00 -0.22 0.11 -0.01 0.00 0.00 0.00

29 1 0.03 -0.08 0.00 -0.22 -0.11 -0.01 0.00 0.00 0.00

30 1 -0.08 0.03 0.00 0.11 0.22 -0.01 0.00 0.00 0.00

31 1 0.08 0.03 0.00 -0.11 0.22 -0.01 0.00 0.00 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 -0.21 0.21 0.00 0.07 0.07 0.00 0.03 0.03 0.00

34 6 0.01 -0.01 0.00 0.00 0.00 0.00 -0.19 -0.19 0.01

35 6 -0.01 0.01 0.00 0.00 0.00 0.00 0.19 0.19 0.01

36 6 0.00 0.00 0.00 -0.01 -0.01 0.00 0.14 0.14 0.00

37 6 0.00 0.00 0.00 0.01 0.01 0.00 -0.14 -0.14 0.00

38 6 0.01 0.01 0.00 0.00 0.00 0.00 0.19 -0.19 -0.01

39 6 0.00 0.00 0.00 -0.01 0.01 0.00 -0.14 0.14 0.00

40 6 -0.01 -0.01 0.00 0.00 0.00 0.00 -0.19 0.19 -0.01

41 6 0.00 0.00 0.00 0.01 -0.01 0.00 0.14 -0.14 0.00

42 1 0.02 0.02 0.00 0.01 -0.01 0.00 0.26 -0.26 0.01

43 1 -0.02 0.02 0.00 -0.01 -0.01 0.00 0.26 0.26 -0.01

44 1 -0.02 -0.02 0.00 -0.01 0.01 0.00 -0.26 0.26 0.01

45 1 0.02 -0.02 0.00 0.01 0.01 0.00 -0.26 -0.26 -0.01

115 116 117

E E A1

Frequencies -- 2189.4503 2189.4503 2189.9173

Red. masses -- 6.0078 6.0078 5.9966

Frc consts -- 16.9683 16.9683 16.9437

IR Inten -- 123.1293 123.1293 0.0048

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

2 6 0.00 0.00 0.00 -0.01 0.00 0.00 0.01 0.00 0.00

3 7 0.00 0.00 0.00 0.01 0.00 0.00 0.00 0.00 0.00

4 6 0.00 0.00 0.00 -0.01 0.00 0.00 -0.01 0.00 0.00

5 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

6 6 0.03 -0.03 0.00 -0.03 0.03 0.00 -0.03 0.03 0.00

7 6 0.00 -0.01 0.00 0.00 0.00 0.00 0.00 0.01 0.00

8 7 0.00 0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00

9 6 0.00 -0.01 0.00 0.00 0.00 0.00 0.00 -0.01 0.00

10 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

11 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

12 6 -0.03 -0.03 0.00 -0.03 -0.03 0.00 0.03 0.03 0.00

13 6 0.00 -0.01 0.00 0.00 0.00 0.00 0.00 0.01 0.00

14 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

15 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

16 6 0.00 -0.01 0.00 0.00 0.00 0.00 0.00 -0.01 0.00

17 7 0.00 0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00

18 6 0.03 -0.03 0.00 -0.03 0.03 0.00 0.03 -0.03 0.00

19 6 0.00 0.00 0.00 -0.01 0.00 0.00 0.01 0.00 0.00

20 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

21 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

22 6 0.00 0.00 0.00 -0.01 0.00 0.00 -0.01 0.00 0.00

23 7 0.00 0.00 0.00 0.01 0.00 0.00 0.00 0.00 0.00

24 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

25 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

26 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

27 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

28 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

29 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

30 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

31 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 -0.03 -0.03 0.00 -0.03 -0.03 0.00 -0.03 -0.03 0.00

34 6 0.19 0.19 -0.01 0.19 0.19 -0.01 0.19 0.19 -0.01

35 6 0.19 0.19 0.01 0.19 0.19 0.01 -0.19 -0.19 -0.01

36 6 -0.14 -0.14 0.00 -0.14 -0.14 0.00 -0.14 -0.14 0.00

37 6 -0.14 -0.14 0.00 -0.14 -0.14 0.00 0.14 0.14 0.00

38 6 -0.19 0.19 0.01 0.19 -0.19 -0.01 0.19 -0.19 -0.01

39 6 0.14 -0.14 0.00 -0.14 0.14 0.00 -0.14 0.14 0.00

40 6 -0.19 0.19 -0.01 0.19 -0.19 0.01 -0.19 0.19 -0.01

41 6 0.14 -0.14 0.00 -0.14 0.14 0.00 0.14 -0.14 0.00

42 1 0.26 -0.26 0.01 -0.26 0.26 -0.01 0.26 -0.26 0.01

43 1 -0.26 -0.26 0.01 -0.26 -0.26 0.01 -0.26 -0.26 0.01

44 1 0.26 -0.26 -0.01 -0.26 0.26 0.01 -0.26 0.26 0.01

45 1 -0.26 -0.26 -0.01 -0.26 -0.26 -0.01 0.26 0.26 0.01

118 119 120

A2 E E

Frequencies -- 3240.7049 3240.8596 3240.8596

Red. masses -- 1.0907 1.0908 1.0908

Frc consts -- 6.7489 6.7503 6.7503

IR Inten -- 0.0000 2.5590 2.5590

Atom AN X Y Z X Y Z X Y Z

1 6 -0.02 -0.02 0.00 0.03 0.04 0.00 0.00 0.00 0.00

2 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

3 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

4 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

5 6 -0.02 0.02 0.00 0.03 -0.04 0.00 0.00 0.00 0.00

6 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

7 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

8 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

9 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

10 6 -0.02 -0.02 0.00 0.00 0.00 0.00 -0.04 -0.03 0.00

11 6 0.02 -0.02 0.00 0.00 0.00 0.00 0.04 -0.03 0.00

12 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

13 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

14 6 0.02 0.02 0.00 0.00 0.00 0.00 -0.04 -0.03 0.00

15 6 -0.02 0.02 0.00 0.00 0.00 0.00 0.04 -0.03 0.00

16 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

17 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

18 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

19 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

20 6 0.02 -0.02 0.00 0.03 -0.04 0.00 0.00 0.00 0.00

21 6 0.02 0.02 0.00 0.03 0.04 0.00 0.00 0.00 0.00

22 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

23 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

24 1 0.21 0.28 0.01 -0.30 -0.40 -0.01 0.00 0.00 0.00

25 1 0.21 -0.28 -0.01 -0.30 0.40 0.01 0.00 0.00 0.00

26 1 0.28 0.21 -0.01 0.00 0.00 0.00 0.40 0.30 -0.01

27 1 -0.28 0.21 0.01 0.00 0.00 0.00 -0.40 0.30 0.01

28 1 -0.28 -0.21 -0.01 0.00 0.00 0.00 0.40 0.30 0.01

29 1 0.28 -0.21 0.01 0.00 0.00 0.00 -0.40 0.30 -0.01

30 1 -0.21 0.28 -0.01 -0.30 0.40 -0.01 0.00 0.00 0.00

31 1 -0.21 -0.28 0.01 -0.30 -0.40 0.01 0.00 0.00 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

34 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

35 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

36 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

37 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

38 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

39 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

40 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

41 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

42 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

43 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

44 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

45 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

121 122 123

B1 B2 E

Frequencies -- 3241.0047 3256.9585 3257.0998

Red. masses -- 1.0909 1.1045 1.1045

Frc consts -- 6.7513 6.9031 6.9038

IR Inten -- 0.0000 0.0000 21.5254

Atom AN X Y Z X Y Z X Y Z

1 6 -0.02 -0.02 0.00 -0.02 -0.02 0.00 0.00 0.00 0.00

2 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

3 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

4 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

5 6 -0.02 0.02 0.00 0.02 -0.02 0.00 0.00 0.00 0.00

6 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

7 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

8 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

9 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

10 6 0.02 0.02 0.00 -0.02 -0.02 0.00 -0.04 -0.03 0.00

11 6 -0.02 0.02 0.00 -0.02 0.02 0.00 -0.04 0.03 0.00

12 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

13 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

14 6 -0.02 -0.02 0.00 0.02 0.02 0.00 -0.04 -0.03 0.00

15 6 0.02 -0.02 0.00 0.02 -0.02 0.00 -0.04 0.03 0.00

16 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

17 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

18 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

19 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

20 6 0.02 -0.02 0.00 -0.02 0.02 0.00 0.00 0.00 0.00

21 6 0.02 0.02 0.00 0.02 0.02 0.00 0.00 0.00 0.00

22 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

23 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

24 1 0.21 0.28 0.01 0.22 0.28 0.01 0.00 0.00 0.00

25 1 0.21 -0.28 -0.01 -0.22 0.28 0.01 0.00 0.00 0.00

26 1 -0.28 -0.21 0.01 0.28 0.22 -0.01 0.39 0.30 -0.01

27 1 0.28 -0.21 -0.01 0.28 -0.22 -0.01 0.39 -0.30 -0.01

28 1 0.28 0.21 0.01 -0.28 -0.22 -0.01 0.39 0.30 0.01

29 1 -0.28 0.21 -0.01 -0.28 0.22 -0.01 0.39 -0.30 0.01

30 1 -0.21 0.28 -0.01 0.22 -0.28 0.01 0.00 0.00 0.00

31 1 -0.21 -0.28 0.01 -0.22 -0.28 0.01 0.00 0.00 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

34 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

35 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

36 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

37 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

38 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

39 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

40 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

41 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

42 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

43 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

44 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

45 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

124 125 126

E A1 B1

Frequencies -- 3257.0998 3257.3486 3432.8177

Red. masses -- 1.1045 1.1045 1.1625

Frc consts -- 6.9038 6.9047 8.0710

IR Inten -- 21.5254 0.0004 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 -0.04 0.00 0.02 0.02 0.00 0.00 0.00 0.00

2 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

3 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

4 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

5 6 0.03 -0.04 0.00 -0.02 0.02 0.00 0.00 0.00 0.00

6 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

7 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

8 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

9 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

10 6 0.00 0.00 0.00 -0.02 -0.02 0.00 0.00 0.00 0.00

11 6 0.00 0.00 0.00 -0.02 0.02 0.00 0.00 0.00 0.00

12 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

13 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

14 6 0.00 0.00 0.00 0.02 0.02 0.00 0.00 0.00 0.00

15 6 0.00 0.00 0.00 0.02 -0.02 0.00 0.00 0.00 0.00

16 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

17 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

18 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

19 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

20 6 0.03 -0.04 0.00 0.02 -0.02 0.00 0.00 0.00 0.00

21 6 -0.03 -0.04 0.00 -0.02 -0.02 0.00 0.00 0.00 0.00

22 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

23 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

24 1 0.30 0.39 0.01 -0.22 -0.28 -0.01 0.00 0.00 0.00

25 1 -0.30 0.39 0.01 0.22 -0.28 -0.01 0.00 0.00 0.00

26 1 0.00 0.00 0.00 0.28 0.22 -0.01 0.00 0.00 0.00

27 1 0.00 0.00 0.00 0.28 -0.22 -0.01 0.00 0.00 0.00

28 1 0.00 0.00 0.00 -0.28 -0.22 -0.01 0.00 0.00 0.00

29 1 0.00 0.00 0.00 -0.28 0.22 -0.01 0.00 0.00 0.00

30 1 -0.30 0.39 -0.01 -0.22 0.28 -0.01 0.00 0.00 0.00

31 1 0.30 0.39 -0.01 0.22 0.28 -0.01 0.00 0.00 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

34 6 0.00 0.00 0.00 0.00 0.00 0.00 0.01 0.01 0.00

35 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.01 -0.01 0.00

36 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.04 -0.04 0.00

37 6 0.00 0.00 0.00 0.00 0.00 0.00 0.04 0.04 0.00

38 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.01 0.01 0.00

39 6 0.00 0.00 0.00 0.00 0.00 0.00 0.04 -0.04 0.00

40 6 0.00 0.00 0.00 0.00 0.00 0.00 0.01 -0.01 0.00

41 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.04 0.04 0.00

42 1 0.00 0.00 0.00 0.00 0.00 0.00 0.35 -0.35 0.01

43 1 0.00 0.00 0.00 0.00 0.00 0.00 0.35 0.35 -0.01

44 1 0.00 0.00 0.00 0.00 0.00 0.00 -0.35 0.35 0.01

45 1 0.00 0.00 0.00 0.00 0.00 0.00 -0.35 -0.35 -0.01

127 128 129

E E A1

Frequencies -- 3432.8370 3432.8370 3433.2880

Red. masses -- 1.1625 1.1625 1.1629

Frc consts -- 8.0717 8.0717 8.0764

IR Inten -- 623.6870 623.6872 0.2828

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

2 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

3 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

4 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

5 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

6 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

7 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

8 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

9 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

10 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

11 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

12 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

13 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

14 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

15 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

16 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

17 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

18 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

19 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

20 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

21 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

22 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

23 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

24 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

25 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

26 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

27 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

28 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

29 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

30 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

31 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

34 6 -0.01 -0.01 0.00 -0.01 -0.01 0.00 0.01 0.01 0.00

35 6 -0.01 -0.01 0.00 -0.01 -0.01 0.00 -0.01 -0.01 0.00

36 6 0.04 0.04 0.00 0.04 0.04 0.00 -0.04 -0.04 0.00

37 6 0.04 0.04 0.00 0.04 0.04 0.00 0.04 0.04 0.00

38 6 -0.01 0.01 0.00 0.01 -0.01 0.00 0.01 -0.01 0.00

39 6 0.04 -0.04 0.00 -0.04 0.04 0.00 -0.04 0.04 0.00

40 6 -0.01 0.01 0.00 0.01 -0.01 0.00 -0.01 0.01 0.00

41 6 0.04 -0.04 0.00 -0.04 0.04 0.00 0.04 -0.04 0.00

42 1 -0.35 0.35 -0.01 0.35 -0.35 0.01 -0.35 0.35 -0.01

43 1 -0.35 -0.35 0.01 -0.35 -0.35 0.01 0.35 0.35 -0.01

44 1 -0.35 0.35 0.01 0.35 -0.35 -0.01 0.35 -0.35 -0.01

45 1 -0.35 -0.35 -0.01 -0.35 -0.35 -0.01 -0.35 -0.35 -0.01

-------------------

- Thermochemistry -

-------------------

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Atom 1 has atomic number 6 and mass 12.00000

Atom 2 has atomic number 6 and mass 12.00000

Atom 3 has atomic number 7 and mass 14.00307

Atom 4 has atomic number 6 and mass 12.00000

Atom 5 has atomic number 6 and mass 12.00000

Atom 6 has atomic number 6 and mass 12.00000

Atom 7 has atomic number 6 and mass 12.00000

Atom 8 has atomic number 7 and mass 14.00307

Atom 9 has atomic number 6 and mass 12.00000

Atom 10 has atomic number 6 and mass 12.00000

Atom 11 has atomic number 6 and mass 12.00000

Atom 12 has atomic number 6 and mass 12.00000

Atom 13 has atomic number 6 and mass 12.00000

Atom 14 has atomic number 6 and mass 12.00000

Atom 15 has atomic number 6 and mass 12.00000

Atom 16 has atomic number 6 and mass 12.00000

Atom 17 has atomic number 7 and mass 14.00307

Atom 18 has atomic number 6 and mass 12.00000

Atom 19 has atomic number 6 and mass 12.00000

Atom 20 has atomic number 6 and mass 12.00000

Atom 21 has atomic number 6 and mass 12.00000

Atom 22 has atomic number 6 and mass 12.00000

Atom 23 has atomic number 7 and mass 14.00307

Atom 24 has atomic number 1 and mass 1.00783

Atom 25 has atomic number 1 and mass 1.00783

Atom 26 has atomic number 1 and mass 1.00783

Atom 27 has atomic number 1 and mass 1.00783

Atom 28 has atomic number 1 and mass 1.00783

Atom 29 has atomic number 1 and mass 1.00783

Atom 30 has atomic number 1 and mass 1.00783

Atom 31 has atomic number 1 and mass 1.00783

Atom 32 has atomic number 30 and mass 63.92915

Atom 33 has atomic number 6 and mass 12.00000

Atom 34 has atomic number 6 and mass 12.00000

Atom 35 has atomic number 6 and mass 12.00000

Atom 36 has atomic number 6 and mass 12.00000

Atom 37 has atomic number 6 and mass 12.00000

Atom 38 has atomic number 6 and mass 12.00000

Atom 39 has atomic number 6 and mass 12.00000

Atom 40 has atomic number 6 and mass 12.00000

Atom 41 has atomic number 6 and mass 12.00000

Atom 42 has atomic number 1 and mass 1.00783

Atom 43 has atomic number 1 and mass 1.00783

Atom 44 has atomic number 1 and mass 1.00783

Atom 45 has atomic number 1 and mass 1.00783

Molecular mass: 468.03534 amu.

Principal axes and moments of inertia in atomic units:

1 2 3

Eigenvalues -- \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

X 0.96562 0.25997 0.00000

Y -0.25997 0.96562 0.00000

Z 0.00000 0.00000 1.00000

This molecule is an oblate symmetric top.

Rotational symmetry number 4.

Warning -- assumption of classical behavior for rotation

may cause significant error

Rotational temperatures (Kelvin) 0.00703 0.00703 0.00352

Rotational constants (GHZ): 0.14652 0.14652 0.07332

Zero-point vibrational energy 802623.6 (Joules/Mol)

191.83163 (Kcal/Mol)

Warning -- explicit consideration of 49 degrees of freedom as

vibrations may cause significant error

Vibrational temperatures: 11.69 56.73 73.29 85.19 85.19

(Kelvin) 127.54 156.16 160.85 160.85 184.93

184.93 200.37 208.36 237.24 242.63

275.88 296.76 311.68 311.68 347.98

347.98 415.62 457.23 461.69 461.69

476.43 537.12 537.12 541.58 541.58

577.00 580.47 620.74 652.62 655.14

687.50 687.50 793.67 806.66 806.66

822.72 833.96 858.54 858.54 878.42

880.10 880.10 883.33 890.94 968.62

982.07 982.14 982.14 982.17 983.26

983.26 991.11 1043.72 1062.67 1062.67

1086.01 1150.12 1158.69 1158.69 1165.57

1210.43 1221.67 1221.67 1258.69 1322.79

1325.44 1325.44 1327.72 1344.62 1379.52

1379.52 1418.45 1468.34 1474.50 1474.50

1486.68 1554.74 1554.74 1563.42 1569.48

1637.47 1673.59 1673.59 1700.60 1777.68

1781.75 1781.75 1837.08 1884.11 1884.11

1904.83 1938.33 1950.12 1950.12 1980.04

1982.50 2083.87 2083.87 2124.51 2125.42

2177.68 2189.84 2189.84 2199.58 2239.04

2239.04 2271.86 2273.01 3148.98 3150.13

3150.13 3150.80 4662.65 4662.87 4662.87

4663.08 4686.03 4686.23 4686.23 4686.59

4939.05 4939.08 4939.08 4939.73

Zero-point correction= 0.305703 (Hartree/Particle)

Thermal correction to Energy= 0.332803

Thermal correction to Enthalpy= 0.333747

Thermal correction to Gibbs Free Energy= 0.249662

Sum of electronic and zero-point Energies= -1358.757343

Sum of electronic and thermal Energies= -1358.730243

Sum of electronic and thermal Enthalpies= -1358.729299

Sum of electronic and thermal Free Energies= -1358.813384

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 208.837 106.969 176.972

Electronic 0.000 0.000 0.000

Translational 0.889 2.981 44.319

Rotational 0.889 2.981 33.812

Vibrational 207.059 101.008 98.842

Vibration 1 0.593 1.987 8.424

Vibration 2 0.594 1.981 5.287

Vibration 3 0.595 1.977 4.781

Vibration 4 0.597 1.974 4.483

Vibration 5 0.597 1.974 4.483

Vibration 6 0.601 1.957 3.690

Vibration 7 0.606 1.942 3.295

Vibration 8 0.607 1.940 3.237

Vibration 9 0.607 1.940 3.237

Vibration 10 0.611 1.925 2.968

Vibration 11 0.611 1.925 2.968

Vibration 12 0.615 1.914 2.814

Vibration 13 0.616 1.908 2.739

Vibration 14 0.623 1.886 2.493

Vibration 15 0.625 1.881 2.451

Vibration 16 0.634 1.851 2.211

Vibration 17 0.641 1.831 2.077

Vibration 18 0.645 1.816 1.987

Vibration 19 0.645 1.816 1.987

Vibration 20 0.658 1.776 1.789

Vibration 21 0.658 1.776 1.789

Vibration 22 0.685 1.694 1.481

Vibration 23 0.704 1.640 1.321

Vibration 24 0.706 1.634 1.306

Vibration 25 0.706 1.634 1.306

Vibration 26 0.714 1.613 1.255

Vibration 27 0.745 1.527 1.066

Vibration 28 0.745 1.527 1.066

Vibration 29 0.747 1.520 1.054

Vibration 30 0.747 1.520 1.054

Vibration 31 0.767 1.468 0.959

Vibration 32 0.769 1.463 0.950

Vibration 33 0.792 1.402 0.854

Vibration 34 0.812 1.353 0.785

Vibration 35 0.814 1.349 0.780

Vibration 36 0.834 1.299 0.716

Vibration 37 0.834 1.299 0.716

Vibration 38 0.907 1.136 0.541

Vibration 39 0.916 1.116 0.523

Vibration 40 0.916 1.116 0.523

Vibration 41 0.928 1.092 0.501

Vibration 42 0.936 1.075 0.486

Vibration 43 0.955 1.039 0.455

Vibration 44 0.955 1.039 0.455

Vibration 45 0.970 1.010 0.432

Vibration 46 0.971 1.007 0.430

Vibration 47 0.971 1.007 0.430

Vibration 48 0.973 1.002 0.426

Vibration 49 0.979 0.991 0.418

Q Log10(Q) Ln(Q)

Total Bot 0.145769-114 -114.836335 -264.420433

Total V=0 0.598497D+26 25.777062 59.353878

Vib (Bot) 0.669698-130 -130.174121 -299.736990

Vib (Bot) 1 0.255116D+02 1.406738 3.239134

Vib (Bot) 2 0.524742D+01 0.719946 1.657736

Vib (Bot) 3 0.405805D+01 0.608317 1.400702

Vib (Bot) 4 0.348790D+01 0.542564 1.249300

Vib (Bot) 5 0.348790D+01 0.542564 1.249300

Vib (Bot) 6 0.231997D+01 0.365482 0.841553

Vib (Bot) 7 0.188763D+01 0.275916 0.635320

Vib (Bot) 8 0.183130D+01 0.262759 0.605026

Vib (Bot) 9 0.183130D+01 0.262759 0.605026

Vib (Bot) 10 0.158669D+01 0.200491 0.461648

Vib (Bot) 11 0.158669D+01 0.200491 0.461648

Vib (Bot) 12 0.146033D+01 0.164450 0.378660

Vib (Bot) 13 0.140222D+01 0.146816 0.338056

Vib (Bot) 14 0.122418D+01 0.087845 0.202270

Vib (Bot) 15 0.119555D+01 0.077568 0.178607

Vib (Bot) 16 0.104309D+01 0.018322 0.042188

Vib (Bot) 17 0.964379D+00 -0.015752 -0.036271

Vib (Bot) 18 0.914394D+00 -0.038867 -0.089493

Vib (Bot) 19 0.914394D+00 -0.038867 -0.089493

Vib (Bot) 20 0.810033D+00 -0.091497 -0.210680

Vib (Bot) 21 0.810033D+00 -0.091497 -0.210680

Vib (Bot) 22 0.662417D+00 -0.178869 -0.411861

Vib (Bot) 23 0.592301D+00 -0.227458 -0.523741

Vib (Bot) 24 0.585498D+00 -0.232475 -0.535293

Vib (Bot) 25 0.585498D+00 -0.232475 -0.535293

Vib (Bot) 26 0.563866D+00 -0.248824 -0.572938

Vib (Bot) 27 0.486574D+00 -0.312851 -0.720366

Vib (Bot) 28 0.486574D+00 -0.312851 -0.720366

Vib (Bot) 29 0.481531D+00 -0.317376 -0.730786

Vib (Bot) 30 0.481531D+00 -0.317376 -0.730786

Vib (Bot) 31 0.444107D+00 -0.352513 -0.811691

Vib (Bot) 32 0.440669D+00 -0.355887 -0.819460

Vib (Bot) 33 0.403403D+00 -0.394261 -0.907818

Vib (Bot) 34 0.376956D+00 -0.423710 -0.975628

Vib (Bot) 35 0.374973D+00 -0.426000 -0.980901

Vib (Bot) 36 0.350660D+00 -0.455114 -1.047939

Vib (Bot) 37 0.350660D+00 -0.455114 -1.047939

Vib (Bot) 38 0.284044D+00 -0.546614 -1.258625

Vib (Bot) 39 0.277039D+00 -0.557458 -1.283595

Vib (Bot) 40 0.277039D+00 -0.557458 -1.283595

Vib (Bot) 41 0.268667D+00 -0.570786 -1.314284

Vib (Bot) 42 0.262990D+00 -0.580060 -1.335638

Vib (Bot) 43 0.251079D+00 -0.600190 -1.381988

Vib (Bot) 44 0.251079D+00 -0.600190 -1.381988

Vib (Bot) 45 0.241919D+00 -0.616331 -1.419154

Vib (Bot) 46 0.241164D+00 -0.617687 -1.422277

Vib (Bot) 47 0.241164D+00 -0.617687 -1.422277

Vib (Bot) 48 0.239720D+00 -0.620295 -1.428282

Vib (Bot) 49 0.236354D+00 -0.626437 -1.442424

Vib (V=0) 0.274964D+11 10.439276 24.037321

Vib (V=0) 1 0.260165D+02 1.415249 3.258731

Vib (V=0) 2 0.577118D+01 0.761265 1.752877

Vib (V=0) 3 0.458873D+01 0.661693 1.523604

Vib (V=0) 4 0.402356D+01 0.604610 1.392167

Vib (V=0) 5 0.402356D+01 0.604610 1.392167

Vib (V=0) 6 0.287324D+01 0.458371 1.055439

Vib (V=0) 7 0.245272D+01 0.389649 0.897199

Vib (V=0) 8 0.239833D+01 0.379909 0.874773

Vib (V=0) 9 0.239833D+01 0.379909 0.874773

Vib (V=0) 10 0.216360D+01 0.335177 0.771775

Vib (V=0) 11 0.216360D+01 0.335177 0.771775

Vib (V=0) 12 0.204355D+01 0.310386 0.714690

Vib (V=0) 13 0.198870D+01 0.298569 0.687480

Vib (V=0) 14 0.182235D+01 0.260632 0.600127

Vib (V=0) 15 0.179589D+01 0.254281 0.585503

Vib (V=0) 16 0.165674D+01 0.219253 0.504850

Vib (V=0) 17 0.158629D+01 0.200383 0.461398

Vib (V=0) 18 0.154217D+01 0.188132 0.433190

Vib (V=0) 19 0.154217D+01 0.188132 0.433190

Vib (V=0) 20 0.145192D+01 0.161943 0.372887

Vib (V=0) 21 0.145192D+01 0.161943 0.372887

Vib (V=0) 22 0.132994D+01 0.123831 0.285132

Vib (V=0) 23 0.127513D+01 0.105553 0.243045

Vib (V=0) 24 0.126994D+01 0.103783 0.238970

Vib (V=0) 25 0.126994D+01 0.103783 0.238970

Vib (V=0) 26 0.125362D+01 0.098166 0.226037

Vib (V=0) 27 0.119768D+01 0.078340 0.180385

Vib (V=0) 28 0.119768D+01 0.078340 0.180385

Vib (V=0) 29 0.119417D+01 0.077066 0.177451

Vib (V=0) 30 0.119417D+01 0.077066 0.177451

Vib (V=0) 31 0.116875D+01 0.067723 0.155937

Vib (V=0) 32 0.116648D+01 0.066876 0.153987

Vib (V=0) 33 0.114244D+01 0.057835 0.133170

Vib (V=0) 34 0.112618D+01 0.051606 0.118827

Vib (V=0) 35 0.112498D+01 0.051146 0.117769

Vib (V=0) 36 0.111071D+01 0.045599 0.104996

Vib (V=0) 37 0.111071D+01 0.045599 0.104996

Vib (V=0) 38 0.107505D+01 0.031428 0.072366

Vib (V=0) 39 0.107162D+01 0.030041 0.069173

Vib (V=0) 40 0.107162D+01 0.030041 0.069173

Vib (V=0) 41 0.106761D+01 0.028413 0.065423

Vib (V=0) 42 0.106495D+01 0.027328 0.062924

Vib (V=0) 43 0.105950D+01 0.025101 0.057797

Vib (V=0) 44 0.105950D+01 0.025101 0.057797

Vib (V=0) 45 0.105545D+01 0.023438 0.053967

Vib (V=0) 46 0.105512D+01 0.023303 0.053656

Vib (V=0) 47 0.105512D+01 0.023303 0.053656

Vib (V=0) 48 0.105450D+01 0.023045 0.053063

Vib (V=0) 49 0.105305D+01 0.022449 0.051690

Electronic 0.100000D+01 0.000000 0.000000

Translational 0.397991D+09 8.599873 19.801940

Rotational 0.546906D+07 6.737913 15.514617

ZnTSPsim0

IR Spectrum

333 333333 222111111111111111111111111111

444 222222 11155555544433333322211100000099999988888777766666666665555544444433333222211111111

333 555444 988875221774775421733863988322853221744109532888887111198765755300773218410966432108553

333 777111 0990969247788657407862381713516953195910595959333339421702128541316311892762955992999198

XX X X X X X X X X XX X X XX XX X XX X X XX X X X X X X XX XXXXX XX X XX XX X

X X X X X X X X X X X X X X

X X X X X X X X X X

X X X X X X X

X X X X X

X

X

X

X

X

X

X

X

X

X

X

X

X

X

X

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000004178 -0.000001495 -0.000001669

2 6 -0.000005455 0.000001598 0.000001922

3 7 0.000000000 -0.000009299 0.000003007

4 6 0.000005455 0.000001598 0.000001922

5 6 -0.000004178 -0.000001495 -0.000001669

6 6 -0.000001995 0.000001995 -0.000004948

7 6 -0.000001598 -0.000005455 0.000001922

8 7 0.000009299 0.000000000 0.000003007

9 6 -0.000001598 0.000005455 0.000001922

10 6 0.000001495 -0.000004178 -0.000001669

11 6 0.000001495 0.000004178 -0.000001669

12 6 0.000001995 0.000001995 -0.000004948

13 6 0.000001598 -0.000005455 0.000001922

14 6 -0.000001495 0.000004178 -0.000001669

15 6 -0.000001495 -0.000004178 -0.000001669

16 6 0.000001598 0.000005455 0.000001922

17 7 -0.000009299 0.000000000 0.000003007

18 6 0.000001995 -0.000001995 -0.000004948

19 6 -0.000005455 -0.000001598 0.000001922

20 6 0.000004178 0.000001495 -0.000001669

21 6 -0.000004178 0.000001495 -0.000001669

22 6 0.000005455 -0.000001598 0.000001922

23 7 0.000000000 0.000009299 0.000003007

24 1 0.000000660 0.000000211 0.000001399

25 1 -0.000000660 0.000000211 0.000001399

26 1 -0.000000211 -0.000000660 0.000001399

27 1 -0.000000211 0.000000660 0.000001399

28 1 0.000000211 0.000000660 0.000001399

29 1 0.000000211 -0.000000660 0.000001399

30 1 0.000000660 -0.000000211 0.000001399

31 1 -0.000000660 -0.000000211 0.000001399

32 30 0.000000000 0.000000000 -0.000004847

33 6 -0.000001995 -0.000001995 -0.000004948

34 6 -0.000000415 -0.000000415 0.000000130

35 6 0.000000415 0.000000415 0.000000130

36 6 0.000001354 0.000001354 -0.000000129

37 6 -0.000001354 -0.000001354 -0.000000129

38 6 -0.000000415 0.000000415 0.000000130

39 6 0.000001354 -0.000001354 -0.000000129

40 6 0.000000415 -0.000000415 0.000000130

41 6 -0.000001354 0.000001354 -0.000000129

42 1 0.000000102 -0.000000102 -0.000000151

43 1 -0.000000102 -0.000000102 -0.000000151

44 1 -0.000000102 0.000000102 -0.000000151

45 1 0.000000102 0.000000102 -0.000000151

-------------------------------------------------------------------

Cartesian Forces: Max 0.000009299 RMS 0.000002774

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Fri Jul 26 14:36:19 2019, MaxMem= 1342177280 cpu: 2.7

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000006472 RMS 0.000001289

Search for a local minimum.

Step number 1 out of a maximum of 2

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Second derivative matrix not updated -- analytic derivatives used.

ITU= 0

Eigenvalues --- 0.00050 0.00195 0.00195 0.00393 0.00477

Eigenvalues --- 0.00477 0.00514 0.00834 0.00985 0.00991

Eigenvalues --- 0.00991 0.01140 0.01234 0.01234 0.01249

Eigenvalues --- 0.01501 0.01521 0.01534 0.01534 0.01586

Eigenvalues --- 0.01735 0.01735 0.01776 0.01954 0.02164

Eigenvalues --- 0.02164 0.02335 0.02398 0.02763 0.02763

Eigenvalues --- 0.02771 0.02787 0.02864 0.03166 0.03166

Eigenvalues --- 0.03567 0.04079 0.04112 0.04112 0.04121

Eigenvalues --- 0.04137 0.04242 0.04242 0.04328 0.07288

Eigenvalues --- 0.08599 0.08606 0.08606 0.08822 0.09002

Eigenvalues --- 0.09060 0.09133 0.09133 0.09486 0.09486

Eigenvalues --- 0.09557 0.09557 0.09722 0.10355 0.10355

Eigenvalues --- 0.10363 0.10412 0.10812 0.10812 0.12889

Eigenvalues --- 0.14783 0.16216 0.16216 0.16939 0.18709

Eigenvalues --- 0.18709 0.19425 0.20111 0.20398 0.20838

Eigenvalues --- 0.20838 0.21763 0.21821 0.21836 0.21864

Eigenvalues --- 0.21864 0.26223 0.26223 0.26405 0.29445

Eigenvalues --- 0.29506 0.29600 0.30120 0.30120 0.32939

Eigenvalues --- 0.32939 0.34376 0.35261 0.35376 0.36091

Eigenvalues --- 0.36091 0.36175 0.36769 0.37224 0.37230

Eigenvalues --- 0.37230 0.37321 0.37571 0.37571 0.37800

Eigenvalues --- 0.38684 0.39389 0.39389 0.39974 0.40186

Eigenvalues --- 0.40186 0.40191 0.40193 0.42404 0.42404

Eigenvalues --- 0.43200 0.43524 0.44420 0.44650 0.44650

Eigenvalues --- 0.46308 0.52624 0.52656 0.52747 0.52747

Eigenvalues --- 1.06103 1.06123 1.06123 1.06283

Angle between quadratic step and forces= 64.15 degrees.

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.00016318 RMS(Int)= 0.00000001

Iteration 2 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000000

ITry= 1 IFail=0 DXMaxC= 9.72D-04 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.68D-08 for atom 25.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73461 0.00000 0.00000 -0.00001 -0.00001 2.73460

R2 2.57442 0.00000 0.00000 0.00001 0.00001 2.57443

R3 2.04039 0.00000 0.00000 0.00000 0.00000 2.04039

R4 2.58205 0.00000 0.00000 0.00000 0.00000 2.58205

R5 2.67450 0.00000 0.00000 0.00000 0.00000 2.67450

R6 2.58205 0.00000 0.00000 0.00000 0.00000 2.58205

R7 3.94732 -0.00001 0.00000 -0.00004 -0.00004 3.94727

R8 2.73461 0.00000 0.00000 -0.00001 -0.00001 2.73460

R9 2.67450 0.00000 0.00000 0.00000 0.00000 2.67450

R10 2.04039 0.00000 0.00000 0.00000 0.00000 2.04039

R11 2.67450 0.00000 0.00000 0.00000 0.00000 2.67450

R12 2.69670 0.00000 0.00000 0.00000 0.00000 2.69669

R13 2.58205 0.00000 0.00000 0.00000 0.00000 2.58205

R14 2.73461 0.00000 0.00000 -0.00001 -0.00001 2.73460

R15 2.58205 0.00000 0.00000 0.00000 0.00000 2.58205

R16 3.94732 -0.00001 0.00000 -0.00004 -0.00004 3.94727

R17 2.73461 0.00000 0.00000 -0.00001 -0.00001 2.73460

R18 2.67450 0.00000 0.00000 0.00000 0.00000 2.67450

R19 2.57442 0.00000 0.00000 0.00001 0.00001 2.57443

R20 2.04039 0.00000 0.00000 0.00000 0.00000 2.04039

R21 2.04039 0.00000 0.00000 0.00000 0.00000 2.04039

R22 2.67450 0.00000 0.00000 0.00000 0.00000 2.67450

R23 2.69670 0.00000 0.00000 0.00000 0.00000 2.69669

R24 2.73461 0.00000 0.00000 -0.00001 -0.00001 2.73460

R25 2.58205 0.00000 0.00000 0.00000 0.00000 2.58205

R26 2.57442 0.00000 0.00000 0.00001 0.00001 2.57443

R27 2.04039 0.00000 0.00000 0.00000 0.00000 2.04039

R28 2.73461 0.00000 0.00000 -0.00001 -0.00001 2.73460

R29 2.04039 0.00000 0.00000 0.00000 0.00000 2.04039

R30 2.58205 0.00000 0.00000 0.00000 0.00000 2.58205

R31 2.67450 0.00000 0.00000 0.00000 0.00000 2.67450

R32 3.94732 -0.00001 0.00000 -0.00004 -0.00004 3.94727

R33 2.67450 0.00000 0.00000 0.00000 0.00000 2.67450

R34 2.69670 0.00000 0.00000 0.00000 0.00000 2.69669

R35 2.73461 0.00000 0.00000 -0.00001 -0.00001 2.73460

R36 2.58205 0.00000 0.00000 0.00000 0.00000 2.58205

R37 2.57442 0.00000 0.00000 0.00001 0.00001 2.57443

R38 2.04039 0.00000 0.00000 0.00000 0.00000 2.04039

R39 2.73461 0.00000 0.00000 -0.00001 -0.00001 2.73460

R40 2.04039 0.00000 0.00000 0.00000 0.00000 2.04039

R41 2.58205 0.00000 0.00000 0.00000 0.00000 2.58205

R42 2.67450 0.00000 0.00000 0.00000 0.00000 2.67450

R43 3.94732 -0.00001 0.00000 -0.00004 -0.00004 3.94727

R44 2.69670 0.00000 0.00000 0.00000 0.00000 2.69669

R45 2.27864 0.00000 0.00000 0.00000 0.00000 2.27864

R46 2.27864 0.00000 0.00000 0.00000 0.00000 2.27864

R47 2.01698 0.00000 0.00000 0.00000 0.00000 2.01698

R48 2.01698 0.00000 0.00000 0.00000 0.00000 2.01698

R49 2.27864 0.00000 0.00000 0.00000 0.00000 2.27864

R50 2.01698 0.00000 0.00000 0.00000 0.00000 2.01698

R51 2.27864 0.00000 0.00000 0.00000 0.00000 2.27864

R52 2.01698 0.00000 0.00000 0.00000 0.00000 2.01698

A1 1.86587 0.00000 0.00000 0.00000 0.00000 1.86587

A2 2.19058 0.00000 0.00000 0.00000 0.00000 2.19057

A3 2.22672 0.00000 0.00000 0.00001 0.00001 2.22673

A4 1.90828 0.00000 0.00000 0.00001 0.00001 1.90829

A5 2.18404 0.00000 0.00000 -0.00001 -0.00001 2.18403

A6 2.19079 0.00000 0.00000 0.00000 0.00000 2.19079

A7 1.87647 0.00000 0.00000 -0.00002 -0.00002 1.87645

A8 2.20226 0.00000 0.00000 0.00001 0.00001 2.20227

A9 2.20226 0.00000 0.00000 0.00001 0.00001 2.20227

A10 1.90828 0.00000 0.00000 0.00001 0.00001 1.90829

A11 2.19079 0.00000 0.00000 0.00000 0.00000 2.19079

A12 2.18404 0.00000 0.00000 -0.00001 -0.00001 2.18403

A13 1.86587 0.00000 0.00000 0.00000 0.00000 1.86587

A14 2.22672 0.00000 0.00000 0.00001 0.00001 2.22673

A15 2.19058 0.00000 0.00000 0.00000 0.00000 2.19057

A16 2.20757 0.00000 0.00000 -0.00001 -0.00001 2.20756

A17 2.03777 0.00000 0.00000 0.00001 0.00001 2.03777

A18 2.03777 0.00000 0.00000 0.00001 0.00001 2.03777

A19 2.19079 0.00000 0.00000 0.00000 0.00000 2.19079

A20 2.18404 0.00000 0.00000 -0.00001 -0.00001 2.18403

A21 1.90828 0.00000 0.00000 0.00001 0.00001 1.90829

A22 1.87647 0.00000 0.00000 -0.00002 -0.00002 1.87645

A23 2.20226 0.00000 0.00000 0.00001 0.00001 2.20227

A24 2.20226 0.00000 0.00000 0.00001 0.00001 2.20227

A25 1.90828 0.00000 0.00000 0.00001 0.00001 1.90829

A26 2.19079 0.00000 0.00000 0.00000 0.00000 2.19079

A27 2.18404 0.00000 0.00000 -0.00001 -0.00001 2.18403

A28 1.86587 0.00000 0.00000 0.00000 0.00000 1.86587

A29 2.19058 0.00000 0.00000 0.00000 0.00000 2.19057

A30 2.22672 0.00000 0.00000 0.00001 0.00001 2.22673

A31 1.86587 0.00000 0.00000 0.00000 0.00000 1.86587

A32 2.19058 0.00000 0.00000 0.00000 0.00000 2.19057

A33 2.22672 0.00000 0.00000 0.00001 0.00001 2.22673

A34 2.20757 0.00000 0.00000 -0.00001 -0.00001 2.20756

A35 2.03777 0.00000 0.00000 0.00001 0.00001 2.03777

A36 2.03777 0.00000 0.00000 0.00001 0.00001 2.03777

A37 2.18404 0.00000 0.00000 -0.00001 -0.00001 2.18403

A38 2.19079 0.00000 0.00000 0.00000 0.00000 2.19079

A39 1.90828 0.00000 0.00000 0.00001 0.00001 1.90829

A40 1.86587 0.00000 0.00000 0.00000 0.00000 1.86587

A41 2.19058 0.00000 0.00000 0.00000 0.00000 2.19057

A42 2.22672 0.00000 0.00000 0.00001 0.00001 2.22673

A43 1.86587 0.00000 0.00000 0.00000 0.00000 1.86587

A44 2.22672 0.00000 0.00000 0.00001 0.00001 2.22673

A45 2.19058 0.00000 0.00000 0.00000 0.00000 2.19057

A46 1.90828 0.00000 0.00000 0.00001 0.00001 1.90829

A47 2.18404 0.00000 0.00000 -0.00001 -0.00001 2.18403

A48 2.19079 0.00000 0.00000 0.00000 0.00000 2.19079

A49 1.87647 0.00000 0.00000 -0.00002 -0.00002 1.87645

A50 2.20226 0.00000 0.00000 0.00001 0.00001 2.20227

A51 2.20226 0.00000 0.00000 0.00001 0.00001 2.20227

A52 2.20757 0.00000 0.00000 -0.00001 -0.00001 2.20756

A53 2.03777 0.00000 0.00000 0.00001 0.00001 2.03777

A54 2.03777 0.00000 0.00000 0.00001 0.00001 2.03777

A55 2.18404 0.00000 0.00000 -0.00001 -0.00001 2.18403

A56 2.19079 0.00000 0.00000 0.00000 0.00000 2.19079

A57 1.90828 0.00000 0.00000 0.00001 0.00001 1.90829

A58 1.86587 0.00000 0.00000 0.00000 0.00000 1.86587

A59 2.19058 0.00000 0.00000 0.00000 0.00000 2.19057

A60 2.22672 0.00000 0.00000 0.00001 0.00001 2.22673

A61 1.86587 0.00000 0.00000 0.00000 0.00000 1.86587

A62 2.22672 0.00000 0.00000 0.00001 0.00001 2.22673

A63 2.19058 0.00000 0.00000 0.00000 0.00000 2.19057

A64 1.90828 0.00000 0.00000 0.00001 0.00001 1.90829

A65 2.18404 0.00000 0.00000 -0.00001 -0.00001 2.18403

A66 2.19079 0.00000 0.00000 0.00000 0.00000 2.19079

A67 1.87647 0.00000 0.00000 -0.00002 -0.00002 1.87645

A68 2.20226 0.00000 0.00000 0.00001 0.00001 2.20227

A69 2.20226 0.00000 0.00000 0.00001 0.00001 2.20227

A70 1.56397 0.00000 0.00000 0.00000 0.00000 1.56397

A71 1.56397 0.00000 0.00000 0.00000 0.00000 1.56397

A72 2.97619 0.00000 0.00000 0.00002 0.00002 2.97621

A73 2.97619 0.00000 0.00000 0.00002 0.00002 2.97621

A74 1.56397 0.00000 0.00000 0.00000 0.00000 1.56397

A75 1.56397 0.00000 0.00000 0.00000 0.00000 1.56397

A76 2.20757 0.00000 0.00000 -0.00001 -0.00001 2.20756

A77 2.03777 0.00000 0.00000 0.00001 0.00001 2.03777

A78 2.03777 0.00000 0.00000 0.00001 0.00001 2.03777

A79 3.14154 0.00000 0.00000 0.00000 0.00000 3.14154

A80 3.14154 0.00000 0.00000 0.00000 0.00000 3.14154

A81 3.14162 0.00000 0.00000 0.00000 0.00000 3.14162

A82 3.14162 0.00000 0.00000 0.00000 0.00000 3.14162

A83 3.14154 0.00000 0.00000 0.00000 0.00000 3.14154

A84 3.14162 0.00000 0.00000 0.00000 0.00000 3.14162

A85 3.14154 0.00000 0.00000 0.00000 0.00000 3.14154

A86 3.14162 0.00000 0.00000 0.00000 0.00000 3.14162

A87 3.13776 0.00000 0.00000 -0.00005 -0.00005 3.13770

A88 3.14543 0.00000 0.00000 0.00005 0.00005 3.14548

A89 3.14440 0.00000 0.00000 0.00002 0.00002 3.14442

A90 3.13878 0.00000 0.00000 -0.00002 -0.00002 3.13876

A91 3.13776 0.00000 0.00000 -0.00005 -0.00005 3.13770

A92 3.14440 0.00000 0.00000 0.00002 0.00002 3.14442

A93 3.14543 0.00000 0.00000 0.00005 0.00005 3.14548

A94 3.13878 0.00000 0.00000 -0.00002 -0.00002 3.13876

D1 -0.00170 0.00000 0.00000 -0.00002 -0.00002 -0.00172

D2 3.12742 0.00000 0.00000 -0.00007 -0.00007 3.12735

D3 -3.13812 0.00000 0.00000 -0.00007 -0.00007 -3.13818

D4 -0.00899 0.00000 0.00000 -0.00012 -0.00012 -0.00911

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13628 0.00000 0.00000 -0.00005 -0.00005 -3.13632

D7 3.13628 0.00000 0.00000 0.00005 0.00005 3.13632

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00275 0.00000 0.00000 0.00003 0.00003 0.00278

D10 -3.07094 0.00000 0.00000 -0.00005 -0.00005 -3.07099

D11 -3.12632 0.00000 0.00000 0.00009 0.00009 -3.12623

D12 0.08319 0.00000 0.00000 0.00000 0.00000 0.08319

D13 -3.11685 0.00000 0.00000 -0.00003 -0.00003 -3.11688

D14 0.01113 0.00000 0.00000 -0.00005 -0.00005 0.01108

D15 0.01028 0.00000 0.00000 -0.00009 -0.00009 0.01019

D16 3.13827 0.00000 0.00000 -0.00011 -0.00011 3.13816

D17 -0.00275 0.00000 0.00000 -0.00003 -0.00003 -0.00278

D18 3.12632 0.00000 0.00000 -0.00009 -0.00009 3.12623

D19 3.07094 0.00000 0.00000 0.00005 0.00005 3.07099

D20 -0.08319 0.00000 0.00000 0.00000 0.00000 -0.08319

D21 -3.09930 0.00000 0.00000 0.00004 0.00004 -3.09926

D22 -0.12255 0.00000 0.00000 0.00006 0.00006 -0.12249

D23 -1.61093 0.00000 0.00000 0.00005 0.00005 -1.61087

D24 0.12255 0.00000 0.00000 -0.00006 -0.00006 0.12249

D25 3.09930 0.00000 0.00000 -0.00004 -0.00004 3.09926

D26 1.61093 0.00000 0.00000 -0.00005 -0.00005 1.61087

D27 0.00170 0.00000 0.00000 0.00002 0.00002 0.00172

D28 3.13812 0.00000 0.00000 0.00007 0.00007 3.13818

D29 -3.12742 0.00000 0.00000 0.00007 0.00007 -3.12735

D30 0.00899 0.00000 0.00000 0.00012 0.00012 0.00911

D31 -0.01028 0.00000 0.00000 0.00009 0.00009 -0.01019

D32 -3.13827 0.00000 0.00000 0.00011 0.00011 -3.13816

D33 3.11685 0.00000 0.00000 0.00003 0.00003 3.11688

D34 -0.01113 0.00000 0.00000 0.00005 0.00005 -0.01108

D35 0.01028 0.00000 0.00000 -0.00009 -0.00009 0.01019

D36 -3.11685 0.00000 0.00000 -0.00003 -0.00003 -3.11688

D37 3.13827 0.00000 0.00000 -0.00011 -0.00011 3.13816

D38 0.01113 0.00000 0.00000 -0.00005 -0.00005 0.01108

D39 -3.12632 0.00000 0.00000 0.00009 0.00009 -3.12623

D40 0.08319 0.00000 0.00000 0.00000 0.00000 0.08319

D41 0.00275 0.00000 0.00000 0.00003 0.00003 0.00278

D42 -3.07094 0.00000 0.00000 -0.00005 -0.00005 -3.07099

D43 3.12742 0.00000 0.00000 -0.00007 -0.00007 3.12735

D44 -0.00899 0.00000 0.00000 -0.00012 -0.00012 -0.00911

D45 -0.00170 0.00000 0.00000 -0.00002 -0.00002 -0.00172

D46 -3.13812 0.00000 0.00000 -0.00007 -0.00007 -3.13818

D47 -0.00275 0.00000 0.00000 -0.00003 -0.00003 -0.00278

D48 3.12632 0.00000 0.00000 -0.00009 -0.00009 3.12623

D49 3.07094 0.00000 0.00000 0.00005 0.00005 3.07099

D50 -0.08319 0.00000 0.00000 0.00000 0.00000 -0.08319

D51 -0.12255 0.00000 0.00000 0.00006 0.00006 -0.12249

D52 -1.61093 0.00000 0.00000 0.00005 0.00005 -1.61087

D53 -3.09930 0.00000 0.00000 0.00004 0.00004 -3.09926

D54 3.09930 0.00000 0.00000 -0.00004 -0.00004 3.09926

D55 1.61093 0.00000 0.00000 -0.00005 -0.00005 1.61087

D56 0.12255 0.00000 0.00000 -0.00006 -0.00006 0.12249

D57 0.00170 0.00000 0.00000 0.00002 0.00002 0.00172

D58 3.13812 0.00000 0.00000 0.00007 0.00007 3.13818

D59 -3.12742 0.00000 0.00000 0.00007 0.00007 -3.12735

D60 0.00899 0.00000 0.00000 0.00012 0.00012 0.00911

D61 -0.01028 0.00000 0.00000 0.00009 0.00009 -0.01019

D62 -3.13827 0.00000 0.00000 0.00011 0.00011 -3.13816

D63 3.11685 0.00000 0.00000 0.00003 0.00003 3.11688

D64 -0.01113 0.00000 0.00000 0.00005 0.00005 -0.01108

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13628 0.00000 0.00000 0.00005 0.00005 3.13632

D67 -3.13628 0.00000 0.00000 -0.00005 -0.00005 -3.13632

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.11685 0.00000 0.00000 0.00003 0.00003 3.11688

D70 -0.01028 0.00000 0.00000 0.00009 0.00009 -0.01019

D71 -0.01113 0.00000 0.00000 0.00005 0.00005 -0.01108

D72 -3.13827 0.00000 0.00000 0.00011 0.00011 -3.13816

D73 -3.12742 0.00000 0.00000 0.00007 0.00007 -3.12735

D74 0.00899 0.00000 0.00000 0.00012 0.00012 0.00911

D75 0.00170 0.00000 0.00000 0.00002 0.00002 0.00172

D76 3.13812 0.00000 0.00000 0.00007 0.00007 3.13818

D77 3.12632 0.00000 0.00000 -0.00009 -0.00009 3.12623

D78 -0.08319 0.00000 0.00000 0.00000 0.00000 -0.08319

D79 -0.00275 0.00000 0.00000 -0.00003 -0.00003 -0.00278

D80 3.07094 0.00000 0.00000 0.00005 0.00005 3.07099

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 3.13628 0.00000 0.00000 0.00005 0.00005 3.13632

D83 -3.13628 0.00000 0.00000 -0.00005 -0.00005 -3.13632

D84 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D85 -0.00170 0.00000 0.00000 -0.00002 -0.00002 -0.00172

D86 3.12742 0.00000 0.00000 -0.00007 -0.00007 3.12735

D87 -3.13812 0.00000 0.00000 -0.00007 -0.00007 -3.13818

D88 -0.00899 0.00000 0.00000 -0.00012 -0.00012 -0.00911

D89 0.00275 0.00000 0.00000 0.00003 0.00003 0.00278

D90 -3.07094 0.00000 0.00000 -0.00005 -0.00005 -3.07099

D91 -3.12632 0.00000 0.00000 0.00009 0.00009 -3.12623

D92 0.08319 0.00000 0.00000 0.00000 0.00000 0.08319

D93 -3.11685 0.00000 0.00000 -0.00003 -0.00003 -3.11688

D94 0.01113 0.00000 0.00000 -0.00005 -0.00005 0.01108

D95 0.01028 0.00000 0.00000 -0.00009 -0.00009 0.01019

D96 3.13827 0.00000 0.00000 -0.00011 -0.00011 3.13816

D97 0.12255 0.00000 0.00000 -0.00006 -0.00006 0.12249

D98 1.61093 0.00000 0.00000 -0.00005 -0.00005 1.61087

D99 3.09930 0.00000 0.00000 -0.00004 -0.00004 3.09926

D100 -3.09930 0.00000 0.00000 0.00004 0.00004 -3.09926

D101 -1.61093 0.00000 0.00000 0.00005 0.00005 -1.61087

D102 -0.12255 0.00000 0.00000 0.00006 0.00006 -0.12249

D103 3.11685 0.00000 0.00000 0.00003 0.00003 3.11688

D104 -0.01028 0.00000 0.00000 0.00009 0.00009 -0.01019

D105 -0.01113 0.00000 0.00000 0.00005 0.00005 -0.01108

D106 -3.13827 0.00000 0.00000 0.00011 0.00011 -3.13816

D107 -3.12742 0.00000 0.00000 0.00007 0.00007 -3.12735

D108 0.00899 0.00000 0.00000 0.00012 0.00012 0.00911

D109 0.00170 0.00000 0.00000 0.00002 0.00002 0.00172

D110 3.13812 0.00000 0.00000 0.00007 0.00007 3.13818

D111 3.12632 0.00000 0.00000 -0.00009 -0.00009 3.12623

D112 -0.08319 0.00000 0.00000 0.00000 0.00000 -0.08319

D113 -0.00275 0.00000 0.00000 -0.00003 -0.00003 -0.00278

D114 3.07094 0.00000 0.00000 0.00005 0.00005 3.07099

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.13628 0.00000 0.00000 0.00005 0.00005 3.13632

D117 -3.13628 0.00000 0.00000 -0.00005 -0.00005 -3.13632

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 -0.00170 0.00000 0.00000 -0.00002 -0.00002 -0.00172

D120 3.12742 0.00000 0.00000 -0.00007 -0.00007 3.12735

D121 -3.13812 0.00000 0.00000 -0.00007 -0.00007 -3.13818

D122 -0.00899 0.00000 0.00000 -0.00012 -0.00012 -0.00911

D123 0.00275 0.00000 0.00000 0.00003 0.00003 0.00278

D124 -3.07094 0.00000 0.00000 -0.00005 -0.00005 -3.07099

D125 -3.12632 0.00000 0.00000 0.00009 0.00009 -3.12623

D126 0.08319 0.00000 0.00000 0.00000 0.00000 0.08319

D127 -3.11685 0.00000 0.00000 -0.00003 -0.00003 -3.11688

D128 0.01113 0.00000 0.00000 -0.00005 -0.00005 0.01108

D129 0.01028 0.00000 0.00000 -0.00009 -0.00009 0.01019

D130 3.13827 0.00000 0.00000 -0.00011 -0.00011 3.13816

D131 1.61093 0.00000 0.00000 -0.00005 -0.00005 1.61087

D132 3.09930 0.00000 0.00000 -0.00004 -0.00004 3.09926

D133 0.12255 0.00000 0.00000 -0.00006 -0.00006 0.12249

D134 -1.61093 0.00000 0.00000 0.00005 0.00005 -1.61087

D135 -0.12255 0.00000 0.00000 0.00006 0.00006 -0.12249

D136 -3.09930 0.00000 0.00000 0.00004 0.00004 -3.09926

Item Value Threshold Converged?

Maximum Force 0.000006 0.000450 YES

RMS Force 0.000001 0.000300 YES

Maximum Displacement 0.000972 0.001800 YES

RMS Displacement 0.000163 0.001200 YES

Predicted change in Energy=-3.629141D-09

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) 1.4471 -DE/DX = 0.0 !

! R2 R(1,5) 1.3623 -DE/DX = 0.0 !

! R3 R(1,24) 1.0797 -DE/DX = 0.0 !

! R4 R(2,3) 1.3664 -DE/DX = 0.0 !

! R5 R(2,12) 1.4153 -DE/DX = 0.0 !

! R6 R(3,4) 1.3664 -DE/DX = 0.0 !

! R7 R(3,32) 2.0888 -DE/DX = 0.0 !

! R8 R(4,5) 1.4471 -DE/DX = 0.0 !

! R9 R(4,6) 1.4153 -DE/DX = 0.0 !

! R10 R(5,25) 1.0797 -DE/DX = 0.0 !

! R11 R(6,7) 1.4153 -DE/DX = 0.0 !

! R12 R(6,38) 1.427 -DE/DX = 0.0 !

! R13 R(7,8) 1.3664 -DE/DX = 0.0 !

! R14 R(7,11) 1.4471 -DE/DX = 0.0 !

! R15 R(8,9) 1.3664 -DE/DX = 0.0 !

! R16 R(8,32) 2.0888 -DE/DX = 0.0 !

! R17 R(9,10) 1.4471 -DE/DX = 0.0 !

! R18 R(9,33) 1.4153 -DE/DX = 0.0 !

! R19 R(10,11) 1.3623 -DE/DX = 0.0 !

! R20 R(10,26) 1.0797 -DE/DX = 0.0 !

! R21 R(11,27) 1.0797 -DE/DX = 0.0 !

! R22 R(12,13) 1.4153 -DE/DX = 0.0 !

! R23 R(12,35) 1.427 -DE/DX = 0.0 !

! R24 R(13,14) 1.4471 -DE/DX = 0.0 !

! R25 R(13,17) 1.3664 -DE/DX = 0.0 !

! R26 R(14,15) 1.3623 -DE/DX = 0.0 !

! R27 R(14,28) 1.0797 -DE/DX = 0.0 !

! R28 R(15,16) 1.4471 -DE/DX = 0.0 !

! R29 R(15,29) 1.0797 -DE/DX = 0.0 !

! R30 R(16,17) 1.3664 -DE/DX = 0.0 !

! R31 R(16,18) 1.4153 -DE/DX = 0.0 !

! R32 R(17,32) 2.0888 -DE/DX = 0.0 !

! R33 R(18,19) 1.4153 -DE/DX = 0.0 !

! R34 R(18,40) 1.427 -DE/DX = 0.0 !

! R35 R(19,20) 1.4471 -DE/DX = 0.0 !

! R36 R(19,23) 1.3664 -DE/DX = 0.0 !

! R37 R(20,21) 1.3623 -DE/DX = 0.0 !

! R38 R(20,30) 1.0797 -DE/DX = 0.0 !

! R39 R(21,22) 1.4471 -DE/DX = 0.0 !

! R40 R(21,31) 1.0797 -DE/DX = 0.0 !

! R41 R(22,23) 1.3664 -DE/DX = 0.0 !

! R42 R(22,33) 1.4153 -DE/DX = 0.0 !

! R43 R(23,32) 2.0888 -DE/DX = 0.0 !

! R44 R(33,34) 1.427 -DE/DX = 0.0 !

! R45 R(34,36) 1.2058 -DE/DX = 0.0 !

! R46 R(35,37) 1.2058 -DE/DX = 0.0 !

! R47 R(36,43) 1.0673 -DE/DX = 0.0 !

! R48 R(37,45) 1.0673 -DE/DX = 0.0 !

! R49 R(38,39) 1.2058 -DE/DX = 0.0 !

! R50 R(39,44) 1.0673 -DE/DX = 0.0 !

! R51 R(40,41) 1.2058 -DE/DX = 0.0 !

! R52 R(41,42) 1.0673 -DE/DX = 0.0 !

! A1 A(2,1,5) 106.9066 -DE/DX = 0.0 !

! A2 A(2,1,24) 125.5108 -DE/DX = 0.0 !

! A3 A(5,1,24) 127.5819 -DE/DX = 0.0 !

! A4 A(1,2,3) 109.3363 -DE/DX = 0.0 !

! A5 A(1,2,12) 125.1365 -DE/DX = 0.0 !

! A6 A(3,2,12) 125.5229 -DE/DX = 0.0 !

! A7 A(2,3,4) 107.5139 -DE/DX = 0.0 !

! A8 A(2,3,32) 126.18 -DE/DX = 0.0 !

! A9 A(4,3,32) 126.18 -DE/DX = 0.0 !

! A10 A(3,4,5) 109.3363 -DE/DX = 0.0 !

! A11 A(3,4,6) 125.5229 -DE/DX = 0.0 !

! A12 A(5,4,6) 125.1365 -DE/DX = 0.0 !

! A13 A(1,5,4) 106.9066 -DE/DX = 0.0 !

! A14 A(1,5,25) 127.5819 -DE/DX = 0.0 !

! A15 A(4,5,25) 125.5108 -DE/DX = 0.0 !

! A16 A(4,6,7) 126.4847 -DE/DX = 0.0 !

! A17 A(4,6,38) 116.7555 -DE/DX = 0.0 !

! A18 A(7,6,38) 116.7555 -DE/DX = 0.0 !

! A19 A(6,7,8) 125.5229 -DE/DX = 0.0 !

! A20 A(6,7,11) 125.1365 -DE/DX = 0.0 !

! A21 A(8,7,11) 109.3363 -DE/DX = 0.0 !

! A22 A(7,8,9) 107.5139 -DE/DX = 0.0 !

! A23 A(7,8,32) 126.18 -DE/DX = 0.0 !

! A24 A(9,8,32) 126.18 -DE/DX = 0.0 !

! A25 A(8,9,10) 109.3363 -DE/DX = 0.0 !

! A26 A(8,9,33) 125.5229 -DE/DX = 0.0 !

! A27 A(10,9,33) 125.1365 -DE/DX = 0.0 !

! A28 A(9,10,11) 106.9066 -DE/DX = 0.0 !

! A29 A(9,10,26) 125.5108 -DE/DX = 0.0 !

! A30 A(11,10,26) 127.5819 -DE/DX = 0.0 !

! A31 A(7,11,10) 106.9066 -DE/DX = 0.0 !

! A32 A(7,11,27) 125.5108 -DE/DX = 0.0 !

! A33 A(10,11,27) 127.5819 -DE/DX = 0.0 !

! A34 A(2,12,13) 126.4847 -DE/DX = 0.0 !

! A35 A(2,12,35) 116.7555 -DE/DX = 0.0 !

! A36 A(13,12,35) 116.7555 -DE/DX = 0.0 !

! A37 A(12,13,14) 125.1365 -DE/DX = 0.0 !

! A38 A(12,13,17) 125.5229 -DE/DX = 0.0 !

! A39 A(14,13,17) 109.3363 -DE/DX = 0.0 !

! A40 A(13,14,15) 106.9066 -DE/DX = 0.0 !

! A41 A(13,14,28) 125.5108 -DE/DX = 0.0 !

! A42 A(15,14,28) 127.5819 -DE/DX = 0.0 !

! A43 A(14,15,16) 106.9066 -DE/DX = 0.0 !

! A44 A(14,15,29) 127.5819 -DE/DX = 0.0 !

! A45 A(16,15,29) 125.5108 -DE/DX = 0.0 !

! A46 A(15,16,17) 109.3363 -DE/DX = 0.0 !

! A47 A(15,16,18) 125.1365 -DE/DX = 0.0 !

! A48 A(17,16,18) 125.5229 -DE/DX = 0.0 !

! A49 A(13,17,16) 107.5139 -DE/DX = 0.0 !

! A50 A(13,17,32) 126.18 -DE/DX = 0.0 !

! A51 A(16,17,32) 126.18 -DE/DX = 0.0 !

! A52 A(16,18,19) 126.4847 -DE/DX = 0.0 !

! A53 A(16,18,40) 116.7555 -DE/DX = 0.0 !

! A54 A(19,18,40) 116.7555 -DE/DX = 0.0 !

! A55 A(18,19,20) 125.1365 -DE/DX = 0.0 !

! A56 A(18,19,23) 125.5229 -DE/DX = 0.0 !

! A57 A(20,19,23) 109.3363 -DE/DX = 0.0 !

! A58 A(19,20,21) 106.9066 -DE/DX = 0.0 !

! A59 A(19,20,30) 125.5108 -DE/DX = 0.0 !

! A60 A(21,20,30) 127.5819 -DE/DX = 0.0 !

! A61 A(20,21,22) 106.9066 -DE/DX = 0.0 !

! A62 A(20,21,31) 127.5819 -DE/DX = 0.0 !

! A63 A(22,21,31) 125.5108 -DE/DX = 0.0 !

! A64 A(21,22,23) 109.3363 -DE/DX = 0.0 !

! A65 A(21,22,33) 125.1365 -DE/DX = 0.0 !

! A66 A(23,22,33) 125.5229 -DE/DX = 0.0 !

! A67 A(19,23,22) 107.5139 -DE/DX = 0.0 !

! A68 A(19,23,32) 126.18 -DE/DX = 0.0 !

! A69 A(22,23,32) 126.18 -DE/DX = 0.0 !

! A70 A(3,32,8) 89.609 -DE/DX = 0.0 !

! A71 A(3,32,17) 89.609 -DE/DX = 0.0 !

! A72 A(3,32,23) 170.5231 -DE/DX = 0.0 !

! A73 A(8,32,17) 170.5231 -DE/DX = 0.0 !

! A74 A(8,32,23) 89.609 -DE/DX = 0.0 !

! A75 A(17,32,23) 89.609 -DE/DX = 0.0 !

! A76 A(9,33,22) 126.4847 -DE/DX = 0.0 !

! A77 A(9,33,34) 116.7555 -DE/DX = 0.0 !

! A78 A(22,33,34) 116.7555 -DE/DX = 0.0 !

! A79 L(33,34,36,26,-1) 179.9973 -DE/DX = 0.0 !

! A80 L(12,35,37,24,-1) 179.9973 -DE/DX = 0.0 !

! A81 L(34,36,43,26,-1) 180.0017 -DE/DX = 0.0 !

! A82 L(35,37,45,24,-1) 180.0017 -DE/DX = 0.0 !

! A83 L(6,38,39,25,-1) 179.9973 -DE/DX = 0.0 !

! A84 L(38,39,44,25,-1) 180.0017 -DE/DX = 0.0 !

! A85 L(18,40,41,29,-1) 179.9973 -DE/DX = 0.0 !

! A86 L(40,41,42,29,-1) 180.0017 -DE/DX = 0.0 !

! A87 L(33,34,36,26,-2) 179.7801 -DE/DX = 0.0 !

! A88 L(12,35,37,24,-2) 180.2199 -DE/DX = 0.0 !

! A89 L(34,36,43,26,-2) 180.1609 -DE/DX = 0.0 !

! A90 L(35,37,45,24,-2) 179.8391 -DE/DX = 0.0 !

! A91 L(6,38,39,25,-2) 179.7801 -DE/DX = 0.0 !

! A92 L(38,39,44,25,-2) 180.1609 -DE/DX = 0.0 !

! A93 L(18,40,41,29,-2) 180.2199 -DE/DX = 0.0 !

! A94 L(40,41,42,29,-2) 179.8391 -DE/DX = 0.0 !

! D1 D(5,1,2,3) -0.0972 -DE/DX = 0.0 !

! D2 D(5,1,2,12) 179.1882 -DE/DX = 0.0 !

! D3 D(24,1,2,3) -179.8008 -DE/DX = 0.0 !

! D4 D(24,1,2,12) -0.5153 -DE/DX = 0.0 !

! D5 D(2,1,5,4) 0.0 -DE/DX = 0.0 !

! D6 D(2,1,5,25) -179.6955 -DE/DX = 0.0 !

! D7 D(24,1,5,4) 179.6955 -DE/DX = 0.0 !

! D8 D(24,1,5,25) 0.0 -DE/DX = 0.0 !

! D9 D(1,2,3,4) 0.1573 -DE/DX = 0.0 !

! D10 D(1,2,3,32) -175.9517 -DE/DX = 0.0 !

! D11 D(12,2,3,4) -179.1247 -DE/DX = 0.0 !

! D12 D(12,2,3,32) 4.7663 -DE/DX = 0.0 !

! D13 D(1,2,12,13) -178.5823 -DE/DX = 0.0 !

! D14 D(1,2,12,35) 0.638 -DE/DX = 0.0 !

! D15 D(3,2,12,13) 0.5893 -DE/DX = 0.0 !

! D16 D(3,2,12,35) 179.8095 -DE/DX = 0.0 !

! D17 D(2,3,4,5) -0.1573 -DE/DX = 0.0 !

! D18 D(2,3,4,6) 179.1247 -DE/DX = 0.0 !

! D19 D(32,3,4,5) 175.9517 -DE/DX = 0.0 !

! D20 D(32,3,4,6) -4.7663 -DE/DX = 0.0 !

! D21 D(2,3,32,8) -177.5769 -DE/DX = 0.0 !

! D22 D(2,3,32,17) -7.0216 -DE/DX = 0.0 !

! D23 D(2,3,32,23) -92.2992 -DE/DX = 0.0 !

! D24 D(4,3,32,8) 7.0216 -DE/DX = 0.0 !

! D25 D(4,3,32,17) 177.5769 -DE/DX = 0.0 !

! D26 D(4,3,32,23) 92.2992 -DE/DX = 0.0 !

! D27 D(3,4,5,1) 0.0972 -DE/DX = 0.0 !

! D28 D(3,4,5,25) 179.8008 -DE/DX = 0.0 !

! D29 D(6,4,5,1) -179.1882 -DE/DX = 0.0 !

! D30 D(6,4,5,25) 0.5153 -DE/DX = 0.0 !

! D31 D(3,4,6,7) -0.5893 -DE/DX = 0.0 !

! D32 D(3,4,6,38) -179.8095 -DE/DX = 0.0 !

! D33 D(5,4,6,7) 178.5823 -DE/DX = 0.0 !

! D34 D(5,4,6,38) -0.638 -DE/DX = 0.0 !

! D35 D(4,6,7,8) 0.5893 -DE/DX = 0.0 !

! D36 D(4,6,7,11) -178.5823 -DE/DX = 0.0 !

! D37 D(38,6,7,8) 179.8095 -DE/DX = 0.0 !

! D38 D(38,6,7,11) 0.638 -DE/DX = 0.0 !

! D39 D(6,7,8,9) -179.1247 -DE/DX = 0.0 !

! D40 D(6,7,8,32) 4.7663 -DE/DX = 0.0 !

! D41 D(11,7,8,9) 0.1573 -DE/DX = 0.0 !

! D42 D(11,7,8,32) -175.9517 -DE/DX = 0.0 !

! D43 D(6,7,11,10) 179.1882 -DE/DX = 0.0 !

! D44 D(6,7,11,27) -0.5153 -DE/DX = 0.0 !

! D45 D(8,7,11,10) -0.0972 -DE/DX = 0.0 !

! D46 D(8,7,11,27) -179.8008 -DE/DX = 0.0 !

! D47 D(7,8,9,10) -0.1573 -DE/DX = 0.0 !

! D48 D(7,8,9,33) 179.1247 -DE/DX = 0.0 !

! D49 D(32,8,9,10) 175.9517 -DE/DX = 0.0 !

! D50 D(32,8,9,33) -4.7663 -DE/DX = 0.0 !

! D51 D(7,8,32,3) -7.0216 -DE/DX = 0.0 !

! D52 D(7,8,32,17) -92.2992 -DE/DX = 0.0 !

! D53 D(7,8,32,23) -177.5769 -DE/DX = 0.0 !

! D54 D(9,8,32,3) 177.5769 -DE/DX = 0.0 !

! D55 D(9,8,32,17) 92.2992 -DE/DX = 0.0 !

! D56 D(9,8,32,23) 7.0216 -DE/DX = 0.0 !

! D57 D(8,9,10,11) 0.0972 -DE/DX = 0.0 !

! D58 D(8,9,10,26) 179.8008 -DE/DX = 0.0 !

! D59 D(33,9,10,11) -179.1882 -DE/DX = 0.0 !

! D60 D(33,9,10,26) 0.5153 -DE/DX = 0.0 !

! D61 D(8,9,33,22) -0.5893 -DE/DX = 0.0 !

! D62 D(8,9,33,34) -179.8095 -DE/DX = 0.0 !

! D63 D(10,9,33,22) 178.5823 -DE/DX = 0.0 !

! D64 D(10,9,33,34) -0.638 -DE/DX = 0.0 !

! D65 D(9,10,11,7) 0.0 -DE/DX = 0.0 !

! D66 D(9,10,11,27) 179.6955 -DE/DX = 0.0 !

! D67 D(26,10,11,7) -179.6955 -DE/DX = 0.0 !

! D68 D(26,10,11,27) 0.0 -DE/DX = 0.0 !

! D69 D(2,12,13,14) 178.5823 -DE/DX = 0.0 !

! D70 D(2,12,13,17) -0.5893 -DE/DX = 0.0 !

! D71 D(35,12,13,14) -0.638 -DE/DX = 0.0 !

! D72 D(35,12,13,17) -179.8095 -DE/DX = 0.0 !

! D73 D(12,13,14,15) -179.1882 -DE/DX = 0.0 !

! D74 D(12,13,14,28) 0.5153 -DE/DX = 0.0 !

! D75 D(17,13,14,15) 0.0972 -DE/DX = 0.0 !

! D76 D(17,13,14,28) 179.8008 -DE/DX = 0.0 !

! D77 D(12,13,17,16) 179.1247 -DE/DX = 0.0 !

! D78 D(12,13,17,32) -4.7663 -DE/DX = 0.0 !

! D79 D(14,13,17,16) -0.1573 -DE/DX = 0.0 !

! D80 D(14,13,17,32) 175.9517 -DE/DX = 0.0 !

! D81 D(13,14,15,16) 0.0 -DE/DX = 0.0 !

! D82 D(13,14,15,29) 179.6955 -DE/DX = 0.0 !

! D83 D(28,14,15,16) -179.6955 -DE/DX = 0.0 !

! D84 D(28,14,15,29) 0.0 -DE/DX = 0.0 !

! D85 D(14,15,16,17) -0.0972 -DE/DX = 0.0 !

! D86 D(14,15,16,18) 179.1882 -DE/DX = 0.0 !

! D87 D(29,15,16,17) -179.8008 -DE/DX = 0.0 !

! D88 D(29,15,16,18) -0.5153 -DE/DX = 0.0 !

! D89 D(15,16,17,13) 0.1573 -DE/DX = 0.0 !

! D90 D(15,16,17,32) -175.9517 -DE/DX = 0.0 !

! D91 D(18,16,17,13) -179.1247 -DE/DX = 0.0 !

! D92 D(18,16,17,32) 4.7663 -DE/DX = 0.0 !

! D93 D(15,16,18,19) -178.5823 -DE/DX = 0.0 !

! D94 D(15,16,18,40) 0.638 -DE/DX = 0.0 !

! D95 D(17,16,18,19) 0.5893 -DE/DX = 0.0 !

! D96 D(17,16,18,40) 179.8095 -DE/DX = 0.0 !

! D97 D(13,17,32,3) 7.0216 -DE/DX = 0.0 !

! D98 D(13,17,32,8) 92.2992 -DE/DX = 0.0 !

! D99 D(13,17,32,23) 177.5769 -DE/DX = 0.0 !

! D100 D(16,17,32,3) -177.5769 -DE/DX = 0.0 !

! D101 D(16,17,32,8) -92.2992 -DE/DX = 0.0 !

! D102 D(16,17,32,23) -7.0216 -DE/DX = 0.0 !

! D103 D(16,18,19,20) 178.5823 -DE/DX = 0.0 !

! D104 D(16,18,19,23) -0.5893 -DE/DX = 0.0 !

! D105 D(40,18,19,20) -0.638 -DE/DX = 0.0 !

! D106 D(40,18,19,23) -179.8095 -DE/DX = 0.0 !

! D107 D(18,19,20,21) -179.1882 -DE/DX = 0.0 !

! D108 D(18,19,20,30) 0.5153 -DE/DX = 0.0 !

! D109 D(23,19,20,21) 0.0972 -DE/DX = 0.0 !

! D110 D(23,19,20,30) 179.8008 -DE/DX = 0.0 !

! D111 D(18,19,23,22) 179.1247 -DE/DX = 0.0 !

! D112 D(18,19,23,32) -4.7663 -DE/DX = 0.0 !

! D113 D(20,19,23,22) -0.1573 -DE/DX = 0.0 !

! D114 D(20,19,23,32) 175.9517 -DE/DX = 0.0 !

! D115 D(19,20,21,22) 0.0 -DE/DX = 0.0 !

! D116 D(19,20,21,31) 179.6955 -DE/DX = 0.0 !

! D117 D(30,20,21,22) -179.6955 -DE/DX = 0.0 !

! D118 D(30,20,21,31) 0.0 -DE/DX = 0.0 !

! D119 D(20,21,22,23) -0.0972 -DE/DX = 0.0 !

! D120 D(20,21,22,33) 179.1882 -DE/DX = 0.0 !

! D121 D(31,21,22,23) -179.8008 -DE/DX = 0.0 !

! D122 D(31,21,22,33) -0.5153 -DE/DX = 0.0 !

! D123 D(21,22,23,19) 0.1573 -DE/DX = 0.0 !

! D124 D(21,22,23,32) -175.9517 -DE/DX = 0.0 !

! D125 D(33,22,23,19) -179.1247 -DE/DX = 0.0 !

! D126 D(33,22,23,32) 4.7663 -DE/DX = 0.0 !

! D127 D(21,22,33,9) -178.5823 -DE/DX = 0.0 !

! D128 D(21,22,33,34) 0.638 -DE/DX = 0.0 !

! D129 D(23,22,33,9) 0.5893 -DE/DX = 0.0 !

! D130 D(23,22,33,34) 179.8095 -DE/DX = 0.0 !

! D131 D(19,23,32,3) 92.2992 -DE/DX = 0.0 !

! D132 D(19,23,32,8) 177.5769 -DE/DX = 0.0 !

! D133 D(19,23,32,17) 7.0216 -DE/DX = 0.0 !

! D134 D(22,23,32,3) -92.2992 -DE/DX = 0.0 !

! D135 D(22,23,32,8) -7.0216 -DE/DX = 0.0 !

! D136 D(22,23,32,17) -177.5769 -DE/DX = 0.0 !

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GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 26 14:36:20 2019, MaxMem= 1342177280 cpu: 5.7

(Enter /apps/gaussian/g09d01/g09/l9999.exe)

1\1\GINC-K009\Freq\RB3LYP\GenECP\C28H12N4Zn1\Z5105842\26-Jul-2019\0\\#

P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/GenECP Freq\\ZnT

SPsim0\\0,1\C,0.6811632879,4.2732946298,-0.0396282291\C,1.101995218,2.

8891864292,-0.0047490578\N,0.,2.0816904415,0.0177872219\C,-1.101995218

,2.8891864292,-0.0047490578\C,-0.6811632879,4.2732946298,-0.0396282291

\C,-2.4461346812,2.4461346812,-0.0099866712\C,-2.8891864292,1.10199521

8,-0.0047490578\N,-2.0816904415,0.,0.0177872219\C,-2.8891864292,-1.101

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59,0.00001244,-0.00000868,0.00005239,-0.00000082,0.00001264,-0.0000126

6,0.00000024,-0.00000055,-0.00000188,0.00000048,0.00000075,-0.00000019

,-0.00000200,-0.00000138,-0.00000038,-0.00000273,-0.00000458,0.0000027

1,0.00000096,-0.00000096,-0.00000187,0.00000138,0.00000200,-0.00000038

,-0.00000075,-0.00000048,-0.00000019,0.00000055,-0.00000024,-0.0000018

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0.00000023,-0.00000056,-0.00002526,-0.00000044,0.00000127,0.00005254,0

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00269,0.00000269,0.00001515,0.00000868,-0.00001244,0.00005239,0.000001

54,0.00000082,0.00002391,-0.00000082,-0.00000154,0.00002391,-0.0000018

6,-0.00000133,-0.00000984,0.00000133,0.00000186,-0.00000984,-0.0000300

2,0.00003002,-0.00029270,-0.00620692,0.00620692,-0.01699073,-0.0000013

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3,0.00000023,0.00000061,0.00000016,0.00000011,0.00000218,0.00627733,-0

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7,-0.00000007,-0.00000054,0.00000551,-0.00000070,0.00364025,-0.0026266

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096,-0.00000187,0.00000130,0.00000130,-0.00000068,0.00003002,0.0000300

2,-0.00029270,-0.00000199,-0.00000199,-0.00000038,0.00620692,0.0062069

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.00000015,0.00000010,0.00000010,0.00000015,0.00000010,-0.00000010,0.00

000015,-0.00000010,-0.00000010,0.00000015\\\@

I DON'T PRETEND TO UNDERSTAND THE UNIVERSE --

IT'S A GREAT DEAL BIGGER THAN I AM.

-- ATTR. TO WILLIAM ALLINGHAM (1828-89)

Job cpu time: 0 days 2 hours 19 minutes 56.0 seconds.

File lengths (MBytes): RWF= 1097 Int= 0 D2E= 0 Chk= 43 Scr= 2

Normal termination of Gaussian 09 at Fri Jul 26 14:36:21 2019.