Entering Gaussian System, Link 0=g09

Initial command:

/apps/gaussian/g09d01/g09/l1.exe "/srv/scratch/z5105842/Gau-68446.inp" -scrdir="/srv/scratch/z5105842/"

Entering Link 1 = /apps/gaussian/g09d01/g09/l1.exe PID= 68465.

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Cite this work as:

Gaussian 09, Revision D.01,

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,

M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,

G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,

A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,

M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,

Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,

J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,

K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand,

K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,

M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,

V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,

O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,

R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,

P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,

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

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

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

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

5-Jul-2019

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

%nprocshared=12

Will use up to 12 processors via shared memory.

%mem=10GB

%chk=ZntAzPcation.chk

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

#p opt b3lyp/genecp scrf=(solvent=dmso,smd) empiricaldispersion=gd3bj

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

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

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

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

4//1;

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

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

7//1,2,3,16;

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

2/9=110/2;

99//99;

2/9=110/2;

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

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

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

7//1,2,3,16;

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

2/9=110/2;

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

99/9=1/99;

Leave Link 1 at Fri Jul 5 21:06:56 2019, MaxMem= 1342177280 cpu: 1.5

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

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

ZntAzPcation

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

Symbolic Z-matrix:

Charge = 1 Multiplicity = 2

C -2.06677 -2.19041 0.

N -0.7423 -1.86521 0.

C 0. -3.00728 0.

C -0.9161 -4.16652 0.

C -2.18334 -3.64784 0.

N 1.33695 -3.10409 0.

C 2.19041 -2.06677 0.

N 1.86521 -0.7423 0.

C 3.00728 0. 0.

C 4.16652 -0.9161 0.

C 3.64784 -2.18334 0.

N -3.10409 -1.33695 0.

C -4.16652 0.9161 0.

C -3.64784 2.18334 0.

C -2.19041 2.06677 0.

N -1.86521 0.7423 0.

C -3.00728 0. 0.

N -1.33695 3.10409 0.

N 0.7423 1.86521 0.

C 0. 3.00728 0.

C 0.9161 4.16652 0.

C 2.18334 3.64784 0.

C 2.06677 2.19041 0.

N 3.10409 1.33695 0.

Zn 0. 0. 0.

C -0.48237 -5.59359 0.

H -3.11869 -4.19296 0.

C 5.59359 -0.48237 0.

H 4.19296 -3.11869 0.

C -5.59359 0.48237 0.

H -4.19296 3.11869 0.

C 0.48237 5.59359 0.

H 3.11869 4.19296 0.

H -1.34628 -6.26359 0.

H 0.1302 -5.81848 0.88508

H 0.1302 -5.81848 -0.88508

H 5.81848 0.1302 0.88508

H 5.81848 0.1302 -0.88508

H 6.26359 -1.34628 0.

H -5.81848 -0.1302 0.88508

H -5.81848 -0.1302 -0.88508

H -6.26359 1.34628 0.

H -0.1302 5.81848 0.88508

H -0.1302 5.81848 -0.88508

H 1.34628 6.26359 0.

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

NMic= 0 NMicF= 0.

Isotopes and Nuclear Properties:

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

in nuclear magnetons)

Atom 1 2 3 4 5 6 7 8 9 10

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

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

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

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

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

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

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

Atom 11 12 13 14 15 16 17 18 19 20

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

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

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

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

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

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

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

Atom 21 22 23 24 25 26 27 28 29 30

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

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

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

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

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

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

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

Atom 31 32 33 34 35 36 37 38 39 40

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

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

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

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

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

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

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

Atom 41 42 43 44 45

IAtWgt= 1 1 1 1 1

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 1 1 1 1 1

AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Leave Link 101 at Fri Jul 5 21:06:57 2019, MaxMem= 1342177280 cpu: 2.7

(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) 1.3638 estimate D2E/DX2 !

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 5 21:06:57 2019, MaxMem= 1342177280 cpu: 0.2

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.066774 -2.190409 0.000000

2 7 0 -0.742302 -1.865213 0.000000

3 6 0 0.000000 -3.007280 0.000000

4 6 0 -0.916097 -4.166516 0.000000

5 6 0 -2.183341 -3.647838 0.000000

6 7 0 1.336945 -3.104087 0.000000

7 6 0 2.190409 -2.066774 0.000000

8 7 0 1.865213 -0.742302 0.000000

9 6 0 3.007280 0.000000 0.000000

10 6 0 4.166516 -0.916097 0.000000

11 6 0 3.647838 -2.183341 0.000000

12 7 0 -3.104087 -1.336945 0.000000

13 6 0 -4.166516 0.916097 0.000000

14 6 0 -3.647838 2.183341 0.000000

15 6 0 -2.190409 2.066774 0.000000

16 7 0 -1.865213 0.742302 0.000000

17 6 0 -3.007280 0.000000 0.000000

18 7 0 -1.336945 3.104087 0.000000

19 7 0 0.742302 1.865213 0.000000

20 6 0 0.000000 3.007280 0.000000

21 6 0 0.916097 4.166516 0.000000

22 6 0 2.183341 3.647838 0.000000

23 6 0 2.066774 2.190409 0.000000

24 7 0 3.104087 1.336945 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.482366 -5.593592 0.000000

27 1 0 -3.118690 -4.192956 0.000000

28 6 0 5.593592 -0.482366 0.000000

29 1 0 4.192956 -3.118690 0.000000

30 6 0 -5.593592 0.482366 0.000000

31 1 0 -4.192956 3.118690 0.000000

32 6 0 0.482366 5.593592 0.000000

33 1 0 3.118690 4.192956 0.000000

34 1 0 -1.346284 -6.263586 0.000000

35 1 0 0.130195 -5.818475 0.885075

36 1 0 0.130195 -5.818475 -0.885075

37 1 0 5.818475 0.130195 0.885075

38 1 0 5.818475 0.130195 -0.885075

39 1 0 6.263586 -1.346284 0.000000

40 1 0 -5.818475 -0.130195 0.885075

41 1 0 -5.818475 -0.130195 -0.885075

42 1 0 -6.263586 1.346284 0.000000

43 1 0 -0.130195 5.818475 0.885075

44 1 0 -0.130195 5.818475 -0.885075

45 1 0 1.346284 6.263586 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.363810 0.000000

3 C 2.222349 1.362105 0.000000

4 C 2.286713 2.307856 1.477519 0.000000

5 C 1.462083 2.292236 2.275366 1.369282 0.000000

6 N 3.524218 2.420346 1.340445 2.490974 3.562033

7 C 4.258978 2.939629 2.383788 3.749573 4.650748

8 N 4.190171 2.839025 2.934134 4.411454 4.983265

9 C 5.526655 4.187885 4.252936 5.723001 6.344231

10 C 6.362215 4.999732 4.661856 6.033090 6.912532

11 C 5.714616 4.401651 3.739732 4.976192 6.012271

12 N 1.343287 2.420144 3.524965 3.576838 2.487569

13 C 3.749573 4.411454 5.723001 6.033090 4.976192

14 C 4.650748 4.983265 6.344231 6.912532 6.012271

15 C 4.258978 4.190171 5.526655 6.362215 5.714616

16 N 2.939629 2.839025 4.187885 4.999732 4.401651

17 C 2.383788 2.934134 4.252936 4.661856 3.739732

18 N 5.344562 5.004752 6.255896 7.282773 6.804769

19 N 4.933455 4.014988 4.928712 6.255561 6.241243

20 C 5.593525 4.928712 6.014560 7.232052 7.004111

21 C 7.021967 6.255561 7.232052 8.532078 8.406583

22 C 7.221399 6.241243 7.004111 8.406583 8.502635

23 C 6.023104 4.933455 5.593525 7.021967 7.221399

24 N 6.259395 5.004850 5.339255 6.815421 7.266702

25 Zn 3.011552 2.007494 3.007280 4.266039 4.251317

26 C 3.753932 3.737429 2.630910 1.491532 2.584429

27 H 2.262017 3.326501 3.336473 2.202752 1.082604

28 C 7.848479 6.485046 6.137056 7.479907 8.396481

29 H 6.328185 5.091952 4.194436 5.215397 6.398215

30 C 4.425175 5.389447 6.592867 6.594775 5.356155

31 H 5.719019 6.061873 7.423502 7.988243 7.058644

32 C 8.190774 7.558676 8.614388 9.859787 9.618213

33 H 8.224134 7.183918 7.846631 9.282256 9.465177

34 H 4.136409 4.439649 3.523636 2.140739 2.746416

35 H 4.332770 4.144018 2.950106 2.146405 3.293550

36 H 4.332770 4.144018 2.950106 2.146405 3.293550

37 H 8.267147 6.914391 6.669465 8.037384 8.893028

38 H 8.267147 6.914391 6.669465 8.037384 8.893028

39 H 8.373019 7.025080 6.480078 7.713725 8.754869

40 H 4.370709 5.437019 6.551002 6.411595 5.135306

41 H 4.370709 5.437019 6.551002 6.411595 5.135306

42 H 5.488299 6.387354 7.627977 7.680274 6.449004

43 H 8.287094 7.758679 8.870979 10.054902 9.726759

44 H 8.287094 7.758679 8.870979 10.054902 9.726759

45 H 9.116962 8.392828 9.368107 10.672647 10.521149

6 7 8 9 10

6 N 0.000000

7 C 1.343287 0.000000

8 N 2.420144 1.363810 0.000000

9 C 3.524965 2.222349 1.362105 0.000000

10 C 3.576838 2.286713 2.307856 1.477519 0.000000

11 C 2.487569 1.462083 2.292236 2.275366 1.369282

12 N 4.779703 5.344562 5.004752 6.255896 7.282773

13 C 6.815421 7.021967 6.255561 7.232052 8.532078

14 C 7.266702 7.221399 6.241243 7.004111 8.406583

15 C 6.259395 6.023104 4.933455 5.593525 7.021967

16 N 5.004850 4.933455 4.014988 4.928712 6.255561

17 C 5.339255 5.593525 4.928712 6.014560 7.232052

18 N 6.759520 6.259395 5.004850 5.339255 6.815421

19 N 5.004752 4.190171 2.839025 2.934134 4.411454

20 C 6.255896 5.526655 4.187885 4.252936 5.723001

21 C 7.282773 6.362215 4.999732 4.661856 6.033090

22 C 6.804769 5.714616 4.401651 3.739732 4.976192

23 C 5.344562 4.258978 2.939629 2.383788 3.749573

24 N 4.779703 3.524218 2.420346 1.340445 2.490974

25 Zn 3.379760 3.011552 2.007494 3.007280 4.266039

26 C 3.083428 4.425175 5.389447 6.592867 6.594775

27 H 4.586755 5.719019 6.061873 7.423502 7.988243

28 C 4.999246 3.753932 3.737429 2.630910 1.491532

29 H 2.856048 2.262017 3.326501 3.336473 2.202752

30 C 7.803524 8.190774 7.558676 8.614388 9.859787

31 H 8.324828 8.224134 7.183918 7.846631 9.282256

32 C 8.739561 7.848479 6.485046 6.137056 7.479907

33 H 7.511421 6.328185 5.091952 4.194436 5.215397

34 H 4.145136 5.488299 6.387354 7.627977 7.680274

35 H 3.099598 4.370709 5.437019 6.551002 6.411595

36 H 3.099598 4.370709 5.437019 6.551002 6.411595

37 H 5.597147 4.332770 4.144018 2.950106 2.146405

38 H 5.597147 4.332770 4.144018 2.950106 2.146405

39 H 5.230838 4.136409 4.439649 3.523636 2.140739

40 H 7.799194 8.287094 7.758679 8.870979 10.054902

41 H 7.799194 8.287094 7.758679 8.870979 10.054902

42 H 8.807603 9.116962 8.392828 9.368107 10.672647

43 H 9.085591 8.267147 6.914391 6.669465 8.037384

44 H 9.085591 8.267147 6.914391 6.669465 8.037384

45 H 9.367678 8.373019 7.025080 6.480078 7.713725

11 12 13 14 15

11 C 0.000000

12 N 6.804769 0.000000

13 C 8.406583 2.490974 0.000000

14 C 8.502635 3.562033 1.369282 0.000000

15 C 7.221399 3.524218 2.286713 1.462083 0.000000

16 N 6.241243 2.420346 2.307856 2.292236 1.363810

17 C 7.004111 1.340445 1.477519 2.275366 2.222349

18 N 7.266702 4.779703 3.576838 2.487569 1.343287

19 N 4.983265 5.004850 4.999732 4.401651 2.939629

20 C 6.344231 5.339255 4.661856 3.739732 2.383788

21 C 6.912532 6.815421 6.033090 4.976192 3.749573

22 C 6.012271 7.266702 6.912532 6.012271 4.650748

23 C 4.650748 6.259395 6.362215 5.714616 4.258978

24 N 3.562033 6.759520 7.282773 6.804769 5.344562

25 Zn 4.251317 3.379760 4.266039 4.251317 3.011552

26 C 5.356155 4.999246 7.479907 8.396481 7.848479

27 H 7.058644 2.856048 5.215397 6.398215 6.328185

28 C 2.584429 8.739561 9.859787 9.618213 8.190774

29 H 1.082604 7.511421 9.282256 9.465177 8.224134

30 C 9.618213 3.083428 1.491532 2.584429 3.753932

31 H 9.465177 4.586755 2.202752 1.082604 2.262017

32 C 8.396481 7.803524 6.594775 5.356155 4.425175

33 H 6.398215 8.324828 7.988243 7.058644 5.719019

34 H 6.449004 5.230838 7.713725 8.754869 8.373019

35 H 5.135306 5.597147 8.037384 8.893028 8.267147

36 H 5.135306 5.597147 8.037384 8.893028 8.267147

37 H 3.293550 9.085591 10.054902 9.726759 8.287094

38 H 3.293550 9.085591 10.054902 9.726759 8.287094

39 H 2.746416 9.367678 10.672647 10.521149 9.116962

40 H 9.726759 3.099598 2.146405 3.293550 4.332770

41 H 9.726759 3.099598 2.146405 3.293550 4.332770

42 H 10.521149 4.145136 2.140739 2.746416 4.136409

43 H 8.893028 7.799194 6.411595 5.135306 4.370709

44 H 8.893028 7.799194 6.411595 5.135306 4.370709

45 H 8.754869 8.807603 7.680274 6.449004 5.488299

16 17 18 19 20

16 N 0.000000

17 C 1.362105 0.000000

18 N 2.420144 3.524965 0.000000

19 N 2.839025 4.187885 2.420346 0.000000

20 C 2.934134 4.252936 1.340445 1.362105 0.000000

21 C 4.411454 5.723001 2.490974 2.307856 1.477519

22 C 4.983265 6.344231 3.562033 2.292236 2.275366

23 C 4.190171 5.526655 3.524218 1.363810 2.222349

24 N 5.004752 6.255896 4.779703 2.420144 3.524965

25 Zn 2.007494 3.007280 3.379760 2.007494 3.007280

26 C 6.485046 6.137056 8.739561 7.558676 8.614388

27 H 5.091952 4.194436 7.511421 7.183918 7.846631

28 C 7.558676 8.614388 7.803524 5.389447 6.592867

29 H 7.183918 7.846631 8.324828 6.061873 7.423502

30 C 3.737429 2.630910 4.999246 6.485046 6.137056

31 H 3.326501 3.336473 2.856048 5.091952 4.194436

32 C 5.389447 6.592867 3.083428 3.737429 2.630910

33 H 6.061873 7.423502 4.586755 3.326501 3.336473

34 H 7.025080 6.480078 9.367678 8.392828 9.368107

35 H 6.914391 6.669465 9.085591 7.758679 8.870979

36 H 6.914391 6.669465 9.085591 7.758679 8.870979

37 H 7.758679 8.870979 7.799194 5.437019 6.551002

38 H 7.758679 8.870979 7.799194 5.437019 6.551002

39 H 8.392828 9.368107 8.807603 6.387354 7.627977

40 H 4.144018 2.950106 5.597147 6.914391 6.669465

41 H 4.144018 2.950106 5.597147 6.914391 6.669465

42 H 4.439649 3.523636 5.230838 7.025080 6.480078

43 H 5.437019 6.551002 3.099598 4.144018 2.950106

44 H 5.437019 6.551002 3.099598 4.144018 2.950106

45 H 6.387354 7.627977 4.145136 4.439649 3.523636

21 22 23 24 25

21 C 0.000000

22 C 1.369282 0.000000

23 C 2.286713 1.462083 0.000000

24 N 3.576838 2.487569 1.343287 0.000000

25 Zn 4.266039 4.251317 3.011552 3.379760 0.000000

26 C 9.859787 9.618213 8.190774 7.803524 5.614352

27 H 9.282256 9.465177 8.224134 8.324828 5.225620

28 C 6.594775 5.356155 4.425175 3.083428 5.614352

29 H 7.988243 7.058644 5.719019 4.586755 5.225620

30 C 7.479907 8.396481 7.848479 8.739561 5.614352

31 H 5.215397 6.398215 6.328185 7.511421 5.225620

32 C 1.491532 2.584429 3.753932 4.999246 5.614352

33 H 2.202752 1.082604 2.262017 2.856048 5.225620

34 H 10.672647 10.521149 9.116962 8.807603 6.406636

35 H 10.054902 9.726759 8.287094 7.799194 5.886846

36 H 10.054902 9.726759 8.287094 7.799194 5.886846

37 H 6.411595 5.135306 4.370709 3.099598 5.886846

38 H 6.411595 5.135306 4.370709 3.099598 5.886846

39 H 7.680274 6.449004 5.488299 4.145136 6.406636

40 H 8.037384 8.893028 8.267147 9.085591 5.886846

41 H 8.037384 8.893028 8.267147 9.085591 5.886846

42 H 7.713725 8.754869 8.373019 9.367678 6.406636

43 H 2.146405 3.293550 4.332770 5.597147 5.886846

44 H 2.146405 3.293550 4.332770 5.597147 5.886846

45 H 2.140739 2.746416 4.136409 5.230838 6.406636

26 27 28 29 30

26 C 0.000000

27 H 2.985295 0.000000

28 C 7.939893 9.469548 0.000000

29 H 5.289969 7.390143 2.985295 0.000000

30 C 7.939893 5.289969 11.228704 10.428045 0.000000

31 H 9.469548 7.390143 10.428045 10.451241 2.985295

32 C 11.228704 10.428045 7.939893 9.469548 7.939893

33 H 10.428045 10.451241 5.289969 7.390143 9.469548

34 H 1.093273 2.725607 9.032407 6.369737 7.971668

35 H 1.099619 3.739107 7.688051 4.957643 8.558370

36 H 1.099619 3.739107 7.688051 4.957643 8.558370

37 H 8.558370 9.967242 1.099619 3.739107 11.451753

38 H 8.558370 9.967242 1.099619 3.739107 11.451753

39 H 7.971668 9.804624 1.093273 2.725607 11.997359

40 H 7.688051 4.957643 11.451753 10.485381 1.099619

41 H 7.688051 4.957643 11.451753 10.485381 1.099619

42 H 9.032407 6.369737 11.997359 11.369928 1.093273

43 H 11.451753 10.485381 8.558370 9.967242 7.688051

44 H 11.451753 10.485381 8.558370 9.967242 7.688051

45 H 11.997359 11.369928 7.971668 9.804624 9.032407

31 32 33 34 35

31 H 0.000000

32 C 5.289969 0.000000

33 H 7.390143 2.985295 0.000000

34 H 9.804624 11.997359 11.369928 0.000000

35 H 9.967242 11.451753 10.485381 1.778053 0.000000

36 H 9.967242 11.451753 10.485381 1.778053 1.770150

37 H 10.485381 7.688051 4.957643 9.643524 8.230626

38 H 10.485381 7.688051 4.957643 9.643524 8.418826

39 H 11.369928 9.032407 6.369737 9.060352 7.642142

40 H 3.739107 8.558370 9.967242 7.642142 8.230626

41 H 3.739107 8.558370 9.967242 7.642142 8.418826

42 H 2.725607 7.971668 9.804624 9.060352 9.643524

43 H 4.957643 1.099619 3.739107 12.175320 11.639863

44 H 4.957643 1.099619 3.739107 12.175320 11.773693

45 H 6.369737 1.093273 2.725607 12.813273 12.175320

36 37 38 39 40

36 H 0.000000

37 H 8.418826 0.000000

38 H 8.230626 1.770150 0.000000

39 H 7.642142 1.778053 1.778053 0.000000

40 H 8.418826 11.639863 11.773693 12.175320 0.000000

41 H 8.230626 11.773693 11.639863 12.175320 1.770150

42 H 9.643524 12.175320 12.175320 12.813273 1.778053

43 H 11.773693 8.230626 8.418826 9.643524 8.230626

44 H 11.639863 8.418826 8.230626 9.643524 8.418826

45 H 12.175320 7.642142 7.642142 9.060352 9.643524

41 42 43 44 45

41 H 0.000000

42 H 1.778053 0.000000

43 H 8.418826 7.642142 0.000000

44 H 8.230626 7.642142 1.770150 0.000000

45 H 9.643524 9.060352 1.778053 1.778053 0.000000

Stoichiometry C20H16N8Zn(1+,2)

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

Deg. of freedom 20

Full point group C4H NOp 8

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.190409 2.066774 0.000000

2 7 0 -1.865213 0.742302 0.000000

3 6 0 -3.007280 0.000000 0.000000

4 6 0 -4.166516 0.916097 0.000000

5 6 0 -3.647838 2.183341 0.000000

6 7 0 -3.104087 -1.336945 0.000000

7 6 0 -2.066774 -2.190409 0.000000

8 7 0 -0.742302 -1.865213 0.000000

9 6 0 0.000000 -3.007280 0.000000

10 6 0 -0.916097 -4.166516 0.000000

11 6 0 -2.183341 -3.647838 0.000000

12 7 0 -1.336945 3.104087 0.000000

13 6 0 0.916097 4.166516 0.000000

14 6 0 2.183341 3.647838 0.000000

15 6 0 2.066774 2.190409 0.000000

16 7 0 0.742302 1.865213 0.000000

17 6 0 0.000000 3.007280 0.000000

18 7 0 3.104087 1.336945 0.000000

19 7 0 1.865213 -0.742302 0.000000

20 6 0 3.007280 0.000000 0.000000

21 6 0 4.166516 -0.916097 0.000000

22 6 0 3.647838 -2.183341 0.000000

23 6 0 2.190409 -2.066774 0.000000

24 7 0 1.336945 -3.104087 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.593592 0.482366 0.000000

27 1 0 -4.192956 3.118690 0.000000

28 6 0 -0.482366 -5.593592 0.000000

29 1 0 -3.118690 -4.192956 0.000000

30 6 0 0.482366 5.593592 0.000000

31 1 0 3.118690 4.192956 0.000000

32 6 0 5.593592 -0.482366 0.000000

33 1 0 4.192956 -3.118690 0.000000

34 1 0 -6.263586 1.346284 0.000000

35 1 0 -5.818475 -0.130195 0.885075

36 1 0 -5.818475 -0.130195 -0.885075

37 1 0 0.130195 -5.818475 0.885075

38 1 0 0.130195 -5.818475 -0.885075

39 1 0 -1.346284 -6.263586 0.000000

40 1 0 -0.130195 5.818475 0.885075

41 1 0 -0.130195 5.818475 -0.885075

42 1 0 1.346284 6.263586 0.000000

43 1 0 5.818475 0.130195 0.885075

44 1 0 5.818475 0.130195 -0.885075

45 1 0 6.263586 -1.346284 0.000000

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

Rotational constants (GHZ): 0.1821070 0.1821070 0.0912612

Leave Link 202 at Fri Jul 5 21:06:57 2019, MaxMem= 1342177280 cpu: 0.2

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

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

Centers: 25

S 1 1.00

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

S 1 1.00

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

S 1 1.00

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

P 1 1.00

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

P 1 1.00

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

D 3 1.00

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

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

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

D 1 1.00

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

D 1 1.00

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

\*\*\*\*

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

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

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

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

Centers: 16 18 19 24

6-311G\*

\*\*\*\*

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

Pseudopotential Parameters

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

Center Atomic Valence Angular Power

Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

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

1 6

No pseudopotential on this center.

2 7

No pseudopotential on this center.

3 6

No pseudopotential on this center.

4 6

No pseudopotential on this center.

5 6

No pseudopotential on this center.

6 7

No pseudopotential on this center.

7 6

No pseudopotential on this center.

8 7

No pseudopotential on this center.

9 6

No pseudopotential on this center.

10 6

No pseudopotential on this center.

11 6

No pseudopotential on this center.

12 7

No pseudopotential on this center.

13 6

No pseudopotential on this center.

14 6

No pseudopotential on this center.

15 6

No pseudopotential on this center.

16 7

No pseudopotential on this center.

17 6

No pseudopotential on this center.

18 7

No pseudopotential on this center.

19 7

No pseudopotential on this center.

20 6

No pseudopotential on this center.

21 6

No pseudopotential on this center.

22 6

No pseudopotential on this center.

23 6

No pseudopotential on this center.

24 7

No pseudopotential on this center.

25 30 12

F and up

1 386.7379660 -18.00000000 0.00000000

2 72.8587359 -124.35274030 0.00000000

2 15.9066170 -30.66018220 0.00000000

2 4.3502340 -10.63589890 0.00000000

2 1.2842199 -0.76836230 0.00000000

S - F

0 19.0867858 3.00000000 0.00000000

1 5.0231080 22.52342250 0.00000000

2 1.2701744 48.44659420 0.00000000

2 1.0671287 -44.55601190 0.00000000

2 0.9264190 12.99839580 0.00000000

P - F

0 43.4927750 5.00000000 0.00000000

1 20.8692669 20.74355890 0.00000000

2 21.7118378 90.30271580 0.00000000

2 6.3616915 74.66103160 0.00000000

2 1.2291195 9.88944240 0.00000000

D - F

2 13.5851800 -4.84903590 0.00000000

2 9.8373050 3.69133790 0.00000000

2 0.8373113 -0.50373190 0.00000000

26 6

No pseudopotential on this center.

27 1

No pseudopotential on this center.

28 6

No pseudopotential on this center.

29 1

No pseudopotential on this center.

30 6

No pseudopotential on this center.

31 1

No pseudopotential on this center.

32 6

No pseudopotential on this center.

33 1

No pseudopotential on this center.

34 1

No pseudopotential on this center.

35 1

No pseudopotential on this center.

36 1

No pseudopotential on this center.

37 1

No pseudopotential on this center.

38 1

No pseudopotential on this center.

39 1

No pseudopotential on this center.

40 1

No pseudopotential on this center.

41 1

No pseudopotential on this center.

42 1

No pseudopotential on this center.

43 1

No pseudopotential on this center.

44 1

No pseudopotential on this center.

45 1

No pseudopotential on this center.

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

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

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

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

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

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

There are 212 symmetry adapted basis functions of AG symmetry.

There are 82 symmetry adapted basis functions of BG symmetry.

There are 78 symmetry adapted basis functions of AU symmetry.

There are 204 symmetry adapted basis functions of BU symmetry.

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

102 alpha electrons 101 beta electrons

nuclear repulsion energy 2759.9985592461 Hartrees.

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

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

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

NAtoms= 45 NActive= 45 NUniq= 11 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

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

Nuclear repulsion after empirical dispersion term = 2759.8845224332 Hartrees.

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Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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

Smoothing algorithm: 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 = 3558

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.58D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 180

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

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

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

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

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PCM non-electrostatic energy = -0.0109045791 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2759.8736178541 Hartrees.

Leave Link 301 at Fri Jul 5 21:06:57 2019, MaxMem= 1342177280 cpu: 1.4

(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= 19306 NPrTT= 91506 LenC2= 15315 LenP2D= 41224.

LDataN: DoStor=T MaxTD1= 5 Len= 102

GSVD: received Info= 1 from GESDD.

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

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

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Fri Jul 5 21:06:58 2019, MaxMem= 1342177280 cpu: 8.1

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 5 21:06:58 2019, MaxMem= 1342177280 cpu: 1.0

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

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1275.92411446635

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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

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Beta Orbitals:

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

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

Leave Link 401 at Fri Jul 5 21:07:00 2019, MaxMem= 1342177280 cpu: 16.4

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1138797 IEndB= 1138797 NGot= 1342177280 MDV= 1341424180

LenX= 1341424180 LenY= 1341055124

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

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

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 37978092.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.22D-15 for 3557.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.66D-15 for 3205 2074.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.44D-15 for 3557.

Iteration 1 A^-1\*A deviation from orthogonality is 2.47D-12 for 1595 1524.

E= -1275.03904728182

DIIS: error= 9.30D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.03904728182 IErMin= 1 ErrMin= 9.30D-02

ErrMax= 9.30D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.85D+00 BMatP= 3.85D+00

IDIUse=3 WtCom= 7.05D-02 WtEn= 9.30D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.103 Goal= None Shift= 0.000

Gap= 0.017 Goal= None Shift= 0.000

GapD= 0.017 DampG=0.250 DampE=0.250 DampFc=0.1250 IDamp=-1.

Damping current iteration by 1.25D-01

RMSDP=2.64D-03 MaxDP=1.27D-01 OVMax= 2.36D-01

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.28D-04 CP: 9.96D-01

E= -1275.17953494205 Delta-E= -0.140487660222 Rises=F Damp=T

DIIS: error= 6.15D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.17953494205 IErMin= 2 ErrMin= 6.15D-02

ErrMax= 6.15D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.06D+00 BMatP= 3.85D+00

IDIUse=3 WtCom= 3.85D-01 WtEn= 6.15D-01

Coeff-Com: -0.243D+01 0.343D+01

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

Coeff: -0.937D+00 0.194D+01

Gap= 0.117 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 21319 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

Gap= 0.041 Goal= None Shift= 0.000

RMSDP=1.45D-03 MaxDP=8.05D-02 DE=-1.40D-01 OVMax= 1.31D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.01D-03 CP: 9.83D-01 3.00D+00

E= -1275.55572764664 Delta-E= -0.376192704595 Rises=F Damp=F

DIIS: error= 2.70D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.55572764664 IErMin= 3 ErrMin= 2.70D-02

ErrMax= 2.70D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.50D-01 BMatP= 2.06D+00

IDIUse=3 WtCom= 7.30D-01 WtEn= 2.70D-01

EnCoef did 100 forward-backward iterations

Coeff-Com: -0.949D-01 0.470D+00 0.625D+00

Coeff-En: 0.117D+00 0.275D-03 0.883D+00

Coeff: -0.377D-01 0.343D+00 0.695D+00

Gap= 0.098 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=7.33D-04 MaxDP=4.36D-02 DE=-3.76D-01 OVMax= 6.44D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.23D-04 CP: 9.89D-01 2.81D+00 4.67D-01

E= -1275.67723827422 Delta-E= -0.121510627578 Rises=F Damp=F

DIIS: error= 7.31D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.67723827422 IErMin= 4 ErrMin= 7.31D-03

ErrMax= 7.31D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.50D-02 BMatP= 6.50D-01

IDIUse=3 WtCom= 9.27D-01 WtEn= 7.31D-02

Coeff-Com: 0.151D+00-0.880D-01 0.371D+00 0.566D+00

Coeff-En: 0.000D+00 0.000D+00 0.447D-01 0.955D+00

Coeff: 0.140D+00-0.816D-01 0.347D+00 0.595D+00

Gap= 0.103 Goal= None Shift= 0.000

Gap= 0.074 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 31774 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

RMSDP=2.17D-04 MaxDP=1.16D-02 DE=-1.22D-01 OVMax= 3.04D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.29D-04 CP: 9.88D-01 3.00D+00 5.61D-01 7.65D-01

E= -1275.69472607475 Delta-E= -0.017487800534 Rises=F Damp=F

DIIS: error= 3.15D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.69472607475 IErMin= 5 ErrMin= 3.15D-03

ErrMax= 3.15D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.84D-03 BMatP= 8.50D-02

IDIUse=3 WtCom= 9.69D-01 WtEn= 3.15D-02

Coeff-Com: 0.103D+00-0.105D+00 0.152D+00 0.349D+00 0.500D+00

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

Coeff: 0.100D+00-0.101D+00 0.147D+00 0.338D+00 0.516D+00

Gap= 0.102 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 31774 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

Gap= 0.075 Goal= None Shift= 0.000

RMSDP=6.92D-05 MaxDP=3.14D-03 DE=-1.75D-02 OVMax= 1.30D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.41D-05 CP: 9.88D-01 3.00D+00 5.52D-01 8.18D-01 6.31D-01

E= -1275.69664644001 Delta-E= -0.001920365252 Rises=F Damp=F

DIIS: error= 1.18D-03 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.69664644001 IErMin= 6 ErrMin= 1.18D-03

ErrMax= 1.18D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-03 BMatP= 9.84D-03

IDIUse=3 WtCom= 9.88D-01 WtEn= 1.18D-02

Coeff-Com: 0.626D-01-0.733D-01 0.484D-01 0.119D+00 0.293D+00 0.550D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.214D-01 0.979D+00

Coeff: 0.619D-01-0.725D-01 0.478D-01 0.118D+00 0.290D+00 0.555D+00

Gap= 0.103 Goal= None Shift= 0.000

Gap= 0.076 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

RMSDP=2.61D-05 MaxDP=1.31D-03 DE=-1.92D-03 OVMax= 4.69D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.11D-05 CP: 9.88D-01 3.00D+00 5.59D-01 8.10D-01 6.88D-01

CP: 7.56D-01

E= -1275.69690169596 Delta-E= -0.000255255955 Rises=F Damp=F

DIIS: error= 5.01D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.69690169596 IErMin= 7 ErrMin= 5.01D-04

ErrMax= 5.01D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.69D-05 BMatP= 1.05D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.01D-03

Coeff-Com: 0.148D-01-0.185D-01-0.528D-02-0.251D-01 0.557D-04 0.164D+00

Coeff-Com: 0.869D+00

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

Coeff-En: 0.100D+01

Coeff: 0.148D-01-0.184D-01-0.525D-02-0.250D-01 0.554D-04 0.164D+00

Coeff: 0.870D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.076 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 31774 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

RMSDP=1.17D-05 MaxDP=6.78D-04 DE=-2.55D-04 OVMax= 3.21D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.38D-06 CP: 9.88D-01 3.00D+00 5.60D-01 8.10D-01 7.18D-01

CP: 9.09D-01 1.12D+00

E= -1275.69694911512 Delta-E= -0.000047419157 Rises=F Damp=F

DIIS: error= 1.47D-04 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.69694911512 IErMin= 8 ErrMin= 1.47D-04

ErrMax= 1.47D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.29D-05 BMatP= 7.69D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.47D-03

Coeff-Com: -0.136D-01 0.159D-01-0.126D-01-0.333D-01-0.850D-01-0.148D+00

Coeff-Com: 0.799D-01 0.120D+01

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

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

Coeff: -0.136D-01 0.159D-01-0.126D-01-0.332D-01-0.849D-01-0.147D+00

Coeff: 0.798D-01 0.120D+01

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=9.18D-06 MaxDP=5.47D-04 DE=-4.74D-05 OVMax= 2.92D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.43D-06 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.27D-01

CP: 9.85D-01 1.40D+00 1.49D+00

E= -1275.69696601495 Delta-E= -0.000016899835 Rises=F Damp=F

DIIS: error= 1.02D-04 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.69696601495 IErMin= 9 ErrMin= 1.02D-04

ErrMax= 1.02D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.59D-06 BMatP= 1.29D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.02D-03

Coeff-Com: -0.113D-01 0.133D-01-0.655D-02-0.138D-01-0.476D-01-0.111D+00

Coeff-Com: -0.846D-01 0.699D+00 0.563D+00

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

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

Coeff: -0.113D-01 0.133D-01-0.654D-02-0.138D-01-0.475D-01-0.111D+00

Coeff: -0.845D-01 0.698D+00 0.563D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=2.64D-06 MaxDP=1.46D-04 DE=-1.69D-05 OVMax= 7.27D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.90D-06 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.30D-01

CP: 1.01D+00 1.44D+00 1.63D+00 1.04D+00

E= -1275.69696834906 Delta-E= -0.000002334111 Rises=F Damp=F

DIIS: error= 3.26D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.69696834906 IErMin=10 ErrMin= 3.26D-05

ErrMax= 3.26D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.32D-07 BMatP= 6.59D-06

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

Coeff-Com: -0.456D-02 0.525D-02-0.117D-02 0.713D-03-0.257D-02-0.162D-01

Coeff-Com: -0.505D-01 0.184D-01 0.218D+00 0.833D+00

Coeff: -0.456D-02 0.525D-02-0.117D-02 0.713D-03-0.257D-02-0.162D-01

Coeff: -0.505D-01 0.184D-01 0.218D+00 0.833D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=1.43D-06 MaxDP=7.15D-05 DE=-2.33D-06 OVMax= 4.57D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 7.23D-07 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.30D-01

CP: 1.01D+00 1.47D+00 1.70D+00 1.23D+00 1.07D+00

E= -1275.69696875272 Delta-E= -0.000000403659 Rises=F Damp=F

DIIS: error= 2.47D-05 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.69696875272 IErMin=11 ErrMin= 2.47D-05

ErrMax= 2.47D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.15D-07 BMatP= 9.32D-07

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

Coeff-Com: -0.212D-02 0.241D-02-0.188D-03 0.196D-02 0.380D-02 0.279D-02

Coeff-Com: -0.201D-01-0.708D-01 0.588D-01 0.509D+00 0.514D+00

Coeff: -0.212D-02 0.241D-02-0.188D-03 0.196D-02 0.380D-02 0.279D-02

Coeff: -0.201D-01-0.708D-01 0.588D-01 0.509D+00 0.514D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=4.69D-07 MaxDP=2.49D-05 DE=-4.04D-07 OVMax= 1.75D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.04D-07 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.30D-01

CP: 1.01D+00 1.47D+00 1.72D+00 1.27D+00 1.18D+00

CP: 8.17D-01

E= -1275.69696884611 Delta-E= -0.000000093384 Rises=F Damp=F

DIIS: error= 1.16D-05 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.69696884611 IErMin=12 ErrMin= 1.16D-05

ErrMax= 1.16D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.43D-08 BMatP= 3.15D-07

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

Coeff-Com: -0.507D-03 0.579D-03-0.107D-03 0.249D-03 0.798D-03 0.207D-02

Coeff-Com: 0.227D-02-0.143D-01-0.175D-01-0.158D-01 0.112D+00 0.931D+00

Coeff: -0.507D-03 0.579D-03-0.107D-03 0.249D-03 0.798D-03 0.207D-02

Coeff: 0.227D-02-0.143D-01-0.175D-01-0.158D-01 0.112D+00 0.931D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=2.94D-07 MaxDP=1.74D-05 DE=-9.34D-08 OVMax= 1.49D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.47D-07 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.31D-01

CP: 1.01D+00 1.47D+00 1.72D+00 1.29D+00 1.23D+00

CP: 1.02D+00 1.43D+00

E= -1275.69696886903 Delta-E= -0.000000022923 Rises=F Damp=F

DIIS: error= 3.90D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1275.69696886903 IErMin=13 ErrMin= 3.90D-06

ErrMax= 3.90D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.08D-08 BMatP= 3.43D-08

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

Coeff-Com: 0.979D-04-0.106D-03-0.856D-04-0.457D-03-0.810D-03-0.120D-03

Coeff-Com: 0.687D-02 0.134D-01-0.235D-01-0.154D+00-0.750D-01 0.507D+00

Coeff-Com: 0.726D+00

Coeff: 0.979D-04-0.106D-03-0.856D-04-0.457D-03-0.810D-03-0.120D-03

Coeff: 0.687D-02 0.134D-01-0.235D-01-0.154D+00-0.750D-01 0.507D+00

Coeff: 0.726D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=2.00D-07 MaxDP=1.24D-05 DE=-2.29D-08 OVMax= 1.11D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 7.80D-08 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.31D-01

CP: 1.01D+00 1.47D+00 1.73D+00 1.31D+00 1.27D+00

CP: 1.13D+00 1.85D+00 1.33D+00

E= -1275.69696887968 Delta-E= -0.000000010655 Rises=F Damp=F

DIIS: error= 2.47D-06 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1275.69696887968 IErMin=14 ErrMin= 2.47D-06

ErrMax= 2.47D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.40D-09 BMatP= 1.08D-08

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

Coeff-Com: 0.373D-03-0.427D-03 0.867D-04-0.152D-03-0.400D-03-0.724D-03

Coeff-Com: 0.151D-02 0.653D-02 0.436D-02-0.346D-01-0.651D-01-0.370D+00

Coeff-Com: 0.182D+00 0.128D+01

Coeff: 0.373D-03-0.427D-03 0.867D-04-0.152D-03-0.400D-03-0.724D-03

Coeff: 0.151D-02 0.653D-02 0.436D-02-0.346D-01-0.651D-01-0.370D+00

Coeff: 0.182D+00 0.128D+01

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=2.30D-07 MaxDP=1.37D-05 DE=-1.07D-08 OVMax= 1.26D-04

Cycle 15 Pass 1 IDiag 1:

RMSU= 4.09D-08 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.31D-01

CP: 1.01D+00 1.47D+00 1.73D+00 1.32D+00 1.30D+00

CP: 1.26D+00 2.31D+00 2.11D+00 1.62D+00

E= -1275.69696888545 Delta-E= -0.000000005770 Rises=F Damp=F

DIIS: error= 3.03D-06 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1275.69696888545 IErMin=14 ErrMin= 2.47D-06

ErrMax= 3.03D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D-09 BMatP= 2.40D-09

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

Coeff-Com: 0.212D-03-0.243D-03 0.705D-04 0.482D-05-0.273D-04-0.228D-03

Coeff-Com: -0.760D-03-0.657D-05 0.799D-02 0.139D-01-0.851D-02-0.233D+00

Coeff-Com: -0.689D-01 0.552D+00 0.737D+00

Coeff: 0.212D-03-0.243D-03 0.705D-04 0.482D-05-0.273D-04-0.228D-03

Coeff: -0.760D-03-0.657D-05 0.799D-02 0.139D-01-0.851D-02-0.233D+00

Coeff: -0.689D-01 0.552D+00 0.737D+00

Gap= 0.104 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 21319 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=5.76D-08 MaxDP=3.93D-06 DE=-5.77D-09 OVMax= 3.00D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.83D-08 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.31D-01

CP: 1.01D+00 1.47D+00 1.73D+00 1.32D+00 1.30D+00

CP: 1.29D+00 2.42D+00 2.33D+00 1.91D+00 1.10D+00

E= -1275.69696888598 Delta-E= -0.000000000529 Rises=F Damp=F

DIIS: error= 1.30D-06 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1275.69696888598 IErMin=16 ErrMin= 1.30D-06

ErrMax= 1.30D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.08D-10 BMatP= 1.37D-09

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

Coeff-Com: 0.697D-04-0.809D-04 0.389D-04 0.763D-04 0.189D-03 0.296D-03

Coeff-Com: -0.107D-02-0.316D-02 0.392D-02 0.217D-01 0.203D-01-0.706D-02

Coeff-Com: -0.129D+00-0.134D+00 0.390D+00 0.838D+00

Coeff: 0.697D-04-0.809D-04 0.389D-04 0.763D-04 0.189D-03 0.296D-03

Coeff: -0.107D-02-0.316D-02 0.392D-02 0.217D-01 0.203D-01-0.706D-02

Coeff: -0.129D+00-0.134D+00 0.390D+00 0.838D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=4.16D-08 MaxDP=2.68D-06 DE=-5.29D-10 OVMax= 1.81D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 8.50D-09 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.31D-01

CP: 1.01D+00 1.47D+00 1.73D+00 1.32D+00 1.30D+00

CP: 1.30D+00 2.49D+00 2.49D+00 2.12D+00 1.42D+00

CP: 1.02D+00

E= -1275.69696888627 Delta-E= -0.000000000290 Rises=F Damp=F

DIIS: error= 5.29D-07 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1275.69696888627 IErMin=17 ErrMin= 5.29D-07

ErrMax= 5.29D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.46D-11 BMatP= 5.08D-10

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

Coeff-Com: 0.498D-05-0.573D-05 0.371D-05 0.115D-04 0.302D-04 0.868D-04

Coeff-Com: -0.492D-04-0.384D-03-0.354D-03 0.469D-03 0.327D-02 0.275D-01

Coeff-Com: -0.857D-02-0.646D-01-0.866D-01 0.113D+00 0.102D+01

Coeff: 0.498D-05-0.573D-05 0.371D-05 0.115D-04 0.302D-04 0.868D-04

Coeff: -0.492D-04-0.384D-03-0.354D-03 0.469D-03 0.327D-02 0.275D-01

Coeff: -0.857D-02-0.646D-01-0.866D-01 0.113D+00 0.102D+01

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.077 Goal= None Shift= 0.000

RMSDP=8.93D-09 MaxDP=6.21D-07 DE=-2.90D-10 OVMax= 2.43D-06

Error on total polarization charges = 0.06047

SCF Done: E(UB3LYP) = -1275.69696889 A.U. after 17 cycles

NFock= 17 Conv=0.89D-08 -V/T= 1.9662

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7830 S= 0.5163

<L.S>= 0.000000000000E+00

KE= 1.320283431434D+03 PE=-8.543513833603D+03 EE= 3.187659815428D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.84

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7830, after 0.7509

Leave Link 502 at Fri Jul 5 21:08:40 2019, MaxMem= 1342177280 cpu: 1163.5

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

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

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Population analysis using the SCF density.

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Orbital symmetries:

Alpha Orbitals:

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The electronic state is 2-AU.

Alpha occ. eigenvalues -- -14.34377 -14.34377 -14.34377 -14.34377 -14.32908

Alpha occ. eigenvalues -- -14.32908 -14.32908 -14.32908 -10.28532 -10.28532

Alpha occ. eigenvalues -- -10.28532 -10.28532 -10.28465 -10.28465 -10.28465

Alpha occ. eigenvalues -- -10.28464 -10.21460 -10.21460 -10.21460 -10.21460

Alpha occ. eigenvalues -- -10.19491 -10.19491 -10.19491 -10.19491 -10.17347

Alpha occ. eigenvalues -- -10.17347 -10.17347 -10.17347 -1.03087 -1.01677

Alpha occ. eigenvalues -- -1.01677 -0.98939 -0.96701 -0.92500 -0.92500

Alpha occ. eigenvalues -- -0.89115 -0.81830 -0.81283 -0.81283 -0.81020

Alpha occ. eigenvalues -- -0.77823 -0.74039 -0.74039 -0.71814 -0.70638

Alpha occ. eigenvalues -- -0.69914 -0.69914 -0.65837 -0.63385 -0.60995

Alpha occ. eigenvalues -- -0.59651 -0.59237 -0.58967 -0.58967 -0.57246

Alpha occ. eigenvalues -- -0.57246 -0.56589 -0.56373 -0.56373 -0.56070

Alpha occ. eigenvalues -- -0.53700 -0.52495 -0.52495 -0.51657 -0.50524

Alpha occ. eigenvalues -- -0.48544 -0.46883 -0.46883 -0.45886 -0.44911

Alpha occ. eigenvalues -- -0.44911 -0.44540 -0.44283 -0.41754 -0.41648

Alpha occ. eigenvalues -- -0.41648 -0.41638 -0.41245 -0.41184 -0.40828

Alpha occ. eigenvalues -- -0.40828 -0.39708 -0.39588 -0.39069 -0.39069

Alpha occ. eigenvalues -- -0.38366 -0.38225 -0.34962 -0.34962 -0.34318

Alpha occ. eigenvalues -- -0.34318 -0.32934 -0.30163 -0.30163 -0.28408

Alpha occ. eigenvalues -- -0.27963 -0.27944 -0.26908 -0.26908 -0.26767

Alpha occ. eigenvalues -- -0.26644 -0.23988

Alpha virt. eigenvalues -- -0.13559 -0.13559 -0.07014 0.00088 0.02359

Alpha virt. eigenvalues -- 0.02359 0.02725 0.03823 0.04049 0.04049

Alpha virt. eigenvalues -- 0.04879 0.06466 0.06634 0.07391 0.07784

Alpha virt. eigenvalues -- 0.07784 0.08501 0.08852 0.08885 0.08885

Alpha virt. eigenvalues -- 0.09527 0.09527 0.09585 0.12426 0.13025

Alpha virt. eigenvalues -- 0.13057 0.13057 0.13123 0.13216 0.13216

Alpha virt. eigenvalues -- 0.13613 0.16627 0.18773 0.19065 0.19386

Alpha virt. eigenvalues -- 0.19386 0.19469 0.19921 0.19921 0.21002

Alpha virt. eigenvalues -- 0.21032 0.21172 0.21468 0.21468 0.24237

Alpha virt. eigenvalues -- 0.25505 0.26359 0.26359 0.27130 0.27304

Alpha virt. eigenvalues -- 0.27787 0.27787 0.28120 0.30523 0.30523

Alpha virt. eigenvalues -- 0.30585 0.30798 0.30974 0.30974 0.31411

Alpha virt. eigenvalues -- 0.31481 0.33581 0.33979 0.33979 0.34608

Alpha virt. eigenvalues -- 0.35980 0.35980 0.36192 0.37172 0.37550

Alpha virt. eigenvalues -- 0.37550 0.38456 0.38765 0.38765 0.39350

Alpha virt. eigenvalues -- 0.40416 0.41975 0.41975 0.42168 0.42241

Alpha virt. eigenvalues -- 0.42805 0.43988 0.45197 0.45197 0.45330

Alpha virt. eigenvalues -- 0.46484 0.47467 0.47467 0.47798 0.47907

Alpha virt. eigenvalues -- 0.47907 0.48176 0.49542 0.50326 0.50530

Alpha virt. eigenvalues -- 0.50530 0.51881 0.52143 0.52775 0.52775

Alpha virt. eigenvalues -- 0.53357 0.54837 0.54837 0.55167 0.55242

Alpha virt. eigenvalues -- 0.56244 0.56244 0.56595 0.57555 0.57624

Alpha virt. eigenvalues -- 0.57624 0.57727 0.58470 0.58470 0.58851

Alpha virt. eigenvalues -- 0.59780 0.59799 0.61316 0.61454 0.61454

Alpha virt. eigenvalues -- 0.62266 0.62294 0.62294 0.63359 0.63838

Alpha virt. eigenvalues -- 0.63838 0.66775 0.66888 0.67551 0.67622

Alpha virt. eigenvalues -- 0.67622 0.68084 0.68084 0.68352 0.69389

Alpha virt. eigenvalues -- 0.70318 0.71895 0.71988 0.71988 0.73123

Alpha virt. eigenvalues -- 0.73888 0.74532 0.74532 0.76442 0.76442

Alpha virt. eigenvalues -- 0.77838 0.78306 0.78619 0.79541 0.79541

Alpha virt. eigenvalues -- 0.79893 0.80090 0.80090 0.80933 0.81330

Alpha virt. eigenvalues -- 0.83973 0.84208 0.84208 0.86051 0.87242

Alpha virt. eigenvalues -- 0.87667 0.87667 0.88560 0.93122 0.95498

Alpha virt. eigenvalues -- 0.95498 0.96375 0.96415 0.98659 0.98659

Alpha virt. eigenvalues -- 0.98683 1.01550 1.01550 1.02890 1.03680

Alpha virt. eigenvalues -- 1.03680 1.05126 1.06637 1.06637 1.06722

Alpha virt. eigenvalues -- 1.08623 1.09007 1.11602 1.11602 1.11803

Alpha virt. eigenvalues -- 1.11804 1.11881 1.12272 1.12272 1.12378

Alpha virt. eigenvalues -- 1.12986 1.16360 1.16612 1.17604 1.17604

Alpha virt. eigenvalues -- 1.19005 1.19005 1.19301 1.21863 1.22349

Alpha virt. eigenvalues -- 1.25914 1.26453 1.27723 1.27723 1.28775

Alpha virt. eigenvalues -- 1.34262 1.34262 1.35571 1.36205 1.37567

Alpha virt. eigenvalues -- 1.38415 1.39295 1.39295 1.40480 1.40480

Alpha virt. eigenvalues -- 1.42429 1.43470 1.47881 1.48396 1.48396

Alpha virt. eigenvalues -- 1.50276 1.50303 1.50303 1.50498 1.50559

Alpha virt. eigenvalues -- 1.50614 1.50614 1.51602 1.51976 1.53457

Alpha virt. eigenvalues -- 1.53457 1.54177 1.54578 1.54578 1.55609

Alpha virt. eigenvalues -- 1.56793 1.58928 1.59281 1.59281 1.60606

Alpha virt. eigenvalues -- 1.61360 1.61360 1.61539 1.65664 1.66509

Alpha virt. eigenvalues -- 1.66614 1.66614 1.67468 1.67468 1.67798

Alpha virt. eigenvalues -- 1.69103 1.69888 1.69888 1.72086 1.73839

Alpha virt. eigenvalues -- 1.73839 1.73884 1.78096 1.78203 1.78203

Alpha virt. eigenvalues -- 1.78309 1.83124 1.84562 1.84562 1.85273

Alpha virt. eigenvalues -- 1.86812 1.88363 1.88363 1.88741 1.89652

Alpha virt. eigenvalues -- 1.92088 1.93428 1.94668 1.94668 1.94908

Alpha virt. eigenvalues -- 1.98963 1.99083 1.99083 1.99151 1.99738

Alpha virt. eigenvalues -- 1.99919 2.00089 2.00089 2.03412 2.04312

Alpha virt. eigenvalues -- 2.05938 2.06833 2.06833 2.10564 2.10564

Alpha virt. eigenvalues -- 2.13244 2.13788 2.13788 2.15034 2.15449

Alpha virt. eigenvalues -- 2.18074 2.25799 2.26795 2.27309 2.27602

Alpha virt. eigenvalues -- 2.27602 2.28197 2.31073 2.31073 2.33928

Alpha virt. eigenvalues -- 2.34173 2.34173 2.35344 2.35344 2.35380

Alpha virt. eigenvalues -- 2.36249 2.37004 2.37677 2.37677 2.37859

Alpha virt. eigenvalues -- 2.42057 2.45972 2.46177 2.46177 2.46230

Alpha virt. eigenvalues -- 2.46329 2.46329 2.47225 2.47423 2.53431

Alpha virt. eigenvalues -- 2.53533 2.53533 2.54113 2.55831 2.55831

Alpha virt. eigenvalues -- 2.57206 2.58208 2.58208 2.60992 2.61397

Alpha virt. eigenvalues -- 2.62415 2.63956 2.65092 2.68148 2.68148

Alpha virt. eigenvalues -- 2.69426 2.70128 2.70255 2.70255 2.73227

Alpha virt. eigenvalues -- 2.73227 2.74036 2.77047 2.80668 2.81527

Alpha virt. eigenvalues -- 2.81527 2.81813 2.81895 2.82483 2.82483

Alpha virt. eigenvalues -- 2.82649 2.89295 2.89295 2.90535 2.91567

Alpha virt. eigenvalues -- 2.93648 2.94775 2.94775 2.99077 3.01204

Alpha virt. eigenvalues -- 3.02412 3.02412 3.03677 3.10292 3.10778

Alpha virt. eigenvalues -- 3.11702 3.12036 3.12036 3.12214 3.12214

Alpha virt. eigenvalues -- 3.12532 3.13590 3.15004 3.15004 3.16576

Alpha virt. eigenvalues -- 3.18485 3.18485 3.18843 3.19960 3.22231

Alpha virt. eigenvalues -- 3.24717 3.25998 3.25998 3.26337 3.28451

Alpha virt. eigenvalues -- 3.28451 3.34185 3.35659 3.36902 3.36902

Alpha virt. eigenvalues -- 3.37400 3.50865 3.55032 3.55032 3.67530

Alpha virt. eigenvalues -- 3.69824 3.69971 3.69971 3.73889 3.75448

Alpha virt. eigenvalues -- 3.75948 3.75948 3.76552 3.78866 3.79684

Alpha virt. eigenvalues -- 3.79684 3.84990 3.85672 3.85807 3.85807

Alpha virt. eigenvalues -- 3.89007 4.02773 4.02773 4.03385 4.03449

Alpha virt. eigenvalues -- 4.09202 4.10238 4.10238 4.16380 4.25941

Alpha virt. eigenvalues -- 4.32919 4.32919 4.35320 4.43637 4.49194

Alpha virt. eigenvalues -- 4.59142 4.59142 4.97083 5.00327 5.00327

Alpha virt. eigenvalues -- 5.08892 5.12385 5.30431 5.30431 5.47645

Alpha virt. eigenvalues -- 7.76867 7.76867 7.88056 7.93529 8.21149

Alpha virt. eigenvalues -- 11.17965 23.41511 23.44044 23.44044 23.45459

Alpha virt. eigenvalues -- 23.65108 23.65687 23.65687 23.65802 23.78269

Alpha virt. eigenvalues -- 23.79126 23.79126 23.80222 23.82697 23.83841

Alpha virt. eigenvalues -- 23.83841 23.84026 24.07298 24.07784 24.07784

Alpha virt. eigenvalues -- 24.08486 35.53841 35.58427 35.58427 35.59601

Alpha virt. eigenvalues -- 35.64821 35.66068 35.66068 35.66385

Beta occ. eigenvalues -- -14.34525 -14.34525 -14.34525 -14.34524 -14.33007

Beta occ. eigenvalues -- -14.33007 -14.33007 -14.33007 -10.28263 -10.28262

Beta occ. eigenvalues -- -10.28262 -10.28262 -10.28194 -10.28194 -10.28194

Beta occ. eigenvalues -- -10.28194 -10.21392 -10.21392 -10.21392 -10.21392

Beta occ. eigenvalues -- -10.19511 -10.19511 -10.19511 -10.19510 -10.17348

Beta occ. eigenvalues -- -10.17348 -10.17348 -10.17348 -1.02885 -1.01475

Beta occ. eigenvalues -- -1.01475 -0.98722 -0.96616 -0.92480 -0.92480

Beta occ. eigenvalues -- -0.89295 -0.81713 -0.81203 -0.81203 -0.80949

Beta occ. eigenvalues -- -0.77249 -0.73749 -0.73749 -0.71769 -0.70506

Beta occ. eigenvalues -- -0.69704 -0.69704 -0.65554 -0.63123 -0.60939

Beta occ. eigenvalues -- -0.59580 -0.59195 -0.58802 -0.58802 -0.57267

Beta occ. eigenvalues -- -0.57267 -0.56480 -0.56220 -0.56220 -0.56037

Beta occ. eigenvalues -- -0.53577 -0.52403 -0.52403 -0.51553 -0.50450

Beta occ. eigenvalues -- -0.47803 -0.46126 -0.46126 -0.45852 -0.44874

Beta occ. eigenvalues -- -0.44874 -0.44232 -0.43899 -0.41600 -0.41525

Beta occ. eigenvalues -- -0.41445 -0.41445 -0.41245 -0.40717 -0.40717

Beta occ. eigenvalues -- -0.40516 -0.39586 -0.39105 -0.39032 -0.39032

Beta occ. eigenvalues -- -0.38318 -0.38162 -0.34965 -0.34965 -0.33555

Beta occ. eigenvalues -- -0.33555 -0.33023 -0.30261 -0.30261 -0.28526

Beta occ. eigenvalues -- -0.27994 -0.27891 -0.27627 -0.26894 -0.26894

Beta occ. eigenvalues -- -0.26630

Beta virt. eigenvalues -- -0.18906 -0.12186 -0.12186 -0.06360 0.01283

Beta virt. eigenvalues -- 0.02967 0.03232 0.03232 0.04101 0.04101

Beta virt. eigenvalues -- 0.04635 0.04886 0.06468 0.06649 0.07815

Beta virt. eigenvalues -- 0.07815 0.08161 0.08869 0.08891 0.09541

Beta virt. eigenvalues -- 0.09541 0.09634 0.09634 0.09635 0.12433

Beta virt. eigenvalues -- 0.13073 0.13073 0.13132 0.13137 0.13390

Beta virt. eigenvalues -- 0.13390 0.13786 0.16848 0.19002 0.19291

Beta virt. eigenvalues -- 0.19539 0.19539 0.19717 0.20203 0.20203

Beta virt. eigenvalues -- 0.21111 0.21114 0.21394 0.21747 0.21747

Beta virt. eigenvalues -- 0.24522 0.25794 0.26473 0.26473 0.27216

Beta virt. eigenvalues -- 0.27780 0.28019 0.28019 0.28274 0.30662

Beta virt. eigenvalues -- 0.30684 0.30684 0.30867 0.31039 0.31039

Beta virt. eigenvalues -- 0.31509 0.31571 0.33640 0.34185 0.34185

Beta virt. eigenvalues -- 0.34779 0.36114 0.36114 0.36399 0.37456

Beta virt. eigenvalues -- 0.38214 0.38214 0.38605 0.38916 0.38916

Beta virt. eigenvalues -- 0.39512 0.40869 0.42115 0.42115 0.42355

Beta virt. eigenvalues -- 0.42924 0.43314 0.44142 0.45428 0.45428

Beta virt. eigenvalues -- 0.45517 0.46617 0.47634 0.47634 0.48049

Beta virt. eigenvalues -- 0.48049 0.48084 0.48304 0.49683 0.50611

Beta virt. eigenvalues -- 0.50881 0.50881 0.52273 0.52322 0.52843

Beta virt. eigenvalues -- 0.52843 0.53414 0.54907 0.54907 0.55243

Beta virt. eigenvalues -- 0.55335 0.56331 0.56331 0.56905 0.57598

Beta virt. eigenvalues -- 0.57750 0.57750 0.57782 0.58546 0.58546

Beta virt. eigenvalues -- 0.58898 0.59870 0.59880 0.61452 0.61632

Beta virt. eigenvalues -- 0.61632 0.62311 0.62656 0.62656 0.63446

Beta virt. eigenvalues -- 0.63893 0.63893 0.67031 0.67075 0.67622

Beta virt. eigenvalues -- 0.67753 0.67753 0.67928 0.67928 0.68506

Beta virt. eigenvalues -- 0.69525 0.70333 0.72019 0.72141 0.72141

Beta virt. eigenvalues -- 0.73210 0.74082 0.74621 0.74621 0.76577

Beta virt. eigenvalues -- 0.76577 0.77821 0.78196 0.78822 0.79448

Beta virt. eigenvalues -- 0.79448 0.79699 0.80199 0.80199 0.81011

Beta virt. eigenvalues -- 0.81400 0.84048 0.84311 0.84311 0.86129

Beta virt. eigenvalues -- 0.87297 0.87738 0.87738 0.88660 0.93273

Beta virt. eigenvalues -- 0.95552 0.95552 0.96453 0.96616 0.98766

Beta virt. eigenvalues -- 0.98766 0.99097 1.01872 1.01872 1.02953

Beta virt. eigenvalues -- 1.03846 1.03846 1.05308 1.06826 1.07074

Beta virt. eigenvalues -- 1.07074 1.08979 1.09018 1.11856 1.11858

Beta virt. eigenvalues -- 1.12245 1.12245 1.12379 1.12379 1.12392

Beta virt. eigenvalues -- 1.12910 1.13481 1.16823 1.16974 1.17638

Beta virt. eigenvalues -- 1.17638 1.19464 1.19464 1.19486 1.21897

Beta virt. eigenvalues -- 1.22396 1.25997 1.26894 1.27861 1.27861

Beta virt. eigenvalues -- 1.28820 1.34752 1.34752 1.35737 1.36801

Beta virt. eigenvalues -- 1.37646 1.38872 1.39368 1.39368 1.40600

Beta virt. eigenvalues -- 1.40600 1.42662 1.43611 1.47878 1.48443

Beta virt. eigenvalues -- 1.48443 1.50343 1.50367 1.50367 1.50516

Beta virt. eigenvalues -- 1.50546 1.50598 1.50598 1.51690 1.52420

Beta virt. eigenvalues -- 1.53565 1.53565 1.54245 1.54742 1.54742

Beta virt. eigenvalues -- 1.55836 1.57035 1.59027 1.59574 1.59574

Beta virt. eigenvalues -- 1.60685 1.61484 1.61484 1.61752 1.65731

Beta virt. eigenvalues -- 1.66786 1.66786 1.66882 1.67561 1.67561

Beta virt. eigenvalues -- 1.67993 1.69212 1.70390 1.70390 1.72230

Beta virt. eigenvalues -- 1.74000 1.74000 1.74531 1.78400 1.78428

Beta virt. eigenvalues -- 1.78428 1.78493 1.83244 1.84714 1.84714

Beta virt. eigenvalues -- 1.85528 1.86936 1.88718 1.88718 1.88886

Beta virt. eigenvalues -- 1.90008 1.92428 1.93738 1.95006 1.95006

Beta virt. eigenvalues -- 1.95013 1.99141 1.99253 1.99253 1.99311

Beta virt. eigenvalues -- 2.00090 2.00160 2.00614 2.00614 2.03481

Beta virt. eigenvalues -- 2.04721 2.05943 2.06868 2.06868 2.10613

Beta virt. eigenvalues -- 2.10613 2.13368 2.14100 2.14100 2.15149

Beta virt. eigenvalues -- 2.15894 2.18220 2.25851 2.27065 2.27355

Beta virt. eigenvalues -- 2.27636 2.27636 2.28229 2.31157 2.31157

Beta virt. eigenvalues -- 2.33973 2.34231 2.34231 2.35428 2.35683

Beta virt. eigenvalues -- 2.35683 2.36286 2.37074 2.37709 2.37709

Beta virt. eigenvalues -- 2.38248 2.42104 2.45893 2.46348 2.46348

Beta virt. eigenvalues -- 2.46358 2.46358 2.46364 2.47480 2.47510

Beta virt. eigenvalues -- 2.53355 2.53422 2.53422 2.54111 2.55816

Beta virt. eigenvalues -- 2.55816 2.57651 2.58628 2.58628 2.61301

Beta virt. eigenvalues -- 2.61312 2.62292 2.64286 2.65088 2.68359

Beta virt. eigenvalues -- 2.68359 2.69590 2.70087 2.70191 2.70191

Beta virt. eigenvalues -- 2.74010 2.74010 2.74778 2.77950 2.81223

Beta virt. eigenvalues -- 2.81856 2.82199 2.82199 2.82553 2.82553

Beta virt. eigenvalues -- 2.82677 2.82716 2.89375 2.89375 2.90647

Beta virt. eigenvalues -- 2.92023 2.93709 2.95383 2.95383 2.99808

Beta virt. eigenvalues -- 3.01293 3.02491 3.02491 3.03759 3.10337

Beta virt. eigenvalues -- 3.10834 3.11778 3.12106 3.12106 3.12308

Beta virt. eigenvalues -- 3.12308 3.12630 3.13724 3.15062 3.15062

Beta virt. eigenvalues -- 3.16614 3.18551 3.18551 3.18903 3.19977

Beta virt. eigenvalues -- 3.22299 3.24774 3.26059 3.26059 3.26423

Beta virt. eigenvalues -- 3.28532 3.28532 3.34270 3.35689 3.36942

Beta virt. eigenvalues -- 3.36942 3.37454 3.51013 3.55165 3.55165

Beta virt. eigenvalues -- 3.67641 3.69951 3.70117 3.70117 3.73995

Beta virt. eigenvalues -- 3.75621 3.76082 3.76082 3.76693 3.78376

Beta virt. eigenvalues -- 3.79292 3.79292 3.84676 3.85205 3.85414

Beta virt. eigenvalues -- 3.85414 3.88685 4.02884 4.02884 4.03491

Beta virt. eigenvalues -- 4.03568 4.09199 4.10283 4.10283 4.16492

Beta virt. eigenvalues -- 4.26002 4.33087 4.33087 4.35562 4.43693

Beta virt. eigenvalues -- 4.49204 4.59167 4.59167 4.97258 5.00504

Beta virt. eigenvalues -- 5.00504 5.09087 5.12541 5.30612 5.30612

Beta virt. eigenvalues -- 5.47827 7.76849 7.76849 7.88056 7.93524

Beta virt. eigenvalues -- 8.21145 11.17955 23.41569 23.44093 23.44093

Beta virt. eigenvalues -- 23.45503 23.65136 23.65709 23.65709 23.65821

Beta virt. eigenvalues -- 23.78523 23.79401 23.79401 23.80504 23.83010

Beta virt. eigenvalues -- 23.84150 23.84150 23.84337 24.07330 24.07816

Beta virt. eigenvalues -- 24.07816 24.08517 35.53715 35.58313 35.58313

Beta virt. eigenvalues -- 35.59500 35.64668 35.65927 35.65927 35.66255

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 4.563057 0.401781 -0.125072 -0.046360 0.403509 -0.001839

2 N 0.401781 7.123694 0.386031 -0.063158 -0.093413 -0.077438

3 C -0.125072 0.386031 4.599754 0.378724 -0.065400 0.553895

4 C -0.046360 -0.063158 0.378724 5.030078 0.628331 -0.069071

5 C 0.403509 -0.093413 -0.065400 0.628331 5.085094 0.004185

6 N -0.001839 -0.077438 0.553895 -0.069071 0.004185 6.574328

7 C -0.001037 -0.004590 -0.088060 0.004303 -0.000302 0.511057

8 N 0.000675 -0.018506 -0.005334 -0.000123 -0.000192 -0.070768

9 C -0.000005 0.000578 -0.000855 0.000022 -0.000003 0.000087

10 C -0.000003 -0.000101 0.000041 0.000014 0.000000 0.003239

11 C 0.000022 0.000213 0.004004 -0.000253 0.000010 -0.040211

12 N 0.511057 -0.070768 0.000087 0.003239 -0.040211 -0.000146

13 C 0.004303 -0.000123 0.000022 0.000014 -0.000253 0.000000

14 C -0.000302 -0.000192 -0.000003 0.000000 0.000010 0.000000

15 C -0.001037 0.000675 -0.000005 -0.000003 0.000022 -0.000001

16 N -0.004590 -0.018506 0.000578 -0.000101 0.000213 -0.000005

17 C -0.088060 -0.005334 -0.000855 0.000041 0.004004 -0.000024

18 N -0.000018 -0.000004 -0.000001 0.000000 0.000000 0.000000

19 N 0.000153 -0.003445 0.000205 0.000002 0.000003 -0.000004

20 C -0.000048 0.000205 -0.000010 0.000000 0.000000 -0.000001

21 C 0.000000 0.000002 0.000000 0.000000 0.000000 0.000000

22 C 0.000000 0.000003 0.000000 0.000000 0.000000 0.000000

23 C -0.000004 0.000153 -0.000048 0.000000 0.000000 -0.000018

24 N -0.000001 -0.000005 -0.000024 0.000000 0.000000 -0.000146

25 Zn -0.015245 0.106371 -0.016060 -0.001148 -0.001056 -0.004692

26 C 0.008714 0.008230 -0.067873 0.271487 -0.052204 0.012814

27 H -0.045762 0.005683 0.008982 -0.039659 0.394018 -0.000010

28 C 0.000000 0.000000 0.000002 0.000000 0.000000 -0.000019

29 H 0.000001 0.000065 -0.000206 -0.000126 -0.000003 0.005429

30 C -0.000458 0.000054 0.000000 0.000000 -0.000045 0.000000

31 H 0.000010 0.000001 0.000000 0.000000 0.000000 0.000000

32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

33 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

34 H 0.000274 -0.000225 0.006143 -0.040049 -0.005591 0.000052

35 H -0.000200 0.000371 -0.005175 -0.041871 -0.000130 0.003338

36 H -0.000200 0.000371 -0.005175 -0.041871 -0.000130 0.003338

37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000007

38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000007

39 H 0.000000 0.000000 0.000001 0.000000 0.000000 -0.000011

40 H -0.000035 0.000011 0.000000 0.000000 -0.000018 0.000000

41 H -0.000035 0.000011 0.000000 0.000000 -0.000018 0.000000

42 H 0.000034 0.000000 0.000000 0.000000 -0.000001 0.000000

43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 8 9 10 11 12

1 C -0.001037 0.000675 -0.000005 -0.000003 0.000022 0.511057

2 N -0.004590 -0.018506 0.000578 -0.000101 0.000213 -0.070768

3 C -0.088060 -0.005334 -0.000855 0.000041 0.004004 0.000087

4 C 0.004303 -0.000123 0.000022 0.000014 -0.000253 0.003239

5 C -0.000302 -0.000192 -0.000003 0.000000 0.000010 -0.040211

6 N 0.511057 -0.070768 0.000087 0.003239 -0.040211 -0.000146

7 C 4.563057 0.401781 -0.125072 -0.046360 0.403509 -0.000018

8 N 0.401781 7.123694 0.386031 -0.063158 -0.093413 -0.000004

9 C -0.125072 0.386031 4.599754 0.378724 -0.065400 -0.000001

10 C -0.046360 -0.063158 0.378724 5.030078 0.628331 0.000000

11 C 0.403509 -0.093413 -0.065400 0.628331 5.085094 0.000000

12 N -0.000018 -0.000004 -0.000001 0.000000 0.000000 6.574328

13 C 0.000000 0.000002 0.000000 0.000000 0.000000 -0.069071

14 C 0.000000 0.000003 0.000000 0.000000 0.000000 0.004185

15 C -0.000004 0.000153 -0.000048 0.000000 0.000000 -0.001839

16 N 0.000153 -0.003445 0.000205 0.000002 0.000003 -0.077438

17 C -0.000048 0.000205 -0.000010 0.000000 0.000000 0.553895

18 N -0.000001 -0.000005 -0.000024 0.000000 0.000000 -0.000146

19 N 0.000675 -0.018506 -0.005334 -0.000123 -0.000192 -0.000005

20 C -0.000005 0.000578 -0.000855 0.000022 -0.000003 -0.000024

21 C -0.000003 -0.000101 0.000041 0.000014 0.000000 0.000000

22 C 0.000022 0.000213 0.004004 -0.000253 0.000010 0.000000

23 C -0.001037 -0.004590 -0.088060 0.004303 -0.000302 -0.000001

24 N -0.001839 -0.077438 0.553895 -0.069071 0.004185 0.000000

25 Zn -0.015245 0.106371 -0.016060 -0.001148 -0.001056 -0.004692

26 C -0.000458 0.000054 0.000000 0.000000 -0.000045 -0.000019

27 H 0.000010 0.000001 0.000000 0.000000 0.000000 0.005429

28 C 0.008714 0.008230 -0.067873 0.271487 -0.052204 0.000000

29 H -0.045762 0.005683 0.008982 -0.039659 0.394018 0.000000

30 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.012814

31 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000010

32 C 0.000000 0.000000 0.000002 0.000000 0.000000 0.000000

33 H 0.000001 0.000065 -0.000206 -0.000126 -0.000003 0.000000

34 H 0.000034 0.000000 0.000000 0.000000 -0.000001 -0.000011

35 H -0.000035 0.000011 0.000000 0.000000 -0.000018 0.000007

36 H -0.000035 0.000011 0.000000 0.000000 -0.000018 0.000007

37 H -0.000200 0.000371 -0.005175 -0.041871 -0.000130 0.000000

38 H -0.000200 0.000371 -0.005175 -0.041871 -0.000130 0.000000

39 H 0.000274 -0.000225 0.006143 -0.040049 -0.005591 0.000000

40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.003338

41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.003338

42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000052

43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

45 H 0.000000 0.000000 0.000001 0.000000 0.000000 0.000000

13 14 15 16 17 18

1 C 0.004303 -0.000302 -0.001037 -0.004590 -0.088060 -0.000018

2 N -0.000123 -0.000192 0.000675 -0.018506 -0.005334 -0.000004

3 C 0.000022 -0.000003 -0.000005 0.000578 -0.000855 -0.000001

4 C 0.000014 0.000000 -0.000003 -0.000101 0.000041 0.000000

5 C -0.000253 0.000010 0.000022 0.000213 0.004004 0.000000

6 N 0.000000 0.000000 -0.000001 -0.000005 -0.000024 0.000000

7 C 0.000000 0.000000 -0.000004 0.000153 -0.000048 -0.000001

8 N 0.000002 0.000003 0.000153 -0.003445 0.000205 -0.000005

9 C 0.000000 0.000000 -0.000048 0.000205 -0.000010 -0.000024

10 C 0.000000 0.000000 0.000000 0.000002 0.000000 0.000000

11 C 0.000000 0.000000 0.000000 0.000003 0.000000 0.000000

12 N -0.069071 0.004185 -0.001839 -0.077438 0.553895 -0.000146

13 C 5.030078 0.628331 -0.046360 -0.063158 0.378724 0.003239

14 C 0.628331 5.085094 0.403509 -0.093413 -0.065400 -0.040211

15 C -0.046360 0.403509 4.563057 0.401781 -0.125072 0.511057

16 N -0.063158 -0.093413 0.401781 7.123694 0.386031 -0.070768

17 C 0.378724 -0.065400 -0.125072 0.386031 4.599754 0.000087

18 N 0.003239 -0.040211 0.511057 -0.070768 0.000087 6.574328

19 N -0.000101 0.000213 -0.004590 -0.018506 0.000578 -0.077438

20 C 0.000041 0.004004 -0.088060 -0.005334 -0.000855 0.553895

21 C 0.000014 -0.000253 0.004303 -0.000123 0.000022 -0.069071

22 C 0.000000 0.000010 -0.000302 -0.000192 -0.000003 0.004185

23 C -0.000003 0.000022 -0.001037 0.000675 -0.000005 -0.001839

24 N 0.000000 0.000000 -0.000018 -0.000004 -0.000001 -0.000146

25 Zn -0.001148 -0.001056 -0.015245 0.106371 -0.016060 -0.004692

26 C 0.000000 0.000000 0.000000 0.000000 0.000002 0.000000

27 H -0.000126 -0.000003 0.000001 0.000065 -0.000206 0.000000

28 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

29 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

30 C 0.271487 -0.052204 0.008714 0.008230 -0.067873 -0.000019

31 H -0.039659 0.394018 -0.045762 0.005683 0.008982 0.005429

32 C 0.000000 -0.000045 -0.000458 0.000054 0.000000 0.012814

33 H 0.000000 0.000000 0.000010 0.000001 0.000000 -0.000010

34 H 0.000000 0.000000 0.000000 0.000000 0.000001 0.000000

35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

40 H -0.041871 -0.000130 -0.000200 0.000371 -0.005175 0.000007

41 H -0.041871 -0.000130 -0.000200 0.000371 -0.005175 0.000007

42 H -0.040049 -0.005591 0.000274 -0.000225 0.006143 -0.000011

43 H 0.000000 -0.000018 -0.000035 0.000011 0.000000 0.003338

44 H 0.000000 -0.000018 -0.000035 0.000011 0.000000 0.003338

45 H 0.000000 -0.000001 0.000034 0.000000 0.000000 0.000052

19 20 21 22 23 24

1 C 0.000153 -0.000048 0.000000 0.000000 -0.000004 -0.000001

2 N -0.003445 0.000205 0.000002 0.000003 0.000153 -0.000005

3 C 0.000205 -0.000010 0.000000 0.000000 -0.000048 -0.000024

4 C 0.000002 0.000000 0.000000 0.000000 0.000000 0.000000

5 C 0.000003 0.000000 0.000000 0.000000 0.000000 0.000000

6 N -0.000004 -0.000001 0.000000 0.000000 -0.000018 -0.000146

7 C 0.000675 -0.000005 -0.000003 0.000022 -0.001037 -0.001839

8 N -0.018506 0.000578 -0.000101 0.000213 -0.004590 -0.077438

9 C -0.005334 -0.000855 0.000041 0.004004 -0.088060 0.553895

10 C -0.000123 0.000022 0.000014 -0.000253 0.004303 -0.069071

11 C -0.000192 -0.000003 0.000000 0.000010 -0.000302 0.004185

12 N -0.000005 -0.000024 0.000000 0.000000 -0.000001 0.000000

13 C -0.000101 0.000041 0.000014 0.000000 -0.000003 0.000000

14 C 0.000213 0.004004 -0.000253 0.000010 0.000022 0.000000

15 C -0.004590 -0.088060 0.004303 -0.000302 -0.001037 -0.000018

16 N -0.018506 -0.005334 -0.000123 -0.000192 0.000675 -0.000004

17 C 0.000578 -0.000855 0.000022 -0.000003 -0.000005 -0.000001

18 N -0.077438 0.553895 -0.069071 0.004185 -0.001839 -0.000146

19 N 7.123694 0.386031 -0.063158 -0.093413 0.401781 -0.070768

20 C 0.386031 4.599754 0.378724 -0.065400 -0.125072 0.000087

21 C -0.063158 0.378724 5.030078 0.628331 -0.046360 0.003239

22 C -0.093413 -0.065400 0.628331 5.085094 0.403509 -0.040211

23 C 0.401781 -0.125072 -0.046360 0.403509 4.563057 0.511057

24 N -0.070768 0.000087 0.003239 -0.040211 0.511057 6.574328

25 Zn 0.106371 -0.016060 -0.001148 -0.001056 -0.015245 -0.004692

26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

28 C 0.000054 0.000000 0.000000 -0.000045 -0.000458 0.012814

29 H 0.000001 0.000000 0.000000 0.000000 0.000010 -0.000010

30 C 0.000000 0.000002 0.000000 0.000000 0.000000 0.000000

31 H 0.000065 -0.000206 -0.000126 -0.000003 0.000001 0.000000

32 C 0.008230 -0.067873 0.271487 -0.052204 0.008714 -0.000019

33 H 0.005683 0.008982 -0.039659 0.394018 -0.045762 0.005429

34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 H 0.000011 0.000000 0.000000 -0.000018 -0.000035 0.003338

38 H 0.000011 0.000000 0.000000 -0.000018 -0.000035 0.003338

39 H 0.000000 0.000000 0.000000 -0.000001 0.000034 0.000052

40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

42 H 0.000000 0.000001 0.000000 0.000000 0.000000 0.000000

43 H 0.000371 -0.005175 -0.041871 -0.000130 -0.000200 0.000007

44 H 0.000371 -0.005175 -0.041871 -0.000130 -0.000200 0.000007

45 H -0.000225 0.006143 -0.040049 -0.005591 0.000274 -0.000011

25 26 27 28 29 30

1 C -0.015245 0.008714 -0.045762 0.000000 0.000001 -0.000458

2 N 0.106371 0.008230 0.005683 0.000000 0.000065 0.000054

3 C -0.016060 -0.067873 0.008982 0.000002 -0.000206 0.000000

4 C -0.001148 0.271487 -0.039659 0.000000 -0.000126 0.000000

5 C -0.001056 -0.052204 0.394018 0.000000 -0.000003 -0.000045

6 N -0.004692 0.012814 -0.000010 -0.000019 0.005429 0.000000

7 C -0.015245 -0.000458 0.000010 0.008714 -0.045762 0.000000

8 N 0.106371 0.000054 0.000001 0.008230 0.005683 0.000000

9 C -0.016060 0.000000 0.000000 -0.067873 0.008982 0.000000

10 C -0.001148 0.000000 0.000000 0.271487 -0.039659 0.000000

11 C -0.001056 -0.000045 0.000000 -0.052204 0.394018 0.000000

12 N -0.004692 -0.000019 0.005429 0.000000 0.000000 0.012814

13 C -0.001148 0.000000 -0.000126 0.000000 0.000000 0.271487

14 C -0.001056 0.000000 -0.000003 0.000000 0.000000 -0.052204

15 C -0.015245 0.000000 0.000001 0.000000 0.000000 0.008714

16 N 0.106371 0.000000 0.000065 0.000000 0.000000 0.008230

17 C -0.016060 0.000002 -0.000206 0.000000 0.000000 -0.067873

18 N -0.004692 0.000000 0.000000 0.000000 0.000000 -0.000019

19 N 0.106371 0.000000 0.000000 0.000054 0.000001 0.000000

20 C -0.016060 0.000000 0.000000 0.000000 0.000000 0.000002

21 C -0.001148 0.000000 0.000000 0.000000 0.000000 0.000000

22 C -0.001056 0.000000 0.000000 -0.000045 0.000000 0.000000

23 C -0.015245 0.000000 0.000000 -0.000458 0.000010 0.000000

24 N -0.004692 0.000000 0.000000 0.012814 -0.000010 0.000000

25 Zn 10.187981 0.000379 0.000005 0.000379 0.000005 0.000379

26 C 0.000379 5.357363 -0.004195 0.000000 0.000055 0.000000

27 H 0.000005 -0.004195 0.425541 0.000000 0.000000 0.000055

28 C 0.000379 0.000000 0.000000 5.357363 -0.004195 0.000000

29 H 0.000005 0.000055 0.000000 -0.004195 0.425541 0.000000

30 C 0.000379 0.000000 0.000055 0.000000 0.000000 5.357363

31 H 0.000005 0.000000 0.000000 0.000000 0.000000 -0.004195

32 C 0.000379 0.000000 0.000000 0.000000 0.000000 0.000000

33 H 0.000005 0.000000 0.000000 0.000055 0.000000 0.000000

34 H 0.000046 0.388258 0.001216 0.000000 0.000000 0.000000

35 H 0.000074 0.385664 -0.000087 0.000000 0.000028 0.000000

36 H 0.000074 0.385664 -0.000087 0.000000 0.000028 0.000000

37 H 0.000074 0.000000 0.000000 0.385664 -0.000087 0.000000

38 H 0.000074 0.000000 0.000000 0.385664 -0.000087 0.000000

39 H 0.000046 0.000000 0.000000 0.388258 0.001216 0.000000

40 H 0.000074 0.000000 0.000028 0.000000 0.000000 0.385664

41 H 0.000074 0.000000 0.000028 0.000000 0.000000 0.385664

42 H 0.000046 0.000000 0.000000 0.000000 0.000000 0.388258

43 H 0.000074 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000074 0.000000 0.000000 0.000000 0.000000 0.000000

45 H 0.000046 0.000000 0.000000 0.000000 0.000000 0.000000

31 32 33 34 35 36

1 C 0.000010 0.000000 0.000000 0.000274 -0.000200 -0.000200

2 N 0.000001 0.000000 0.000000 -0.000225 0.000371 0.000371

3 C 0.000000 0.000000 0.000000 0.006143 -0.005175 -0.005175

4 C 0.000000 0.000000 0.000000 -0.040049 -0.041871 -0.041871

5 C 0.000000 0.000000 0.000000 -0.005591 -0.000130 -0.000130

6 N 0.000000 0.000000 0.000000 0.000052 0.003338 0.003338

7 C 0.000000 0.000000 0.000001 0.000034 -0.000035 -0.000035

8 N 0.000000 0.000000 0.000065 0.000000 0.000011 0.000011

9 C 0.000000 0.000002 -0.000206 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 -0.000126 0.000000 0.000000 0.000000

11 C 0.000000 0.000000 -0.000003 -0.000001 -0.000018 -0.000018

12 N -0.000010 0.000000 0.000000 -0.000011 0.000007 0.000007

13 C -0.039659 0.000000 0.000000 0.000000 0.000000 0.000000

14 C 0.394018 -0.000045 0.000000 0.000000 0.000000 0.000000

15 C -0.045762 -0.000458 0.000010 0.000000 0.000000 0.000000

16 N 0.005683 0.000054 0.000001 0.000000 0.000000 0.000000

17 C 0.008982 0.000000 0.000000 0.000001 0.000000 0.000000

18 N 0.005429 0.012814 -0.000010 0.000000 0.000000 0.000000

19 N 0.000065 0.008230 0.005683 0.000000 0.000000 0.000000

20 C -0.000206 -0.067873 0.008982 0.000000 0.000000 0.000000

21 C -0.000126 0.271487 -0.039659 0.000000 0.000000 0.000000

22 C -0.000003 -0.052204 0.394018 0.000000 0.000000 0.000000

23 C 0.000001 0.008714 -0.045762 0.000000 0.000000 0.000000

24 N 0.000000 -0.000019 0.005429 0.000000 0.000000 0.000000

25 Zn 0.000005 0.000379 0.000005 0.000046 0.000074 0.000074

26 C 0.000000 0.000000 0.000000 0.388258 0.385664 0.385664

27 H 0.000000 0.000000 0.000000 0.001216 -0.000087 -0.000087

28 C 0.000000 0.000000 0.000055 0.000000 0.000000 0.000000

29 H 0.000000 0.000000 0.000000 0.000000 0.000028 0.000028

30 C -0.004195 0.000000 0.000000 0.000000 0.000000 0.000000

31 H 0.425541 0.000055 0.000000 0.000000 0.000000 0.000000

32 C 0.000055 5.357363 -0.004195 0.000000 0.000000 0.000000

33 H 0.000000 -0.004195 0.425541 0.000000 0.000000 0.000000

34 H 0.000000 0.000000 0.000000 0.448379 -0.024293 -0.024293

35 H 0.000000 0.000000 0.000000 -0.024293 0.458233 -0.026445

36 H 0.000000 0.000000 0.000000 -0.024293 -0.026445 0.458233

37 H 0.000000 0.000000 0.000028 0.000000 0.000000 0.000000

38 H 0.000000 0.000000 0.000028 0.000000 0.000000 0.000000

39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

40 H -0.000087 0.000000 0.000000 0.000000 0.000000 0.000000

41 H -0.000087 0.000000 0.000000 0.000000 0.000000 0.000000

42 H 0.001216 0.000000 0.000000 0.000000 0.000000 0.000000

43 H 0.000028 0.385664 -0.000087 0.000000 0.000000 0.000000

44 H 0.000028 0.385664 -0.000087 0.000000 0.000000 0.000000

45 H 0.000000 0.388258 0.001216 0.000000 0.000000 0.000000

37 38 39 40 41 42

1 C 0.000000 0.000000 0.000000 -0.000035 -0.000035 0.000034

2 N 0.000000 0.000000 0.000000 0.000011 0.000011 0.000000

3 C 0.000000 0.000000 0.000001 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 C 0.000000 0.000000 0.000000 -0.000018 -0.000018 -0.000001

6 N 0.000007 0.000007 -0.000011 0.000000 0.000000 0.000000

7 C -0.000200 -0.000200 0.000274 0.000000 0.000000 0.000000

8 N 0.000371 0.000371 -0.000225 0.000000 0.000000 0.000000

9 C -0.005175 -0.005175 0.006143 0.000000 0.000000 0.000000

10 C -0.041871 -0.041871 -0.040049 0.000000 0.000000 0.000000

11 C -0.000130 -0.000130 -0.005591 0.000000 0.000000 0.000000

12 N 0.000000 0.000000 0.000000 0.003338 0.003338 0.000052

13 C 0.000000 0.000000 0.000000 -0.041871 -0.041871 -0.040049

14 C 0.000000 0.000000 0.000000 -0.000130 -0.000130 -0.005591

15 C 0.000000 0.000000 0.000000 -0.000200 -0.000200 0.000274

16 N 0.000000 0.000000 0.000000 0.000371 0.000371 -0.000225

17 C 0.000000 0.000000 0.000000 -0.005175 -0.005175 0.006143

18 N 0.000000 0.000000 0.000000 0.000007 0.000007 -0.000011

19 N 0.000011 0.000011 0.000000 0.000000 0.000000 0.000000

20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000001

21 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

22 C -0.000018 -0.000018 -0.000001 0.000000 0.000000 0.000000

23 C -0.000035 -0.000035 0.000034 0.000000 0.000000 0.000000

24 N 0.003338 0.003338 0.000052 0.000000 0.000000 0.000000

25 Zn 0.000074 0.000074 0.000046 0.000074 0.000074 0.000046

26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000 0.000028 0.000028 0.000000

28 C 0.385664 0.385664 0.388258 0.000000 0.000000 0.000000

29 H -0.000087 -0.000087 0.001216 0.000000 0.000000 0.000000

30 C 0.000000 0.000000 0.000000 0.385664 0.385664 0.388258

31 H 0.000000 0.000000 0.000000 -0.000087 -0.000087 0.001216

32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

33 H 0.000028 0.000028 0.000000 0.000000 0.000000 0.000000

34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 H 0.458233 -0.026445 -0.024293 0.000000 0.000000 0.000000

38 H -0.026445 0.458233 -0.024293 0.000000 0.000000 0.000000

39 H -0.024293 -0.024293 0.448379 0.000000 0.000000 0.000000

40 H 0.000000 0.000000 0.000000 0.458233 -0.026445 -0.024293

41 H 0.000000 0.000000 0.000000 -0.026445 0.458233 -0.024293

42 H 0.000000 0.000000 0.000000 -0.024293 -0.024293 0.448379

43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

43 44 45

1 C 0.000000 0.000000 0.000000

2 N 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000

5 C 0.000000 0.000000 0.000000

6 N 0.000000 0.000000 0.000000

7 C 0.000000 0.000000 0.000000

8 N 0.000000 0.000000 0.000000

9 C 0.000000 0.000000 0.000001

10 C 0.000000 0.000000 0.000000

11 C 0.000000 0.000000 0.000000

12 N 0.000000 0.000000 0.000000

13 C 0.000000 0.000000 0.000000

14 C -0.000018 -0.000018 -0.000001

15 C -0.000035 -0.000035 0.000034

16 N 0.000011 0.000011 0.000000

17 C 0.000000 0.000000 0.000000

18 N 0.003338 0.003338 0.000052

19 N 0.000371 0.000371 -0.000225

20 C -0.005175 -0.005175 0.006143

21 C -0.041871 -0.041871 -0.040049

22 C -0.000130 -0.000130 -0.005591

23 C -0.000200 -0.000200 0.000274

24 N 0.000007 0.000007 -0.000011

25 Zn 0.000074 0.000074 0.000046

26 C 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000

28 C 0.000000 0.000000 0.000000

29 H 0.000000 0.000000 0.000000

30 C 0.000000 0.000000 0.000000

31 H 0.000028 0.000028 0.000000

32 C 0.385664 0.385664 0.388258

33 H -0.000087 -0.000087 0.001216

34 H 0.000000 0.000000 0.000000

35 H 0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000

37 H 0.000000 0.000000 0.000000

38 H 0.000000 0.000000 0.000000

39 H 0.000000 0.000000 0.000000

40 H 0.000000 0.000000 0.000000

41 H 0.000000 0.000000 0.000000

42 H 0.000000 0.000000 0.000000

43 H 0.458233 -0.026445 -0.024293

44 H -0.026445 0.458233 -0.024293

45 H -0.024293 -0.024293 0.448379

Atomic-Atomic Spin Densities.

1 2 3 4 5 6

1 C 0.183879 0.003437 -0.011952 -0.008579 0.013738 0.000170

2 N 0.003437 -0.058671 -0.001081 -0.001522 0.000311 0.001058

3 C -0.011952 -0.001081 0.186096 0.021388 -0.006149 -0.000491

4 C -0.008579 -0.001522 0.021388 0.051698 -0.008656 -0.000676

5 C 0.013738 0.000311 -0.006149 -0.008656 -0.016380 -0.000071

6 N 0.000170 0.001058 -0.000491 -0.000676 -0.000071 -0.083734

7 C 0.000174 0.000009 -0.010915 -0.000416 0.000034 0.002644

8 N 0.000030 0.000207 -0.000270 -0.000012 0.000000 0.000690

9 C -0.000007 0.000022 0.000182 0.000002 0.000000 0.000071

10 C 0.000000 -0.000002 0.000054 0.000000 0.000000 0.000015

11 C 0.000001 -0.000004 -0.000292 0.000009 0.000000 0.000241

12 N 0.002644 0.000690 0.000071 0.000015 0.000241 0.000001

13 C -0.000416 -0.000012 0.000002 0.000000 0.000009 0.000000

14 C 0.000034 0.000000 0.000000 0.000000 0.000000 0.000000

15 C 0.000174 0.000030 -0.000007 0.000000 0.000001 0.000000

16 N 0.000009 0.000207 0.000022 -0.000002 -0.000004 0.000000

17 C -0.010915 -0.000270 0.000182 0.000054 -0.000292 0.000000

18 N 0.000000 -0.000001 0.000000 0.000000 0.000000 0.000000

19 N 0.000001 0.000013 0.000000 0.000000 0.000000 -0.000001

20 C -0.000007 0.000000 0.000002 0.000000 0.000000 0.000000

21 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

22 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

23 C 0.000001 0.000001 -0.000007 0.000000 0.000000 0.000000

24 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000001

25 Zn 0.000198 0.001147 -0.000427 -0.000047 0.000011 -0.000109

26 C -0.000002 0.000003 -0.001189 -0.003477 0.001229 0.000297

27 H 0.000037 -0.000020 -0.000087 0.000299 0.000341 -0.000002

28 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000001

29 H 0.000000 0.000001 -0.000005 0.000000 0.000000 0.000082

30 C 0.000032 0.000000 0.000000 0.000000 0.000001 0.000000

31 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

33 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

34 H 0.000011 0.000000 0.000032 -0.000178 0.000014 -0.000001

35 H 0.000024 0.000007 -0.000439 -0.001119 0.000078 0.000023

36 H 0.000024 0.000007 -0.000439 -0.001119 0.000078 0.000023

37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

40 H 0.000025 0.000000 0.000000 0.000000 0.000002 0.000000

41 H 0.000025 0.000000 0.000000 0.000000 0.000002 0.000000

42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 8 9 10 11 12

1 C 0.000174 0.000030 -0.000007 0.000000 0.000001 0.002644

2 N 0.000009 0.000207 0.000022 -0.000002 -0.000004 0.000690

3 C -0.010915 -0.000270 0.000182 0.000054 -0.000292 0.000071

4 C -0.000416 -0.000012 0.000002 0.000000 0.000009 0.000015

5 C 0.000034 0.000000 0.000000 0.000000 0.000000 0.000241

6 N 0.002644 0.000690 0.000071 0.000015 0.000241 0.000001

7 C 0.183879 0.003437 -0.011952 -0.008579 0.013738 0.000000

8 N 0.003437 -0.058671 -0.001081 -0.001522 0.000311 -0.000001

9 C -0.011952 -0.001081 0.186096 0.021388 -0.006149 0.000000

10 C -0.008579 -0.001522 0.021388 0.051698 -0.008656 0.000000

11 C 0.013738 0.000311 -0.006149 -0.008656 -0.016380 0.000000

12 N 0.000000 -0.000001 0.000000 0.000000 0.000000 -0.083734

13 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000676

14 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000071

15 C 0.000001 0.000001 -0.000007 0.000000 0.000000 0.000170

16 N 0.000001 0.000013 0.000000 0.000000 0.000000 0.001058

17 C -0.000007 0.000000 0.000002 0.000000 0.000000 -0.000491

18 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000001

19 N 0.000030 0.000207 -0.000270 -0.000012 0.000000 0.000000

20 C -0.000007 0.000022 0.000182 0.000002 0.000000 0.000000

21 C 0.000000 -0.000002 0.000054 0.000000 0.000000 0.000000

22 C 0.000001 -0.000004 -0.000292 0.000009 0.000000 0.000000

23 C 0.000174 0.000009 -0.010915 -0.000416 0.000034 0.000000

24 N 0.000170 0.001058 -0.000491 -0.000676 -0.000071 0.000000

25 Zn 0.000198 0.001147 -0.000427 -0.000047 0.000011 -0.000109

26 C 0.000032 0.000000 0.000000 0.000000 0.000001 0.000001

27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000082

28 C -0.000002 0.000003 -0.001189 -0.003477 0.001229 0.000000

29 H 0.000037 -0.000020 -0.000087 0.000299 0.000341 0.000000

30 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000297

31 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

33 H 0.000000 0.000001 -0.000005 0.000000 0.000000 0.000000

34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 H 0.000025 0.000000 0.000000 0.000000 0.000002 0.000000

36 H 0.000025 0.000000 0.000000 0.000000 0.000002 0.000000

37 H 0.000024 0.000007 -0.000439 -0.001119 0.000078 0.000000

38 H 0.000024 0.000007 -0.000439 -0.001119 0.000078 0.000000

39 H 0.000011 0.000000 0.000032 -0.000178 0.000014 0.000000

40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000023

41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000023

42 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000001

43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

13 14 15 16 17 18

1 C -0.000416 0.000034 0.000174 0.000009 -0.010915 0.000000

2 N -0.000012 0.000000 0.000030 0.000207 -0.000270 -0.000001

3 C 0.000002 0.000000 -0.000007 0.000022 0.000182 0.000000

4 C 0.000000 0.000000 0.000000 -0.000002 0.000054 0.000000

5 C 0.000009 0.000000 0.000001 -0.000004 -0.000292 0.000000

6 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 C 0.000000 0.000000 0.000001 0.000001 -0.000007 0.000000

8 N 0.000000 0.000000 0.000001 0.000013 0.000000 0.000000

9 C 0.000000 0.000000 -0.000007 0.000000 0.000002 0.000000

10 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

11 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

12 N -0.000676 -0.000071 0.000170 0.001058 -0.000491 0.000001

13 C 0.051698 -0.008656 -0.008579 -0.001522 0.021388 0.000015

14 C -0.008656 -0.016380 0.013738 0.000311 -0.006149 0.000241

15 C -0.008579 0.013738 0.183879 0.003437 -0.011952 0.002644

16 N -0.001522 0.000311 0.003437 -0.058671 -0.001081 0.000690

17 C 0.021388 -0.006149 -0.011952 -0.001081 0.186096 0.000071

18 N 0.000015 0.000241 0.002644 0.000690 0.000071 -0.083734

19 N -0.000002 -0.000004 0.000009 0.000207 0.000022 0.001058

20 C 0.000054 -0.000292 -0.010915 -0.000270 0.000182 -0.000491

21 C 0.000000 0.000009 -0.000416 -0.000012 0.000002 -0.000676

22 C 0.000000 0.000000 0.000034 0.000000 0.000000 -0.000071

23 C 0.000000 0.000001 0.000174 0.000030 -0.000007 0.000170

24 N 0.000000 0.000000 0.000000 -0.000001 0.000000 0.000001

25 Zn -0.000047 0.000011 0.000198 0.001147 -0.000427 -0.000109

26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000 0.000001 -0.000005 0.000000

28 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

29 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

30 C -0.003477 0.001229 -0.000002 0.000003 -0.001189 0.000001

31 H 0.000299 0.000341 0.000037 -0.000020 -0.000087 0.000082

32 C 0.000000 0.000001 0.000032 0.000000 0.000000 0.000297

33 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

40 H -0.001119 0.000078 0.000024 0.000007 -0.000439 0.000000

41 H -0.001119 0.000078 0.000024 0.000007 -0.000439 0.000000

42 H -0.000178 0.000014 0.000011 0.000000 0.000032 0.000000

43 H 0.000000 0.000002 0.000025 0.000000 0.000000 0.000023

44 H 0.000000 0.000002 0.000025 0.000000 0.000000 0.000023

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000001

19 20 21 22 23 24

1 C 0.000001 -0.000007 0.000000 0.000000 0.000001 0.000000

2 N 0.000013 0.000000 0.000000 0.000000 0.000001 0.000000

3 C 0.000000 0.000002 0.000000 0.000000 -0.000007 0.000000

4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

6 N -0.000001 0.000000 0.000000 0.000000 0.000000 0.000001

7 C 0.000030 -0.000007 0.000000 0.000001 0.000174 0.000170

8 N 0.000207 0.000022 -0.000002 -0.000004 0.000009 0.001058

9 C -0.000270 0.000182 0.000054 -0.000292 -0.010915 -0.000491

10 C -0.000012 0.000002 0.000000 0.000009 -0.000416 -0.000676

11 C 0.000000 0.000000 0.000000 0.000000 0.000034 -0.000071

12 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

13 C -0.000002 0.000054 0.000000 0.000000 0.000000 0.000000

14 C -0.000004 -0.000292 0.000009 0.000000 0.000001 0.000000

15 C 0.000009 -0.010915 -0.000416 0.000034 0.000174 0.000000

16 N 0.000207 -0.000270 -0.000012 0.000000 0.000030 -0.000001

17 C 0.000022 0.000182 0.000002 0.000000 -0.000007 0.000000

18 N 0.001058 -0.000491 -0.000676 -0.000071 0.000170 0.000001

19 N -0.058671 -0.001081 -0.001522 0.000311 0.003437 0.000690

20 C -0.001081 0.186096 0.021388 -0.006149 -0.011952 0.000071

21 C -0.001522 0.021388 0.051698 -0.008656 -0.008579 0.000015

22 C 0.000311 -0.006149 -0.008656 -0.016380 0.013738 0.000241

23 C 0.003437 -0.011952 -0.008579 0.013738 0.183879 0.002644

24 N 0.000690 0.000071 0.000015 0.000241 0.002644 -0.083734

25 Zn 0.001147 -0.000427 -0.000047 0.000011 0.000198 -0.000109

26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

28 C 0.000000 0.000000 0.000000 0.000001 0.000032 0.000297

29 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

30 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

31 H 0.000001 -0.000005 0.000000 0.000000 0.000000 0.000000

32 C 0.000003 -0.001189 -0.003477 0.001229 -0.000002 0.000001

33 H -0.000020 -0.000087 0.000299 0.000341 0.000037 0.000082

34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 H 0.000000 0.000000 0.000000 0.000002 0.000025 0.000023

38 H 0.000000 0.000000 0.000000 0.000002 0.000025 0.000023

39 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000001

40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

43 H 0.000007 -0.000439 -0.001119 0.000078 0.000024 0.000000

44 H 0.000007 -0.000439 -0.001119 0.000078 0.000024 0.000000

45 H 0.000000 0.000032 -0.000178 0.000014 0.000011 0.000000

25 26 27 28 29 30

1 C 0.000198 -0.000002 0.000037 0.000000 0.000000 0.000032

2 N 0.001147 0.000003 -0.000020 0.000000 0.000001 0.000000

3 C -0.000427 -0.001189 -0.000087 0.000000 -0.000005 0.000000

4 C -0.000047 -0.003477 0.000299 0.000000 0.000000 0.000000

5 C 0.000011 0.001229 0.000341 0.000000 0.000000 0.000001

6 N -0.000109 0.000297 -0.000002 0.000001 0.000082 0.000000

7 C 0.000198 0.000032 0.000000 -0.000002 0.000037 0.000000

8 N 0.001147 0.000000 0.000000 0.000003 -0.000020 0.000000

9 C -0.000427 0.000000 0.000000 -0.001189 -0.000087 0.000000

10 C -0.000047 0.000000 0.000000 -0.003477 0.000299 0.000000

11 C 0.000011 0.000001 0.000000 0.001229 0.000341 0.000000

12 N -0.000109 0.000001 0.000082 0.000000 0.000000 0.000297

13 C -0.000047 0.000000 0.000000 0.000000 0.000000 -0.003477

14 C 0.000011 0.000000 0.000000 0.000000 0.000000 0.001229

15 C 0.000198 0.000000 0.000000 0.000000 0.000000 -0.000002

16 N 0.001147 0.000000 0.000001 0.000000 0.000000 0.000003

17 C -0.000427 0.000000 -0.000005 0.000000 0.000000 -0.001189

18 N -0.000109 0.000000 0.000000 0.000000 0.000000 0.000001

19 N 0.001147 0.000000 0.000000 0.000000 0.000000 0.000000

20 C -0.000427 0.000000 0.000000 0.000000 0.000000 0.000000

21 C -0.000047 0.000000 0.000000 0.000000 0.000000 0.000000

22 C 0.000011 0.000000 0.000000 0.000001 0.000000 0.000000

23 C 0.000198 0.000000 0.000000 0.000032 0.000000 0.000000

24 N -0.000109 0.000000 0.000000 0.000297 -0.000002 0.000000

25 Zn -0.000445 0.000000 0.000000 0.000000 0.000000 0.000000

26 C 0.000000 -0.002708 0.000124 0.000000 0.000000 0.000000

27 H 0.000000 0.000124 -0.000667 0.000000 0.000000 0.000000

28 C 0.000000 0.000000 0.000000 -0.002708 0.000124 0.000000

29 H 0.000000 0.000000 0.000000 0.000124 -0.000667 0.000000

30 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.002708

31 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000124

32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

33 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

34 H 0.000002 0.000264 -0.000036 0.000000 0.000000 0.000000

35 H 0.000000 0.001627 0.000001 0.000000 0.000000 0.000000

36 H 0.000000 0.001627 0.000001 0.000000 0.000000 0.000000

37 H 0.000000 0.000000 0.000000 0.001627 0.000001 0.000000

38 H 0.000000 0.000000 0.000000 0.001627 0.000001 0.000000

39 H 0.000002 0.000000 0.000000 0.000264 -0.000036 0.000000

40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.001627

41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.001627

42 H 0.000002 0.000000 0.000000 0.000000 0.000000 0.000264

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 0.000002 0.000000 0.000000 0.000000 0.000000 0.000000

31 32 33 34 35 36

1 C 0.000000 0.000000 0.000000 0.000011 0.000024 0.000024

2 N 0.000000 0.000000 0.000000 0.000000 0.000007 0.000007

3 C 0.000000 0.000000 0.000000 0.000032 -0.000439 -0.000439

4 C 0.000000 0.000000 0.000000 -0.000178 -0.001119 -0.001119

5 C 0.000000 0.000000 0.000000 0.000014 0.000078 0.000078

6 N 0.000000 0.000000 0.000000 -0.000001 0.000023 0.000023

7 C 0.000000 0.000000 0.000000 0.000000 0.000025 0.000025

8 N 0.000000 0.000000 0.000001 0.000000 0.000000 0.000000

9 C 0.000000 0.000000 -0.000005 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

11 C 0.000000 0.000000 0.000000 0.000000 0.000002 0.000002

12 N -0.000002 0.000000 0.000000 0.000000 0.000000 0.000000

13 C 0.000299 0.000000 0.000000 0.000000 0.000000 0.000000

14 C 0.000341 0.000001 0.000000 0.000000 0.000000 0.000000

15 C 0.000037 0.000032 0.000000 0.000000 0.000000 0.000000

16 N -0.000020 0.000000 0.000000 0.000000 0.000000 0.000000

17 C -0.000087 0.000000 0.000000 0.000000 0.000000 0.000000

18 N 0.000082 0.000297 -0.000002 0.000000 0.000000 0.000000

19 N 0.000001 0.000003 -0.000020 0.000000 0.000000 0.000000

20 C -0.000005 -0.001189 -0.000087 0.000000 0.000000 0.000000

21 C 0.000000 -0.003477 0.000299 0.000000 0.000000 0.000000

22 C 0.000000 0.001229 0.000341 0.000000 0.000000 0.000000

23 C 0.000000 -0.000002 0.000037 0.000000 0.000000 0.000000

24 N 0.000000 0.000001 0.000082 0.000000 0.000000 0.000000

25 Zn 0.000000 0.000000 0.000000 0.000002 0.000000 0.000000

26 C 0.000000 0.000000 0.000000 0.000264 0.001627 0.001627

27 H 0.000000 0.000000 0.000000 -0.000036 0.000001 0.000001

28 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

29 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

30 C 0.000124 0.000000 0.000000 0.000000 0.000000 0.000000

31 H -0.000667 0.000000 0.000000 0.000000 0.000000 0.000000

32 C 0.000000 -0.002708 0.000124 0.000000 0.000000 0.000000

33 H 0.000000 0.000124 -0.000667 0.000000 0.000000 0.000000

34 H 0.000000 0.000000 0.000000 -0.000376 -0.000004 -0.000004

35 H 0.000000 0.000000 0.000000 -0.000004 0.003885 -0.000788

36 H 0.000000 0.000000 0.000000 -0.000004 -0.000788 0.003885

37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

40 H 0.000001 0.000000 0.000000 0.000000 0.000000 0.000000

41 H 0.000001 0.000000 0.000000 0.000000 0.000000 0.000000

42 H -0.000036 0.000000 0.000000 0.000000 0.000000 0.000000

43 H 0.000000 0.001627 0.000001 0.000000 0.000000 0.000000

44 H 0.000000 0.001627 0.000001 0.000000 0.000000 0.000000

45 H 0.000000 0.000264 -0.000036 0.000000 0.000000 0.000000

37 38 39 40 41 42

1 C 0.000000 0.000000 0.000000 0.000025 0.000025 0.000000

2 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 C 0.000000 0.000000 0.000000 0.000002 0.000002 0.000000

6 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 C 0.000024 0.000024 0.000011 0.000000 0.000000 0.000000

8 N 0.000007 0.000007 0.000000 0.000000 0.000000 0.000000

9 C -0.000439 -0.000439 0.000032 0.000000 0.000000 0.000000

10 C -0.001119 -0.001119 -0.000178 0.000000 0.000000 0.000000

11 C 0.000078 0.000078 0.000014 0.000000 0.000000 0.000000

12 N 0.000000 0.000000 0.000000 0.000023 0.000023 -0.000001

13 C 0.000000 0.000000 0.000000 -0.001119 -0.001119 -0.000178

14 C 0.000000 0.000000 0.000000 0.000078 0.000078 0.000014

15 C 0.000000 0.000000 0.000000 0.000024 0.000024 0.000011

16 N 0.000000 0.000000 0.000000 0.000007 0.000007 0.000000

17 C 0.000000 0.000000 0.000000 -0.000439 -0.000439 0.000032

18 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

19 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

21 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

22 C 0.000002 0.000002 0.000000 0.000000 0.000000 0.000000

23 C 0.000025 0.000025 0.000000 0.000000 0.000000 0.000000

24 N 0.000023 0.000023 -0.000001 0.000000 0.000000 0.000000

25 Zn 0.000000 0.000000 0.000002 0.000000 0.000000 0.000002

26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

28 C 0.001627 0.001627 0.000264 0.000000 0.000000 0.000000

29 H 0.000001 0.000001 -0.000036 0.000000 0.000000 0.000000

30 C 0.000000 0.000000 0.000000 0.001627 0.001627 0.000264

31 H 0.000000 0.000000 0.000000 0.000001 0.000001 -0.000036

32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

33 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 H 0.003885 -0.000788 -0.000004 0.000000 0.000000 0.000000

38 H -0.000788 0.003885 -0.000004 0.000000 0.000000 0.000000

39 H -0.000004 -0.000004 -0.000376 0.000000 0.000000 0.000000

40 H 0.000000 0.000000 0.000000 0.003885 -0.000788 -0.000004

41 H 0.000000 0.000000 0.000000 -0.000788 0.003885 -0.000004

42 H 0.000000 0.000000 0.000000 -0.000004 -0.000004 -0.000376

43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

43 44 45

1 C 0.000000 0.000000 0.000000

2 N 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000

5 C 0.000000 0.000000 0.000000

6 N 0.000000 0.000000 0.000000

7 C 0.000000 0.000000 0.000000

8 N 0.000000 0.000000 0.000000

9 C 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 0.000000

11 C 0.000000 0.000000 0.000000

12 N 0.000000 0.000000 0.000000

13 C 0.000000 0.000000 0.000000

14 C 0.000002 0.000002 0.000000

15 C 0.000025 0.000025 0.000000

16 N 0.000000 0.000000 0.000000

17 C 0.000000 0.000000 0.000000

18 N 0.000023 0.000023 -0.000001

19 N 0.000007 0.000007 0.000000

20 C -0.000439 -0.000439 0.000032

21 C -0.001119 -0.001119 -0.000178

22 C 0.000078 0.000078 0.000014

23 C 0.000024 0.000024 0.000011

24 N 0.000000 0.000000 0.000000

25 Zn 0.000000 0.000000 0.000002

26 C 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000

28 C 0.000000 0.000000 0.000000

29 H 0.000000 0.000000 0.000000

30 C 0.000000 0.000000 0.000000

31 H 0.000000 0.000000 0.000000

32 C 0.001627 0.001627 0.000264

33 H 0.000001 0.000001 -0.000036

34 H 0.000000 0.000000 0.000000

35 H 0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000

37 H 0.000000 0.000000 0.000000

38 H 0.000000 0.000000 0.000000

39 H 0.000000 0.000000 0.000000

40 H 0.000000 0.000000 0.000000

41 H 0.000000 0.000000 0.000000

42 H 0.000000 0.000000 0.000000

43 H 0.003885 -0.000788 -0.000004

44 H -0.000788 0.003885 -0.000004

45 H -0.000004 -0.000004 -0.000376

Mulliken charges and spin densities:

1 2

1 C 0.436720 0.172790

2 N -0.678698 -0.054430

3 C 0.441688 0.174281

4 C 0.027539 0.047662

5 C -0.260428 -0.015462

6 N -0.407373 -0.079767

7 C 0.436720 0.172790

8 N -0.678698 -0.054430

9 C 0.441688 0.174281

10 C 0.027539 0.047662

11 C -0.260428 -0.015462

12 N -0.407373 -0.079767

13 C 0.027539 0.047662

14 C -0.260428 -0.015462

15 C 0.436720 0.172790

16 N -0.678698 -0.054430

17 C 0.441688 0.174281

18 N -0.407373 -0.079767

19 N -0.678698 -0.054430

20 C 0.441688 0.174281

21 C 0.027539 0.047662

22 C -0.260428 -0.015462

23 C 0.436720 0.172790

24 N -0.407373 -0.079767

25 Zn 1.537029 0.002655

26 C -0.693889 -0.002172

27 H 0.249072 0.000070

28 C -0.693889 -0.002172

29 H 0.249072 0.000070

30 C -0.693889 -0.002172

31 H 0.249072 0.000070

32 C -0.693889 -0.002172

33 H 0.249072 0.000070

34 H 0.250059 -0.000277

35 H 0.250526 0.003320

36 H 0.250526 0.003320

37 H 0.250526 0.003320

38 H 0.250526 0.003320

39 H 0.250059 -0.000277

40 H 0.250526 0.003320

41 H 0.250526 0.003320

42 H 0.250059 -0.000277

43 H 0.250526 0.003320

44 H 0.250526 0.003320

45 H 0.250059 -0.000277

Sum of Mulliken charges = 1.00000 1.00000

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

1 2

1 C 0.436720 0.172790

2 N -0.678698 -0.054430

3 C 0.441688 0.174281

4 C 0.027539 0.047662

5 C -0.011356 -0.015392

6 N -0.407373 -0.079767

7 C 0.436720 0.172790

8 N -0.678698 -0.054430

9 C 0.441688 0.174281

10 C 0.027539 0.047662

11 C -0.011356 -0.015392

12 N -0.407373 -0.079767

13 C 0.027539 0.047662

14 C -0.011356 -0.015392

15 C 0.436720 0.172790

16 N -0.678698 -0.054430

17 C 0.441688 0.174281

18 N -0.407373 -0.079767

19 N -0.678698 -0.054430

20 C 0.441688 0.174281

21 C 0.027539 0.047662

22 C -0.011356 -0.015392

23 C 0.436720 0.172790

24 N -0.407373 -0.079767

25 Zn 1.537029 0.002655

26 C 0.057223 0.004192

28 C 0.057223 0.004192

30 C 0.057223 0.004192

32 C 0.057223 0.004192

Electronic spatial extent (au): <R\*\*2>= 11176.5599

Charge= 1.0000 electrons

Dipole moment (field-independent basis, Debye):

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

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

XX= -119.6138 YY= -119.6138 ZZ= -167.4250

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XX= 15.9371 YY= 15.9371 ZZ= -31.8741

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

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

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

YYZ= 0.0000 XYZ= 0.0000

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

XXXX= -6213.2124 YYYY= -6213.2124 ZZZZ= -198.2630 XXXY= -323.0018

XXXZ= 0.0000 YYYX= 323.0018 YYYZ= 0.0000 ZZZX= 0.0000

ZZZY= 0.0000 XXYY= -2267.1181 XXZZ= -1323.6280 YYZZ= -1323.6280

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 2.759873617854D+03 E-N=-8.543513847690D+03 KE= 1.320283431434D+03

Symmetry AG KE= 6.512722584995D+02

Symmetry BG KE= 6.558854295226D+01

Symmetry AU KE= 2.126547440389D+01

Symmetry BU KE= 5.821571555787D+02

Isotropic Fermi Contact Couplings

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

1 C(13) 0.01407 15.81600 5.64354 5.27565

2 N(14) -0.00842 -2.71954 -0.97040 -0.90714

3 C(13) 0.01283 14.42151 5.14595 4.81050

4 C(13) -0.00079 -0.89029 -0.31768 -0.29697

5 C(13) -0.00576 -6.47782 -2.31145 -2.16077

6 N(14) -0.01208 -3.90455 -1.39324 -1.30242

7 C(13) 0.01407 15.81600 5.64354 5.27565

8 N(14) -0.00842 -2.71954 -0.97040 -0.90714

9 C(13) 0.01283 14.42151 5.14595 4.81050

10 C(13) -0.00079 -0.89029 -0.31768 -0.29697

11 C(13) -0.00576 -6.47782 -2.31145 -2.16077

12 N(14) -0.01208 -3.90455 -1.39324 -1.30242

13 C(13) -0.00079 -0.89029 -0.31768 -0.29697

14 C(13) -0.00576 -6.47782 -2.31145 -2.16077

15 C(13) 0.01407 15.81600 5.64354 5.27565

16 N(14) -0.00842 -2.71954 -0.97040 -0.90714

17 C(13) 0.01283 14.42151 5.14595 4.81050

18 N(14) -0.01208 -3.90455 -1.39324 -1.30242

19 N(14) -0.00842 -2.71954 -0.97040 -0.90714

20 C(13) 0.01283 14.42151 5.14595 4.81050

21 C(13) -0.00079 -0.89029 -0.31768 -0.29697

22 C(13) -0.00576 -6.47782 -2.31145 -2.16077

23 C(13) 0.01407 15.81600 5.64354 5.27565

24 N(14) -0.01208 -3.90455 -1.39324 -1.30242

25 Zn(67) 0.00000 0.00000 0.00000 0.00000

26 C(13) -0.00200 -2.24679 -0.80171 -0.74945

27 H(1) -0.00009 -0.38395 -0.13700 -0.12807

28 C(13) -0.00200 -2.24679 -0.80171 -0.74945

29 H(1) -0.00009 -0.38395 -0.13700 -0.12807

30 C(13) -0.00200 -2.24679 -0.80171 -0.74945

31 H(1) -0.00009 -0.38395 -0.13700 -0.12807

32 C(13) -0.00200 -2.24679 -0.80171 -0.74945

33 H(1) -0.00009 -0.38395 -0.13700 -0.12807

34 H(1) -0.00009 -0.41764 -0.14903 -0.13931

35 H(1) 0.00208 9.30324 3.31963 3.10323

36 H(1) 0.00208 9.30324 3.31963 3.10323

37 H(1) 0.00208 9.30324 3.31963 3.10323

38 H(1) 0.00208 9.30324 3.31963 3.10323

39 H(1) -0.00009 -0.41764 -0.14903 -0.13931

40 H(1) 0.00208 9.30324 3.31963 3.10323

41 H(1) 0.00208 9.30324 3.31963 3.10323

42 H(1) -0.00009 -0.41764 -0.14903 -0.13931

43 H(1) 0.00208 9.30324 3.31963 3.10323

44 H(1) 0.00208 9.30324 3.31963 3.10323

45 H(1) -0.00009 -0.41764 -0.14903 -0.13931

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

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

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

1 Atom -0.103334 -0.108220 0.211554

2 Atom 0.045221 0.046859 -0.092080

3 Atom -0.107158 -0.109045 0.216203

4 Atom -0.029869 -0.035414 0.065284

5 Atom 0.002165 0.003315 -0.005480

6 Atom 0.065585 0.076684 -0.142269

7 Atom -0.108220 -0.103334 0.211554

8 Atom 0.046859 0.045221 -0.092080

9 Atom -0.109045 -0.107158 0.216203

10 Atom -0.035414 -0.029869 0.065284

11 Atom 0.003315 0.002165 -0.005480

12 Atom 0.076684 0.065585 -0.142269

13 Atom -0.035414 -0.029869 0.065284

14 Atom 0.003315 0.002165 -0.005480

15 Atom -0.108220 -0.103334 0.211554

16 Atom 0.046859 0.045221 -0.092080

17 Atom -0.109045 -0.107158 0.216203

18 Atom 0.065585 0.076684 -0.142269

19 Atom 0.045221 0.046859 -0.092080

20 Atom -0.107158 -0.109045 0.216203

21 Atom -0.029869 -0.035414 0.065284

22 Atom 0.002165 0.003315 -0.005480

23 Atom -0.103334 -0.108220 0.211554

24 Atom 0.076684 0.065585 -0.142269

25 Atom 0.003474 0.003474 -0.006948

26 Atom 0.000722 -0.004147 0.003425

27 Atom 0.001858 0.000114 -0.001972

28 Atom -0.004147 0.000722 0.003425

29 Atom 0.000114 0.001858 -0.001972

30 Atom -0.004147 0.000722 0.003425

31 Atom 0.000114 0.001858 -0.001972

32 Atom 0.000722 -0.004147 0.003425

33 Atom 0.001858 0.000114 -0.001972

34 Atom 0.001806 -0.000700 -0.001106

35 Atom 0.001949 -0.000864 -0.001084

36 Atom 0.001949 -0.000864 -0.001084

37 Atom -0.000864 0.001949 -0.001084

38 Atom -0.000864 0.001949 -0.001084

39 Atom -0.000700 0.001806 -0.001106

40 Atom -0.000864 0.001949 -0.001084

41 Atom -0.000864 0.001949 -0.001084

42 Atom -0.000700 0.001806 -0.001106

43 Atom 0.001949 -0.000864 -0.001084

44 Atom 0.001949 -0.000864 -0.001084

45 Atom 0.001806 -0.000700 -0.001106

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XY XZ YZ

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

1 Atom -0.000159 0.000000 0.000000

2 Atom 0.001301 0.000000 0.000000

3 Atom -0.003886 0.000000 0.000000

4 Atom -0.000804 0.000000 0.000000

5 Atom -0.001411 0.000000 0.000000

6 Atom -0.005870 0.000000 0.000000

7 Atom 0.000159 0.000000 0.000000

8 Atom -0.001301 0.000000 0.000000

9 Atom 0.003886 0.000000 0.000000

10 Atom 0.000804 0.000000 0.000000

11 Atom 0.001411 0.000000 0.000000

12 Atom 0.005870 0.000000 0.000000

13 Atom 0.000804 0.000000 0.000000

14 Atom 0.001411 0.000000 0.000000

15 Atom 0.000159 0.000000 0.000000

16 Atom -0.001301 0.000000 0.000000

17 Atom 0.003886 0.000000 0.000000

18 Atom -0.005870 0.000000 0.000000

19 Atom 0.001301 0.000000 0.000000

20 Atom -0.003886 0.000000 0.000000

21 Atom -0.000804 0.000000 0.000000

22 Atom -0.001411 0.000000 0.000000

23 Atom -0.000159 0.000000 0.000000

24 Atom 0.005870 0.000000 0.000000

25 Atom 0.000000 0.000000 0.000000

26 Atom -0.000305 0.000000 0.000000

27 Atom -0.002300 0.000000 0.000000

28 Atom 0.000305 0.000000 0.000000

29 Atom 0.002300 0.000000 0.000000

30 Atom 0.000305 0.000000 0.000000

31 Atom 0.002300 0.000000 0.000000

32 Atom -0.000305 0.000000 0.000000

33 Atom -0.002300 0.000000 0.000000

34 Atom -0.000969 0.000000 0.000000

35 Atom 0.000814 -0.001059 -0.000844

36 Atom 0.000814 0.001059 0.000844

37 Atom -0.000814 0.000844 -0.001059

38 Atom -0.000814 -0.000844 0.001059

39 Atom 0.000969 0.000000 0.000000

40 Atom -0.000814 -0.000844 0.001059

41 Atom -0.000814 0.000844 -0.001059

42 Atom 0.000969 0.000000 0.000000

43 Atom 0.000814 0.001059 0.000844

44 Atom 0.000814 -0.001059 -0.000844

45 Atom -0.000969 0.000000 0.000000

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Anisotropic Spin Dipole Couplings in Principal Axis System

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

Baa -0.1082 -14.523 -5.182 -4.844 0.0325 0.9995 0.0000

1 C(13) Bbb -0.1033 -13.866 -4.948 -4.625 0.9995 -0.0325 0.0000

Bcc 0.2116 28.389 10.130 9.469 0.0000 0.0000 1.0000

Baa -0.0921 -3.551 -1.267 -1.185 0.0000 0.0000 1.0000

2 N(14) Bbb 0.0445 1.716 0.612 0.573 0.8754 -0.4834 0.0000

Bcc 0.0476 1.835 0.655 0.612 0.4834 0.8754 0.0000

Baa -0.1121 -15.043 -5.368 -5.018 0.6181 0.7861 0.0000

3 C(13) Bbb -0.1041 -13.970 -4.985 -4.660 0.7861 -0.6181 0.0000

Bcc 0.2162 29.012 10.352 9.678 0.0000 0.0000 1.0000

Baa -0.0355 -4.768 -1.701 -1.590 0.1407 0.9900 0.0000

4 C(13) Bbb -0.0298 -3.993 -1.425 -1.332 0.9900 -0.1407 0.0000

Bcc 0.0653 8.760 3.126 2.922 0.0000 0.0000 1.0000

Baa -0.0055 -0.735 -0.262 -0.245 0.0000 0.0000 1.0000

5 C(13) Bbb 0.0012 0.163 0.058 0.054 0.8298 0.5580 0.0000

Bcc 0.0043 0.572 0.204 0.191 -0.5580 0.8298 0.0000

Baa -0.1423 -5.487 -1.958 -1.830 0.0000 0.0000 1.0000

6 N(14) Bbb 0.0631 2.432 0.868 0.811 0.9184 0.3956 0.0000

Bcc 0.0792 3.055 1.090 1.019 -0.3956 0.9184 0.0000

Baa -0.1082 -14.523 -5.182 -4.844 0.9995 -0.0325 0.0000

7 C(13) Bbb -0.1033 -13.866 -4.948 -4.625 0.0325 0.9995 0.0000

Bcc 0.2116 28.389 10.130 9.469 0.0000 0.0000 1.0000

Baa -0.0921 -3.551 -1.267 -1.185 0.0000 0.0000 1.0000

8 N(14) Bbb 0.0445 1.716 0.612 0.573 0.4834 0.8754 0.0000

Bcc 0.0476 1.835 0.655 0.612 0.8754 -0.4834 0.0000

Baa -0.1121 -15.043 -5.368 -5.018 0.7861 -0.6181 0.0000

9 C(13) Bbb -0.1041 -13.970 -4.985 -4.660 0.6181 0.7861 0.0000

Bcc 0.2162 29.012 10.352 9.678 0.0000 0.0000 1.0000

Baa -0.0355 -4.768 -1.701 -1.590 0.9900 -0.1407 0.0000

10 C(13) Bbb -0.0298 -3.993 -1.425 -1.332 0.1407 0.9900 0.0000

Bcc 0.0653 8.760 3.126 2.922 0.0000 0.0000 1.0000

Baa -0.0055 -0.735 -0.262 -0.245 0.0000 0.0000 1.0000

11 C(13) Bbb 0.0012 0.163 0.058 0.054 -0.5580 0.8298 0.0000

Bcc 0.0043 0.572 0.204 0.191 0.8298 0.5580 0.0000

Baa -0.1423 -5.487 -1.958 -1.830 0.0000 0.0000 1.0000

12 N(14) Bbb 0.0631 2.432 0.868 0.811 -0.3956 0.9184 0.0000

Bcc 0.0792 3.055 1.090 1.019 0.9184 0.3956 0.0000

Baa -0.0355 -4.768 -1.701 -1.590 0.9900 -0.1407 0.0000

13 C(13) Bbb -0.0298 -3.993 -1.425 -1.332 0.1407 0.9900 0.0000

Bcc 0.0653 8.760 3.126 2.922 0.0000 0.0000 1.0000

Baa -0.0055 -0.735 -0.262 -0.245 0.0000 0.0000 1.0000

14 C(13) Bbb 0.0012 0.163 0.058 0.054 -0.5580 0.8298 0.0000

Bcc 0.0043 0.572 0.204 0.191 0.8298 0.5580 0.0000

Baa -0.1082 -14.523 -5.182 -4.844 0.9995 -0.0325 0.0000

15 C(13) Bbb -0.1033 -13.866 -4.948 -4.625 0.0325 0.9995 0.0000

Bcc 0.2116 28.389 10.130 9.469 0.0000 0.0000 1.0000

Baa -0.0921 -3.551 -1.267 -1.185 0.0000 0.0000 1.0000

16 N(14) Bbb 0.0445 1.716 0.612 0.573 0.4834 0.8754 0.0000

Bcc 0.0476 1.835 0.655 0.612 0.8754 -0.4834 0.0000

Baa -0.1121 -15.043 -5.368 -5.018 0.7861 -0.6181 0.0000

17 C(13) Bbb -0.1041 -13.970 -4.985 -4.660 0.6181 0.7861 0.0000

Bcc 0.2162 29.012 10.352 9.678 0.0000 0.0000 1.0000

Baa -0.1423 -5.487 -1.958 -1.830 0.0000 0.0000 1.0000

18 N(14) Bbb 0.0631 2.432 0.868 0.811 0.9184 0.3956 0.0000

Bcc 0.0792 3.055 1.090 1.019 -0.3956 0.9184 0.0000

Baa -0.0921 -3.551 -1.267 -1.185 0.0000 0.0000 1.0000

19 N(14) Bbb 0.0445 1.716 0.612 0.573 0.8754 -0.4834 0.0000

Bcc 0.0476 1.835 0.655 0.612 0.4834 0.8754 0.0000

Baa -0.1121 -15.043 -5.368 -5.018 0.6181 0.7861 0.0000

20 C(13) Bbb -0.1041 -13.970 -4.985 -4.660 0.7861 -0.6181 0.0000

Bcc 0.2162 29.012 10.352 9.678 0.0000 0.0000 1.0000

Baa -0.0355 -4.768 -1.701 -1.590 0.1407 0.9900 0.0000

21 C(13) Bbb -0.0298 -3.993 -1.425 -1.332 0.9900 -0.1407 0.0000

Bcc 0.0653 8.760 3.126 2.922 0.0000 0.0000 1.0000

Baa -0.0055 -0.735 -0.262 -0.245 0.0000 0.0000 1.0000

22 C(13) Bbb 0.0012 0.163 0.058 0.054 0.8298 0.5580 0.0000

Bcc 0.0043 0.572 0.204 0.191 -0.5580 0.8298 0.0000

Baa -0.1082 -14.523 -5.182 -4.844 0.0325 0.9995 0.0000

23 C(13) Bbb -0.1033 -13.866 -4.948 -4.625 0.9995 -0.0325 0.0000

Bcc 0.2116 28.389 10.130 9.469 0.0000 0.0000 1.0000

Baa -0.1423 -5.487 -1.958 -1.830 0.0000 0.0000 1.0000

24 N(14) Bbb 0.0631 2.432 0.868 0.811 -0.3956 0.9184 0.0000

Bcc 0.0792 3.055 1.090 1.019 0.9184 0.3956 0.0000

Baa -0.0069 -0.232 -0.083 -0.078 0.0000 0.0000 1.0000

25 Zn(67) Bbb 0.0035 0.116 0.041 0.039 -0.0039 1.0000 0.0000

Bcc 0.0035 0.116 0.041 0.039 1.0000 0.0039 0.0000

Baa -0.0042 -0.559 -0.199 -0.186 0.0623 0.9981 0.0000

26 C(13) Bbb 0.0007 0.099 0.035 0.033 0.9981 -0.0623 0.0000

Bcc 0.0034 0.460 0.164 0.153 0.0000 0.0000 1.0000

Baa -0.0020 -1.052 -0.375 -0.351 0.0000 0.0000 1.0000

27 H(1) Bbb -0.0015 -0.786 -0.281 -0.262 0.5681 0.8230 0.0000

Bcc 0.0034 1.838 0.656 0.613 0.8230 -0.5681 0.0000

Baa -0.0042 -0.559 -0.199 -0.186 0.9981 -0.0623 0.0000

28 C(13) Bbb 0.0007 0.099 0.035 0.033 0.0623 0.9981 0.0000

Bcc 0.0034 0.460 0.164 0.153 0.0000 0.0000 1.0000

Baa -0.0020 -1.052 -0.375 -0.351 0.0000 0.0000 1.0000

29 H(1) Bbb -0.0015 -0.786 -0.281 -0.262 0.8230 -0.5681 0.0000

Bcc 0.0034 1.838 0.656 0.613 0.5681 0.8230 0.0000

Baa -0.0042 -0.559 -0.199 -0.186 0.9981 -0.0623 0.0000

30 C(13) Bbb 0.0007 0.099 0.035 0.033 0.0623 0.9981 0.0000

Bcc 0.0034 0.460 0.164 0.153 0.0000 0.0000 1.0000

Baa -0.0020 -1.052 -0.375 -0.351 0.0000 0.0000 1.0000

31 H(1) Bbb -0.0015 -0.786 -0.281 -0.262 0.8230 -0.5681 0.0000

Bcc 0.0034 1.838 0.656 0.613 0.5681 0.8230 0.0000

Baa -0.0042 -0.559 -0.199 -0.186 0.0623 0.9981 0.0000

32 C(13) Bbb 0.0007 0.099 0.035 0.033 0.9981 -0.0623 0.0000

Bcc 0.0034 0.460 0.164 0.153 0.0000 0.0000 1.0000

Baa -0.0020 -1.052 -0.375 -0.351 0.0000 0.0000 1.0000

33 H(1) Bbb -0.0015 -0.786 -0.281 -0.262 0.5681 0.8230 0.0000

Bcc 0.0034 1.838 0.656 0.613 0.8230 -0.5681 0.0000

Baa -0.0011 -0.590 -0.211 -0.197 0.0000 0.0000 1.0000

34 H(1) Bbb -0.0010 -0.550 -0.196 -0.183 0.3233 0.9463 0.0000

Bcc 0.0021 1.140 0.407 0.380 0.9463 -0.3233 0.0000

Baa -0.0018 -0.987 -0.352 -0.329 0.0916 0.6032 0.7923

35 H(1) Bbb -0.0007 -0.398 -0.142 -0.133 -0.4270 0.7426 -0.5160

Bcc 0.0026 1.385 0.494 0.462 0.8996 0.2910 -0.3256

Baa -0.0018 -0.987 -0.352 -0.329 -0.0916 -0.6032 0.7923

36 H(1) Bbb -0.0007 -0.398 -0.142 -0.133 -0.4270 0.7426 0.5160

Bcc 0.0026 1.385 0.494 0.462 0.8996 0.2910 0.3256

Baa -0.0018 -0.987 -0.352 -0.329 -0.6032 0.0916 0.7923

37 H(1) Bbb -0.0007 -0.398 -0.142 -0.133 0.7426 0.4270 0.5160

Bcc 0.0026 1.385 0.494 0.462 -0.2910 0.8996 -0.3256

Baa -0.0018 -0.987 -0.352 -0.329 0.6032 -0.0916 0.7923

38 H(1) Bbb -0.0007 -0.398 -0.142 -0.133 0.7426 0.4270 -0.5160

Bcc 0.0026 1.385 0.494 0.462 -0.2910 0.8996 0.3256

Baa -0.0011 -0.590 -0.211 -0.197 0.0000 0.0000 1.0000

39 H(1) Bbb -0.0010 -0.550 -0.196 -0.183 0.9463 -0.3233 0.0000

Bcc 0.0021 1.140 0.407 0.380 0.3233 0.9463 0.0000

Baa -0.0018 -0.987 -0.352 -0.329 0.6032 -0.0916 0.7923

40 H(1) Bbb -0.0007 -0.398 -0.142 -0.133 0.7426 0.4270 -0.5160

Bcc 0.0026 1.385 0.494 0.462 -0.2910 0.8996 0.3256

Baa -0.0018 -0.987 -0.352 -0.329 -0.6032 0.0916 0.7923

41 H(1) Bbb -0.0007 -0.398 -0.142 -0.133 0.7426 0.4270 0.5160

Bcc 0.0026 1.385 0.494 0.462 -0.2910 0.8996 -0.3256

Baa -0.0011 -0.590 -0.211 -0.197 0.0000 0.0000 1.0000

42 H(1) Bbb -0.0010 -0.550 -0.196 -0.183 0.9463 -0.3233 0.0000

Bcc 0.0021 1.140 0.407 0.380 0.3233 0.9463 0.0000

Baa -0.0018 -0.987 -0.352 -0.329 -0.0916 -0.6032 0.7923

43 H(1) Bbb -0.0007 -0.398 -0.142 -0.133 -0.4270 0.7426 0.5160

Bcc 0.0026 1.385 0.494 0.462 0.8996 0.2910 0.3256

Baa -0.0018 -0.987 -0.352 -0.329 0.0916 0.6032 0.7923

44 H(1) Bbb -0.0007 -0.398 -0.142 -0.133 -0.4270 0.7426 -0.5160

Bcc 0.0026 1.385 0.494 0.462 0.8996 0.2910 -0.3256

Baa -0.0011 -0.590 -0.211 -0.197 0.0000 0.0000 1.0000

45 H(1) Bbb -0.0010 -0.550 -0.196 -0.183 0.3233 0.9463 0.0000

Bcc 0.0021 1.140 0.407 0.380 0.9463 -0.3233 0.0000

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No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Fri Jul 5 21:08:41 2019, MaxMem= 1342177280 cpu: 16.6

(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= 19306 NPrTT= 91506 LenC2= 15315 LenP2D= 41224.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 254

Leave Link 701 at Fri Jul 5 21:08:46 2019, MaxMem= 1342177280 cpu: 54.2

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

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

Leave Link 702 at Fri Jul 5 21:08:46 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= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Fri Jul 5 21:08:54 2019, MaxMem= 1342177280 cpu: 91.6

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

Dipole =-1.40332190D-13 1.33226763D-15-4.44089210D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.002910864 0.007310752 0.000000000

2 7 0.000680794 -0.003050920 0.000000000

3 6 0.007020202 0.014221933 0.000000000

4 6 -0.015410626 -0.006780355 0.000000000

5 6 0.007985139 -0.009773662 0.000000000

6 7 -0.002170522 0.000597974 0.000000000

7 6 -0.007310752 0.002910864 0.000000000

8 7 0.003050920 0.000680794 0.000000000

9 6 -0.014221933 0.007020202 0.000000000

10 6 0.006780355 -0.015410626 0.000000000

11 6 0.009773662 0.007985139 0.000000000

12 7 0.000597974 0.002170522 0.000000000

13 6 -0.006780355 0.015410626 0.000000000

14 6 -0.009773662 -0.007985139 0.000000000

15 6 0.007310752 -0.002910864 0.000000000

16 7 -0.003050920 -0.000680794 0.000000000

17 6 0.014221933 -0.007020202 0.000000000

18 7 0.002170522 -0.000597974 0.000000000

19 7 -0.000680794 0.003050920 0.000000000

20 6 -0.007020202 -0.014221933 0.000000000

21 6 0.015410626 0.006780355 0.000000000

22 6 -0.007985139 0.009773662 0.000000000

23 6 -0.002910864 -0.007310752 0.000000000

24 7 -0.000597974 -0.002170522 0.000000000

25 30 0.000000000 0.000000000 0.000000000

26 6 0.000208115 0.001267614 0.000000000

27 1 0.001315226 0.001055427 0.000000000

28 6 -0.001267614 0.000208115 0.000000000

29 1 -0.001055427 0.001315226 0.000000000

30 6 0.001267614 -0.000208115 0.000000000

31 1 0.001055427 -0.001315226 0.000000000

32 6 -0.000208115 -0.001267614 0.000000000

33 1 -0.001315226 -0.001055427 0.000000000

34 1 0.001411382 0.001182284 0.000000000

35 1 -0.001205848 0.001010923 -0.003187130

36 1 -0.001205848 0.001010923 0.003187130

37 1 -0.001010923 -0.001205848 -0.003187130

38 1 -0.001010923 -0.001205848 0.003187130

39 1 -0.001182284 0.001411382 0.000000000

40 1 0.001010923 0.001205848 -0.003187130

41 1 0.001010923 0.001205848 0.003187130

42 1 0.001182284 -0.001411382 0.000000000

43 1 0.001205848 -0.001010923 -0.003187130

44 1 0.001205848 -0.001010923 0.003187130

45 1 -0.001411382 -0.001182284 0.000000000

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

Cartesian Forces: Max 0.015410626 RMS 0.004881427

Leave Link 716 at Fri Jul 5 21:08:54 2019, MaxMem= 1342177280 cpu: 0.4

(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 0.010999812 RMS 0.002346279

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 = .23463D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Second derivative matrix not updated -- first step.

ITU= 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01333

Eigenvalues --- 0.01336 0.01336 0.01336 0.01604 0.01623

Eigenvalues --- 0.01636 0.01636 0.01772 0.01788 0.01811

Eigenvalues --- 0.01811 0.01885 0.01901 0.01940 0.01940

Eigenvalues --- 0.01997 0.01998 0.02045 0.02045 0.02070

Eigenvalues --- 0.02086 0.02100 0.02111 0.02111 0.02205

Eigenvalues --- 0.02317 0.02317 0.02353 0.02374 0.07287

Eigenvalues --- 0.07287 0.07287 0.07287 0.07341 0.07341

Eigenvalues --- 0.07341 0.07341 0.14497 0.14497 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16499 0.18264 0.22088 0.22088 0.23816

Eigenvalues --- 0.23854 0.23854 0.23879 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.33191 0.33191 0.33222 0.33234

Eigenvalues --- 0.33282 0.33282 0.33282 0.33282 0.33724

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.34437 0.34437 0.34437

Eigenvalues --- 0.34437 0.35364 0.35417 0.35563 0.35563

Eigenvalues --- 0.35682 0.35682 0.35682 0.35682 0.39288

Eigenvalues --- 0.41735 0.41735 0.42785 0.47883 0.48973

Eigenvalues --- 0.48973 0.49843 0.50268 0.50571 0.51360

Eigenvalues --- 0.51360 0.51797 0.53989 0.53989 0.54934

Eigenvalues --- 0.56287 0.56340 0.56340 0.56414

RFO step: Lambda=-3.99587473D-03 EMin= 8.77959372D-03

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.01151218 RMS(Int)= 0.00003262

Iteration 2 RMS(Cart)= 0.00004150 RMS(Int)= 0.00000525

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000525

ITry= 1 IFail=0 DXMaxC= 4.83D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.10D-10 for atom 37.

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

(Linear) (Quad) (Total)

R1 2.57723 -0.00384 0.00000 -0.00659 -0.00660 2.57063

R2 2.76294 0.00473 0.00000 0.01239 0.01239 2.77533

R3 2.53844 -0.00244 0.00000 -0.00624 -0.00624 2.53220

R4 2.57400 -0.00713 0.00000 -0.01321 -0.01321 2.56079

R5 3.79361 -0.00485 0.00000 -0.02108 -0.02109 3.77253

R6 2.79211 0.00863 0.00000 0.02391 0.02391 2.81601

R7 2.53307 -0.00383 0.00000 -0.00875 -0.00875 2.52433

R8 2.58757 -0.01100 0.00000 -0.02248 -0.02248 2.56509

R9 2.81859 -0.00446 0.00000 -0.01325 -0.01325 2.80534

R10 2.04583 -0.00168 0.00000 -0.00465 -0.00465 2.04117

R11 2.53844 -0.00244 0.00000 -0.00624 -0.00624 2.53220

R12 2.57723 -0.00384 0.00000 -0.00659 -0.00660 2.57063

R13 2.76294 0.00473 0.00000 0.01239 0.01239 2.77533

R14 2.57400 -0.00713 0.00000 -0.01321 -0.01321 2.56079

R15 3.79361 -0.00485 0.00000 -0.02108 -0.02109 3.77253

R16 2.79211 0.00863 0.00000 0.02391 0.02391 2.81601

R17 2.53307 -0.00383 0.00000 -0.00875 -0.00875 2.52433

R18 2.58757 -0.01100 0.00000 -0.02248 -0.02248 2.56509

R19 2.81859 -0.00446 0.00000 -0.01325 -0.01325 2.80534

R20 2.04583 -0.00168 0.00000 -0.00465 -0.00465 2.04117

R21 2.53307 -0.00383 0.00000 -0.00875 -0.00875 2.52433

R22 2.58757 -0.01100 0.00000 -0.02248 -0.02248 2.56509

R23 2.79211 0.00863 0.00000 0.02391 0.02391 2.81601

R24 2.81859 -0.00446 0.00000 -0.01325 -0.01325 2.80534

R25 2.76294 0.00473 0.00000 0.01239 0.01239 2.77533

R26 2.04583 -0.00168 0.00000 -0.00465 -0.00465 2.04117

R27 2.57723 -0.00384 0.00000 -0.00659 -0.00660 2.57063

R28 2.53844 -0.00244 0.00000 -0.00624 -0.00624 2.53220

R29 2.57400 -0.00713 0.00000 -0.01321 -0.01321 2.56079

R30 3.79361 -0.00485 0.00000 -0.02108 -0.02109 3.77253

R31 2.53307 -0.00383 0.00000 -0.00875 -0.00875 2.52433

R32 2.57400 -0.00713 0.00000 -0.01321 -0.01321 2.56079

R33 2.57723 -0.00384 0.00000 -0.00659 -0.00660 2.57063

R34 3.79361 -0.00485 0.00000 -0.02108 -0.02109 3.77253

R35 2.79211 0.00863 0.00000 0.02391 0.02391 2.81601

R36 2.58757 -0.01100 0.00000 -0.02248 -0.02248 2.56509

R37 2.81859 -0.00446 0.00000 -0.01325 -0.01325 2.80534

R38 2.76294 0.00473 0.00000 0.01239 0.01239 2.77533

R39 2.04583 -0.00168 0.00000 -0.00465 -0.00465 2.04117

R40 2.53844 -0.00244 0.00000 -0.00624 -0.00624 2.53220

R41 2.06599 -0.00186 0.00000 -0.00535 -0.00535 2.06064

R42 2.07798 -0.00343 0.00000 -0.01004 -0.01004 2.06794

R43 2.07798 -0.00343 0.00000 -0.01004 -0.01004 2.06794

R44 2.07798 -0.00343 0.00000 -0.01004 -0.01004 2.06794

R45 2.07798 -0.00343 0.00000 -0.01004 -0.01004 2.06794

R46 2.06599 -0.00186 0.00000 -0.00535 -0.00535 2.06064

R47 2.07798 -0.00343 0.00000 -0.01004 -0.01004 2.06794

R48 2.07798 -0.00343 0.00000 -0.01004 -0.01004 2.06794

R49 2.06599 -0.00186 0.00000 -0.00535 -0.00535 2.06064

R50 2.07798 -0.00343 0.00000 -0.01004 -0.01004 2.06794

R51 2.07798 -0.00343 0.00000 -0.01004 -0.01004 2.06794

R52 2.06599 -0.00186 0.00000 -0.00535 -0.00535 2.06064

A1 1.89137 0.00057 0.00000 0.00500 0.00500 1.89637

A2 2.21236 -0.00033 0.00000 -0.00114 -0.00114 2.21121

A3 2.17945 -0.00024 0.00000 -0.00386 -0.00385 2.17560

A4 1.90638 0.00059 0.00000 -0.00200 -0.00200 1.90438

A5 2.19032 -0.00015 0.00000 0.00260 0.00259 2.19291

A6 2.18649 -0.00044 0.00000 -0.00060 -0.00060 2.18589

A7 1.89647 -0.00081 0.00000 -0.00029 -0.00030 1.89617

A8 2.21943 0.00174 0.00000 0.00609 0.00610 2.22553

A9 2.16729 -0.00093 0.00000 -0.00580 -0.00580 2.16149

A10 1.85108 0.00018 0.00000 0.00006 0.00006 1.85113

A11 2.17776 -0.00165 0.00000 -0.00618 -0.00618 2.17158

A12 2.25435 0.00147 0.00000 0.00612 0.00612 2.26047

A13 1.87948 -0.00053 0.00000 -0.00276 -0.00276 1.87672

A14 2.17828 0.00004 0.00000 -0.00001 -0.00001 2.17827

A15 2.22542 0.00050 0.00000 0.00277 0.00277 2.22820

A16 2.18698 -0.00082 0.00000 -0.00695 -0.00695 2.18003

A17 2.21236 -0.00033 0.00000 -0.00114 -0.00114 2.21121

A18 2.17945 -0.00024 0.00000 -0.00386 -0.00385 2.17560

A19 1.89137 0.00057 0.00000 0.00500 0.00500 1.89637

A20 1.90638 0.00059 0.00000 -0.00200 -0.00200 1.90438

A21 2.19032 -0.00015 0.00000 0.00260 0.00259 2.19291

A22 2.18649 -0.00044 0.00000 -0.00060 -0.00060 2.18589

A23 1.89647 -0.00081 0.00000 -0.00029 -0.00030 1.89617

A24 2.21943 0.00174 0.00000 0.00609 0.00610 2.22553

A25 2.16729 -0.00093 0.00000 -0.00580 -0.00580 2.16149

A26 1.85108 0.00018 0.00000 0.00006 0.00006 1.85113

A27 2.17776 -0.00165 0.00000 -0.00618 -0.00618 2.17158

A28 2.25435 0.00147 0.00000 0.00612 0.00612 2.26047

A29 1.87948 -0.00053 0.00000 -0.00276 -0.00276 1.87672

A30 2.17828 0.00004 0.00000 -0.00001 -0.00001 2.17827

A31 2.22542 0.00050 0.00000 0.00277 0.00277 2.22820

A32 2.18698 -0.00082 0.00000 -0.00695 -0.00695 2.18003

A33 1.85108 0.00018 0.00000 0.00006 0.00006 1.85113

A34 2.25435 0.00147 0.00000 0.00612 0.00612 2.26047

A35 2.17776 -0.00165 0.00000 -0.00618 -0.00618 2.17158

A36 1.87948 -0.00053 0.00000 -0.00276 -0.00276 1.87672

A37 2.22542 0.00050 0.00000 0.00277 0.00277 2.22820

A38 2.17828 0.00004 0.00000 -0.00001 -0.00001 2.17827

A39 1.89137 0.00057 0.00000 0.00500 0.00500 1.89637

A40 2.17945 -0.00024 0.00000 -0.00386 -0.00385 2.17560

A41 2.21236 -0.00033 0.00000 -0.00114 -0.00114 2.21121

A42 1.90638 0.00059 0.00000 -0.00200 -0.00200 1.90438

A43 2.19032 -0.00015 0.00000 0.00260 0.00259 2.19291

A44 2.18649 -0.00044 0.00000 -0.00060 -0.00060 2.18589

A45 2.16729 -0.00093 0.00000 -0.00580 -0.00580 2.16149

A46 2.21943 0.00174 0.00000 0.00609 0.00610 2.22553

A47 1.89647 -0.00081 0.00000 -0.00029 -0.00030 1.89617

A48 2.18698 -0.00082 0.00000 -0.00695 -0.00695 2.18003

A49 1.90638 0.00059 0.00000 -0.00200 -0.00200 1.90438

A50 2.18649 -0.00044 0.00000 -0.00060 -0.00060 2.18589

A51 2.19032 -0.00015 0.00000 0.00260 0.00259 2.19291

A52 2.21943 0.00174 0.00000 0.00609 0.00610 2.22553

A53 2.16729 -0.00093 0.00000 -0.00580 -0.00580 2.16149

A54 1.89647 -0.00081 0.00000 -0.00029 -0.00030 1.89617

A55 1.85108 0.00018 0.00000 0.00006 0.00006 1.85113

A56 2.17776 -0.00165 0.00000 -0.00618 -0.00618 2.17158

A57 2.25435 0.00147 0.00000 0.00612 0.00612 2.26047

A58 1.87948 -0.00053 0.00000 -0.00276 -0.00276 1.87672

A59 2.22542 0.00050 0.00000 0.00277 0.00277 2.22820

A60 2.17828 0.00004 0.00000 -0.00001 -0.00001 2.17827

A61 1.89137 0.00057 0.00000 0.00500 0.00500 1.89637

A62 2.21236 -0.00033 0.00000 -0.00114 -0.00114 2.21121

A63 2.17945 -0.00024 0.00000 -0.00386 -0.00385 2.17560

A64 2.18698 -0.00082 0.00000 -0.00695 -0.00695 2.18003

A65 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A66 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A67 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A68 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A69 1.93538 0.00031 0.00000 0.00419 0.00419 1.93957

A70 1.93656 -0.00027 0.00000 -0.00275 -0.00277 1.93379

A71 1.93656 -0.00027 0.00000 -0.00275 -0.00277 1.93379

A72 1.89112 0.00038 0.00000 0.00446 0.00446 1.89557

A73 1.89112 0.00038 0.00000 0.00446 0.00446 1.89557

A74 1.87099 -0.00054 0.00000 -0.00765 -0.00768 1.86331

A75 1.93656 -0.00027 0.00000 -0.00275 -0.00277 1.93379

A76 1.93656 -0.00027 0.00000 -0.00275 -0.00277 1.93379

A77 1.93538 0.00031 0.00000 0.00419 0.00419 1.93957

A78 1.87099 -0.00054 0.00000 -0.00765 -0.00768 1.86331

A79 1.89112 0.00038 0.00000 0.00446 0.00446 1.89557

A80 1.89112 0.00038 0.00000 0.00446 0.00446 1.89557

A81 1.93656 -0.00027 0.00000 -0.00275 -0.00277 1.93379

A82 1.93656 -0.00027 0.00000 -0.00275 -0.00277 1.93379

A83 1.93538 0.00031 0.00000 0.00419 0.00419 1.93957

A84 1.87099 -0.00054 0.00000 -0.00765 -0.00768 1.86331

A85 1.89112 0.00038 0.00000 0.00446 0.00446 1.89557

A86 1.89112 0.00038 0.00000 0.00446 0.00446 1.89557

A87 1.93656 -0.00027 0.00000 -0.00275 -0.00277 1.93379

A88 1.93656 -0.00027 0.00000 -0.00275 -0.00277 1.93379

A89 1.93538 0.00031 0.00000 0.00419 0.00419 1.93957

A90 1.87099 -0.00054 0.00000 -0.00765 -0.00768 1.86331

A91 1.89112 0.00038 0.00000 0.00446 0.00446 1.89557

A92 1.89112 0.00038 0.00000 0.00446 0.00446 1.89557

A93 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A94 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A95 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A96 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D2 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D3 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D4 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D7 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D10 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D11 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D12 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D13 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D18 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D24 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D25 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D26 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D27 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D28 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D29 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D30 1.03902 -0.00051 0.00000 -0.00659 -0.00658 1.03244

D31 -1.03902 0.00051 0.00000 0.00659 0.00658 -1.03244

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10257 -0.00051 0.00000 -0.00659 -0.00658 -2.10915

D34 2.10257 0.00051 0.00000 0.00659 0.00658 2.10915

D35 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D36 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D37 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D38 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D39 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D40 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D41 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D42 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D43 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D44 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D45 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D46 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D47 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D48 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D49 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D50 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D51 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D52 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D56 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D57 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D58 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D59 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D60 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D61 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D62 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D63 1.03902 -0.00051 0.00000 -0.00659 -0.00658 1.03244

D64 -1.03902 0.00051 0.00000 0.00659 0.00658 -1.03244

D65 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.10257 -0.00051 0.00000 -0.00659 -0.00658 -2.10915

D67 2.10257 0.00051 0.00000 0.00659 0.00658 2.10915

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D70 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D71 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D72 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D73 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D74 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D75 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D76 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D77 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D78 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D79 -2.10257 -0.00051 0.00000 -0.00659 -0.00658 -2.10915

D80 2.10257 0.00051 0.00000 0.00659 0.00658 2.10915

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.03902 -0.00051 0.00000 -0.00659 -0.00658 1.03244

D83 -1.03902 0.00051 0.00000 0.00659 0.00658 -1.03244

D84 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D85 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D86 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D87 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D88 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D89 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D90 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D91 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D92 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D93 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D94 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D95 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D96 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D97 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D98 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D99 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D100 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D101 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D102 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D103 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D104 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D105 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D106 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D107 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D108 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D109 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D110 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D111 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D112 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D113 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D114 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D117 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D120 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D121 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D122 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D123 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D124 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D125 1.03902 -0.00051 0.00000 -0.00659 -0.00658 1.03244

D126 -1.03902 0.00051 0.00000 0.00659 0.00658 -1.03244

D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D128 -2.10257 -0.00051 0.00000 -0.00659 -0.00658 -2.10915

D129 2.10257 0.00051 0.00000 0.00659 0.00658 2.10915

D130 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D131 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D132 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D133 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D134 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.011000 0.000450 NO

RMS Force 0.002346 0.000300 NO

Maximum Displacement 0.048338 0.001800 NO

RMS Displacement 0.011520 0.001200 NO

Predicted change in Energy=-2.021879D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 5 21:08:54 2019, MaxMem= 1342177280 cpu: 1.6

(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 -2.059287 -2.181809 0.000000

2 7 0 -0.738920 -1.854548 0.000000

3 6 0 -0.000206 -2.990610 0.000000

4 6 0 -0.924270 -4.159674 0.000000

5 6 0 -2.180482 -3.645442 0.000000

6 7 0 1.331529 -3.094943 0.000000

7 6 0 2.181809 -2.059287 0.000000

8 7 0 1.854548 -0.738920 0.000000

9 6 0 2.990610 -0.000206 0.000000

10 6 0 4.159674 -0.924270 0.000000

11 6 0 3.645442 -2.180482 0.000000

12 7 0 -3.094943 -1.331529 0.000000

13 6 0 -4.159674 0.924270 0.000000

14 6 0 -3.645442 2.180482 0.000000

15 6 0 -2.181809 2.059287 0.000000

16 7 0 -1.854548 0.738920 0.000000

17 6 0 -2.990610 0.000206 0.000000

18 7 0 -1.331529 3.094943 0.000000

19 7 0 0.738920 1.854548 0.000000

20 6 0 0.000206 2.990610 0.000000

21 6 0 0.924270 4.159674 0.000000

22 6 0 2.180482 3.645442 0.000000

23 6 0 2.059287 2.181809 0.000000

24 7 0 3.094943 1.331529 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.483956 -5.577392 0.000000

27 1 0 -3.115233 -4.186688 0.000000

28 6 0 5.577392 -0.483956 0.000000

29 1 0 4.186688 -3.115233 0.000000

30 6 0 -5.577392 0.483956 0.000000

31 1 0 -4.186688 3.115233 0.000000

32 6 0 0.483956 5.577392 0.000000

33 1 0 3.115233 4.186688 0.000000

34 1 0 -1.338734 -6.254460 0.000000

35 1 0 0.132206 -5.792895 0.878298

36 1 0 0.132206 -5.792895 -0.878298

37 1 0 5.792895 0.132206 0.878298

38 1 0 5.792895 0.132206 -0.878298

39 1 0 6.254460 -1.338734 0.000000

40 1 0 -5.792895 -0.132206 0.878298

41 1 0 -5.792895 -0.132206 -0.878298

42 1 0 -6.254460 1.338734 0.000000

43 1 0 -0.132206 5.792895 0.878298

44 1 0 -0.132206 5.792895 -0.878298

45 1 0 1.338734 6.254460 0.000000

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Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.360320 0.000000

3 C 2.212233 1.355114 0.000000

4 C 2.280398 2.312565 1.490169 0.000000

5 C 1.468642 2.299001 2.276491 1.357389 0.000000

6 N 3.511616 2.413574 1.335816 2.494450 3.554894

7 C 4.242866 2.927896 2.372457 3.749580 4.641711

8 N 4.171336 2.823244 2.917229 4.407197 4.972861

9 C 5.500987 4.165090 4.229361 5.712045 6.326764

10 C 6.344831 4.986145 4.644821 6.026137 6.899447

11 C 5.704730 4.396460 3.734576 4.979906 6.007288

12 N 1.339985 2.413379 3.511402 3.565141 2.488058

13 C 3.749580 4.407197 5.712045 6.026137 4.979906

14 C 4.641711 4.972861 6.326764 6.899447 6.007288

15 C 4.242866 4.171336 5.500987 6.344831 5.704730

16 N 2.927896 2.823244 4.165090 4.986145 4.396460

17 C 2.372457 2.917229 4.229361 4.644821 3.734576

18 N 5.326702 4.984843 6.229477 7.266040 6.793638

19 N 4.911430 3.992670 4.901211 6.239958 6.226782

20 C 5.567354 4.901211 5.981220 7.209800 6.985169

21 C 7.008282 6.239958 7.209800 8.522244 8.399960

22 C 7.206421 6.226782 6.985169 8.399960 8.495588

23 C 6.000319 4.911430 5.567354 7.008282 7.206421

24 N 6.237759 4.984937 5.316092 6.804953 7.252611

25 Zn 3.000159 1.996335 2.990610 4.261122 4.247794

26 C 3.743213 3.731564 2.631626 1.484520 2.571115

27 H 2.265957 3.329525 3.336764 2.191130 1.080142

28 C 7.823143 6.463305 6.114974 7.468768 8.377327

29 H 6.315337 5.084382 4.188748 5.216583 6.389208

30 C 4.413996 5.373957 6.570967 6.573800 5.347048

31 H 5.708283 6.048622 7.403239 7.972932 7.052063

32 C 8.165371 7.531876 8.581670 9.838371 9.599995

33 H 8.205694 7.165963 7.824293 9.272504 9.454463

34 H 4.135902 4.440608 3.527659 2.135395 2.741444

35 H 4.314394 4.128056 2.939684 2.134235 3.275895

36 H 4.314394 4.128056 2.939684 2.134235 3.275895

37 H 8.233034 6.883546 6.639534 8.019473 8.866611

38 H 8.233034 6.883546 6.639534 8.019473 8.866611

39 H 8.356385 7.012377 6.469122 7.713097 8.744665

40 H 4.348806 5.411149 6.518982 6.379296 5.115053

41 H 4.348806 5.411149 6.518982 6.379296 5.115053

42 H 5.476651 6.373244 7.606505 7.657900 6.437338

43 H 8.251119 7.721587 8.828295 10.022595 9.697889

44 H 8.251119 7.721587 8.828295 10.022595 9.697889

45 H 9.094900 8.370942 9.341525 10.657175 10.506805

6 7 8 9 10

6 N 0.000000

7 C 1.339985 0.000000

8 N 2.413379 1.360320 0.000000

9 C 3.511402 2.212233 1.355114 0.000000

10 C 3.565141 2.280398 2.312565 1.490169 0.000000

11 C 2.488058 1.468642 2.299001 2.276491 1.357389

12 N 4.764797 5.326702 4.984843 6.229477 7.266040

13 C 6.804953 7.008282 6.239958 7.209800 8.522244

14 C 7.252611 7.206421 6.226782 6.985169 8.399960

15 C 6.237759 6.000319 4.911430 5.567354 7.008282

16 N 4.984937 4.911430 3.992670 4.901211 6.239958

17 C 5.316092 5.567354 4.901211 5.981220 7.209800

18 N 6.738440 6.237759 4.984937 5.316092 6.804953

19 N 4.984843 4.171336 2.823244 2.917229 4.407197

20 C 6.229477 5.500987 4.165090 4.229361 5.712045

21 C 7.266040 6.344831 4.986145 4.644821 6.026137

22 C 6.793638 5.704730 4.396460 3.734576 4.979906

23 C 5.326702 4.242866 2.927896 2.372457 3.749580

24 N 4.764797 3.511616 2.413574 1.335816 2.494450

25 Zn 3.369220 3.000159 1.996335 2.990610 4.261122

26 C 3.075473 4.413996 5.373957 6.570967 6.573800

27 H 4.578821 5.708283 6.048622 7.403239 7.972932

28 C 4.984436 3.743213 3.731564 2.631626 1.484520

29 H 2.855231 2.265957 3.329525 3.336764 2.191130

30 C 7.780855 8.165371 7.531876 8.581670 9.838371

31 H 8.307648 8.205694 7.165963 7.824293 9.272504

32 C 8.713655 7.823143 6.463305 6.114974 7.468768

33 H 7.496916 6.315337 5.084382 4.188748 5.216583

34 H 4.136769 5.476651 6.373244 7.606505 7.657900

35 H 3.080378 4.348806 5.411149 6.518982 6.379296

36 H 3.080378 4.348806 5.411149 6.518982 6.379296

37 H 5.575813 4.314394 4.128056 2.939684 2.134235

38 H 5.575813 4.314394 4.128056 2.939684 2.134235

39 H 5.226808 4.135902 4.440608 3.527659 2.135395

40 H 7.765735 8.251119 7.721587 8.828295 10.022595

41 H 7.765735 8.251119 7.721587 8.828295 10.022595

42 H 8.786623 9.094900 8.370942 9.341525 10.657175

43 H 9.050282 8.233034 6.883546 6.639534 8.019473

44 H 9.050282 8.233034 6.883546 6.639534 8.019473

45 H 9.349407 8.356385 7.012377 6.469122 7.713097

11 12 13 14 15

11 C 0.000000

12 N 6.793638 0.000000

13 C 8.399960 2.494450 0.000000

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16 N 6.226782 2.413574 2.312565 2.299001 1.360320

17 C 6.985169 1.335816 1.490169 2.276491 2.212233

18 N 7.252611 4.764797 3.565141 2.488058 1.339985

19 N 4.972861 4.984937 4.986145 4.396460 2.927896

20 C 6.326764 5.316092 4.644821 3.734576 2.372457

21 C 6.899447 6.804953 6.026137 4.979906 3.749580

22 C 6.007288 7.252611 6.899447 6.007288 4.641711

23 C 4.641711 6.237759 6.344831 5.704730 4.242866

24 N 3.554894 6.738440 7.266040 6.793638 5.326702

25 Zn 4.247794 3.369220 4.261122 4.247794 3.000159

26 C 5.347048 4.984436 7.468768 8.377327 7.823143

27 H 7.052063 2.855231 5.216583 6.389208 6.315337

28 C 2.571115 8.713655 9.838371 9.599995 8.165371

29 H 1.080142 7.496916 9.272504 9.454463 8.205694

30 C 9.599995 3.075473 1.484520 2.571115 3.743213

31 H 9.454463 4.578821 2.191130 1.080142 2.265957

32 C 8.377327 7.780855 6.573800 5.347048 4.413996

33 H 6.389208 8.307648 7.972932 7.052063 5.708283

34 H 6.437338 5.226808 7.713097 8.744665 8.356385

35 H 5.115053 5.575813 8.019473 8.866611 8.233034

36 H 5.115053 5.575813 8.019473 8.866611 8.233034

37 H 3.275895 9.050282 10.022595 9.697889 8.251119

38 H 3.275895 9.050282 10.022595 9.697889 8.251119

39 H 2.741444 9.349407 10.657175 10.506805 9.094900

40 H 9.697889 3.080378 2.134235 3.275895 4.314394

41 H 9.697889 3.080378 2.134235 3.275895 4.314394

42 H 10.506805 4.136769 2.135395 2.741444 4.135902

43 H 8.866611 7.765735 6.379296 5.115053 4.348806

44 H 8.866611 7.765735 6.379296 5.115053 4.348806

45 H 8.744665 8.786623 7.657900 6.437338 5.476651

16 17 18 19 20

16 N 0.000000

17 C 1.355114 0.000000

18 N 2.413379 3.511402 0.000000

19 N 2.823244 4.165090 2.413574 0.000000

20 C 2.917229 4.229361 1.335816 1.355114 0.000000

21 C 4.407197 5.712045 2.494450 2.312565 1.490169

22 C 4.972861 6.326764 3.554894 2.299001 2.276491

23 C 4.171336 5.500987 3.511616 1.360320 2.212233

24 N 4.984843 6.229477 4.764797 2.413379 3.511402

25 Zn 1.996335 2.990610 3.369220 1.996335 2.990610

26 C 6.463305 6.114974 8.713655 7.531876 8.581670

27 H 5.084382 4.188748 7.496916 7.165963 7.824293

28 C 7.531876 8.581670 7.780855 5.373957 6.570967

29 H 7.165963 7.824293 8.307648 6.048622 7.403239

30 C 3.731564 2.631626 4.984436 6.463305 6.114974

31 H 3.329525 3.336764 2.855231 5.084382 4.188748

32 C 5.373957 6.570967 3.075473 3.731564 2.631626

33 H 6.048622 7.403239 4.578821 3.329525 3.336764

34 H 7.012377 6.469122 9.349407 8.370942 9.341525

35 H 6.883546 6.639534 9.050282 7.721587 8.828295

36 H 6.883546 6.639534 9.050282 7.721587 8.828295

37 H 7.721587 8.828295 7.765735 5.411149 6.518982

38 H 7.721587 8.828295 7.765735 5.411149 6.518982

39 H 8.370942 9.341525 8.786623 6.373244 7.606505

40 H 4.128056 2.939684 5.575813 6.883546 6.639534

41 H 4.128056 2.939684 5.575813 6.883546 6.639534

42 H 4.440608 3.527659 5.226808 7.012377 6.469122

43 H 5.411149 6.518982 3.080378 4.128056 2.939684

44 H 5.411149 6.518982 3.080378 4.128056 2.939684

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21 22 23 24 25

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22 C 1.357389 0.000000

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27 H 9.272504 9.454463 8.205694 8.307648 5.218528

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29 H 7.972932 7.052063 5.708283 4.578821 5.218528

30 C 7.468768 8.377327 7.823143 8.713655 5.598349

31 H 5.216583 6.389208 6.315337 7.496916 5.218528

32 C 1.484520 2.571115 3.743213 4.984436 5.598349

33 H 2.191130 1.080142 2.265957 2.855231 5.218528

34 H 10.657175 10.506805 9.094900 8.786623 6.396130

35 H 10.022595 9.697889 8.251119 7.765735 5.860591

36 H 10.022595 9.697889 8.251119 7.765735 5.860591

37 H 6.379296 5.115053 4.348806 3.080378 5.860591

38 H 6.379296 5.115053 4.348806 3.080378 5.860591

39 H 7.657900 6.437338 5.476651 4.136769 6.396130

40 H 8.019473 8.866611 8.233034 9.050282 5.860591

41 H 8.019473 8.866611 8.233034 9.050282 5.860591

42 H 7.713097 8.744665 8.356385 9.349407 6.396130

43 H 2.134235 3.275895 4.314394 5.575813 5.860591

44 H 2.134235 3.275895 4.314394 5.575813 5.860591

45 H 2.135395 2.741444 4.135902 5.226808 6.396130

26 27 28 29 30

26 C 0.000000

27 H 2.976185 0.000000

28 C 7.917261 9.448383 0.000000

29 H 5.279881 7.380113 2.976185 0.000000

30 C 7.917261 5.279881 11.196698 10.406316 0.000000

31 H 9.448383 7.380113 10.406316 10.437056 2.976185

32 C 11.196698 10.406316 7.917261 9.448383 7.917261

33 H 10.406316 10.437056 5.279881 7.380113 9.448383

34 H 1.090444 2.726102 9.007304 6.354923 7.960683

35 H 1.094305 3.727891 7.655474 4.937621 8.530520

36 H 1.094305 3.727891 7.655474 4.937621 8.530520

37 H 8.530520 9.938763 1.094305 3.727891 11.409582

38 H 8.530520 9.938763 1.094305 3.727891 11.409582

39 H 7.960683 9.792956 1.090444 2.726102 11.971421

40 H 7.655474 4.937621 11.409582 10.452844 1.094305

41 H 7.655474 4.937621 11.409582 10.452844 1.094305

42 H 9.007304 6.354923 11.971421 11.351449 1.090444

43 H 11.409582 10.452844 8.530520 9.938763 7.655474

44 H 11.409582 10.452844 8.530520 9.938763 7.655474

45 H 11.971421 11.351449 7.960683 9.792956 9.007304

31 32 33 34 35

31 H 0.000000

32 C 5.279881 0.000000

33 H 7.380113 2.976185 0.000000

34 H 9.792956 11.971421 11.351449 0.000000

35 H 9.938763 11.409582 10.452844 1.774293 0.000000

36 H 9.938763 11.409582 10.452844 1.774293 1.756595

37 H 10.452844 7.655474 4.937621 9.613587 8.194524

38 H 10.452844 7.655474 4.937621 9.613587 8.380684

39 H 11.351449 9.007304 6.354923 9.045494 7.621873

40 H 3.727891 8.530520 9.938763 7.621873 8.194524

41 H 3.727891 8.530520 9.938763 7.621873 8.380684

42 H 2.726102 7.960683 9.792956 9.045494 9.613587

43 H 4.937621 1.094305 3.727891 12.139436 11.588808

44 H 4.937621 1.094305 3.727891 12.139436 11.721181

45 H 6.354923 1.090444 2.726102 12.792261 12.139436

36 37 38 39 40

36 H 0.000000

37 H 8.380684 0.000000

38 H 8.194524 1.756595 0.000000

39 H 7.621873 1.774293 1.774293 0.000000

40 H 8.380684 11.588808 11.721181 12.139436 0.000000

41 H 8.194524 11.721181 11.588808 12.139436 1.756595

42 H 9.613587 12.139436 12.139436 12.792261 1.774293

43 H 11.721181 8.194524 8.380684 9.613587 8.194524

44 H 11.588808 8.380684 8.194524 9.613587 8.380684

45 H 12.139436 7.621873 7.621873 9.045494 9.613587

41 42 43 44 45

41 H 0.000000

42 H 1.774293 0.000000

43 H 8.380684 7.621873 0.000000

44 H 8.194524 7.621873 1.756595 0.000000

45 H 9.613587 9.045494 1.774293 1.774293 0.000000

Stoichiometry C20H16N8Zn(1+,2)

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

Deg. of freedom 20

Full point group C4H NOp 8

RotChk: IX=0 Diff= 9.74D-05

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H NOp 4

Standard orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 -2.181951 2.059137 0.000000

2 7 0 -1.854599 0.738792 0.000000

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5 6 0 -3.645593 2.180231 0.000000

6 7 0 -3.094852 -1.331743 0.000000

7 6 0 -2.059137 -2.181951 0.000000

8 7 0 -0.738792 -1.854599 0.000000

9 6 0 0.000000 -2.990610 0.000000

10 6 0 -0.923983 -4.159738 0.000000

11 6 0 -2.180231 -3.645593 0.000000

12 7 0 -1.331743 3.094852 0.000000

13 6 0 0.923983 4.159738 0.000000

14 6 0 2.180231 3.645593 0.000000

15 6 0 2.059137 2.181951 0.000000

16 7 0 0.738792 1.854599 0.000000

17 6 0 0.000000 2.990610 0.000000

18 7 0 3.094852 1.331743 0.000000

19 7 0 1.854599 -0.738792 0.000000

20 6 0 2.990610 0.000000 0.000000

21 6 0 4.159738 -0.923983 0.000000

22 6 0 3.645593 -2.180231 0.000000

23 6 0 2.181951 -2.059137 0.000000

24 7 0 1.331743 -3.094852 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.577425 0.483572 0.000000

27 1 0 -4.186903 3.114945 0.000000

28 6 0 -0.483572 -5.577425 0.000000

29 1 0 -3.114945 -4.186903 0.000000

30 6 0 0.483572 5.577425 0.000000

31 1 0 3.114945 4.186903 0.000000

32 6 0 5.577425 -0.483572 0.000000

33 1 0 4.186903 -3.114945 0.000000

34 1 0 -6.254553 1.338304 0.000000

35 1 0 -5.792886 -0.132605 0.878298

36 1 0 -5.792886 -0.132605 -0.878298

37 1 0 0.132605 -5.792886 0.878298

38 1 0 0.132605 -5.792886 -0.878298

39 1 0 -1.338304 -6.254553 0.000000

40 1 0 -0.132605 5.792886 0.878298

41 1 0 -0.132605 5.792886 -0.878298

42 1 0 1.338304 6.254553 0.000000

43 1 0 5.792886 0.132605 0.878298

44 1 0 5.792886 0.132605 -0.878298

45 1 0 6.254553 -1.338304 0.000000

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

Rotational constants (GHZ): 0.1830987 0.1830987 0.0917561

Leave Link 202 at Fri Jul 5 21:08:54 2019, MaxMem= 1342177280 cpu: 0.2

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

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

Pseudo-potential data read from rwf file.

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

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

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

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

There are 212 symmetry adapted basis functions of AG symmetry.

There are 82 symmetry adapted basis functions of BG symmetry.

There are 78 symmetry adapted basis functions of AU symmetry.

There are 204 symmetry adapted basis functions of BU symmetry.

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

102 alpha electrons 101 beta electrons

nuclear repulsion energy 2767.4139286336 Hartrees.

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

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

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

NAtoms= 45 NActive= 45 NUniq= 11 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1141878158 Hartrees.

Nuclear repulsion after empirical dispersion term = 2767.2997408178 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 = 3534

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.55D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 156

GePol: Fraction of low-weight points (<1% of avg) = 4.41%

GePol: Cavity surface area = 381.790 Ang\*\*2

GePol: Cavity volume = 378.632 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0110224291 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2767.2887183886 Hartrees.

Leave Link 301 at Fri Jul 5 21:08:54 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= 19306 NPrTT= 91506 LenC2= 15363 LenP2D= 41360.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.83D-04 NBF= 212 82 78 204

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

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Fri Jul 5 21:08:55 2019, MaxMem= 1342177280 cpu: 7.8

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 5 21:08:55 2019, MaxMem= 1342177280 cpu: 0.8

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

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

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000168 Ang= 0.02 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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

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

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7828 S= 0.5163

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= -1275.93768598349

Leave Link 401 at Fri Jul 5 21:08:58 2019, MaxMem= 1342177280 cpu: 32.8

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1138797 IEndB= 1138797 NGot= 1342177280 MDV= 1341424180

LenX= 1341424180 LenY= 1341055124

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

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

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 37467468.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.55D-15 for 272.

Iteration 1 A\*A^-1 deviation from orthogonality is 6.37D-15 for 3515 2677.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.99D-15 for 3529.

Iteration 1 A^-1\*A deviation from orthogonality is 3.89D-12 for 1538 1510.

E= -1275.69829803588

DIIS: error= 1.34D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.69829803588 IErMin= 1 ErrMin= 1.34D-03

ErrMax= 1.34D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.45D-03 BMatP= 3.45D-03

IDIUse=3 WtCom= 9.87D-01 WtEn= 1.34D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.373 Goal= None Shift= 0.000

Gap= 0.407 Goal= None Shift= 0.000

GapD= 0.373 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

RMSDP=7.41D-05 MaxDP=1.82D-03 OVMax= 6.94D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 7.41D-05 CP: 1.00D+00

E= -1275.69910529858 Delta-E= -0.000807262702 Rises=F Damp=F

DIIS: error= 4.97D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.69910529858 IErMin= 2 ErrMin= 4.97D-04

ErrMax= 4.97D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.61D-04 BMatP= 3.45D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.97D-03

Coeff-Com: 0.185D+00 0.815D+00

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

Coeff: 0.184D+00 0.816D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.081 Goal= None Shift= 0.000

RMSDP=2.47D-05 MaxDP=1.47D-03 DE=-8.07D-04 OVMax= 3.13D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.42D-05 CP: 1.00D+00 9.34D-01

E= -1275.69912140926 Delta-E= -0.000016110675 Rises=F Damp=F

DIIS: error= 5.15D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1275.69912140926 IErMin= 2 ErrMin= 4.97D-04

ErrMax= 5.15D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.18D-04 BMatP= 5.61D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.15D-03

Coeff-Com: -0.423D-02 0.490D+00 0.514D+00

Coeff-En: 0.000D+00 0.466D+00 0.534D+00

Coeff: -0.421D-02 0.490D+00 0.514D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.34D-05 MaxDP=8.10D-04 DE=-1.61D-05 OVMax= 2.18D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.87D-06 CP: 1.00D+00 9.89D-01 5.58D-01

E= -1275.69921748463 Delta-E= -0.000096075374 Rises=F Damp=F

DIIS: error= 1.46D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.69921748463 IErMin= 4 ErrMin= 1.46D-04

ErrMax= 1.46D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.09D-05 BMatP= 5.18D-04

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

Coeff-Com: -0.855D-02 0.219D+00 0.270D+00 0.519D+00

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

Coeff: -0.854D-02 0.219D+00 0.270D+00 0.520D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.92D-06 MaxDP=1.44D-04 DE=-9.61D-05 OVMax= 7.58D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.14D-06 CP: 1.00D+00 9.91D-01 5.83D-01 5.31D-01

E= -1275.69922197889 Delta-E= -0.000004494257 Rises=F Damp=F

DIIS: error= 3.51D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.69922197889 IErMin= 5 ErrMin= 3.51D-05

ErrMax= 3.51D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.92D-06 BMatP= 2.09D-05

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

Coeff-Com: -0.397D-02 0.597D-01 0.822D-01 0.276D+00 0.586D+00

Coeff: -0.397D-02 0.597D-01 0.822D-01 0.276D+00 0.586D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.10D-06 MaxDP=3.86D-05 DE=-4.49D-06 OVMax= 1.86D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 7.25D-07 CP: 1.00D+00 9.93D-01 5.80D-01 6.24D-01 7.74D-01

E= -1275.69922238436 Delta-E= -0.000000405477 Rises=F Damp=F

DIIS: error= 1.36D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.69922238436 IErMin= 6 ErrMin= 1.36D-05

ErrMax= 1.36D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.47D-07 BMatP= 1.92D-06

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

Coeff-Com: -0.116D-02 0.120D-01 0.192D-01 0.101D+00 0.289D+00 0.580D+00

Coeff: -0.116D-02 0.120D-01 0.192D-01 0.101D+00 0.289D+00 0.580D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.31D-07 MaxDP=1.41D-05 DE=-4.05D-07 OVMax= 1.05D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.71D-07 CP: 1.00D+00 9.94D-01 5.82D-01 6.31D-01 8.31D-01

CP: 8.25D-01

E= -1275.69922241599 Delta-E= -0.000000031623 Rises=F Damp=F

DIIS: error= 7.00D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.69922241599 IErMin= 7 ErrMin= 7.00D-06

ErrMax= 7.00D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.07D-08 BMatP= 1.47D-07

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

Coeff-Com: -0.101D-03-0.251D-02-0.162D-02 0.188D-01 0.764D-01 0.341D+00

Coeff-Com: 0.568D+00

Coeff: -0.101D-03-0.251D-02-0.162D-02 0.188D-01 0.764D-01 0.341D+00

Coeff: 0.568D+00

Gap= 0.104 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=1.65D-07 MaxDP=8.65D-06 DE=-3.16D-08 OVMax= 6.78D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.23D-07 CP: 1.00D+00 9.94D-01 5.83D-01 6.36D-01 8.57D-01

CP: 9.11D-01 8.23D-01

E= -1275.69922242469 Delta-E= -0.000000008709 Rises=F Damp=F

DIIS: error= 1.98D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.69922242469 IErMin= 8 ErrMin= 1.98D-06

ErrMax= 1.98D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.34D-09 BMatP= 3.07D-08

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

Coeff-Com: 0.132D-03-0.299D-02-0.377D-02-0.714D-02-0.155D-01 0.582D-01

Coeff-Com: 0.231D+00 0.741D+00

Coeff: 0.132D-03-0.299D-02-0.377D-02-0.714D-02-0.155D-01 0.582D-01

Coeff: 0.231D+00 0.741D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.26D-08 MaxDP=2.97D-06 DE=-8.71D-09 OVMax= 5.13D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.89D-08 CP: 1.00D+00 9.94D-01 5.83D-01 6.38D-01 8.66D-01

CP: 9.59D-01 1.00D+00 1.12D+00

E= -1275.69922242630 Delta-E= -0.000000001603 Rises=F Damp=F

DIIS: error= 8.48D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.69922242630 IErMin= 9 ErrMin= 8.48D-07

ErrMax= 8.48D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.22D-10 BMatP= 2.34D-09

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

Coeff-Com: 0.422D-04-0.108D-03-0.425D-03-0.443D-02-0.165D-01-0.511D-01

Coeff-Com: -0.566D-01 0.158D+00 0.971D+00

Coeff: 0.422D-04-0.108D-03-0.425D-03-0.443D-02-0.165D-01-0.511D-01

Coeff: -0.566D-01 0.158D+00 0.971D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=5.78D-08 MaxDP=2.33D-06 DE=-1.60D-09 OVMax= 3.51D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.36D-08 CP: 1.00D+00 9.94D-01 5.83D-01 6.39D-01 8.73D-01

CP: 9.92D-01 1.08D+00 1.38D+00 1.45D+00

E= -1275.69922242711 Delta-E= -0.000000000810 Rises=F Damp=F

DIIS: error= 5.30D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.69922242711 IErMin=10 ErrMin= 5.30D-07

ErrMax= 5.30D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.77D-10 BMatP= 4.22D-10

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

Coeff-Com: -0.230D-04 0.900D-03 0.998D-03 0.486D-03-0.110D-02-0.366D-01

Coeff-Com: -0.810D-01-0.131D+00 0.459D+00 0.788D+00

Coeff: -0.230D-04 0.900D-03 0.998D-03 0.486D-03-0.110D-02-0.366D-01

Coeff: -0.810D-01-0.131D+00 0.459D+00 0.788D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.16D-08 MaxDP=1.92D-06 DE=-8.10D-10 OVMax= 1.59D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.27D-08 CP: 1.00D+00 9.94D-01 5.83D-01 6.39D-01 8.76D-01

CP: 1.00D+00 1.12D+00 1.52D+00 1.76D+00 1.34D+00

E= -1275.69922242724 Delta-E= -0.000000000137 Rises=F Damp=F

DIIS: error= 3.70D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.69922242724 IErMin=11 ErrMin= 3.70D-07

ErrMax= 3.70D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.61D-11 BMatP= 1.77D-10

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

Coeff-Com: -0.186D-04 0.273D-03 0.387D-03 0.112D-02 0.427D-02 0.738D-03

Coeff-Com: -0.109D-01-0.101D+00-0.165D+00 0.246D+00 0.102D+01

Coeff: -0.186D-04 0.273D-03 0.387D-03 0.112D-02 0.427D-02 0.738D-03

Coeff: -0.109D-01-0.101D+00-0.165D+00 0.246D+00 0.102D+01

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=2.40D-08 MaxDP=1.50D-06 DE=-1.37D-10 OVMax= 1.04D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 8.14D-09 CP: 1.00D+00 9.94D-01 5.83D-01 6.39D-01 8.78D-01

CP: 1.01D+00 1.15D+00 1.60D+00 2.01D+00 1.85D+00

CP: 1.46D+00

E= -1275.69922242749 Delta-E= -0.000000000243 Rises=F Damp=F

DIIS: error= 2.57D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1275.69922242749 IErMin=12 ErrMin= 2.57D-07

ErrMax= 2.57D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.39D-11 BMatP= 4.61D-11

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

Coeff-Com: -0.591D-05-0.866D-04-0.287D-04 0.800D-03 0.363D-02 0.144D-01

Coeff-Com: 0.222D-01-0.134D-01-0.224D+00-0.839D-01 0.617D+00 0.663D+00

Coeff: -0.591D-05-0.866D-04-0.287D-04 0.800D-03 0.363D-02 0.144D-01

Coeff: 0.222D-01-0.134D-01-0.224D+00-0.839D-01 0.617D+00 0.663D+00

Gap= 0.104 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=8.45D-09 MaxDP=6.04D-07 DE=-2.43D-10 OVMax= 4.04D-06

Error on total polarization charges = 0.06020

SCF Done: E(UB3LYP) = -1275.69922243 A.U. after 12 cycles

NFock= 12 Conv=0.84D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7820 S= 0.5159

<L.S>= 0.000000000000E+00

KE= 1.320615687339D+03 PE=-8.558478107178D+03 EE= 3.194874479023D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.92

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7820, after 0.7509

Leave Link 502 at Fri Jul 5 21:10:12 2019, MaxMem= 1342177280 cpu: 852.8

(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= 19306 NPrTT= 91506 LenC2= 15363 LenP2D= 41360.

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 = 252

Leave Link 701 at Fri Jul 5 21:10:17 2019, MaxMem= 1342177280 cpu: 53.4

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

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

Leave Link 702 at Fri Jul 5 21:10:17 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= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Fri Jul 5 21:10:24 2019, MaxMem= 1342177280 cpu: 92.4

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

Dipole =-4.97379915D-14 1.62092562D-13 0.00000000D+00

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.001190550 0.002342220 0.000000000

2 7 -0.001003503 -0.003661979 0.000000000

3 6 0.003363733 0.004087129 0.000000000

4 6 -0.004271749 -0.002580000 0.000000000

5 6 0.002264445 -0.001197823 0.000000000

6 7 -0.000481261 -0.000444642 0.000000000

7 6 -0.002342220 -0.001190550 0.000000000

8 7 0.003661979 -0.001003503 0.000000000

9 6 -0.004087129 0.003363733 0.000000000

10 6 0.002580000 -0.004271749 0.000000000

11 6 0.001197823 0.002264445 0.000000000

12 7 -0.000444642 0.000481261 0.000000000

13 6 -0.002580000 0.004271749 0.000000000

14 6 -0.001197823 -0.002264445 0.000000000

15 6 0.002342220 0.001190550 0.000000000

16 7 -0.003661979 0.001003503 0.000000000

17 6 0.004087129 -0.003363733 0.000000000

18 7 0.000481261 0.000444642 0.000000000

19 7 0.001003503 0.003661979 0.000000000

20 6 -0.003363733 -0.004087129 0.000000000

21 6 0.004271749 0.002580000 0.000000000

22 6 -0.002264445 0.001197823 0.000000000

23 6 0.001190550 -0.002342220 0.000000000

24 7 0.000444642 -0.000481261 0.000000000

25 30 0.000000000 0.000000000 0.000000000

26 6 0.000261417 0.000650376 0.000000000

27 1 -0.000340192 0.000524067 0.000000000

28 6 -0.000650376 0.000261417 0.000000000

29 1 -0.000524067 -0.000340192 0.000000000

30 6 0.000650376 -0.000261417 0.000000000

31 1 0.000524067 0.000340192 0.000000000

32 6 -0.000261417 -0.000650376 0.000000000

33 1 0.000340192 -0.000524067 0.000000000

34 1 0.000063217 -0.000023112 0.000000000

35 1 0.000285590 -0.000084597 -0.000098269

36 1 0.000285590 -0.000084597 0.000098269

37 1 0.000084597 0.000285590 -0.000098269

38 1 0.000084597 0.000285590 0.000098269

39 1 0.000023112 0.000063217 0.000000000

40 1 -0.000084597 -0.000285590 -0.000098269

41 1 -0.000084597 -0.000285590 0.000098269

42 1 -0.000023112 -0.000063217 0.000000000

43 1 -0.000285590 0.000084597 -0.000098269

44 1 -0.000285590 0.000084597 0.000098269

45 1 -0.000063217 0.000023112 0.000000000

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

Cartesian Forces: Max 0.004271749 RMS 0.001561755

Leave Link 716 at Fri Jul 5 21:10:24 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.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.002610598 RMS 0.000577776

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 = .57778D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 2

DE= -2.25D-03 DEPred=-2.02D-03 R= 1.11D+00

TightC=F SS= 1.41D+00 RLast= 1.10D-01 DXNew= 5.0454D-01 3.2880D-01

Trust test= 1.11D+00 RLast= 1.10D-01 DXMaxT set to 3.29D-01

ITU= 1 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01336

Eigenvalues --- 0.01339 0.01339 0.01339 0.01600 0.01618

Eigenvalues --- 0.01631 0.01631 0.01774 0.01789 0.01814

Eigenvalues --- 0.01814 0.01887 0.01903 0.01941 0.01941

Eigenvalues --- 0.01997 0.01997 0.02044 0.02044 0.02070

Eigenvalues --- 0.02085 0.02100 0.02111 0.02111 0.02204

Eigenvalues --- 0.02316 0.02316 0.02352 0.02374 0.07248

Eigenvalues --- 0.07248 0.07248 0.07248 0.07284 0.07387

Eigenvalues --- 0.07387 0.07387 0.14502 0.14502 0.15827

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16005

Eigenvalues --- 0.16516 0.19896 0.21732 0.22078 0.22078

Eigenvalues --- 0.23814 0.23851 0.23851 0.24015 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25013 0.31446 0.33170 0.33170 0.33213

Eigenvalues --- 0.33282 0.33282 0.33282 0.33409 0.33724

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.34318 0.34437 0.34437 0.34437

Eigenvalues --- 0.34613 0.34923 0.35380 0.35572 0.35572

Eigenvalues --- 0.35682 0.35682 0.35682 0.35873 0.39290

Eigenvalues --- 0.41744 0.41744 0.42490 0.47537 0.48960

Eigenvalues --- 0.48960 0.49463 0.50263 0.50556 0.51357

Eigenvalues --- 0.51357 0.52367 0.53983 0.53983 0.54929

Eigenvalues --- 0.56278 0.56331 0.56331 0.56399

RFO step: Lambda=-3.72232765D-04 EMin= 8.77959372D-03

Quartic linear search produced a step of 0.14147.

Iteration 1 RMS(Cart)= 0.00492715 RMS(Int)= 0.00001533

Iteration 2 RMS(Cart)= 0.00002827 RMS(Int)= 0.00000170

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000170

ITry= 1 IFail=0 DXMaxC= 1.54D-02 DCOld= 1.00D+10 DXMaxT= 3.29D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.28D-10 for atom 36.

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

(Linear) (Quad) (Total)

R1 2.57063 -0.00010 -0.00093 0.00004 -0.00089 2.56974

R2 2.77533 0.00106 0.00175 0.00271 0.00447 2.77980

R3 2.53220 -0.00033 -0.00088 -0.00013 -0.00101 2.53120

R4 2.56079 -0.00108 -0.00187 -0.00182 -0.00369 2.55710

R5 3.77253 0.00111 -0.00298 0.00889 0.00590 3.77843

R6 2.81601 0.00261 0.00338 0.00744 0.01082 2.82683

R7 2.52433 -0.00064 -0.00124 -0.00065 -0.00189 2.52244

R8 2.56509 -0.00092 -0.00318 -0.00075 -0.00393 2.56117

R9 2.80534 -0.00012 -0.00187 0.00025 -0.00163 2.80371

R10 2.04117 0.00002 -0.00066 0.00030 -0.00036 2.04081

R11 2.53220 -0.00033 -0.00088 -0.00013 -0.00101 2.53120

R12 2.57063 -0.00010 -0.00093 0.00004 -0.00089 2.56974

R13 2.77533 0.00106 0.00175 0.00271 0.00447 2.77980

R14 2.56079 -0.00108 -0.00187 -0.00182 -0.00369 2.55710

R15 3.77253 0.00111 -0.00298 0.00889 0.00590 3.77843

R16 2.81601 0.00261 0.00338 0.00744 0.01082 2.82683

R17 2.52433 -0.00064 -0.00124 -0.00065 -0.00189 2.52244

R18 2.56509 -0.00092 -0.00318 -0.00075 -0.00393 2.56117

R19 2.80534 -0.00012 -0.00187 0.00025 -0.00163 2.80371

R20 2.04117 0.00002 -0.00066 0.00030 -0.00036 2.04081

R21 2.52433 -0.00064 -0.00124 -0.00065 -0.00189 2.52244

R22 2.56509 -0.00092 -0.00318 -0.00075 -0.00393 2.56117

R23 2.81601 0.00261 0.00338 0.00744 0.01082 2.82683

R24 2.80534 -0.00012 -0.00187 0.00025 -0.00163 2.80371

R25 2.77533 0.00106 0.00175 0.00271 0.00447 2.77980

R26 2.04117 0.00002 -0.00066 0.00030 -0.00036 2.04081

R27 2.57063 -0.00010 -0.00093 0.00004 -0.00089 2.56974

R28 2.53220 -0.00033 -0.00088 -0.00013 -0.00101 2.53120

R29 2.56079 -0.00108 -0.00187 -0.00182 -0.00369 2.55710

R30 3.77253 0.00111 -0.00298 0.00889 0.00590 3.77843

R31 2.52433 -0.00064 -0.00124 -0.00065 -0.00189 2.52244

R32 2.56079 -0.00108 -0.00187 -0.00182 -0.00369 2.55710

R33 2.57063 -0.00010 -0.00093 0.00004 -0.00089 2.56974

R34 3.77253 0.00111 -0.00298 0.00889 0.00590 3.77843

R35 2.81601 0.00261 0.00338 0.00744 0.01082 2.82683

R36 2.56509 -0.00092 -0.00318 -0.00075 -0.00393 2.56117

R37 2.80534 -0.00012 -0.00187 0.00025 -0.00163 2.80371

R38 2.77533 0.00106 0.00175 0.00271 0.00447 2.77980

R39 2.04117 0.00002 -0.00066 0.00030 -0.00036 2.04081

R40 2.53220 -0.00033 -0.00088 -0.00013 -0.00101 2.53120

R41 2.06064 -0.00006 -0.00076 0.00008 -0.00068 2.05996

R42 2.06794 0.00012 -0.00142 0.00091 -0.00051 2.06742

R43 2.06794 0.00012 -0.00142 0.00091 -0.00051 2.06742

R44 2.06794 0.00012 -0.00142 0.00091 -0.00051 2.06742

R45 2.06794 0.00012 -0.00142 0.00091 -0.00051 2.06742

R46 2.06064 -0.00006 -0.00076 0.00008 -0.00068 2.05996

R47 2.06794 0.00012 -0.00142 0.00091 -0.00051 2.06742

R48 2.06794 0.00012 -0.00142 0.00091 -0.00051 2.06742

R49 2.06064 -0.00006 -0.00076 0.00008 -0.00068 2.05996

R50 2.06794 0.00012 -0.00142 0.00091 -0.00051 2.06742

R51 2.06794 0.00012 -0.00142 0.00091 -0.00051 2.06742

R52 2.06064 -0.00006 -0.00076 0.00008 -0.00068 2.05996

A1 1.89637 -0.00069 0.00071 -0.00399 -0.00328 1.89309

A2 2.21121 0.00025 -0.00016 0.00142 0.00125 2.21247

A3 2.17560 0.00044 -0.00055 0.00257 0.00203 2.17763

A4 1.90438 0.00115 -0.00028 0.00561 0.00533 1.90971

A5 2.19291 -0.00041 0.00037 -0.00182 -0.00146 2.19146

A6 2.18589 -0.00074 -0.00008 -0.00379 -0.00388 2.18201

A7 1.89617 -0.00069 -0.00004 -0.00340 -0.00345 1.89272

A8 2.22553 0.00115 0.00086 0.00472 0.00558 2.23111

A9 2.16149 -0.00046 -0.00082 -0.00132 -0.00214 2.15935

A10 1.85113 -0.00024 0.00001 -0.00094 -0.00093 1.85020

A11 2.17158 -0.00156 -0.00087 -0.00688 -0.00775 2.16383

A12 2.26047 0.00180 0.00087 0.00781 0.00868 2.26915

A13 1.87672 0.00048 -0.00039 0.00272 0.00233 1.87905

A14 2.17827 -0.00085 0.00000 -0.00562 -0.00562 2.17264

A15 2.22820 0.00037 0.00039 0.00290 0.00329 2.23149

A16 2.18003 -0.00025 -0.00098 -0.00053 -0.00151 2.17852

A17 2.21121 0.00025 -0.00016 0.00142 0.00125 2.21247

A18 2.17560 0.00044 -0.00055 0.00257 0.00203 2.17763

A19 1.89637 -0.00069 0.00071 -0.00399 -0.00328 1.89309

A20 1.90438 0.00115 -0.00028 0.00561 0.00533 1.90971

A21 2.19291 -0.00041 0.00037 -0.00182 -0.00146 2.19146

A22 2.18589 -0.00074 -0.00008 -0.00379 -0.00388 2.18201

A23 1.89617 -0.00069 -0.00004 -0.00340 -0.00345 1.89272

A24 2.22553 0.00115 0.00086 0.00472 0.00558 2.23111

A25 2.16149 -0.00046 -0.00082 -0.00132 -0.00214 2.15935

A26 1.85113 -0.00024 0.00001 -0.00094 -0.00093 1.85020

A27 2.17158 -0.00156 -0.00087 -0.00688 -0.00775 2.16383

A28 2.26047 0.00180 0.00087 0.00781 0.00868 2.26915

A29 1.87672 0.00048 -0.00039 0.00272 0.00233 1.87905

A30 2.17827 -0.00085 0.00000 -0.00562 -0.00562 2.17264

A31 2.22820 0.00037 0.00039 0.00290 0.00329 2.23149

A32 2.18003 -0.00025 -0.00098 -0.00053 -0.00151 2.17852

A33 1.85113 -0.00024 0.00001 -0.00094 -0.00093 1.85020

A34 2.26047 0.00180 0.00087 0.00781 0.00868 2.26915

A35 2.17158 -0.00156 -0.00087 -0.00688 -0.00775 2.16383

A36 1.87672 0.00048 -0.00039 0.00272 0.00233 1.87905

A37 2.22820 0.00037 0.00039 0.00290 0.00329 2.23149

A38 2.17827 -0.00085 0.00000 -0.00562 -0.00562 2.17264

A39 1.89637 -0.00069 0.00071 -0.00399 -0.00328 1.89309

A40 2.17560 0.00044 -0.00055 0.00257 0.00203 2.17763

A41 2.21121 0.00025 -0.00016 0.00142 0.00125 2.21247

A42 1.90438 0.00115 -0.00028 0.00561 0.00533 1.90971

A43 2.19291 -0.00041 0.00037 -0.00182 -0.00146 2.19146

A44 2.18589 -0.00074 -0.00008 -0.00379 -0.00388 2.18201

A45 2.16149 -0.00046 -0.00082 -0.00132 -0.00214 2.15935

A46 2.22553 0.00115 0.00086 0.00472 0.00558 2.23111

A47 1.89617 -0.00069 -0.00004 -0.00340 -0.00345 1.89272

A48 2.18003 -0.00025 -0.00098 -0.00053 -0.00151 2.17852

A49 1.90438 0.00115 -0.00028 0.00561 0.00533 1.90971

A50 2.18589 -0.00074 -0.00008 -0.00379 -0.00388 2.18201

A51 2.19291 -0.00041 0.00037 -0.00182 -0.00146 2.19146

A52 2.22553 0.00115 0.00086 0.00472 0.00558 2.23111

A53 2.16149 -0.00046 -0.00082 -0.00132 -0.00214 2.15935

A54 1.89617 -0.00069 -0.00004 -0.00340 -0.00345 1.89272

A55 1.85113 -0.00024 0.00001 -0.00094 -0.00093 1.85020

A56 2.17158 -0.00156 -0.00087 -0.00688 -0.00775 2.16383

A57 2.26047 0.00180 0.00087 0.00781 0.00868 2.26915

A58 1.87672 0.00048 -0.00039 0.00272 0.00233 1.87905

A59 2.22820 0.00037 0.00039 0.00290 0.00329 2.23149

A60 2.17827 -0.00085 0.00000 -0.00562 -0.00562 2.17264

A61 1.89637 -0.00069 0.00071 -0.00399 -0.00328 1.89309

A62 2.21121 0.00025 -0.00016 0.00142 0.00125 2.21247

A63 2.17560 0.00044 -0.00055 0.00257 0.00203 2.17763

A64 2.18003 -0.00025 -0.00098 -0.00053 -0.00151 2.17852

A65 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A66 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A67 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A68 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A69 1.93957 0.00015 0.00059 0.00164 0.00223 1.94179

A70 1.93379 0.00011 -0.00039 0.00052 0.00012 1.93391

A71 1.93379 0.00011 -0.00039 0.00052 0.00012 1.93391

A72 1.89557 -0.00002 0.00063 0.00034 0.00097 1.89654

A73 1.89557 -0.00002 0.00063 0.00034 0.00097 1.89654

A74 1.86331 -0.00035 -0.00109 -0.00356 -0.00465 1.85865

A75 1.93379 0.00011 -0.00039 0.00052 0.00012 1.93391

A76 1.93379 0.00011 -0.00039 0.00052 0.00012 1.93391

A77 1.93957 0.00015 0.00059 0.00164 0.00223 1.94179

A78 1.86331 -0.00035 -0.00109 -0.00356 -0.00465 1.85865

A79 1.89557 -0.00002 0.00063 0.00034 0.00097 1.89654

A80 1.89557 -0.00002 0.00063 0.00034 0.00097 1.89654

A81 1.93379 0.00011 -0.00039 0.00052 0.00012 1.93391

A82 1.93379 0.00011 -0.00039 0.00052 0.00012 1.93391

A83 1.93957 0.00015 0.00059 0.00164 0.00223 1.94179

A84 1.86331 -0.00035 -0.00109 -0.00356 -0.00465 1.85865

A85 1.89557 -0.00002 0.00063 0.00034 0.00097 1.89654

A86 1.89557 -0.00002 0.00063 0.00034 0.00097 1.89654

A87 1.93379 0.00011 -0.00039 0.00052 0.00012 1.93391

A88 1.93379 0.00011 -0.00039 0.00052 0.00012 1.93391

A89 1.93957 0.00015 0.00059 0.00164 0.00223 1.94179

A90 1.86331 -0.00035 -0.00109 -0.00356 -0.00465 1.85865

A91 1.89557 -0.00002 0.00063 0.00034 0.00097 1.89654

A92 1.89557 -0.00002 0.00063 0.00034 0.00097 1.89654

A93 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A94 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A95 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A96 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D4 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D28 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D29 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D30 1.03244 -0.00015 -0.00093 -0.00189 -0.00282 1.02962

D31 -1.03244 0.00015 0.00093 0.00189 0.00282 -1.02962

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.10915 -0.00015 -0.00093 -0.00189 -0.00282 -2.11197

D34 2.10915 0.00015 0.00093 0.00189 0.00282 2.11197

D35 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D38 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D39 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D40 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D41 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D42 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D43 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D44 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D60 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D61 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D62 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D63 1.03244 -0.00015 -0.00093 -0.00189 -0.00282 1.02962

D64 -1.03244 0.00015 0.00093 0.00189 0.00282 -1.02962

D65 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.10915 -0.00015 -0.00093 -0.00189 -0.00282 -2.11197

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D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D71 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D73 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D74 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D75 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D76 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D77 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D78 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D79 -2.10915 -0.00015 -0.00093 -0.00189 -0.00282 -2.11197

D80 2.10915 0.00015 0.00093 0.00189 0.00282 2.11197

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.03244 -0.00015 -0.00093 -0.00189 -0.00282 1.02962

D83 -1.03244 0.00015 0.00093 0.00189 0.00282 -1.02962

D84 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D85 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D86 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D101 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D105 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D106 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D107 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D109 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D110 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D111 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D112 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D113 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D114 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D117 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D120 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D121 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D122 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D123 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D124 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D125 1.03244 -0.00015 -0.00093 -0.00189 -0.00282 1.02962

D126 -1.03244 0.00015 0.00093 0.00189 0.00282 -1.02962

D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D128 -2.10915 -0.00015 -0.00093 -0.00189 -0.00282 -2.11197

D129 2.10915 0.00015 0.00093 0.00189 0.00282 2.11197

D130 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D131 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D132 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D133 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D134 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.002611 0.000450 NO

RMS Force 0.000578 0.000300 NO

Maximum Displacement 0.015402 0.001800 NO

RMS Displacement 0.004930 0.001200 NO

Predicted change in Energy=-2.225845D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 5 21:10:25 2019, MaxMem= 1342177280 cpu: 1.5

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.063828 -2.179493 0.000000

2 7 0 -0.742942 -1.856306 0.000000

3 6 0 -0.002647 -2.989006 0.000000

4 6 0 -0.931567 -4.161527 0.000000

5 6 0 -2.184803 -3.645517 0.000000

6 7 0 1.327747 -3.097587 0.000000

7 6 0 2.179493 -2.063828 0.000000

8 7 0 1.856306 -0.742942 0.000000

9 6 0 2.989006 -0.002647 0.000000

10 6 0 4.161527 -0.931567 0.000000

11 6 0 3.645517 -2.184803 0.000000

12 7 0 -3.097587 -1.327747 0.000000

13 6 0 -4.161527 0.931567 0.000000

14 6 0 -3.645517 2.184803 0.000000

15 6 0 -2.179493 2.063828 0.000000

16 7 0 -1.856306 0.742942 0.000000

17 6 0 -2.989006 0.002647 0.000000

18 7 0 -1.327747 3.097587 0.000000

19 7 0 0.742942 1.856306 0.000000

20 6 0 0.002647 2.989006 0.000000

21 6 0 0.931567 4.161527 0.000000

22 6 0 2.184803 3.645517 0.000000

23 6 0 2.063828 2.179493 0.000000

24 7 0 3.097587 1.327747 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.482118 -5.575472 0.000000

27 1 0 -3.122267 -4.181668 0.000000

28 6 0 5.575472 -0.482118 0.000000

29 1 0 4.181668 -3.122267 0.000000

30 6 0 -5.575472 0.482118 0.000000

31 1 0 -4.181668 3.122267 0.000000

32 6 0 0.482118 5.575472 0.000000

33 1 0 3.122267 4.181668 0.000000

34 1 0 -1.330584 -6.259866 0.000000

35 1 0 0.137676 -5.786207 0.876559

36 1 0 0.137676 -5.786207 -0.876559

37 1 0 5.786207 0.137676 0.876559

38 1 0 5.786207 0.137676 -0.876559

39 1 0 6.259866 -1.330584 0.000000

40 1 0 -5.786207 -0.137676 0.876559

41 1 0 -5.786207 -0.137676 -0.876559

42 1 0 -6.259866 1.330584 0.000000

43 1 0 -0.137676 5.786207 0.876559

44 1 0 -0.137676 5.786207 -0.876559

45 1 0 1.330584 6.259866 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.359849 0.000000

3 C 2.214447 1.353161 0.000000

4 C 2.282646 2.312926 1.495894 0.000000

5 C 1.471006 2.297877 2.278774 1.355311 0.000000

6 N 3.513642 2.414235 1.334818 2.497292 3.555029

7 C 4.244897 2.929794 2.370167 3.752204 4.642071

8 N 4.175060 2.827661 2.915563 4.411231 4.975490

9 C 5.501798 4.166951 4.227094 5.715520 6.327621

10 C 6.349202 4.990887 4.644718 6.030941 6.902277

11 C 5.709347 4.400736 3.735752 4.985693 6.010517

12 N 1.339451 2.413240 3.512611 3.566785 2.491030

13 C 3.752204 4.411231 5.715520 6.030941 4.985693

14 C 4.642071 4.975490 6.327621 6.902277 6.010517

15 C 4.244897 4.175060 5.501798 6.349202 5.709347

16 N 2.929794 2.827661 4.166951 4.990887 4.400736

17 C 2.370167 2.915563 4.227094 4.644718 3.735752

18 N 5.328170 4.988291 6.229165 7.269917 6.797352

19 N 4.915855 3.998916 4.902341 6.246462 6.232314

20 C 5.566300 4.902341 5.978014 7.211302 6.985830

21 C 7.012911 6.246462 7.211302 8.529038 8.406051

22 C 7.209827 6.232314 6.985830 8.406051 8.500154

23 C 6.003191 4.915855 5.566300 7.012911 7.209827

24 N 6.240268 4.988773 5.314679 6.809274 7.255136

25 Zn 3.001596 1.999458 2.989007 4.264519 4.250077

26 C 3.746262 3.728301 2.630533 1.483660 2.573687

27 H 2.264729 3.326935 3.339831 2.190793 1.079953

28 C 7.825599 6.466123 6.115546 7.475267 8.380272

29 H 6.316252 5.084726 4.186437 5.217781 6.387937

30 C 4.406339 5.368573 6.565446 6.567290 5.341723

31 H 5.709108 6.050704 7.403504 7.976015 7.056229

32 C 8.162189 7.532071 8.578186 9.839089 9.598912

33 H 8.207311 7.169168 7.821998 9.275908 9.456734

34 H 4.145731 4.442596 3.530147 2.135940 2.750365

35 H 4.315479 4.121647 2.934686 2.133359 3.277929

36 H 4.315479 4.121647 2.934686 2.133359 3.277929

37 H 8.231688 6.882885 6.637419 8.023714 8.866674

38 H 8.231688 6.882885 6.637419 8.023714 8.866674

39 H 8.366870 7.022513 6.478382 7.728579 8.756217

40 H 4.335145 5.399682 6.507534 6.366103 5.103275

41 H 4.335145 5.399682 6.507534 6.366103 5.103275

42 H 5.470592 6.371241 7.603396 7.652062 6.431774

43 H 8.242014 7.716392 8.819918 10.017786 9.691053

44 H 8.242014 7.716392 8.819918 10.017786 9.691053

45 H 9.096417 8.376858 9.344470 10.664087 10.510687

6 7 8 9 10

6 N 0.000000

7 C 1.339451 0.000000

8 N 2.413240 1.359849 0.000000

9 C 3.512611 2.214447 1.353161 0.000000

10 C 3.566785 2.282646 2.312926 1.495894 0.000000

11 C 2.491030 1.471006 2.297877 2.278774 1.355311

12 N 4.766122 5.328170 4.988291 6.229165 7.269917

13 C 6.809274 7.012911 6.246462 7.211302 8.529038

14 C 7.255136 7.209827 6.232314 6.985830 8.406051

15 C 6.240268 6.003191 4.915855 5.566300 7.012911

16 N 4.988773 4.915855 3.998916 4.902341 6.246462

17 C 5.314679 5.566300 4.902341 5.978014 7.211302

18 N 6.740314 6.240268 4.988773 5.314679 6.809274

19 N 4.988291 4.175060 2.827661 2.915563 4.411231

20 C 6.229165 5.501798 4.166951 4.227094 5.715520

21 C 7.269917 6.349202 4.990887 4.644718 6.030941

22 C 6.797352 5.709347 4.400736 3.735752 4.985693

23 C 5.328170 4.244897 2.929794 2.370167 3.752204

24 N 4.766122 3.513642 2.414235 1.334818 2.497292

25 Zn 3.370157 3.001596 1.999458 2.989007 4.264519

26 C 3.068473 4.406339 5.368573 6.565446 6.567290

27 H 4.580159 5.709108 6.050704 7.403504 7.976015

28 C 4.988372 3.746262 3.728301 2.630533 1.483660

29 H 2.854028 2.264729 3.326935 3.339831 2.190793

30 C 7.776164 8.162189 7.532071 8.578186 9.839089

31 H 8.309046 8.207311 7.169168 7.821998 9.275908

32 C 8.714187 7.825599 6.466123 6.115546 7.475267

33 H 7.497190 6.316252 5.084726 4.186437 5.217781

34 H 4.131190 5.470592 6.371241 7.603396 7.652062

35 H 3.068110 4.335145 5.399682 6.507534 6.366103

36 H 3.068110 4.335145 5.399682 6.507534 6.366103

37 H 5.577916 4.315479 4.121647 2.934686 2.133359

38 H 5.577916 4.315479 4.121647 2.934686 2.133359

39 H 5.239093 4.145731 4.442596 3.530147 2.135940

40 H 7.754855 8.242014 7.716392 8.819918 10.017786

41 H 7.754855 8.242014 7.716392 8.819918 10.017786

42 H 8.785247 9.096417 8.376858 9.344470 10.664087

43 H 9.046415 8.231688 6.882885 6.637419 8.023714

44 H 9.046415 8.231688 6.882885 6.637419 8.023714

45 H 9.357453 8.366870 7.022513 6.478382 7.728579

11 12 13 14 15

11 C 0.000000

12 N 6.797352 0.000000

13 C 8.406051 2.497292 0.000000

14 C 8.500154 3.555029 1.355311 0.000000

15 C 7.209827 3.513642 2.282646 1.471006 0.000000

16 N 6.232314 2.414235 2.312926 2.297877 1.359849

17 C 6.985830 1.334818 1.495894 2.278774 2.214447

18 N 7.255136 4.766122 3.566785 2.491030 1.339451

19 N 4.975490 4.988773 4.990887 4.400736 2.929794

20 C 6.327621 5.314679 4.644718 3.735752 2.370167

21 C 6.902277 6.809274 6.030941 4.985693 3.752204

22 C 6.010517 7.255136 6.902277 6.010517 4.642071

23 C 4.642071 6.240268 6.349202 5.709347 4.244897

24 N 3.555029 6.740314 7.269917 6.797352 5.328170

25 Zn 4.250077 3.370157 4.264519 4.250077 3.001596

26 C 5.341723 4.988372 7.475267 8.380272 7.825599

27 H 7.056229 2.854028 5.217781 6.387937 6.316252

28 C 2.573687 8.714187 9.839089 9.598912 8.162189

29 H 1.079953 7.497190 9.275908 9.456734 8.207311

30 C 9.598912 3.068473 1.483660 2.573687 3.746262

31 H 9.456734 4.580159 2.190793 1.079953 2.264729

32 C 8.380272 7.776164 6.567290 5.341723 4.406339

33 H 6.387937 8.309046 7.976015 7.056229 5.709108

34 H 6.431774 5.239093 7.728579 8.756217 8.366870

35 H 5.103275 5.577916 8.023714 8.866674 8.231688

36 H 5.103275 5.577916 8.023714 8.866674 8.231688

37 H 3.277929 9.046415 10.017786 9.691053 8.242014

38 H 3.277929 9.046415 10.017786 9.691053 8.242014

39 H 2.750365 9.357453 10.664087 10.510687 9.096417

40 H 9.691053 3.068110 2.133359 3.277929 4.315479

41 H 9.691053 3.068110 2.133359 3.277929 4.315479

42 H 10.510687 4.131190 2.135940 2.750365 4.145731

43 H 8.866674 7.754855 6.366103 5.103275 4.335145

44 H 8.866674 7.754855 6.366103 5.103275 4.335145

45 H 8.756217 8.785247 7.652062 6.431774 5.470592

16 17 18 19 20

16 N 0.000000

17 C 1.353161 0.000000

18 N 2.413240 3.512611 0.000000

19 N 2.827661 4.166951 2.414235 0.000000

20 C 2.915563 4.227094 1.334818 1.353161 0.000000

21 C 4.411231 5.715520 2.497292 2.312926 1.495894

22 C 4.975490 6.327621 3.555029 2.297877 2.278774

23 C 4.175060 5.501798 3.513642 1.359849 2.214447

24 N 4.988291 6.229165 4.766122 2.413240 3.512611

25 Zn 1.999458 2.989007 3.370157 1.999458 2.989007

26 C 6.466123 6.115546 8.714187 7.532071 8.578186

27 H 5.084726 4.186437 7.497190 7.169168 7.821998

28 C 7.532071 8.578186 7.776164 5.368573 6.565446

29 H 7.169168 7.821998 8.309046 6.050704 7.403504

30 C 3.728301 2.630533 4.988372 6.466123 6.115546

31 H 3.326935 3.339831 2.854028 5.084726 4.186437

32 C 5.368573 6.565446 3.068473 3.728301 2.630533

33 H 6.050704 7.403504 4.580159 3.326935 3.339831

34 H 7.022513 6.478382 9.357453 8.376858 9.344470

35 H 6.882885 6.637419 9.046415 7.716392 8.819918

36 H 6.882885 6.637419 9.046415 7.716392 8.819918

37 H 7.716392 8.819918 7.754855 5.399682 6.507534

38 H 7.716392 8.819918 7.754855 5.399682 6.507534

39 H 8.376858 9.344470 8.785247 6.371241 7.603396

40 H 4.121647 2.934686 5.577916 6.882885 6.637419

41 H 4.121647 2.934686 5.577916 6.882885 6.637419

42 H 4.442596 3.530147 5.239093 7.022513 6.478382

43 H 5.399682 6.507534 3.068110 4.121647 2.934686

44 H 5.399682 6.507534 3.068110 4.121647 2.934686

45 H 6.371241 7.603396 4.131190 4.442596 3.530147

21 22 23 24 25

21 C 0.000000

22 C 1.355311 0.000000

23 C 2.282646 1.471006 0.000000

24 N 3.566785 2.491030 1.339451 0.000000

25 Zn 4.264519 4.250077 3.001596 3.370157 0.000000

26 C 9.839089 9.598912 8.162189 7.776164 5.596278

27 H 9.275908 9.456734 8.207311 8.309046 5.218707

28 C 6.567290 5.341723 4.406339 3.068473 5.596278

29 H 7.976015 7.056229 5.709108 4.580159 5.218707

30 C 7.475267 8.380272 7.825599 8.714187 5.596278

31 H 5.217781 6.387937 6.316252 7.497190 5.218707

32 C 1.483660 2.573687 3.746262 4.988372 5.596278

33 H 2.190793 1.079953 2.264729 2.854028 5.218707

34 H 10.664087 10.510687 9.096417 8.785247 6.399716

35 H 10.017786 9.691053 8.242014 7.754855 5.853845

36 H 10.017786 9.691053 8.242014 7.754855 5.853845

37 H 6.366103 5.103275 4.335145 3.068110 5.853845

38 H 6.366103 5.103275 4.335145 3.068110 5.853845

39 H 7.652062 6.431774 5.470592 4.131190 6.399716

40 H 8.023714 8.866674 8.231688 9.046415 5.853845

41 H 8.023714 8.866674 8.231688 9.046415 5.853845

42 H 7.728579 8.756217 8.366870 9.357453 6.399716

43 H 2.133359 3.277929 4.315479 5.577916 5.853845

44 H 2.133359 3.277929 4.315479 5.577916 5.853845

45 H 2.135940 2.750365 4.145731 5.239093 6.399716

26 27 28 29 30

26 C 0.000000

27 H 2.985478 0.000000

28 C 7.914333 9.451844 0.000000

29 H 5.269641 7.380366 2.985478 0.000000

30 C 7.914333 5.269641 11.192557 10.401605 0.000000

31 H 9.451844 7.380366 10.401605 10.437414 2.985478

32 C 11.192557 10.401605 7.914333 9.451844 7.914333

33 H 10.401605 10.437414 5.269641 7.380366 9.451844

34 H 1.090087 2.743908 9.004220 6.342669 7.967021

35 H 1.094033 3.737664 7.646656 4.921260 8.526448

36 H 1.094033 3.737664 7.646656 4.921260 8.526448

37 H 8.526448 9.939115 1.094033 3.737664 11.400647

38 H 8.526448 9.939115 1.094033 3.737664 11.400647

39 H 7.967021 9.805768 1.090087 2.743908 11.973350

40 H 7.646656 4.921260 11.400647 10.441967 1.094033

41 H 7.646656 4.921260 11.400647 10.441967 1.094033

42 H 9.004220 6.342669 11.973350 11.351366 1.090087

43 H 11.400647 10.441967 8.526448 9.939115 7.646656

44 H 11.400647 10.441967 8.526448 9.939115 7.646656

45 H 11.973350 11.351366 7.967021 9.805768 9.004220

31 32 33 34 35

31 H 0.000000

32 C 5.269641 0.000000

33 H 7.380366 2.985478 0.000000

34 H 9.805768 11.973350 11.351366 0.000000

35 H 9.939115 11.400647 10.441967 1.774400 0.000000

36 H 9.939115 11.400647 10.441967 1.774400 1.753117

37 H 10.441967 7.646656 4.921260 9.609662 8.185249

38 H 10.441967 7.646656 4.921260 9.609662 8.370885

39 H 11.351366 9.004220 6.342669 9.050566 7.622476

40 H 3.737664 8.526448 9.939115 7.622476 8.185249

41 H 3.737664 8.526448 9.939115 7.622476 8.370885

42 H 2.743908 7.967021 9.805768 9.050566 9.609662

43 H 4.921260 1.094033 3.737664 12.136690 11.575690

44 H 4.921260 1.094033 3.737664 12.136690 11.707690

45 H 6.342669 1.090087 2.743908 12.799433 12.136690

36 37 38 39 40

36 H 0.000000

37 H 8.370885 0.000000

38 H 8.185249 1.753117 0.000000

39 H 7.622476 1.774400 1.774400 0.000000

40 H 8.370885 11.575690 11.707690 12.136690 0.000000

41 H 8.185249 11.707690 11.575690 12.136690 1.753117

42 H 9.609662 12.136690 12.136690 12.799433 1.774400

43 H 11.707690 8.185249 8.370885 9.609662 8.185249

44 H 11.575690 8.370885 8.185249 9.609662 8.370885

45 H 12.136690 7.622476 7.622476 9.050566 9.609662

41 42 43 44 45

41 H 0.000000

42 H 1.774400 0.000000

43 H 8.370885 7.622476 0.000000

44 H 8.185249 7.622476 1.753117 0.000000

45 H 9.609662 9.050566 1.774400 1.774400 0.000000

Stoichiometry C20H16N8Zn(1+,2)

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

Deg. of freedom 20

Full point group C4H NOp 8

RotChk: IX=0 Diff= 1.16D-03

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.181320 2.061897 0.000000

2 7 0 -1.856963 0.741298 0.000000

3 6 0 -2.989007 0.000000 0.000000

4 6 0 -4.162350 0.927881 0.000000

5 6 0 -3.647450 2.181573 0.000000

6 7 0 -3.096410 -1.330490 0.000000

7 6 0 -2.061897 -2.181320 0.000000

8 7 0 -0.741298 -1.856963 0.000000

9 6 0 0.000000 -2.989007 0.000000

10 6 0 -0.927881 -4.162350 0.000000

11 6 0 -2.181573 -3.647450 0.000000

12 7 0 -1.330490 3.096410 0.000000

13 6 0 0.927881 4.162350 0.000000

14 6 0 2.181573 3.647450 0.000000

15 6 0 2.061897 2.181320 0.000000

16 7 0 0.741298 1.856963 0.000000

17 6 0 0.000000 2.989007 0.000000

18 7 0 3.096410 1.330490 0.000000

19 7 0 1.856963 -0.741298 0.000000

20 6 0 2.989007 0.000000 0.000000

21 6 0 4.162350 -0.927881 0.000000

22 6 0 3.647450 -2.181573 0.000000

23 6 0 2.181320 -2.061897 0.000000

24 7 0 1.330490 -3.096410 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.575897 0.477180 0.000000

27 1 0 -4.184432 3.118562 0.000000

28 6 0 -0.477180 -5.575897 0.000000

29 1 0 -3.118562 -4.184432 0.000000

30 6 0 0.477180 5.575897 0.000000

31 1 0 3.118562 4.184432 0.000000

32 6 0 5.575897 -0.477180 0.000000

33 1 0 4.184432 -3.118562 0.000000

34 1 0 -6.261042 1.325039 0.000000

35 1 0 -5.786083 -0.142801 0.876559

36 1 0 -5.786083 -0.142801 -0.876559

37 1 0 0.142801 -5.786083 0.876559

38 1 0 0.142801 -5.786083 -0.876559

39 1 0 -1.325039 -6.261042 0.000000

40 1 0 -0.142801 5.786083 0.876559

41 1 0 -0.142801 5.786083 -0.876559

42 1 0 1.325039 6.261042 0.000000

43 1 0 5.786083 0.142801 0.876559

44 1 0 5.786083 0.142801 -0.876559

45 1 0 6.261042 -1.325039 0.000000

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

Rotational constants (GHZ): 0.1830408 0.1830408 0.0917262

Leave Link 202 at Fri Jul 5 21:10:25 2019, MaxMem= 1342177280 cpu: 0.2

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

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

Pseudo-potential data read from rwf file.

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

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

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

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

There are 212 symmetry adapted basis functions of AG symmetry.

There are 82 symmetry adapted basis functions of BG symmetry.

There are 78 symmetry adapted basis functions of AU symmetry.

There are 204 symmetry adapted basis functions of BU symmetry.

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

102 alpha electrons 101 beta electrons

nuclear repulsion energy 2766.8948892811 Hartrees.

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

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

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

NAtoms= 45 NActive= 45 NUniq= 11 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1142324257 Hartrees.

Nuclear repulsion after empirical dispersion term = 2766.7806568554 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 = 3542

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.43D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 164

GePol: Fraction of low-weight points (<1% of avg) = 4.63%

GePol: Cavity surface area = 381.984 Ang\*\*2

GePol: Cavity volume = 378.927 Ang\*\*3

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

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

PCM non-electrostatic energy = -0.0110740564 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2766.7695827990 Hartrees.

Leave Link 301 at Fri Jul 5 21:10:25 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= 19306 NPrTT= 91506 LenC2= 15383 LenP2D= 41368.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.85D-04 NBF= 212 82 78 204

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

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Fri Jul 5 21:10:25 2019, MaxMem= 1342177280 cpu: 7.7

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 5 21:10:26 2019, MaxMem= 1342177280 cpu: 0.8

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

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

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 -0.000135 Ang= -0.02 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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

(AG) (EU) (EU) (AG) (BG) (AU) (EG) (EG) (AG) (EU)

(EU) (BU) (BG) (AU) (EG) (EG) (BG) (AG) (BU) (EU)

(EU) (BU) (AG) (EU) (EU) (BG) (AG) (EU) (EU) (EG)

(EG) (AG) (EU) (EU) (BG) (AU) (BG) (EG) (EG) (AU)

(BU) (AU)

Virtual (AG) (BG) (AG) (BG) (BG) (AG) (AG) (BG) (AG) (BG)

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

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7819 S= 0.5158

Leave Link 401 at Fri Jul 5 21:10:27 2019, MaxMem= 1342177280 cpu: 21.7

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1138797 IEndB= 1138797 NGot= 1342177280 MDV= 1341424180

LenX= 1341424180 LenY= 1341055124

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

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

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 37637292.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.99D-15 for 2086.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.20D-15 for 3536 2658.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.22D-15 for 1785.

Iteration 1 A^-1\*A deviation from orthogonality is 3.67D-09 for 918 847.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.89D-15 for 676.

Iteration 2 A\*A^-1 deviation from orthogonality is 4.22D-15 for 1508 516.

Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 58.

Iteration 2 A^-1\*A deviation from orthogonality is 3.27D-16 for 1743 735.

E= -1275.69927337364

DIIS: error= 4.57D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.69927337364 IErMin= 1 ErrMin= 4.57D-04

ErrMax= 4.57D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.68D-04 BMatP= 5.68D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.57D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.372 Goal= None Shift= 0.000

Gap= 0.406 Goal= None Shift= 0.000

RMSDP=3.24D-05 MaxDP=7.63D-04 OVMax= 2.64D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.23D-05 CP: 1.00D+00

E= -1275.69947027645 Delta-E= -0.000196902809 Rises=F Damp=F

DIIS: error= 1.77D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.69947027645 IErMin= 2 ErrMin= 1.77D-04

ErrMax= 1.77D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.86D-05 BMatP= 5.68D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.77D-03

Coeff-Com: 0.706D-01 0.929D+00

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

Coeff: 0.705D-01 0.930D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=1.00D-05 MaxDP=5.36D-04 DE=-1.97D-04 OVMax= 1.38D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 9.97D-06 CP: 1.00D+00 9.99D-01

E= -1275.69945947479 Delta-E= 0.000010801666 Rises=F Damp=F

DIIS: error= 3.07D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.69947027645 IErMin= 2 ErrMin= 1.77D-04

ErrMax= 3.07D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-04 BMatP= 4.86D-05

IDIUse=3 WtCom= 3.63D-01 WtEn= 6.37D-01

Coeff-Com: -0.278D-01 0.612D+00 0.416D+00

Coeff-En: 0.000D+00 0.648D+00 0.352D+00

Coeff: -0.101D-01 0.635D+00 0.375D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=5.92D-06 MaxDP=3.18D-04 DE= 1.08D-05 OVMax= 9.30D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.07D-06 CP: 1.00D+00 1.03D+00 4.56D-01

E= -1275.69948101980 Delta-E= -0.000021545016 Rises=F Damp=F

DIIS: error= 2.47D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.69948101980 IErMin= 4 ErrMin= 2.47D-05

ErrMax= 2.47D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.41D-07 BMatP= 4.86D-05

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

Coeff-Com: -0.132D-01 0.199D+00 0.110D+00 0.704D+00

Coeff: -0.132D-01 0.199D+00 0.110D+00 0.704D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

RMSDP=7.58D-07 MaxDP=3.58D-05 DE=-2.15D-05 OVMax= 1.55D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 7.11D-07 CP: 1.00D+00 1.04D+00 4.45D-01 9.91D-01

E= -1275.69948114588 Delta-E= -0.000000126081 Rises=F Damp=F

DIIS: error= 1.29D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.69948114588 IErMin= 5 ErrMin= 1.29D-05

ErrMax= 1.29D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.54D-07 BMatP= 7.41D-07

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

Coeff-Com: -0.351D-02 0.358D-01 0.130D-01 0.395D+00 0.560D+00

Coeff: -0.351D-02 0.358D-01 0.130D-01 0.395D+00 0.560D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=3.78D-07 MaxDP=1.94D-05 DE=-1.26D-07 OVMax= 1.19D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.17D-07 CP: 1.00D+00 1.04D+00 4.43D-01 1.06D+00 7.88D-01

E= -1275.69948120125 Delta-E= -0.000000055368 Rises=F Damp=F

DIIS: error= 3.63D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.69948120125 IErMin= 6 ErrMin= 3.63D-06

ErrMax= 3.63D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.04D-08 BMatP= 2.54D-07

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

Coeff-Com: -0.759D-03 0.840D-03-0.426D-03 0.124D+00 0.276D+00 0.600D+00

Coeff: -0.759D-03 0.840D-03-0.426D-03 0.124D+00 0.276D+00 0.600D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

RMSDP=1.61D-07 MaxDP=6.30D-06 DE=-5.54D-08 OVMax= 6.10D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.32D-07 CP: 1.00D+00 1.04D+00 4.45D-01 1.08D+00 8.75D-01

CP: 9.27D-01

E= -1275.69948120888 Delta-E= -0.000000007627 Rises=F Damp=F

DIIS: error= 2.51D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.69948120888 IErMin= 7 ErrMin= 2.51D-06

ErrMax= 2.51D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.64D-09 BMatP= 2.04D-08

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

Coeff-Com: 0.496D-03-0.877D-02-0.252D-02-0.276D-01 0.241D-01 0.319D+00

Coeff-Com: 0.696D+00

Coeff: 0.496D-03-0.877D-02-0.252D-02-0.276D-01 0.241D-01 0.319D+00

Coeff: 0.696D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=1.09D-07 MaxDP=5.54D-06 DE=-7.63D-09 OVMax= 5.16D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.68D-08 CP: 1.00D+00 1.04D+00 4.47D-01 1.10D+00 9.30D-01

CP: 1.14D+00 1.19D+00

E= -1275.69948121270 Delta-E= -0.000000003824 Rises=F Damp=F

DIIS: error= 1.47D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.69948121270 IErMin= 8 ErrMin= 1.47D-06

ErrMax= 1.47D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.87D-10 BMatP= 4.64D-09

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

Coeff-Com: 0.119D-03 0.400D-03 0.938D-03-0.274D-01-0.596D-01-0.151D+00

Coeff-Com: -0.107D-01 0.125D+01

Coeff: 0.119D-03 0.400D-03 0.938D-03-0.274D-01-0.596D-01-0.151D+00

Coeff: -0.107D-01 0.125D+01

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=1.10D-07 MaxDP=6.66D-06 DE=-3.82D-09 OVMax= 5.76D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.43D-08 CP: 1.00D+00 1.04D+00 4.48D-01 1.11D+00 9.76D-01

CP: 1.30D+00 1.69D+00 1.67D+00

E= -1275.69948121477 Delta-E= -0.000000002063 Rises=F Damp=F

DIIS: error= 1.16D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.69948121477 IErMin= 9 ErrMin= 1.16D-06

ErrMax= 1.16D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.44D-10 BMatP= 7.87D-10

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

Coeff-Com: -0.948D-04 0.359D-02 0.138D-02-0.820D-02-0.506D-01-0.227D+00

Coeff-Com: -0.300D+00 0.825D+00 0.756D+00

Coeff: -0.948D-04 0.359D-02 0.138D-02-0.820D-02-0.506D-01-0.227D+00

Coeff: -0.300D+00 0.825D+00 0.756D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=7.08D-08 MaxDP=4.38D-06 DE=-2.06D-09 OVMax= 3.24D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.26D-08 CP: 1.00D+00 1.04D+00 4.48D-01 1.11D+00 1.00D+00

CP: 1.40D+00 1.99D+00 2.21D+00 1.31D+00

E= -1275.69948121529 Delta-E= -0.000000000522 Rises=F Damp=F

DIIS: error= 5.80D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.69948121529 IErMin=10 ErrMin= 5.80D-07

ErrMax= 5.80D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.23D-10 BMatP= 5.44D-10

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

Coeff-Com: -0.894D-04 0.174D-02 0.244D-03 0.663D-02-0.276D-02-0.514D-01

Coeff-Com: -0.141D+00 0.351D-01 0.386D+00 0.765D+00

Coeff: -0.894D-04 0.174D-02 0.244D-03 0.663D-02-0.276D-02-0.514D-01

Coeff: -0.141D+00 0.351D-01 0.386D+00 0.765D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 21319 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

RMSDP=2.37D-08 MaxDP=1.64D-06 DE=-5.22D-10 OVMax= 1.12D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.12D-08 CP: 1.00D+00 1.04D+00 4.48D-01 1.11D+00 1.01D+00

CP: 1.42D+00 2.06D+00 2.41D+00 1.62D+00 1.10D+00

E= -1275.69948121544 Delta-E= -0.000000000151 Rises=F Damp=F

DIIS: error= 1.61D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.69948121544 IErMin=11 ErrMin= 1.61D-07

ErrMax= 1.61D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.38D-11 BMatP= 1.23D-10

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

Coeff-Com: -0.252D-04 0.347D-04-0.250D-03 0.510D-02 0.936D-02 0.273D-01

Coeff-Com: -0.319D-02-0.186D+00 0.242D-01 0.366D+00 0.758D+00

Coeff: -0.252D-04 0.347D-04-0.250D-03 0.510D-02 0.936D-02 0.273D-01

Coeff: -0.319D-02-0.186D+00 0.242D-01 0.366D+00 0.758D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=1.17D-08 MaxDP=7.40D-07 DE=-1.51D-10 OVMax= 4.04D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.84D-09 CP: 1.00D+00 1.04D+00 4.48D-01 1.11D+00 1.01D+00

CP: 1.43D+00 2.09D+00 2.48D+00 1.81D+00 1.38D+00

CP: 1.12D+00

E= -1275.69948121535 Delta-E= 0.000000000087 Rises=F Damp=F

DIIS: error= 8.56D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=11 EnMin= -1275.69948121544 IErMin=12 ErrMin= 8.56D-08

ErrMax= 8.56D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.09D-12 BMatP= 2.38D-11

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

Coeff-Com: 0.722D-05-0.376D-03-0.170D-03 0.106D-02 0.506D-02 0.247D-01

Coeff-Com: 0.311D-01-0.949D-01-0.566D-01 0.159D-02 0.308D+00 0.781D+00

Coeff: 0.722D-05-0.376D-03-0.170D-03 0.106D-02 0.506D-02 0.247D-01

Coeff: 0.311D-01-0.949D-01-0.566D-01 0.159D-02 0.308D+00 0.781D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

RMSDP=4.24D-09 MaxDP=1.83D-07 DE= 8.69D-11 OVMax= 3.43D-06

Error on total polarization charges = 0.06023

SCF Done: E(UB3LYP) = -1275.69948122 A.U. after 12 cycles

NFock= 12 Conv=0.42D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7819 S= 0.5158

<L.S>= 0.000000000000E+00

KE= 1.320618023965D+03 PE=-8.557393733877D+03 EE= 3.194306645898D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.95

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7819, after 0.7509

Leave Link 502 at Fri Jul 5 21:11:43 2019, MaxMem= 1342177280 cpu: 869.5

(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= 19306 NPrTT= 91506 LenC2= 15383 LenP2D= 41368.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 248

Leave Link 701 at Fri Jul 5 21:11:47 2019, MaxMem= 1342177280 cpu: 53.5

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

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

Leave Link 702 at Fri Jul 5 21:11:47 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= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Fri Jul 5 21:11:55 2019, MaxMem= 1342177280 cpu: 92.4

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

Dipole = 1.59872116D-13 3.20188320D-13-6.66133815D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000374068 -0.000168097 0.000000000

2 7 -0.000004292 -0.000609469 0.000000000

3 6 0.000255950 0.000759312 0.000000000

4 6 -0.000726389 -0.000652617 0.000000000

5 6 0.000189040 0.000241380 0.000000000

6 7 0.000047361 0.000141149 0.000000000

7 6 0.000168097 -0.000374068 0.000000000

8 7 0.000609469 -0.000004292 0.000000000

9 6 -0.000759312 0.000255950 0.000000000

10 6 0.000652617 -0.000726389 0.000000000

11 6 -0.000241380 0.000189040 0.000000000

12 7 0.000141149 -0.000047361 0.000000000

13 6 -0.000652617 0.000726389 0.000000000

14 6 0.000241380 -0.000189040 0.000000000

15 6 -0.000168097 0.000374068 0.000000000

16 7 -0.000609469 0.000004292 0.000000000

17 6 0.000759312 -0.000255950 0.000000000

18 7 -0.000047361 -0.000141149 0.000000000

19 7 0.000004292 0.000609469 0.000000000

20 6 -0.000255950 -0.000759312 0.000000000

21 6 0.000726389 0.000652617 0.000000000

22 6 -0.000189040 -0.000241380 0.000000000

23 6 0.000374068 0.000168097 0.000000000

24 7 -0.000141149 0.000047361 0.000000000

25 30 0.000000000 0.000000000 0.000000000

26 6 0.000086281 0.000257548 0.000000000

27 1 -0.000329970 0.000114263 0.000000000

28 6 -0.000257548 0.000086281 0.000000000

29 1 -0.000114263 -0.000329970 0.000000000

30 6 0.000257548 -0.000086281 0.000000000

31 1 0.000114263 0.000329970 0.000000000

32 6 -0.000086281 -0.000257548 0.000000000

33 1 0.000329970 -0.000114263 0.000000000

34 1 -0.000115795 -0.000187393 0.000000000

35 1 0.000157712 -0.000035209 0.000276027

36 1 0.000157712 -0.000035209 -0.000276027

37 1 0.000035209 0.000157712 0.000276027

38 1 0.000035209 0.000157712 -0.000276027

39 1 0.000187393 -0.000115795 0.000000000

40 1 -0.000035209 -0.000157712 0.000276027

41 1 -0.000035209 -0.000157712 -0.000276027

42 1 -0.000187393 0.000115795 0.000000000

43 1 -0.000157712 0.000035209 0.000276027

44 1 -0.000157712 0.000035209 -0.000276027

45 1 0.000115795 0.000187393 0.000000000

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

Cartesian Forces: Max 0.000759312 RMS 0.000282857

Leave Link 716 at Fri Jul 5 21:11:55 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 0.000737236 RMS 0.000178142

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 = .17814D-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= -2.59D-04 DEPred=-2.23D-04 R= 1.16D+00

TightC=F SS= 1.41D+00 RLast= 4.76D-02 DXNew= 5.5297D-01 1.4279D-01

Trust test= 1.16D+00 RLast= 4.76D-02 DXMaxT set to 3.29D-01

ITU= 1 1 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01340

Eigenvalues --- 0.01343 0.01343 0.01343 0.01600 0.01618

Eigenvalues --- 0.01631 0.01631 0.01776 0.01791 0.01817

Eigenvalues --- 0.01817 0.01890 0.01906 0.01943 0.01943

Eigenvalues --- 0.01998 0.01998 0.02045 0.02045 0.02070

Eigenvalues --- 0.02087 0.02101 0.02112 0.02112 0.02205

Eigenvalues --- 0.02316 0.02316 0.02352 0.02373 0.07189

Eigenvalues --- 0.07222 0.07222 0.07222 0.07222 0.07393

Eigenvalues --- 0.07393 0.07393 0.14163 0.14501 0.14501

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16001 0.16087

Eigenvalues --- 0.16517 0.18229 0.20271 0.22082 0.22082

Eigenvalues --- 0.23812 0.23848 0.23848 0.24090 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25005

Eigenvalues --- 0.25827 0.31253 0.33173 0.33173 0.33215

Eigenvalues --- 0.33282 0.33282 0.33282 0.33416 0.33724

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.34275 0.34437 0.34437 0.34437

Eigenvalues --- 0.34536 0.35253 0.35377 0.35572 0.35572

Eigenvalues --- 0.35682 0.35682 0.35682 0.36194 0.39286

Eigenvalues --- 0.41750 0.41750 0.43818 0.47331 0.48967

Eigenvalues --- 0.48967 0.49690 0.50264 0.50565 0.51356

Eigenvalues --- 0.51356 0.53616 0.53986 0.53986 0.54931

Eigenvalues --- 0.56276 0.56330 0.56330 0.56626

En-DIIS/RFO-DIIS IScMMF= 0 using points: 3 2

RFO step: Lambda=-1.99435033D-05.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 2.59D-04 SmlDif= 1.00D-05

RMS Error= 0.4057630061D-03 NUsed= 2 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.25704 -0.25704

Iteration 1 RMS(Cart)= 0.00277940 RMS(Int)= 0.00000457

Iteration 2 RMS(Cart)= 0.00000778 RMS(Int)= 0.00000047

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000047

ITry= 1 IFail=0 DXMaxC= 9.19D-03 DCOld= 1.00D+10 DXMaxT= 3.29D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.96D-10 for atom 33.

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

(Linear) (Quad) (Total)

R1 2.56974 0.00012 -0.00023 0.00018 -0.00005 2.56969

R2 2.77980 -0.00003 0.00115 -0.00054 0.00061 2.78041

R3 2.53120 -0.00009 -0.00026 -0.00003 -0.00029 2.53091

R4 2.55710 -0.00034 -0.00095 -0.00060 -0.00154 2.55556

R5 3.77843 0.00036 0.00152 0.00038 0.00190 3.78033

R6 2.82683 0.00058 0.00278 0.00068 0.00346 2.83029

R7 2.52244 0.00015 -0.00048 0.00056 0.00007 2.52251

R8 2.56117 0.00028 -0.00101 0.00093 -0.00008 2.56108

R9 2.80371 0.00013 -0.00042 0.00040 -0.00002 2.80369

R10 2.04081 0.00022 -0.00009 0.00068 0.00059 2.04141

R11 2.53120 -0.00009 -0.00026 -0.00003 -0.00029 2.53091

R12 2.56974 0.00012 -0.00023 0.00018 -0.00005 2.56969

R13 2.77980 -0.00003 0.00115 -0.00054 0.00061 2.78041

R14 2.55710 -0.00034 -0.00095 -0.00060 -0.00154 2.55556

R15 3.77843 0.00036 0.00152 0.00038 0.00190 3.78033

R16 2.82683 0.00058 0.00278 0.00068 0.00346 2.83029

R17 2.52244 0.00015 -0.00048 0.00056 0.00007 2.52251

R18 2.56117 0.00028 -0.00101 0.00093 -0.00008 2.56108

R19 2.80371 0.00013 -0.00042 0.00040 -0.00002 2.80369

R20 2.04081 0.00022 -0.00009 0.00068 0.00059 2.04141

R21 2.52244 0.00015 -0.00048 0.00056 0.00007 2.52251

R22 2.56117 0.00028 -0.00101 0.00093 -0.00008 2.56108

R23 2.82683 0.00058 0.00278 0.00068 0.00346 2.83029

R24 2.80371 0.00013 -0.00042 0.00040 -0.00002 2.80369

R25 2.77980 -0.00003 0.00115 -0.00054 0.00061 2.78041

R26 2.04081 0.00022 -0.00009 0.00068 0.00059 2.04141

R27 2.56974 0.00012 -0.00023 0.00018 -0.00005 2.56969

R28 2.53120 -0.00009 -0.00026 -0.00003 -0.00029 2.53091

R29 2.55710 -0.00034 -0.00095 -0.00060 -0.00154 2.55556

R30 3.77843 0.00036 0.00152 0.00038 0.00190 3.78033

R31 2.52244 0.00015 -0.00048 0.00056 0.00007 2.52251

R32 2.55710 -0.00034 -0.00095 -0.00060 -0.00154 2.55556

R33 2.56974 0.00012 -0.00023 0.00018 -0.00005 2.56969

R34 3.77843 0.00036 0.00152 0.00038 0.00190 3.78033

R35 2.82683 0.00058 0.00278 0.00068 0.00346 2.83029

R36 2.56117 0.00028 -0.00101 0.00093 -0.00008 2.56108

R37 2.80371 0.00013 -0.00042 0.00040 -0.00002 2.80369

R38 2.77980 -0.00003 0.00115 -0.00054 0.00061 2.78041

R39 2.04081 0.00022 -0.00009 0.00068 0.00059 2.04141

R40 2.53120 -0.00009 -0.00026 -0.00003 -0.00029 2.53091

R41 2.05996 0.00019 -0.00017 0.00064 0.00046 2.06043

R42 2.06742 0.00033 -0.00013 0.00101 0.00088 2.06830

R43 2.06742 0.00033 -0.00013 0.00101 0.00088 2.06830

R44 2.06742 0.00033 -0.00013 0.00101 0.00088 2.06830

R45 2.06742 0.00033 -0.00013 0.00101 0.00088 2.06830

R46 2.05996 0.00019 -0.00017 0.00064 0.00046 2.06043

R47 2.06742 0.00033 -0.00013 0.00101 0.00088 2.06830

R48 2.06742 0.00033 -0.00013 0.00101 0.00088 2.06830

R49 2.05996 0.00019 -0.00017 0.00064 0.00046 2.06043

R50 2.06742 0.00033 -0.00013 0.00101 0.00088 2.06830

R51 2.06742 0.00033 -0.00013 0.00101 0.00088 2.06830

R52 2.05996 0.00019 -0.00017 0.00064 0.00046 2.06043

A1 1.89309 0.00007 -0.00084 0.00086 0.00002 1.89311

A2 2.21247 -0.00017 0.00032 -0.00109 -0.00077 2.21170

A3 2.17763 0.00010 0.00052 0.00023 0.00075 2.17838

A4 1.90971 0.00012 0.00137 -0.00043 0.00094 1.91066

A5 2.19146 0.00000 -0.00037 0.00042 0.00004 2.19150

A6 2.18201 -0.00012 -0.00100 0.00001 -0.00098 2.18103

A7 1.89272 -0.00003 -0.00089 0.00030 -0.00059 1.89214

A8 2.23111 0.00012 0.00144 -0.00040 0.00104 2.23215

A9 2.15935 -0.00010 -0.00055 0.00010 -0.00045 2.15890

A10 1.85020 -0.00012 -0.00024 -0.00019 -0.00043 1.84977

A11 2.16383 -0.00061 -0.00199 -0.00178 -0.00377 2.16006

A12 2.26915 0.00074 0.00223 0.00197 0.00420 2.27335

A13 1.87905 -0.00004 0.00060 -0.00054 0.00005 1.87911

A14 2.17264 -0.00022 -0.00145 -0.00075 -0.00219 2.17045

A15 2.23149 0.00026 0.00085 0.00129 0.00214 2.23363

A16 2.17852 0.00017 -0.00039 0.00106 0.00068 2.17920

A17 2.21247 -0.00017 0.00032 -0.00109 -0.00077 2.21170

A18 2.17763 0.00010 0.00052 0.00023 0.00075 2.17838

A19 1.89309 0.00007 -0.00084 0.00086 0.00002 1.89311

A20 1.90971 0.00012 0.00137 -0.00043 0.00094 1.91066

A21 2.19146 0.00000 -0.00037 0.00042 0.00004 2.19150

A22 2.18201 -0.00012 -0.00100 0.00001 -0.00098 2.18103

A23 1.89272 -0.00003 -0.00089 0.00030 -0.00059 1.89214

A24 2.23111 0.00012 0.00144 -0.00040 0.00104 2.23215

A25 2.15935 -0.00010 -0.00055 0.00010 -0.00045 2.15890

A26 1.85020 -0.00012 -0.00024 -0.00019 -0.00043 1.84977

A27 2.16383 -0.00061 -0.00199 -0.00178 -0.00377 2.16006

A28 2.26915 0.00074 0.00223 0.00197 0.00420 2.27335

A29 1.87905 -0.00004 0.00060 -0.00054 0.00005 1.87911

A30 2.17264 -0.00022 -0.00145 -0.00075 -0.00219 2.17045

A31 2.23149 0.00026 0.00085 0.00129 0.00214 2.23363

A32 2.17852 0.00017 -0.00039 0.00106 0.00068 2.17920

A33 1.85020 -0.00012 -0.00024 -0.00019 -0.00043 1.84977

A34 2.26915 0.00074 0.00223 0.00197 0.00420 2.27335

A35 2.16383 -0.00061 -0.00199 -0.00178 -0.00377 2.16006

A36 1.87905 -0.00004 0.00060 -0.00054 0.00005 1.87911

A37 2.23149 0.00026 0.00085 0.00129 0.00214 2.23363

A38 2.17264 -0.00022 -0.00145 -0.00075 -0.00219 2.17045

A39 1.89309 0.00007 -0.00084 0.00086 0.00002 1.89311

A40 2.17763 0.00010 0.00052 0.00023 0.00075 2.17838

A41 2.21247 -0.00017 0.00032 -0.00109 -0.00077 2.21170

A42 1.90971 0.00012 0.00137 -0.00043 0.00094 1.91066

A43 2.19146 0.00000 -0.00037 0.00042 0.00004 2.19150

A44 2.18201 -0.00012 -0.00100 0.00001 -0.00098 2.18103

A45 2.15935 -0.00010 -0.00055 0.00010 -0.00045 2.15890

A46 2.23111 0.00012 0.00144 -0.00040 0.00104 2.23215

A47 1.89272 -0.00003 -0.00089 0.00030 -0.00059 1.89214

A48 2.17852 0.00017 -0.00039 0.00106 0.00068 2.17920

A49 1.90971 0.00012 0.00137 -0.00043 0.00094 1.91066

A50 2.18201 -0.00012 -0.00100 0.00001 -0.00098 2.18103

A51 2.19146 0.00000 -0.00037 0.00042 0.00004 2.19150

A52 2.23111 0.00012 0.00144 -0.00040 0.00104 2.23215

A53 2.15935 -0.00010 -0.00055 0.00010 -0.00045 2.15890

A54 1.89272 -0.00003 -0.00089 0.00030 -0.00059 1.89214

A55 1.85020 -0.00012 -0.00024 -0.00019 -0.00043 1.84977

A56 2.16383 -0.00061 -0.00199 -0.00178 -0.00377 2.16006

A57 2.26915 0.00074 0.00223 0.00197 0.00420 2.27335

A58 1.87905 -0.00004 0.00060 -0.00054 0.00005 1.87911

A59 2.23149 0.00026 0.00085 0.00129 0.00214 2.23363

A60 2.17264 -0.00022 -0.00145 -0.00075 -0.00219 2.17045

A61 1.89309 0.00007 -0.00084 0.00086 0.00002 1.89311

A62 2.21247 -0.00017 0.00032 -0.00109 -0.00077 2.21170

A63 2.17763 0.00010 0.00052 0.00023 0.00075 2.17838

A64 2.17852 0.00017 -0.00039 0.00106 0.00068 2.17920

A65 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A66 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A67 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A68 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A69 1.94179 0.00017 0.00057 0.00113 0.00170 1.94349

A70 1.93391 -0.00007 0.00003 -0.00071 -0.00068 1.93324

A71 1.93391 -0.00007 0.00003 -0.00071 -0.00068 1.93324

A72 1.89654 -0.00003 0.00025 -0.00017 0.00008 1.89662

A73 1.89654 -0.00003 0.00025 -0.00017 0.00008 1.89662

A74 1.85865 0.00003 -0.00120 0.00062 -0.00058 1.85808

A75 1.93391 -0.00007 0.00003 -0.00071 -0.00068 1.93324

A76 1.93391 -0.00007 0.00003 -0.00071 -0.00068 1.93324

A77 1.94179 0.00017 0.00057 0.00113 0.00170 1.94349

A78 1.85865 0.00003 -0.00120 0.00062 -0.00058 1.85808

A79 1.89654 -0.00003 0.00025 -0.00017 0.00008 1.89662

A80 1.89654 -0.00003 0.00025 -0.00017 0.00008 1.89662

A81 1.93391 -0.00007 0.00003 -0.00071 -0.00068 1.93324

A82 1.93391 -0.00007 0.00003 -0.00071 -0.00068 1.93324

A83 1.94179 0.00017 0.00057 0.00113 0.00170 1.94349

A84 1.85865 0.00003 -0.00120 0.00062 -0.00058 1.85808

A85 1.89654 -0.00003 0.00025 -0.00017 0.00008 1.89662

A86 1.89654 -0.00003 0.00025 -0.00017 0.00008 1.89662

A87 1.93391 -0.00007 0.00003 -0.00071 -0.00068 1.93324

A88 1.93391 -0.00007 0.00003 -0.00071 -0.00068 1.93324

A89 1.94179 0.00017 0.00057 0.00113 0.00170 1.94349

A90 1.85865 0.00003 -0.00120 0.00062 -0.00058 1.85808

A91 1.89654 -0.00003 0.00025 -0.00017 0.00008 1.89662

A92 1.89654 -0.00003 0.00025 -0.00017 0.00008 1.89662

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A95 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A96 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D3 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D4 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D10 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D12 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D14 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D15 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D16 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D17 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D18 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D124 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D125 1.02962 -0.00003 -0.00072 -0.00006 -0.00079 1.02884

D126 -1.02962 0.00003 0.00072 0.00006 0.00079 -1.02884

D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D128 -2.11197 -0.00003 -0.00072 -0.00006 -0.00079 -2.11275

D129 2.11197 0.00003 0.00072 0.00006 0.00079 2.11275

D130 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D131 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D132 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D133 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D134 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.000737 0.000450 NO

RMS Force 0.000178 0.000300 YES

Maximum Displacement 0.009191 0.001800 NO

RMS Displacement 0.002782 0.001200 NO

Predicted change in Energy=-2.338147D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 5 21:11:55 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 -2.065782 -2.178940 0.000000

2 7 0 -0.744697 -1.856686 0.000000

3 6 0 -0.004578 -2.988525 0.000000

4 6 0 -0.935041 -4.162161 0.000000

5 6 0 -2.187838 -3.645198 0.000000

6 7 0 1.325768 -3.098169 0.000000

7 6 0 2.178940 -2.065782 0.000000

8 7 0 1.856686 -0.744697 0.000000

9 6 0 2.988525 -0.004578 0.000000

10 6 0 4.162161 -0.935041 0.000000

11 6 0 3.645198 -2.187838 0.000000

12 7 0 -3.098169 -1.325768 0.000000

13 6 0 -4.162161 0.935041 0.000000

14 6 0 -3.645198 2.187838 0.000000

15 6 0 -2.178940 2.065782 0.000000

16 7 0 -1.856686 0.744697 0.000000

17 6 0 -2.988525 0.004578 0.000000

18 7 0 -1.325768 3.098169 0.000000

19 7 0 0.744697 1.856686 0.000000

20 6 0 0.004578 2.988525 0.000000

21 6 0 0.935041 4.162161 0.000000

22 6 0 2.187838 3.645198 0.000000

23 6 0 2.065782 2.178940 0.000000

24 7 0 3.098169 1.325768 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.480756 -5.574549 0.000000

27 1 0 -3.127131 -4.178773 0.000000

28 6 0 5.574549 -0.480756 0.000000

29 1 0 4.178773 -3.127131 0.000000

30 6 0 -5.574549 0.480756 0.000000

31 1 0 -4.178773 3.127131 0.000000

32 6 0 0.480756 5.574549 0.000000

33 1 0 3.127131 4.178773 0.000000

34 1 0 -1.325896 -6.263435 0.000000

35 1 0 0.140592 -5.782337 0.876742

36 1 0 0.140592 -5.782337 -0.876742

37 1 0 5.782337 0.140592 0.876742

38 1 0 5.782337 0.140592 -0.876742

39 1 0 6.263435 -1.325896 0.000000

40 1 0 -5.782337 -0.140592 0.876742

41 1 0 -5.782337 -0.140592 -0.876742

42 1 0 -6.263435 1.325896 0.000000

43 1 0 -0.140592 5.782337 0.876742

44 1 0 -0.140592 5.782337 -0.876742

45 1 0 1.325896 6.263435 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.359821 0.000000

3 C 2.214496 1.352345 0.000000

4 C 2.282923 2.313319 1.497726 0.000000

5 C 1.471329 2.298137 2.279878 1.355267 0.000000

6 N 3.513915 2.414147 1.334857 2.498668 3.555935

7 C 4.246231 2.931105 2.370487 3.753889 4.643631

8 N 4.176459 2.829083 2.915316 4.412800 4.977056

9 C 5.502170 4.167404 4.226418 5.716631 6.328416

10 C 6.350949 4.992663 4.645267 6.032891 6.904161

11 C 5.710987 4.402368 3.736571 4.987639 6.012338

12 N 1.339300 2.412614 3.512131 3.567106 2.491678

13 C 3.753889 4.412800 5.716631 6.032891 4.987639

14 C 4.643631 4.977056 6.328416 6.904161 6.012338

15 C 4.246231 4.176459 5.502170 6.350949 5.710987

16 N 2.931105 2.829083 4.167404 4.992663 4.402368

17 C 2.370487 2.915316 4.226418 4.645267 3.736571

18 N 5.328743 4.988811 6.228434 7.270836 6.798247

19 N 4.917832 4.000928 4.902804 6.248843 6.234620

20 C 5.566785 4.902804 5.977058 7.212156 6.986628

21 C 7.015305 6.248843 7.212156 8.531796 8.408759

22 C 7.212065 6.234620 6.986628 8.408759 8.502730

23 C 6.005077 4.917832 5.566785 7.015305 7.212065

24 N 6.240944 4.989553 5.314148 6.810591 7.256196

25 Zn 3.002539 2.000464 2.988529 4.265898 4.251365

26 C 3.747328 3.727220 2.629499 1.483649 2.576145

27 H 2.264021 3.326873 3.341710 2.192152 1.080265

28 C 7.826780 6.467306 6.116826 7.478469 8.382622

29 H 6.316133 5.084741 4.185647 5.217508 6.387655

30 C 4.402889 5.365734 6.562050 6.563666 5.337913

31 H 5.711315 6.052381 7.404401 7.978444 7.058914

32 C 8.160972 7.531599 8.576817 9.839106 9.598184

33 H 8.208951 7.170622 7.821622 9.277523 9.458511

34 H 4.150967 4.444910 3.531418 2.137316 2.756467

35 H 4.315233 4.118635 2.931746 2.133222 3.279882

36 H 4.315233 4.118635 2.931746 2.133222 3.279882

37 H 8.230546 6.881858 6.636900 8.025306 8.867050

38 H 8.230546 6.881858 6.636900 8.025306 8.867050

39 H 8.372786 7.028204 6.484776 7.737083 8.763742

40 H 4.328547 5.393651 6.500916 6.359085 5.096211

41 H 4.328547 5.393651 6.500916 6.359085 5.096211

42 H 5.468470 6.370659 7.601810 7.649218 6.428240

43 H 8.237535 7.712865 8.815623 10.014633 9.687018

44 H 8.237535 7.712865 8.815623 10.014633 9.687018

45 H 9.098197 8.379959 9.347135 10.667937 10.513198

6 7 8 9 10

6 N 0.000000

7 C 1.339300 0.000000

8 N 2.412614 1.359821 0.000000

9 C 3.512131 2.214496 1.352345 0.000000

10 C 3.567106 2.282923 2.313319 1.497726 0.000000

11 C 2.491678 1.471329 2.298137 2.279878 1.355267

12 N 4.765777 5.328743 4.988811 6.228434 7.270836

13 C 6.810591 7.015305 6.248843 7.212156 8.531796

14 C 7.256196 7.212065 6.234620 6.986628 8.408759

15 C 6.240944 6.005077 4.917832 5.566785 7.015305

16 N 4.989553 4.917832 4.000928 4.902804 6.248843

17 C 5.314148 5.566785 4.902804 5.977058 7.212156

18 N 6.739826 6.240944 4.989553 5.314148 6.810591

19 N 4.988811 4.176459 2.829083 2.915316 4.412800

20 C 6.228434 5.502170 4.167404 4.226418 5.716631

21 C 7.270836 6.350949 4.992663 4.645267 6.032891

22 C 6.798247 5.710987 4.402368 3.736571 4.987639

23 C 5.328743 4.246231 2.931105 2.370487 3.753889

24 N 4.765777 3.513915 2.414147 1.334857 2.498668

25 Zn 3.369913 3.002539 2.000464 2.988529 4.265898

26 C 3.065288 4.402889 5.365734 6.562050 6.563666

27 H 4.582141 5.711315 6.052381 7.404401 7.978444

28 C 4.990289 3.747328 3.727220 2.629499 1.483649

29 H 2.853152 2.264021 3.326873 3.341710 2.192152

30 C 7.773229 8.160972 7.531599 8.576817 9.839106

31 H 8.309894 8.208951 7.170622 7.821622 9.277523

32 C 8.713787 7.826780 6.467306 6.116826 7.478469

33 H 7.496586 6.316133 5.084741 4.185647 5.217508

34 H 4.129192 5.468470 6.370659 7.601810 7.649218

35 H 3.062365 4.328547 5.393651 6.500916 6.359085

36 H 3.062365 4.328547 5.393651 6.500916 6.359085

37 H 5.578464 4.315233 4.118635 2.931746 2.133222

38 H 5.578464 4.315233 4.118635 2.931746 2.133222

39 H 5.246094 4.150967 4.444910 3.531418 2.137316

40 H 7.748619 8.237535 7.712865 8.815623 10.014633

41 H 7.748619 8.237535 7.712865 8.815623 10.014633

42 H 8.784552 9.098197 8.379959 9.347135 10.667937

43 H 9.043356 8.230546 6.881858 6.636900 8.025306

44 H 9.043356 8.230546 6.881858 6.636900 8.025306

45 H 9.361604 8.372786 7.028204 6.484776 7.737083

11 12 13 14 15

11 C 0.000000

12 N 6.798247 0.000000

13 C 8.408759 2.498668 0.000000

14 C 8.502730 3.555935 1.355267 0.000000

15 C 7.212065 3.513915 2.282923 1.471329 0.000000

16 N 6.234620 2.414147 2.313319 2.298137 1.359821

17 C 6.986628 1.334857 1.497726 2.279878 2.214496

18 N 7.256196 4.765777 3.567106 2.491678 1.339300

19 N 4.977056 4.989553 4.992663 4.402368 2.931105

20 C 6.328416 5.314148 4.645267 3.736571 2.370487

21 C 6.904161 6.810591 6.032891 4.987639 3.753889

22 C 6.012338 7.256196 6.904161 6.012338 4.643631

23 C 4.643631 6.240944 6.350949 5.710987 4.246231

24 N 3.555935 6.739826 7.270836 6.798247 5.328743

25 Zn 4.251365 3.369913 4.265898 4.251365 3.002539

26 C 5.337913 4.990289 7.478469 8.382622 7.826780

27 H 7.058914 2.853152 5.217508 6.387655 6.316133

28 C 2.576145 8.713787 9.839106 9.598184 8.160972

29 H 1.080265 7.496586 9.277523 9.458511 8.208951

30 C 9.598184 3.065288 1.483649 2.576145 3.747328

31 H 9.458511 4.582141 2.192152 1.080265 2.264021

32 C 8.382622 7.773229 6.563666 5.337913 4.402889

33 H 6.387655 8.309894 7.978444 7.058914 5.711315

34 H 6.428240 5.246094 7.737083 8.763742 8.372786

35 H 5.096211 5.578464 8.025306 8.867050 8.230546

36 H 5.096211 5.578464 8.025306 8.867050 8.230546

37 H 3.279882 9.043356 10.014633 9.687018 8.237535

38 H 3.279882 9.043356 10.014633 9.687018 8.237535

39 H 2.756467 9.361604 10.667937 10.513198 9.098197

40 H 9.687018 3.062365 2.133222 3.279882 4.315233

41 H 9.687018 3.062365 2.133222 3.279882 4.315233

42 H 10.513198 4.129192 2.137316 2.756467 4.150967

43 H 8.867050 7.748619 6.359085 5.096211 4.328547

44 H 8.867050 7.748619 6.359085 5.096211 4.328547

45 H 8.763742 8.784552 7.649218 6.428240 5.468470

16 17 18 19 20

16 N 0.000000

17 C 1.352345 0.000000

18 N 2.412614 3.512131 0.000000

19 N 2.829083 4.167404 2.414147 0.000000

20 C 2.915316 4.226418 1.334857 1.352345 0.000000

21 C 4.412800 5.716631 2.498668 2.313319 1.497726

22 C 4.977056 6.328416 3.555935 2.298137 2.279878

23 C 4.176459 5.502170 3.513915 1.359821 2.214496

24 N 4.988811 6.228434 4.765777 2.412614 3.512131

25 Zn 2.000464 2.988529 3.369913 2.000464 2.988529

26 C 6.467306 6.116826 8.713787 7.531599 8.576817

27 H 5.084741 4.185647 7.496586 7.170622 7.821622

28 C 7.531599 8.576817 7.773229 5.365734 6.562050

29 H 7.170622 7.821622 8.309894 6.052381 7.404401

30 C 3.727220 2.629499 4.990289 6.467306 6.116826

31 H 3.326873 3.341710 2.853152 5.084741 4.185647

32 C 5.365734 6.562050 3.065288 3.727220 2.629499

33 H 6.052381 7.404401 4.582141 3.326873 3.341710

34 H 7.028204 6.484776 9.361604 8.379959 9.347135

35 H 6.881858 6.636900 9.043356 7.712865 8.815623

36 H 6.881858 6.636900 9.043356 7.712865 8.815623

37 H 7.712865 8.815623 7.748619 5.393651 6.500916

38 H 7.712865 8.815623 7.748619 5.393651 6.500916

39 H 8.379959 9.347135 8.784552 6.370659 7.601810

40 H 4.118635 2.931746 5.578464 6.881858 6.636900

41 H 4.118635 2.931746 5.578464 6.881858 6.636900

42 H 4.444910 3.531418 5.246094 7.028204 6.484776

43 H 5.393651 6.500916 3.062365 4.118635 2.931746

44 H 5.393651 6.500916 3.062365 4.118635 2.931746

45 H 6.370659 7.601810 4.129192 4.444910 3.531418

21 22 23 24 25

21 C 0.000000

22 C 1.355267 0.000000

23 C 2.282923 1.471329 0.000000

24 N 3.567106 2.491678 1.339300 0.000000

25 Zn 4.265898 4.251365 3.002539 3.369913 0.000000

26 C 9.839106 9.598184 8.160972 7.773229 5.595241

27 H 9.277523 9.458511 8.208951 8.309894 5.219300

28 C 6.563666 5.337913 4.402889 3.065288 5.595241

29 H 7.978444 7.058914 5.711315 4.582141 5.219300

30 C 7.478469 8.382622 7.826780 8.713787 5.595241

31 H 5.217508 6.387655 6.316133 7.496586 5.219300

32 C 1.483649 2.576145 3.747328 4.990289 5.595241

33 H 2.192152 1.080265 2.264021 2.853152 5.219300

34 H 10.667937 10.513198 9.098197 8.784552 6.402235

35 H 10.014633 9.687018 8.237535 7.748619 5.850117

36 H 10.014633 9.687018 8.237535 7.748619 5.850117

37 H 6.359085 5.096211 4.328547 3.062365 5.850117

38 H 6.359085 5.096211 4.328547 3.062365 5.850117

39 H 7.649218 6.428240 5.468470 4.129192 6.402235

40 H 8.025306 8.867050 8.230546 9.043356 5.850117

41 H 8.025306 8.867050 8.230546 9.043356 5.850117

42 H 7.737083 8.763742 8.372786 9.361604 6.402235

43 H 2.133222 3.279882 4.315233 5.578464 5.850117

44 H 2.133222 3.279882 4.315233 5.578464 5.850117

45 H 2.137316 2.756467 4.150967 5.246094 6.402235

26 27 28 29 30

26 C 0.000000

27 H 2.991904 0.000000

28 C 7.912866 9.454870 0.000000

29 H 5.263181 7.381205 2.991904 0.000000

30 C 7.912866 5.263181 11.190482 10.399238 0.000000

31 H 9.454870 7.381205 10.399238 10.438600 2.991904

32 C 11.190482 10.399238 7.912866 9.454870 7.912866

33 H 10.399238 10.438600 5.263181 7.381205 9.454870

34 H 1.090332 2.755043 9.003083 6.335439 7.970895

35 H 1.094498 3.744076 7.642207 4.911792 8.523958

36 H 1.094498 3.744076 7.642207 4.911792 8.523958

37 H 8.523958 9.940031 1.094498 3.744076 11.395756

38 H 8.523958 9.940031 1.094498 3.744076 11.395756

39 H 7.970895 9.814359 1.090332 2.755043 11.975051

40 H 7.642207 4.911792 11.395756 10.436082 1.094498

41 H 7.642207 4.911792 11.395756 10.436082 1.094498

42 H 9.003083 6.335439 11.975051 11.352055 1.090332

43 H 11.395756 10.436082 8.523958 9.940031 7.642207

44 H 11.395756 10.436082 8.523958 9.940031 7.642207

45 H 11.975051 11.352055 7.970895 9.814359 9.003083

31 32 33 34 35

31 H 0.000000

32 C 5.263181 0.000000

33 H 7.381205 2.991904 0.000000

34 H 9.814359 11.975051 11.352055 0.000000

35 H 9.940031 11.395756 10.436082 1.775026 0.000000

36 H 9.940031 11.395756 10.436082 1.775026 1.753485

37 H 10.436082 7.642207 4.911792 9.607664 8.179876

38 H 10.436082 7.642207 4.911792 9.607664 8.365709

39 H 11.352055 9.003083 6.335439 9.054128 7.623500

40 H 3.744076 8.523958 9.940031 7.623500 8.179876

41 H 3.744076 8.523958 9.940031 7.623500 8.365709

42 H 2.755043 7.970895 9.814359 9.054128 9.607664

43 H 4.911792 1.094498 3.744076 12.135660 11.568092

44 H 4.911792 1.094498 3.744076 12.135660 11.700234

45 H 6.335439 1.090332 2.755043 12.804471 12.135660

36 37 38 39 40

36 H 0.000000

37 H 8.365709 0.000000

38 H 8.179876 1.753485 0.000000

39 H 7.623500 1.775026 1.775026 0.000000

40 H 8.365709 11.568092 11.700234 12.135660 0.000000

41 H 8.179876 11.700234 11.568092 12.135660 1.753485

42 H 9.607664 12.135660 12.135660 12.804471 1.775026

43 H 11.700234 8.179876 8.365709 9.607664 8.179876

44 H 11.568092 8.365709 8.179876 9.607664 8.365709

45 H 12.135660 7.623500 7.623500 9.054128 9.607664

41 42 43 44 45

41 H 0.000000

42 H 1.775026 0.000000

43 H 8.365709 7.623500 0.000000

44 H 8.179876 7.623500 1.753485 0.000000

45 H 9.607664 9.054128 1.775026 1.775026 0.000000

Stoichiometry C20H16N8Zn(1+,2)

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

Deg. of freedom 20

Full point group C4H NOp 8

RotChk: IX=0 Diff= 9.14D-04

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.182102 2.062442 0.000000

2 7 0 -1.857824 0.741852 0.000000

3 6 0 -2.988529 0.000000 0.000000

4 6 0 -4.163588 0.928665 0.000000

5 6 0 -3.648545 2.182252 0.000000

6 7 0 -3.096135 -1.330513 0.000000

7 6 0 -2.062442 -2.182102 0.000000

8 7 0 -0.741852 -1.857824 0.000000

9 6 0 0.000000 -2.988529 0.000000

10 6 0 -0.928665 -4.163588 0.000000

11 6 0 -2.182252 -3.648545 0.000000

12 7 0 -1.330513 3.096135 0.000000

13 6 0 0.928665 4.163588 0.000000

14 6 0 2.182252 3.648545 0.000000

15 6 0 2.062442 2.182102 0.000000

16 7 0 0.741852 1.857824 0.000000

17 6 0 0.000000 2.988529 0.000000

18 7 0 3.096135 1.330513 0.000000

19 7 0 1.857824 -0.741852 0.000000

20 6 0 2.988529 0.000000 0.000000

21 6 0 4.163588 -0.928665 0.000000

22 6 0 3.648545 -2.182252 0.000000

23 6 0 2.182102 -2.062442 0.000000

24 7 0 1.330513 -3.096135 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.575279 0.472217 0.000000

27 1 0 -4.183559 3.120726 0.000000

28 6 0 -0.472217 -5.575279 0.000000

29 1 0 -3.120726 -4.183559 0.000000

30 6 0 0.472217 5.575279 0.000000

31 1 0 3.120726 4.183559 0.000000

32 6 0 5.575279 -0.472217 0.000000

33 1 0 4.183559 -3.120726 0.000000

34 1 0 -6.265459 1.316300 0.000000

35 1 0 -5.782115 -0.149449 0.876742

36 1 0 -5.782115 -0.149449 -0.876742

37 1 0 0.149449 -5.782115 0.876742

38 1 0 0.149449 -5.782115 -0.876742

39 1 0 -1.316300 -6.265459 0.000000

40 1 0 -0.149449 5.782115 0.876742

41 1 0 -0.149449 5.782115 -0.876742

42 1 0 1.316300 6.265459 0.000000

43 1 0 5.782115 0.149449 0.876742

44 1 0 5.782115 0.149449 -0.876742

45 1 0 6.265459 -1.316300 0.000000

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

Rotational constants (GHZ): 0.1830207 0.1830207 0.0917162

Leave Link 202 at Fri Jul 5 21:11:55 2019, MaxMem= 1342177280 cpu: 0.2

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

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

Pseudo-potential data read from rwf file.

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

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

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

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

There are 212 symmetry adapted basis functions of AG symmetry.

There are 82 symmetry adapted basis functions of BG symmetry.

There are 78 symmetry adapted basis functions of AU symmetry.

There are 204 symmetry adapted basis functions of BU symmetry.

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

102 alpha electrons 101 beta electrons

nuclear repulsion energy 2766.6354236876 Hartrees.

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

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

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

NAtoms= 45 NActive= 45 NUniq= 11 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1142374744 Hartrees.

Nuclear repulsion after empirical dispersion term = 2766.5211862132 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 = 3538

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.76D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 160

GePol: Fraction of low-weight points (<1% of avg) = 4.52%

GePol: Cavity surface area = 382.113 Ang\*\*2

GePol: Cavity volume = 379.112 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0110968490 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2766.5100893642 Hartrees.

Leave Link 301 at Fri Jul 5 21:11:56 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= 19306 NPrTT= 91506 LenC2= 15383 LenP2D= 41364.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.86D-04 NBF= 212 82 78 204

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

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Fri Jul 5 21:11:56 2019, MaxMem= 1342177280 cpu: 7.8

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 5 21:11:57 2019, MaxMem= 1342177280 cpu: 0.8

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

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

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 -0.000186 Ang= -0.02 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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Beta Orbitals:

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

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7819 S= 0.5158

Leave Link 401 at Fri Jul 5 21:11:59 2019, MaxMem= 1342177280 cpu: 23.1

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1138797 IEndB= 1138797 NGot= 1342177280 MDV= 1341424180

LenX= 1341424180 LenY= 1341055124

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

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

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 37552332.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.11D-15 for 273.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.41D-15 for 3160 849.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.55D-15 for 861.

Iteration 1 A^-1\*A deviation from orthogonality is 2.24D-15 for 1949 1905.

E= -1275.69945994435

DIIS: error= 2.61D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.69945994435 IErMin= 1 ErrMin= 2.61D-04

ErrMax= 2.61D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-04 BMatP= 1.04D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.61D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.372 Goal= None Shift= 0.000

Gap= 0.406 Goal= None Shift= 0.000

RMSDP=1.33D-05 MaxDP=4.39D-04 OVMax= 1.52D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.32D-05 CP: 1.00D+00

E= -1275.69949984038 Delta-E= -0.000039896028 Rises=F Damp=F

DIIS: error= 5.80D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.69949984038 IErMin= 2 ErrMin= 5.80D-05

ErrMax= 5.80D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.23D-06 BMatP= 1.04D-04

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

Coeff-Com: 0.356D-01 0.964D+00

Coeff: 0.356D-01 0.964D+00

Gap= 0.104 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=3.96D-06 MaxDP=1.76D-04 DE=-3.99D-05 OVMax= 5.88D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.95D-06 CP: 1.00D+00 1.00D+00

E= -1275.69949833130 Delta-E= 0.000001509076 Rises=F Damp=F

DIIS: error= 1.01D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.69949984038 IErMin= 2 ErrMin= 5.80D-05

ErrMax= 1.01D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D-05 BMatP= 6.23D-06

IDIUse=3 WtCom= 4.99D-01 WtEn= 5.01D-01

Coeff-Com: -0.313D-01 0.619D+00 0.412D+00

Coeff-En: 0.000D+00 0.646D+00 0.354D+00

Coeff: -0.156D-01 0.633D+00 0.383D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=2.39D-06 MaxDP=1.03D-04 DE= 1.51D-06 OVMax= 4.90D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.01D-06 CP: 1.00D+00 1.03D+00 4.63D-01

E= -1275.69950151749 Delta-E= -0.000003186193 Rises=F Damp=F

DIIS: error= 7.41D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.69950151749 IErMin= 4 ErrMin= 7.41D-06

ErrMax= 7.41D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.99D-08 BMatP= 6.23D-06

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

Coeff-Com: -0.135D-01 0.168D+00 0.120D+00 0.725D+00

Coeff: -0.135D-01 0.168D+00 0.120D+00 0.725D+00

Gap= 0.104 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 31774 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

Gap= 0.083 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

RMSDP=3.42D-07 MaxDP=1.77D-05 DE=-3.19D-06 OVMax= 1.45D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.25D-07 CP: 1.00D+00 1.04D+00 4.61D-01 1.03D+00

E= -1275.69950154127 Delta-E= -0.000000023778 Rises=F Damp=F

DIIS: error= 5.39D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.69950154127 IErMin= 5 ErrMin= 5.39D-06

ErrMax= 5.39D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.83D-08 BMatP= 8.99D-08

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

Coeff-Com: -0.381D-02 0.330D-01 0.313D-01 0.360D+00 0.580D+00

Coeff: -0.381D-02 0.330D-01 0.313D-01 0.360D+00 0.580D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=1.72D-07 MaxDP=6.94D-06 DE=-2.38D-08 OVMax= 8.24D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.54D-07 CP: 1.00D+00 1.04D+00 4.70D-01 1.09D+00 9.23D-01

E= -1275.69950155045 Delta-E= -0.000000009183 Rises=F Damp=F

DIIS: error= 2.44D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.69950155045 IErMin= 6 ErrMin= 2.44D-06

ErrMax= 2.44D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.32D-09 BMatP= 2.83D-08

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

Coeff-Com: 0.163D-04-0.839D-02 0.110D-02 0.538D-01 0.270D+00 0.683D+00

Coeff: 0.163D-04-0.839D-02 0.110D-02 0.538D-01 0.270D+00 0.683D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=9.84D-08 MaxDP=4.00D-06 DE=-9.18D-09 OVMax= 5.67D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 6.32D-08 CP: 1.00D+00 1.04D+00 4.74D-01 1.13D+00 1.10D+00

CP: 1.07D+00

E= -1275.69950155332 Delta-E= -0.000000002867 Rises=F Damp=F

DIIS: error= 1.31D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.69950155332 IErMin= 7 ErrMin= 1.31D-06

ErrMax= 1.31D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.39D-09 BMatP= 4.32D-09

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

Coeff-Com: 0.105D-02-0.141D-01-0.619D-02-0.603D-01 0.255D-01 0.381D+00

Coeff-Com: 0.673D+00

Coeff: 0.105D-02-0.141D-01-0.619D-02-0.603D-01 0.255D-01 0.381D+00

Coeff: 0.673D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=6.92D-08 MaxDP=3.43D-06 DE=-2.87D-09 OVMax= 4.15D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 3.09D-08 CP: 1.00D+00 1.04D+00 4.77D-01 1.16D+00 1.20D+00

CP: 1.34D+00 1.33D+00

E= -1275.69950155474 Delta-E= -0.000000001423 Rises=F Damp=F

DIIS: error= 8.14D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.69950155474 IErMin= 8 ErrMin= 8.14D-07

ErrMax= 8.14D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.50D-10 BMatP= 1.39D-09

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

Coeff-Com: 0.152D-03 0.122D-02-0.538D-03-0.352D-01-0.115D+00-0.262D+00

Coeff-Com: 0.146D+00 0.126D+01

Coeff: 0.152D-03 0.122D-02-0.538D-03-0.352D-01-0.115D+00-0.262D+00

Coeff: 0.146D+00 0.126D+01

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=8.29D-08 MaxDP=4.64D-06 DE=-1.42D-09 OVMax= 4.04D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.12D-08 CP: 1.00D+00 1.04D+00 4.80D-01 1.18D+00 1.31D+00

CP: 1.60D+00 2.08D+00 1.67D+00

E= -1275.69950155563 Delta-E= -0.000000000882 Rises=F Damp=F

DIIS: error= 3.95D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.69950155563 IErMin= 9 ErrMin= 3.95D-07

ErrMax= 3.95D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.56D-10 BMatP= 3.50D-10

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

Coeff-Com: -0.159D-03 0.422D-02 0.111D-02-0.471D-02-0.725D-01-0.239D+00

Coeff-Com: -0.886D-01 0.751D+00 0.648D+00

Coeff: -0.159D-03 0.422D-02 0.111D-02-0.471D-02-0.725D-01-0.239D+00

Coeff: -0.886D-01 0.751D+00 0.648D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=2.84D-08 MaxDP=1.68D-06 DE=-8.82D-10 OVMax= 1.24D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.22D-08 CP: 1.00D+00 1.04D+00 4.80D-01 1.19D+00 1.34D+00

CP: 1.68D+00 2.31D+00 2.05D+00 1.22D+00

E= -1275.69950155563 Delta-E= 0.000000000000 Rises=F Damp=F

DIIS: error= 2.77D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1275.69950155563 IErMin=10 ErrMin= 2.77D-07

ErrMax= 2.77D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.45D-11 BMatP= 1.56D-10

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

Coeff-Com: -0.146D-03 0.181D-02 0.678D-03 0.118D-01 0.841D-02-0.386D-02

Coeff-Com: -0.982D-01-0.897D-01 0.299D+00 0.870D+00

Coeff: -0.146D-03 0.181D-02 0.678D-03 0.118D-01 0.841D-02-0.386D-02

Coeff: -0.982D-01-0.897D-01 0.299D+00 0.870D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=1.41D-08 MaxDP=8.91D-07 DE=-4.55D-13 OVMax= 6.31D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.27D-09 CP: 1.00D+00 1.04D+00 4.80D-01 1.19D+00 1.34D+00

CP: 1.70D+00 2.40D+00 2.25D+00 1.66D+00 1.25D+00

E= -1275.69950155577 Delta-E= -0.000000000141 Rises=F Damp=F

DIIS: error= 1.02D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1275.69950155577 IErMin=11 ErrMin= 1.02D-07

ErrMax= 1.02D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.91D-12 BMatP= 3.45D-11

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

Coeff-Com: -0.327D-04-0.119D-03-0.515D-04 0.625D-02 0.184D-01 0.508D-01

Coeff-Com: -0.340D-01-0.211D+00 0.752D-02 0.447D+00 0.715D+00

Coeff: -0.327D-04-0.119D-03-0.515D-04 0.625D-02 0.184D-01 0.508D-01

Coeff: -0.340D-01-0.211D+00 0.752D-02 0.447D+00 0.715D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=6.66D-09 MaxDP=3.94D-07 DE=-1.41D-10 OVMax= 3.22D-06

Error on total polarization charges = 0.06026

SCF Done: E(UB3LYP) = -1275.69950156 A.U. after 11 cycles

NFock= 11 Conv=0.67D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7819 S= 0.5158

<L.S>= 0.000000000000E+00

KE= 1.320599904401D+03 PE=-8.556853724139D+03 EE= 3.194044228819D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.96

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7819, after 0.7509

Leave Link 502 at Fri Jul 5 21:13:06 2019, MaxMem= 1342177280 cpu: 775.3

(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= 19306 NPrTT= 91506 LenC2= 15383 LenP2D= 41364.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 248

Leave Link 701 at Fri Jul 5 21:13:11 2019, MaxMem= 1342177280 cpu: 53.4

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

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

Leave Link 702 at Fri Jul 5 21:13:11 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= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Fri Jul 5 21:13:18 2019, MaxMem= 1342177280 cpu: 92.4

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

Dipole =-9.23705556D-14 1.32782674D-13-4.44089210D-16

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000315832 -0.000245734 0.000000000

2 7 0.000181903 0.000062597 0.000000000

3 6 -0.000184370 -0.000064551 0.000000000

4 6 0.000037715 -0.000057082 0.000000000

5 6 -0.000060278 0.000311643 0.000000000

6 7 0.000119418 0.000038493 0.000000000

7 6 0.000245734 -0.000315832 0.000000000

8 7 -0.000062597 0.000181903 0.000000000

9 6 0.000064551 -0.000184370 0.000000000

10 6 0.000057082 0.000037715 0.000000000

11 6 -0.000311643 -0.000060278 0.000000000

12 7 0.000038493 -0.000119418 0.000000000

13 6 -0.000057082 -0.000037715 0.000000000

14 6 0.000311643 0.000060278 0.000000000

15 6 -0.000245734 0.000315832 0.000000000

16 7 0.000062597 -0.000181903 0.000000000

17 6 -0.000064551 0.000184370 0.000000000

18 7 -0.000119418 -0.000038493 0.000000000

19 7 -0.000181903 -0.000062597 0.000000000

20 6 0.000184370 0.000064551 0.000000000

21 6 -0.000037715 0.000057082 0.000000000

22 6 0.000060278 -0.000311643 0.000000000

23 6 0.000315832 0.000245734 0.000000000

24 7 -0.000038493 0.000119418 0.000000000

25 30 0.000000000 0.000000000 0.000000000

26 6 0.000069864 0.000021063 0.000000000

27 1 -0.000047920 0.000054089 0.000000000

28 6 -0.000021063 0.000069864 0.000000000

29 1 -0.000054089 -0.000047920 0.000000000

30 6 0.000021063 -0.000069864 0.000000000

31 1 0.000054089 0.000047920 0.000000000

32 6 -0.000069864 -0.000021063 0.000000000

33 1 0.000047920 -0.000054089 0.000000000

34 1 -0.000034500 -0.000025249 0.000000000

35 1 -0.000029083 0.000012860 0.000051071

36 1 -0.000029083 0.000012860 -0.000051071

37 1 -0.000012860 -0.000029083 0.000051071

38 1 -0.000012860 -0.000029083 -0.000051071

39 1 0.000025249 -0.000034500 0.000000000

40 1 0.000012860 0.000029083 0.000051071

41 1 0.000012860 0.000029083 -0.000051071

42 1 -0.000025249 0.000034500 0.000000000

43 1 0.000029083 -0.000012860 0.000051071

44 1 0.000029083 -0.000012860 -0.000051071

45 1 0.000034500 0.000025249 0.000000000

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

Cartesian Forces: Max 0.000315832 RMS 0.000105563

Leave Link 716 at Fri Jul 5 21:13:18 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.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.000207042 RMS 0.000055295

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 = .55295D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4

DE= -2.03D-05 DEPred=-2.34D-05 R= 8.70D-01

TightC=F SS= 1.41D+00 RLast= 1.72D-02 DXNew= 5.5297D-01 5.1496D-02

Trust test= 8.70D-01 RLast= 1.72D-02 DXMaxT set to 3.29D-01

ITU= 1 1 1 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01342

Eigenvalues --- 0.01345 0.01345 0.01345 0.01600 0.01618

Eigenvalues --- 0.01631 0.01631 0.01777 0.01792 0.01819

Eigenvalues --- 0.01819 0.01890 0.01906 0.01943 0.01943

Eigenvalues --- 0.01998 0.01999 0.02045 0.02045 0.02070

Eigenvalues --- 0.02087 0.02102 0.02113 0.02113 0.02205

Eigenvalues --- 0.02316 0.02316 0.02352 0.02374 0.07179

Eigenvalues --- 0.07212 0.07212 0.07212 0.07212 0.07401

Eigenvalues --- 0.07401 0.07401 0.12607 0.14501 0.14501

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16003 0.16087

Eigenvalues --- 0.16516 0.18181 0.20215 0.22084 0.22084

Eigenvalues --- 0.23811 0.23848 0.23848 0.24128 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25002

Eigenvalues --- 0.25887 0.32167 0.33173 0.33173 0.33215

Eigenvalues --- 0.33282 0.33282 0.33282 0.33433 0.33724

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.34154 0.34437 0.34437 0.34437

Eigenvalues --- 0.34493 0.35379 0.35449 0.35574 0.35574

Eigenvalues --- 0.35682 0.35682 0.35682 0.36047 0.39287

Eigenvalues --- 0.41754 0.41754 0.42763 0.47097 0.48969

Eigenvalues --- 0.48969 0.49606 0.50265 0.50567 0.51356

Eigenvalues --- 0.51356 0.52275 0.53984 0.53984 0.54930

Eigenvalues --- 0.56277 0.56331 0.56331 0.56433

En-DIIS/RFO-DIIS IScMMF= 0 using points: 4 3 2

RFO step: Lambda=-1.56511822D-06.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=F DC= 2.59D-04 SmlDif= 1.00D-05

RMS Error= 0.1037808339D-03 NUsed= 3 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.24858 -0.29634 0.04776

Iteration 1 RMS(Cart)= 0.00085191 RMS(Int)= 0.00000035

Iteration 2 RMS(Cart)= 0.00000050 RMS(Int)= 0.00000009

ITry= 1 IFail=0 DXMaxC= 2.90D-03 DCOld= 1.00D+10 DXMaxT= 3.29D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.02D-10 for atom 36.

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

(Linear) (Quad) (Total)

R1 2.56969 0.00018 0.00003 0.00038 0.00041 2.57010

R2 2.78041 -0.00021 -0.00006 -0.00052 -0.00059 2.77982

R3 2.53091 -0.00006 -0.00002 -0.00014 -0.00017 2.53074

R4 2.55556 -0.00001 -0.00021 0.00004 -0.00017 2.55539

R5 3.78033 0.00001 0.00019 -0.00016 0.00003 3.78036

R6 2.83029 -0.00008 0.00034 -0.00036 -0.00002 2.83028

R7 2.52251 0.00012 0.00011 0.00012 0.00023 2.52274

R8 2.56108 0.00017 0.00017 0.00013 0.00030 2.56138

R9 2.80369 0.00002 0.00007 -0.00008 -0.00001 2.80369

R10 2.04141 0.00000 0.00016 -0.00015 0.00001 2.04142

R11 2.53091 -0.00006 -0.00002 -0.00014 -0.00017 2.53074

R12 2.56969 0.00018 0.00003 0.00038 0.00041 2.57010

R13 2.78041 -0.00021 -0.00006 -0.00052 -0.00059 2.77982

R14 2.55556 -0.00001 -0.00021 0.00004 -0.00017 2.55539

R15 3.78033 0.00001 0.00019 -0.00016 0.00003 3.78036

R16 2.83029 -0.00008 0.00034 -0.00036 -0.00002 2.83028

R17 2.52251 0.00012 0.00011 0.00012 0.00023 2.52274

R18 2.56108 0.00017 0.00017 0.00013 0.00030 2.56138

R19 2.80369 0.00002 0.00007 -0.00008 -0.00001 2.80369

R20 2.04141 0.00000 0.00016 -0.00015 0.00001 2.04142

R21 2.52251 0.00012 0.00011 0.00012 0.00023 2.52274

R22 2.56108 0.00017 0.00017 0.00013 0.00030 2.56138

R23 2.83029 -0.00008 0.00034 -0.00036 -0.00002 2.83028

R24 2.80369 0.00002 0.00007 -0.00008 -0.00001 2.80369

R25 2.78041 -0.00021 -0.00006 -0.00052 -0.00059 2.77982

R26 2.04141 0.00000 0.00016 -0.00015 0.00001 2.04142

R27 2.56969 0.00018 0.00003 0.00038 0.00041 2.57010

R28 2.53091 -0.00006 -0.00002 -0.00014 -0.00017 2.53074

R29 2.55556 -0.00001 -0.00021 0.00004 -0.00017 2.55539

R30 3.78033 0.00001 0.00019 -0.00016 0.00003 3.78036

R31 2.52251 0.00012 0.00011 0.00012 0.00023 2.52274

R32 2.55556 -0.00001 -0.00021 0.00004 -0.00017 2.55539

R33 2.56969 0.00018 0.00003 0.00038 0.00041 2.57010

R34 3.78033 0.00001 0.00019 -0.00016 0.00003 3.78036

R35 2.83029 -0.00008 0.00034 -0.00036 -0.00002 2.83028

R36 2.56108 0.00017 0.00017 0.00013 0.00030 2.56138

R37 2.80369 0.00002 0.00007 -0.00008 -0.00001 2.80369

R38 2.78041 -0.00021 -0.00006 -0.00052 -0.00059 2.77982

R39 2.04141 0.00000 0.00016 -0.00015 0.00001 2.04142

R40 2.53091 -0.00006 -0.00002 -0.00014 -0.00017 2.53074

R41 2.06043 0.00002 0.00015 -0.00008 0.00007 2.06050

R42 2.06830 0.00004 0.00024 -0.00012 0.00013 2.06843

R43 2.06830 0.00004 0.00024 -0.00012 0.00013 2.06843

R44 2.06830 0.00004 0.00024 -0.00012 0.00013 2.06843

R45 2.06830 0.00004 0.00024 -0.00012 0.00013 2.06843

R46 2.06043 0.00002 0.00015 -0.00008 0.00007 2.06050

R47 2.06830 0.00004 0.00024 -0.00012 0.00013 2.06843

R48 2.06830 0.00004 0.00024 -0.00012 0.00013 2.06843

R49 2.06043 0.00002 0.00015 -0.00008 0.00007 2.06050

R50 2.06830 0.00004 0.00024 -0.00012 0.00013 2.06843

R51 2.06830 0.00004 0.00024 -0.00012 0.00013 2.06843

R52 2.06043 0.00002 0.00015 -0.00008 0.00007 2.06050

A1 1.89311 0.00000 0.00016 -0.00019 -0.00003 1.89308

A2 2.21170 -0.00004 -0.00025 0.00006 -0.00019 2.21150

A3 2.17838 0.00004 0.00009 0.00013 0.00022 2.17860

A4 1.91066 -0.00002 -0.00002 -0.00001 -0.00003 1.91062

A5 2.19150 0.00001 0.00008 0.00000 0.00008 2.19158

A6 2.18103 0.00001 -0.00006 0.00001 -0.00005 2.18098

A7 1.89214 0.00002 0.00002 0.00002 0.00004 1.89218

A8 2.23215 0.00001 -0.00001 0.00014 0.00013 2.23228

A9 2.15890 -0.00003 -0.00001 -0.00016 -0.00017 2.15873

A10 1.84977 -0.00002 -0.00006 -0.00007 -0.00013 1.84964

A11 2.16006 -0.00017 -0.00057 -0.00046 -0.00103 2.15904

A12 2.27335 0.00019 0.00063 0.00053 0.00116 2.27451

A13 1.87911 0.00002 -0.00010 0.00024 0.00014 1.87925

A14 2.17045 -0.00006 -0.00028 -0.00027 -0.00054 2.16991

A15 2.23363 0.00003 0.00037 0.00003 0.00040 2.23403

A16 2.17920 0.00000 0.00024 -0.00021 0.00003 2.17923

A17 2.21170 -0.00004 -0.00025 0.00006 -0.00019 2.21150

A18 2.17838 0.00004 0.00009 0.00013 0.00022 2.17860

A19 1.89311 0.00000 0.00016 -0.00019 -0.00003 1.89308

A20 1.91066 -0.00002 -0.00002 -0.00001 -0.00003 1.91062

A21 2.19150 0.00001 0.00008 0.00000 0.00008 2.19158

A22 2.18103 0.00001 -0.00006 0.00001 -0.00005 2.18098

A23 1.89214 0.00002 0.00002 0.00002 0.00004 1.89218

A24 2.23215 0.00001 -0.00001 0.00014 0.00013 2.23228

A25 2.15890 -0.00003 -0.00001 -0.00016 -0.00017 2.15873

A26 1.84977 -0.00002 -0.00006 -0.00007 -0.00013 1.84964

A27 2.16006 -0.00017 -0.00057 -0.00046 -0.00103 2.15904

A28 2.27335 0.00019 0.00063 0.00053 0.00116 2.27451

A29 1.87911 0.00002 -0.00010 0.00024 0.00014 1.87925

A30 2.17045 -0.00006 -0.00028 -0.00027 -0.00054 2.16991

A31 2.23363 0.00003 0.00037 0.00003 0.00040 2.23403

A32 2.17920 0.00000 0.00024 -0.00021 0.00003 2.17923

A33 1.84977 -0.00002 -0.00006 -0.00007 -0.00013 1.84964

A34 2.27335 0.00019 0.00063 0.00053 0.00116 2.27451

A35 2.16006 -0.00017 -0.00057 -0.00046 -0.00103 2.15904

A36 1.87911 0.00002 -0.00010 0.00024 0.00014 1.87925

A37 2.23363 0.00003 0.00037 0.00003 0.00040 2.23403

A38 2.17045 -0.00006 -0.00028 -0.00027 -0.00054 2.16991

A39 1.89311 0.00000 0.00016 -0.00019 -0.00003 1.89308

A40 2.17838 0.00004 0.00009 0.00013 0.00022 2.17860

A41 2.21170 -0.00004 -0.00025 0.00006 -0.00019 2.21150

A42 1.91066 -0.00002 -0.00002 -0.00001 -0.00003 1.91062

A43 2.19150 0.00001 0.00008 0.00000 0.00008 2.19158

A44 2.18103 0.00001 -0.00006 0.00001 -0.00005 2.18098

A45 2.15890 -0.00003 -0.00001 -0.00016 -0.00017 2.15873

A46 2.23215 0.00001 -0.00001 0.00014 0.00013 2.23228

A47 1.89214 0.00002 0.00002 0.00002 0.00004 1.89218

A48 2.17920 0.00000 0.00024 -0.00021 0.00003 2.17923

A49 1.91066 -0.00002 -0.00002 -0.00001 -0.00003 1.91062

A50 2.18103 0.00001 -0.00006 0.00001 -0.00005 2.18098

A51 2.19150 0.00001 0.00008 0.00000 0.00008 2.19158

A52 2.23215 0.00001 -0.00001 0.00014 0.00013 2.23228

A53 2.15890 -0.00003 -0.00001 -0.00016 -0.00017 2.15873

A54 1.89214 0.00002 0.00002 0.00002 0.00004 1.89218

A55 1.84977 -0.00002 -0.00006 -0.00007 -0.00013 1.84964

A56 2.16006 -0.00017 -0.00057 -0.00046 -0.00103 2.15904

A57 2.27335 0.00019 0.00063 0.00053 0.00116 2.27451

A58 1.87911 0.00002 -0.00010 0.00024 0.00014 1.87925

A59 2.23363 0.00003 0.00037 0.00003 0.00040 2.23403

A60 2.17045 -0.00006 -0.00028 -0.00027 -0.00054 2.16991

A61 1.89311 0.00000 0.00016 -0.00019 -0.00003 1.89308

A62 2.21170 -0.00004 -0.00025 0.00006 -0.00019 2.21150

A63 2.17838 0.00004 0.00009 0.00013 0.00022 2.17860

A64 2.17920 0.00000 0.00024 -0.00021 0.00003 2.17923

A65 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A66 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A67 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A68 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A69 1.94349 0.00004 0.00032 0.00010 0.00042 1.94391

A70 1.93324 -0.00004 -0.00017 -0.00016 -0.00033 1.93291

A71 1.93324 -0.00004 -0.00017 -0.00016 -0.00033 1.93291

A72 1.89662 0.00000 -0.00003 0.00001 -0.00002 1.89660

A73 1.89662 0.00000 -0.00003 0.00001 -0.00002 1.89660

A74 1.85808 0.00004 0.00008 0.00020 0.00028 1.85835

A75 1.93324 -0.00004 -0.00017 -0.00016 -0.00033 1.93291

A76 1.93324 -0.00004 -0.00017 -0.00016 -0.00033 1.93291

A77 1.94349 0.00004 0.00032 0.00010 0.00042 1.94391

A78 1.85808 0.00004 0.00008 0.00020 0.00028 1.85835

A79 1.89662 0.00000 -0.00003 0.00001 -0.00002 1.89660

A80 1.89662 0.00000 -0.00003 0.00001 -0.00002 1.89660

A81 1.93324 -0.00004 -0.00017 -0.00016 -0.00033 1.93291

A82 1.93324 -0.00004 -0.00017 -0.00016 -0.00033 1.93291

A83 1.94349 0.00004 0.00032 0.00010 0.00042 1.94391

A84 1.85808 0.00004 0.00008 0.00020 0.00028 1.85835

A85 1.89662 0.00000 -0.00003 0.00001 -0.00002 1.89660

A86 1.89662 0.00000 -0.00003 0.00001 -0.00002 1.89660

A87 1.93324 -0.00004 -0.00017 -0.00016 -0.00033 1.93291

A88 1.93324 -0.00004 -0.00017 -0.00016 -0.00033 1.93291

A89 1.94349 0.00004 0.00032 0.00010 0.00042 1.94391

A90 1.85808 0.00004 0.00008 0.00020 0.00028 1.85835

A91 1.89662 0.00000 -0.00003 0.00001 -0.00002 1.89660

A92 1.89662 0.00000 -0.00003 0.00001 -0.00002 1.89660

A93 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A94 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A95 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A96 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D28 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D29 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D30 1.02884 0.00000 -0.00006 0.00002 -0.00004 1.02880

D31 -1.02884 0.00000 0.00006 -0.00002 0.00004 -1.02880

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.11275 0.00000 -0.00006 0.00002 -0.00004 -2.11279

D34 2.11275 0.00000 0.00006 -0.00002 0.00004 2.11279

D35 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D36 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D37 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D61 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D62 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D63 1.02884 0.00000 -0.00006 0.00002 -0.00004 1.02880

D64 -1.02884 0.00000 0.00006 -0.00002 0.00004 -1.02880

D65 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.11275 0.00000 -0.00006 0.00002 -0.00004 -2.11279

D67 2.11275 0.00000 0.00006 -0.00002 0.00004 2.11279

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D70 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D71 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D72 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D73 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D74 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D76 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D77 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D78 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D79 -2.11275 0.00000 -0.00006 0.00002 -0.00004 -2.11279

D80 2.11275 0.00000 0.00006 -0.00002 0.00004 2.11279

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.02884 0.00000 -0.00006 0.00002 -0.00004 1.02880

D83 -1.02884 0.00000 0.00006 -0.00002 0.00004 -1.02880

D84 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D85 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D100 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D101 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D102 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D103 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D104 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D105 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D106 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D107 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D108 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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D111 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D112 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D114 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D117 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D120 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D121 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D122 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D123 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D124 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D125 1.02884 0.00000 -0.00006 0.00002 -0.00004 1.02880

D126 -1.02884 0.00000 0.00006 -0.00002 0.00004 -1.02880

D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D128 -2.11275 0.00000 -0.00006 0.00002 -0.00004 -2.11279

D129 2.11275 0.00000 0.00006 -0.00002 0.00004 2.11279

D130 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D131 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D132 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D133 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D134 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.000207 0.000450 YES

RMS Force 0.000055 0.000300 YES

Maximum Displacement 0.002896 0.001800 NO

RMS Displacement 0.000852 0.001200 YES

Predicted change in Energy=-1.518488D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 5 21:13:19 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 -2.066415 -2.178693 0.000000

2 7 0 -0.745079 -1.856552 0.000000

3 6 0 -0.005184 -2.988429 0.000000

4 6 0 -0.935773 -4.161954 0.000000

5 6 0 -2.188591 -3.644629 0.000000

6 7 0 1.325250 -3.098463 0.000000

7 6 0 2.178693 -2.066415 0.000000

8 7 0 1.856552 -0.745079 0.000000

9 6 0 2.988429 -0.005184 0.000000

10 6 0 4.161954 -0.935773 0.000000

11 6 0 3.644629 -2.188591 0.000000

12 7 0 -3.098463 -1.325250 0.000000

13 6 0 -4.161954 0.935773 0.000000

14 6 0 -3.644629 2.188591 0.000000

15 6 0 -2.178693 2.066415 0.000000

16 7 0 -1.856552 0.745079 0.000000

17 6 0 -2.988429 0.005184 0.000000

18 7 0 -1.325250 3.098463 0.000000

19 7 0 0.745079 1.856552 0.000000

20 6 0 0.005184 2.988429 0.000000

21 6 0 0.935773 4.161954 0.000000

22 6 0 2.188591 3.644629 0.000000

23 6 0 2.066415 2.178693 0.000000

24 7 0 3.098463 1.325250 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.480197 -5.573923 0.000000

27 1 0 -3.128232 -4.177604 0.000000

28 6 0 5.573923 -0.480197 0.000000

29 1 0 4.177604 -3.128232 0.000000

30 6 0 -5.573923 0.480197 0.000000

31 1 0 -4.177604 3.128232 0.000000

32 6 0 0.480197 5.573923 0.000000

33 1 0 3.128232 4.177604 0.000000

34 1 0 -1.324446 -6.263958 0.000000

35 1 0 0.141368 -5.780804 0.876886

36 1 0 0.141368 -5.780804 -0.876886

37 1 0 5.780804 0.141368 0.876886

38 1 0 5.780804 0.141368 -0.876886

39 1 0 6.263958 -1.324446 0.000000

40 1 0 -5.780804 -0.141368 0.876886

41 1 0 -5.780804 -0.141368 -0.876886

42 1 0 -6.263958 1.324446 0.000000

43 1 0 -0.141368 5.780804 0.876886

44 1 0 -0.141368 5.780804 -0.876886

45 1 0 1.324446 6.263958 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.360038 0.000000

3 C 2.214576 1.352254 0.000000

4 C 2.282910 2.313276 1.497717 0.000000

5 C 1.471019 2.298031 2.279882 1.355425 0.000000

6 N 3.514167 2.414251 1.334977 2.498647 3.556033

7 C 4.246592 2.931294 2.370534 3.753822 4.643697

8 N 4.176711 2.829108 2.915250 4.412722 4.977004

9 C 5.502326 4.167330 4.226283 5.716476 6.328277

10 C 6.351176 4.992675 4.645260 6.032832 6.904152

11 C 5.711053 4.402248 3.736426 4.987409 6.012196

12 N 1.339212 2.412613 3.512057 3.567088 2.491463

13 C 3.753822 4.412722 5.716476 6.032832 4.987409

14 C 4.643697 4.977004 6.328277 6.904152 6.012196

15 C 4.246592 4.176711 5.502326 6.351176 5.711053

16 N 2.931294 2.829108 4.167330 4.992675 4.402248

17 C 2.370534 2.915250 4.226283 4.645260 3.736426

18 N 5.328949 4.988865 6.228389 7.270856 6.798136

19 N 4.918099 4.000963 4.902727 6.248814 6.234533

20 C 5.566927 4.902727 5.976867 7.212030 6.986423

21 C 7.015478 6.248814 7.212030 8.531714 8.408590

22 C 7.212222 6.234533 6.986423 8.408590 8.502529

23 C 6.005588 4.918099 5.566927 7.015478 7.212222

24 N 6.241280 4.989657 5.314175 6.810615 7.256214

25 Zn 3.002794 2.000481 2.988434 4.265857 4.251265

26 C 3.747489 3.726797 2.628767 1.483646 2.576972

27 H 2.263427 3.326665 3.341791 2.192515 1.080272

28 C 7.826855 6.467159 6.116998 7.478735 8.382735

29 H 6.315805 5.084287 4.185124 5.216819 6.387104

30 C 4.401399 5.364525 6.560657 6.562165 5.336166

31 H 5.711442 6.052297 7.404231 7.978489 7.058883

32 C 8.160165 7.530820 8.576099 9.838307 9.597090

33 H 8.208950 7.170325 7.821146 9.277088 9.458115

34 H 4.152097 4.445323 3.531223 2.137635 2.758193

35 H 4.314910 4.117582 2.930489 2.133035 3.280378

36 H 4.314910 4.117582 2.930489 2.133035 3.280378

37 H 8.229852 6.880971 6.636432 8.024957 8.866452

38 H 8.229852 6.880971 6.636432 8.024957 8.866452

39 H 8.374058 7.029205 6.486215 7.738706 8.765205

40 H 4.326235 5.391597 6.498652 6.356758 5.093699

41 H 4.326235 5.391597 6.498652 6.356758 5.093699

42 H 5.467298 6.369989 7.600864 7.647884 6.426532

43 H 8.235796 7.711200 8.814019 10.012915 9.684981

44 H 8.235796 7.711200 8.814019 10.012915 9.684981

45 H 9.098147 8.380072 9.347437 10.668094 10.512921

6 7 8 9 10

6 N 0.000000

7 C 1.339212 0.000000

8 N 2.412613 1.360038 0.000000

9 C 3.512057 2.214576 1.352254 0.000000

10 C 3.567088 2.282910 2.313276 1.497717 0.000000

11 C 2.491463 1.471019 2.298031 2.279882 1.355425

12 N 4.765871 5.328949 4.988865 6.228389 7.270856

13 C 6.810615 7.015478 6.248814 7.212030 8.531714

14 C 7.256214 7.212222 6.234533 6.986423 8.408590

15 C 6.241280 6.005588 4.918099 5.566927 7.015478

16 N 4.989657 4.918099 4.000963 4.902727 6.248814

17 C 5.314175 5.566927 4.902727 5.976867 7.212030

18 N 6.739959 6.241280 4.989657 5.314175 6.810615

19 N 4.988865 4.176711 2.829108 2.915250 4.412722

20 C 6.228389 5.502326 4.167330 4.226283 5.716476

21 C 7.270856 6.351176 4.992675 4.645260 6.032832

22 C 6.798136 5.711053 4.402248 3.736426 4.987409

23 C 5.328949 4.246592 2.931294 2.370534 3.753822

24 N 4.765871 3.514167 2.414251 1.334977 2.498647

25 Zn 3.369980 3.002794 2.000481 2.988434 4.265857

26 C 3.063909 4.401399 5.364525 6.560657 6.562165

27 H 4.582363 5.711442 6.052297 7.404231 7.978489

28 C 4.990646 3.747489 3.726797 2.628767 1.483646

29 H 2.852509 2.263427 3.326665 3.341791 2.192515

30 C 7.772091 8.160165 7.530820 8.576099 9.838307

31 H 8.309822 8.208950 7.170325 7.821146 9.277088

32 C 8.713461 7.826855 6.467159 6.116998 7.478735

33 H 7.496125 6.315805 5.084287 4.185124 5.216819

34 H 4.128104 5.467298 6.369989 7.600864 7.647884

35 H 3.060304 4.326235 5.391597 6.498652 6.356758

36 H 3.060304 4.326235 5.391597 6.498652 6.356758

37 H 5.578298 4.314910 4.117582 2.930489 2.133035

38 H 5.578298 4.314910 4.117582 2.930489 2.133035

39 H 5.247664 4.152097 4.445323 3.531223 2.137635

40 H 7.746570 8.235796 7.711200 8.814019 10.012915

41 H 7.746570 8.235796 7.711200 8.814019 10.012915

42 H 8.783974 9.098147 8.380072 9.347437 10.668094

43 H 9.042195 8.229852 6.880971 6.636432 8.024957

44 H 9.042195 8.229852 6.880971 6.636432 8.024957

45 H 9.362421 8.374058 7.029205 6.486215 7.738706

11 12 13 14 15

11 C 0.000000

12 N 6.798136 0.000000

13 C 8.408590 2.498647 0.000000

14 C 8.502529 3.556033 1.355425 0.000000

15 C 7.212222 3.514167 2.282910 1.471019 0.000000

16 N 6.234533 2.414251 2.313276 2.298031 1.360038

17 C 6.986423 1.334977 1.497717 2.279882 2.214576

18 N 7.256214 4.765871 3.567088 2.491463 1.339212

19 N 4.977004 4.989657 4.992675 4.402248 2.931294

20 C 6.328277 5.314175 4.645260 3.736426 2.370534

21 C 6.904152 6.810615 6.032832 4.987409 3.753822

22 C 6.012196 7.256214 6.904152 6.012196 4.643697

23 C 4.643697 6.241280 6.351176 5.711053 4.246592

24 N 3.556033 6.739959 7.270856 6.798136 5.328949

25 Zn 4.251265 3.369980 4.265857 4.251265 3.002794

26 C 5.336166 4.990646 7.478735 8.382735 7.826855

27 H 7.058883 2.852509 5.216819 6.387104 6.315805

28 C 2.576972 8.713461 9.838307 9.597090 8.160165

29 H 1.080272 7.496125 9.277088 9.458115 8.208950

30 C 9.597090 3.063909 1.483646 2.576972 3.747489

31 H 9.458115 4.582363 2.192515 1.080272 2.263427

32 C 8.382735 7.772091 6.562165 5.336166 4.401399

33 H 6.387104 8.309822 7.978489 7.058883 5.711442

34 H 6.426532 5.247664 7.738706 8.765205 8.374058

35 H 5.093699 5.578298 8.024957 8.866452 8.229852

36 H 5.093699 5.578298 8.024957 8.866452 8.229852

37 H 3.280378 9.042195 10.012915 9.684981 8.235796

38 H 3.280378 9.042195 10.012915 9.684981 8.235796

39 H 2.758193 9.362421 10.668094 10.512921 9.098147

40 H 9.684981 3.060304 2.133035 3.280378 4.314910

41 H 9.684981 3.060304 2.133035 3.280378 4.314910

42 H 10.512921 4.128104 2.137635 2.758193 4.152097

43 H 8.866452 7.746570 6.356758 5.093699 4.326235

44 H 8.866452 7.746570 6.356758 5.093699 4.326235

45 H 8.765205 8.783974 7.647884 6.426532 5.467298

16 17 18 19 20

16 N 0.000000

17 C 1.352254 0.000000

18 N 2.412613 3.512057 0.000000

19 N 2.829108 4.167330 2.414251 0.000000

20 C 2.915250 4.226283 1.334977 1.352254 0.000000

21 C 4.412722 5.716476 2.498647 2.313276 1.497717

22 C 4.977004 6.328277 3.556033 2.298031 2.279882

23 C 4.176711 5.502326 3.514167 1.360038 2.214576

24 N 4.988865 6.228389 4.765871 2.412613 3.512057

25 Zn 2.000481 2.988434 3.369980 2.000481 2.988434

26 C 6.467159 6.116998 8.713461 7.530820 8.576099

27 H 5.084287 4.185124 7.496125 7.170325 7.821146

28 C 7.530820 8.576099 7.772091 5.364525 6.560657

29 H 7.170325 7.821146 8.309822 6.052297 7.404231

30 C 3.726797 2.628767 4.990646 6.467159 6.116998

31 H 3.326665 3.341791 2.852509 5.084287 4.185124

32 C 5.364525 6.560657 3.063909 3.726797 2.628767

33 H 6.052297 7.404231 4.582363 3.326665 3.341791

34 H 7.029205 6.486215 9.362421 8.380072 9.347437

35 H 6.880971 6.636432 9.042195 7.711200 8.814019

36 H 6.880971 6.636432 9.042195 7.711200 8.814019

37 H 7.711200 8.814019 7.746570 5.391597 6.498652

38 H 7.711200 8.814019 7.746570 5.391597 6.498652

39 H 8.380072 9.347437 8.783974 6.369989 7.600864

40 H 4.117582 2.930489 5.578298 6.880971 6.636432

41 H 4.117582 2.930489 5.578298 6.880971 6.636432

42 H 4.445323 3.531223 5.247664 7.029205 6.486215

43 H 5.391597 6.498652 3.060304 4.117582 2.930489

44 H 5.391597 6.498652 3.060304 4.117582 2.930489

45 H 6.369989 7.600864 4.128104 4.445323 3.531223

21 22 23 24 25

21 C 0.000000

22 C 1.355425 0.000000

23 C 2.282910 1.471019 0.000000

24 N 3.567088 2.491463 1.339212 0.000000

25 Zn 4.265857 4.251265 3.002794 3.369980 0.000000

26 C 9.838307 9.597090 8.160165 7.772091 5.594570

27 H 9.277088 9.458115 8.208950 8.309822 5.219024

28 C 6.562165 5.336166 4.401399 3.063909 5.594570

29 H 7.978489 7.058883 5.711442 4.582363 5.219024

30 C 7.478735 8.382735 7.826855 8.713461 5.594570

31 H 5.216819 6.387104 6.315805 7.496125 5.219024

32 C 1.483646 2.576972 3.747489 4.990646 5.594570

33 H 2.192515 1.080272 2.263427 2.852509 5.219024

34 H 10.668094 10.512921 9.098147 8.783974 6.402446

35 H 10.012915 9.684981 8.235796 7.746570 5.848642

36 H 10.012915 9.684981 8.235796 7.746570 5.848642

37 H 6.356758 5.093699 4.326235 3.060304 5.848642

38 H 6.356758 5.093699 4.326235 3.060304 5.848642

39 H 7.647884 6.426532 5.467298 4.128104 6.402446

40 H 8.024957 8.866452 8.229852 9.042195 5.848642

41 H 8.024957 8.866452 8.229852 9.042195 5.848642

42 H 7.738706 8.765205 8.374058 9.362421 6.402446

43 H 2.133035 3.280378 4.314910 5.578298 5.848642

44 H 2.133035 3.280378 4.314910 5.578298 5.848642

45 H 2.137635 2.758193 4.152097 5.247664 6.402446

26 27 28 29 30

26 C 0.000000

27 H 2.993627 0.000000

28 C 7.911916 9.455069 0.000000

29 H 5.260847 7.380814 2.993627 0.000000

30 C 7.911916 5.260847 11.189139 10.397742 0.000000

31 H 9.455069 7.380814 10.397742 10.438048 2.993627

32 C 11.189139 10.397742 7.911916 9.455069 7.911916

33 H 10.397742 10.438048 5.260847 7.380814 9.455069

34 H 1.090368 2.757992 9.002188 6.332876 7.971304

35 H 1.094565 3.745594 7.640551 4.908794 8.522536

36 H 1.094565 3.745594 7.640551 4.908794 8.522536

37 H 8.522536 9.939486 1.094565 3.745594 11.393576

38 H 8.522536 9.939486 1.094565 3.745594 11.393576

39 H 7.971304 9.815994 1.090368 2.757992 11.974646

40 H 7.640551 4.908794 11.393576 10.433608 1.094565

41 H 7.640551 4.908794 11.393576 10.433608 1.094565

42 H 9.002188 6.332876 11.974646 11.351323 1.090368

43 H 11.393576 10.433608 8.522536 9.939486 7.640551

44 H 11.393576 10.433608 8.522536 9.939486 7.640551

45 H 11.974646 11.351323 7.971304 9.815994 9.002188

31 32 33 34 35

31 H 0.000000

32 C 5.260847 0.000000

33 H 7.380814 2.993627 0.000000

34 H 9.815994 11.974646 11.351323 0.000000

35 H 9.939486 11.393576 10.433608 1.775099 0.000000

36 H 9.939486 11.393576 10.433608 1.775099 1.753773

37 H 10.433608 7.640551 4.908794 9.606337 8.177736

38 H 10.433608 7.640551 4.908794 9.606337 8.363677

39 H 11.351323 9.002188 6.332876 9.054427 7.623265

40 H 3.745594 8.522536 9.939486 7.623265 8.177736

41 H 3.745594 8.522536 9.939486 7.623265 8.363677

42 H 2.757992 7.971304 9.815994 9.054427 9.606337

43 H 4.908794 1.094565 3.745594 12.134451 11.565066

44 H 4.908794 1.094565 3.745594 12.134451 11.697284

45 H 6.332876 1.090368 2.757992 12.804893 12.134451

36 37 38 39 40

36 H 0.000000

37 H 8.363677 0.000000

38 H 8.177736 1.753773 0.000000

39 H 7.623265 1.775099 1.775099 0.000000

40 H 8.363677 11.565066 11.697284 12.134451 0.000000

41 H 8.177736 11.697284 11.565066 12.134451 1.753773

42 H 9.606337 12.134451 12.134451 12.804893 1.775099

43 H 11.697284 8.177736 8.363677 9.606337 8.177736

44 H 11.565066 8.363677 8.177736 9.606337 8.363677

45 H 12.134451 7.623265 7.623265 9.054427 9.606337

41 42 43 44 45

41 H 0.000000

42 H 1.775099 0.000000

43 H 8.363677 7.623265 0.000000

44 H 8.177736 7.623265 1.753773 0.000000

45 H 9.606337 9.054427 1.775099 1.775099 0.000000

Stoichiometry C20H16N8Zn(1+,2)

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

Deg. of freedom 20

Full point group C4H NOp 8

RotChk: IX=0 Diff= 2.87D-04

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.182274 2.062632 0.000000

2 7 0 -1.857841 0.741857 0.000000

3 6 0 -2.988434 0.000000 0.000000

4 6 0 -4.163571 0.928552 0.000000

5 6 0 -3.648420 2.182265 0.000000

6 7 0 -3.096160 -1.330623 0.000000

7 6 0 -2.062632 -2.182274 0.000000

8 7 0 -0.741857 -1.857841 0.000000

9 6 0 0.000000 -2.988434 0.000000

10 6 0 -0.928552 -4.163571 0.000000

11 6 0 -2.182265 -3.648420 0.000000

12 7 0 -1.330623 3.096160 0.000000

13 6 0 0.928552 4.163571 0.000000

14 6 0 2.182265 3.648420 0.000000

15 6 0 2.062632 2.182274 0.000000

16 7 0 0.741857 1.857841 0.000000

17 6 0 0.000000 2.988434 0.000000

18 7 0 3.096160 1.330623 0.000000

19 7 0 1.857841 -0.741857 0.000000

20 6 0 2.988434 0.000000 0.000000

21 6 0 4.163571 -0.928552 0.000000

22 6 0 3.648420 -2.182265 0.000000

23 6 0 2.182274 -2.062632 0.000000

24 7 0 1.330623 -3.096160 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.574748 0.470527 0.000000

27 1 0 -4.183024 3.120980 0.000000

28 6 0 -0.470527 -5.574748 0.000000

29 1 0 -3.120980 -4.183024 0.000000

30 6 0 0.470527 5.574748 0.000000

31 1 0 3.120980 4.183024 0.000000

32 6 0 5.574748 -0.470527 0.000000

33 1 0 4.183024 -3.120980 0.000000

34 1 0 -6.266246 1.313577 0.000000

35 1 0 -5.780551 -0.151397 0.876886

36 1 0 -5.780551 -0.151397 -0.876886

37 1 0 0.151397 -5.780551 0.876886

38 1 0 0.151397 -5.780551 -0.876886

39 1 0 -1.313577 -6.266246 0.000000

40 1 0 -0.151397 5.780551 0.876886

41 1 0 -0.151397 5.780551 -0.876886

42 1 0 1.313577 6.266246 0.000000

43 1 0 5.780551 0.151397 0.876886

44 1 0 5.780551 0.151397 -0.876886

45 1 0 6.266246 -1.313577 0.000000

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

Rotational constants (GHZ): 0.1830366 0.1830366 0.0917243

Leave Link 202 at Fri Jul 5 21:13:19 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 229 symmetry adapted cartesian basis functions of AG symmetry.

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

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

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

There are 212 symmetry adapted basis functions of AG symmetry.

There are 82 symmetry adapted basis functions of BG symmetry.

There are 78 symmetry adapted basis functions of AU symmetry.

There are 204 symmetry adapted basis functions of BU symmetry.

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

102 alpha electrons 101 beta electrons

nuclear repulsion energy 2766.6963647715 Hartrees.

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

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

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

NAtoms= 45 NActive= 45 NUniq= 11 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1142450957 Hartrees.

Nuclear repulsion after empirical dispersion term = 2766.5821196758 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 = 3538

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.69D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 160

GePol: Fraction of low-weight points (<1% of avg) = 4.52%

GePol: Cavity surface area = 382.114 Ang\*\*2

GePol: Cavity volume = 379.149 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0110998430 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 2766.5710198328 Hartrees.

Leave Link 301 at Fri Jul 5 21:13:19 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= 19306 NPrTT= 91506 LenC2= 15383 LenP2D= 41364.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 576 RedAO= T EigKep= 1.86D-04 NBF= 212 82 78 204

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

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Fri Jul 5 21:13:19 2019, MaxMem= 1342177280 cpu: 7.7

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 5 21:13:20 2019, MaxMem= 1342177280 cpu: 1.1

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

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

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 -0.000064 Ang= -0.01 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7819 S= 0.5158

Leave Link 401 at Fri Jul 5 21:13:21 2019, MaxMem= 1342177280 cpu: 21.7

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1138797 IEndB= 1138797 NGot= 1342177280 MDV= 1341424180

LenX= 1341424180 LenY= 1341055124

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

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

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 37552332.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.55D-15 for 252.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.56D-15 for 3161 850.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.10D-15 for 553.

Iteration 1 A^-1\*A deviation from orthogonality is 1.10D-14 for 1948 1904.

E= -1275.69949886719

DIIS: error= 7.23D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1275.69949886719 IErMin= 1 ErrMin= 7.23D-05

ErrMax= 7.23D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.57D-06 BMatP= 6.57D-06

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

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.372 Goal= None Shift= 0.000

Gap= 0.406 Goal= None Shift= 0.000

RMSDP=3.54D-06 MaxDP=1.19D-04 OVMax= 6.55D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.54D-06 CP: 1.00D+00

E= -1275.69950154482 Delta-E= -0.000002677623 Rises=F Damp=F

DIIS: error= 1.58D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1275.69950154482 IErMin= 2 ErrMin= 1.58D-05

ErrMax= 1.58D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.56D-07 BMatP= 6.57D-06

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

Coeff-Com: 0.271D-01 0.973D+00

Coeff: 0.271D-01 0.973D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=9.14D-07 MaxDP=4.00D-05 DE=-2.68D-06 OVMax= 1.88D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 9.06D-07 CP: 1.00D+00 1.03D+00

E= -1275.69950148951 Delta-E= 0.000000055305 Rises=F Damp=F

DIIS: error= 2.59D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1275.69950154482 IErMin= 2 ErrMin= 1.58D-05

ErrMax= 2.59D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.70D-07 BMatP= 3.56D-07

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

Coeff-Com: -0.290D-01 0.600D+00 0.429D+00

Coeff: -0.290D-01 0.600D+00 0.429D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=5.81D-07 MaxDP=2.59D-05 DE= 5.53D-08 OVMax= 1.42D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.31D-07 CP: 1.00D+00 1.05D+00 4.81D-01

E= -1275.69950164832 Delta-E= -0.000000158807 Rises=F Damp=F

DIIS: error= 4.92D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1275.69950164832 IErMin= 4 ErrMin= 4.92D-06

ErrMax= 4.92D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.27D-08 BMatP= 3.56D-07

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

Coeff-Com: -0.142D-01 0.169D+00 0.205D+00 0.640D+00

Coeff: -0.142D-01 0.169D+00 0.205D+00 0.640D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=1.24D-07 MaxDP=4.52D-06 DE=-1.59D-07 OVMax= 5.73D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.09D-07 CP: 1.00D+00 1.06D+00 5.37D-01 9.46D-01

E= -1275.69950165430 Delta-E= -0.000000005978 Rises=F Damp=F

DIIS: error= 1.24D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1275.69950165430 IErMin= 5 ErrMin= 1.24D-06

ErrMax= 1.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.96D-09 BMatP= 2.27D-08

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

Coeff-Com: -0.468D-02 0.390D-01 0.771D-01 0.297D+00 0.592D+00

Coeff: -0.468D-02 0.390D-01 0.771D-01 0.297D+00 0.592D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=5.11D-08 MaxDP=2.08D-06 DE=-5.98D-09 OVMax= 3.42D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.73D-08 CP: 1.00D+00 1.06D+00 5.54D-01 1.04D+00 1.05D+00

E= -1275.69950165539 Delta-E= -0.000000001096 Rises=F Damp=F

DIIS: error= 8.71D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1275.69950165539 IErMin= 6 ErrMin= 8.71D-07

ErrMax= 8.71D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.54D-10 BMatP= 1.96D-09

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

Coeff-Com: 0.184D-02-0.289D-01-0.142D-01-0.449D-01 0.214D+00 0.872D+00

Coeff: 0.184D-02-0.289D-01-0.142D-01-0.449D-01 0.214D+00 0.872D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=4.69D-08 MaxDP=1.89D-06 DE=-1.10D-09 OVMax= 3.62D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.32D-08 CP: 1.00D+00 1.06D+00 5.69D-01 1.11D+00 1.30D+00

CP: 1.28D+00

E= -1275.69950165571 Delta-E= -0.000000000316 Rises=F Damp=F

DIIS: error= 5.33D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1275.69950165571 IErMin= 7 ErrMin= 5.33D-07

ErrMax= 5.33D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.57D-10 BMatP= 3.54D-10

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

Coeff-Com: 0.203D-02-0.261D-01-0.229D-01-0.859D-01 0.130D-01 0.523D+00

Coeff-Com: 0.597D+00

Coeff: 0.203D-02-0.261D-01-0.229D-01-0.859D-01 0.130D-01 0.523D+00

Coeff: 0.597D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=2.22D-08 MaxDP=1.05D-06 DE=-3.16D-10 OVMax= 1.46D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.07D-08 CP: 1.00D+00 1.06D+00 5.75D-01 1.14D+00 1.40D+00

CP: 1.57D+00 1.16D+00

E= -1275.69950165577 Delta-E= -0.000000000061 Rises=F Damp=F

DIIS: error= 2.49D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1275.69950165577 IErMin= 8 ErrMin= 2.49D-07

ErrMax= 2.49D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.53D-11 BMatP= 1.57D-10

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

Coeff-Com: -0.216D-03 0.635D-02 0.212D-03-0.824D-02-0.123D+00-0.284D+00

Coeff-Com: 0.274D+00 0.113D+01

Coeff: -0.216D-03 0.635D-02 0.212D-03-0.824D-02-0.123D+00-0.284D+00

Coeff: 0.274D+00 0.113D+01

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=2.46D-08 MaxDP=1.33D-06 DE=-6.09D-11 OVMax= 1.35D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 7.17D-09 CP: 1.00D+00 1.06D+00 5.79D-01 1.16D+00 1.50D+00

CP: 1.87D+00 1.70D+00 1.54D+00

E= -1275.69950165586 Delta-E= -0.000000000094 Rises=F Damp=F

DIIS: error= 1.25D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1275.69950165586 IErMin= 9 ErrMin= 1.25D-07

ErrMax= 1.25D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.43D-12 BMatP= 3.53D-11

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

Coeff-Com: -0.394D-03 0.624D-02 0.377D-02 0.112D-01-0.357D-01-0.159D+00

Coeff-Com: 0.135D-01 0.318D+00 0.843D+00

Coeff: -0.394D-03 0.624D-02 0.377D-02 0.112D-01-0.357D-01-0.159D+00

Coeff: 0.135D-01 0.318D+00 0.843D+00

Gap= 0.104 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=6.35D-09 MaxDP=4.11D-07 DE=-9.37D-11 OVMax= 3.11D-06

Error on total polarization charges = 0.06026

SCF Done: E(UB3LYP) = -1275.69950166 A.U. after 9 cycles

NFock= 9 Conv=0.64D-08 -V/T= 1.9660

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7819 S= 0.5158

<L.S>= 0.000000000000E+00

KE= 1.320598028643D+03 PE=-8.556975834555D+03 EE= 3.194107284423D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.97

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7819, after 0.7509

Leave Link 502 at Fri Jul 5 21:14:19 2019, MaxMem= 1342177280 cpu: 657.7

(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= 19306 NPrTT= 91506 LenC2= 15383 LenP2D= 41364.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 248

Leave Link 701 at Fri Jul 5 21:14:24 2019, MaxMem= 1342177280 cpu: 53.3

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

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

Leave Link 702 at Fri Jul 5 21:14:24 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= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Fri Jul 5 21:14:32 2019, MaxMem= 1342177280 cpu: 92.4

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

Dipole = 4.05009359D-13 2.04281037D-13 0.00000000D+00

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000135460 -0.000083215 0.000000000

2 7 0.000147749 0.000070182 0.000000000

3 6 -0.000166317 -0.000012274 0.000000000

4 6 -0.000002228 0.000012154 0.000000000

5 6 -0.000025779 0.000080556 0.000000000

6 7 0.000067498 0.000023114 0.000000000

7 6 0.000083215 -0.000135460 0.000000000

8 7 -0.000070182 0.000147749 0.000000000

9 6 0.000012274 -0.000166317 0.000000000

10 6 -0.000012154 -0.000002228 0.000000000

11 6 -0.000080556 -0.000025779 0.000000000

12 7 0.000023114 -0.000067498 0.000000000

13 6 0.000012154 0.000002228 0.000000000

14 6 0.000080556 0.000025779 0.000000000

15 6 -0.000083215 0.000135460 0.000000000

16 7 0.000070182 -0.000147749 0.000000000

17 6 -0.000012274 0.000166317 0.000000000

18 7 -0.000067498 -0.000023114 0.000000000

19 7 -0.000147749 -0.000070182 0.000000000

20 6 0.000166317 0.000012274 0.000000000

21 6 0.000002228 -0.000012154 0.000000000

22 6 0.000025779 -0.000080556 0.000000000

23 6 0.000135460 0.000083215 0.000000000

24 7 -0.000023114 0.000067498 0.000000000

25 30 0.000000000 0.000000000 0.000000000

26 6 -0.000004128 -0.000010487 0.000000000

27 1 -0.000021841 0.000010315 0.000000000

28 6 0.000010487 -0.000004128 0.000000000

29 1 -0.000010315 -0.000021841 0.000000000

30 6 -0.000010487 0.000004128 0.000000000

31 1 0.000010315 0.000021841 0.000000000

32 6 0.000004128 0.000010487 0.000000000

33 1 0.000021841 -0.000010315 0.000000000

34 1 -0.000029422 0.000005172 0.000000000

35 1 -0.000037997 0.000006278 -0.000002224

36 1 -0.000037997 0.000006278 0.000002224

37 1 -0.000006278 -0.000037997 -0.000002224

38 1 -0.000006278 -0.000037997 0.000002224

39 1 -0.000005172 -0.000029422 0.000000000

40 1 0.000006278 0.000037997 -0.000002224

41 1 0.000006278 0.000037997 0.000002224

42 1 0.000005172 0.000029422 0.000000000

43 1 0.000037997 -0.000006278 -0.000002224

44 1 0.000037997 -0.000006278 0.000002224

45 1 0.000029422 -0.000005172 0.000000000

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

Cartesian Forces: Max 0.000166317 RMS 0.000053560

Leave Link 716 at Fri Jul 5 21:14:32 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.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.000096381 RMS 0.000019584

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 = .19584D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

DE= -1.00D-07 DEPred=-1.52D-06 R= 6.59D-02

Trust test= 6.59D-02 RLast= 4.12D-03 DXMaxT set to 1.64D-01

ITU= -1 1 1 1 0

Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01343

Eigenvalues --- 0.01345 0.01345 0.01345 0.01600 0.01618

Eigenvalues --- 0.01631 0.01631 0.01777 0.01792 0.01819

Eigenvalues --- 0.01819 0.01890 0.01906 0.01943 0.01943

Eigenvalues --- 0.01998 0.01999 0.02045 0.02045 0.02070

Eigenvalues --- 0.02088 0.02102 0.02113 0.02113 0.02205

Eigenvalues --- 0.02316 0.02316 0.02352 0.02374 0.07152

Eigenvalues --- 0.07210 0.07210 0.07210 0.07210 0.07404

Eigenvalues --- 0.07404 0.07404 0.12187 0.14501 0.14501

Eigenvalues --- 0.15897 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16007

Eigenvalues --- 0.16516 0.17929 0.20123 0.22084 0.22084

Eigenvalues --- 0.23767 0.23811 0.23847 0.23847 0.24544

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25058 0.30893 0.33173 0.33173 0.33215

Eigenvalues --- 0.33282 0.33282 0.33282 0.33448 0.33718

Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

Eigenvalues --- 0.33724 0.33724 0.34353 0.34437 0.34437

Eigenvalues --- 0.34437 0.35176 0.35379 0.35573 0.35573

Eigenvalues --- 0.35682 0.35682 0.35682 0.36240 0.39287

Eigenvalues --- 0.41753 0.41753 0.42576 0.45927 0.48969

Eigenvalues --- 0.48969 0.49008 0.50265 0.50567 0.51356

Eigenvalues --- 0.51356 0.52270 0.53984 0.53984 0.54930

Eigenvalues --- 0.56214 0.56277 0.56331 0.56331

En-DIIS/RFO-DIIS IScMMF= 0 using points: 5 4 3 2

RFO step: Lambda=-1.99512507D-07.

NNeg= 0 NP= 4 Switch= 2.50D-03 Rises=F DC= 2.59D-04 SmlDif= 1.00D-05

RMS Error= 0.3698654048D-04 NUsed= 4 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.28243 -0.28403 -0.01157 0.01316

Iteration 1 RMS(Cart)= 0.00021472 RMS(Int)= 0.00000003

Iteration 2 RMS(Cart)= 0.00000003 RMS(Int)= 0.00000003

ITry= 1 IFail=0 DXMaxC= 8.23D-04 DCOld= 1.00D+10 DXMaxT= 1.64D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 5.07D-10 for atom 40.

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

(Linear) (Quad) (Total)

R1 2.57010 0.00010 0.00013 0.00017 0.00029 2.57039

R2 2.77982 -0.00005 -0.00023 0.00001 -0.00022 2.77960

R3 2.53074 -0.00003 -0.00003 -0.00005 -0.00008 2.53066

R4 2.55539 -0.00003 0.00000 -0.00010 -0.00010 2.55529

R5 3.78036 -0.00003 -0.00007 -0.00010 -0.00018 3.78019

R6 2.83028 -0.00003 -0.00015 0.00005 -0.00010 2.83017

R7 2.52274 0.00008 0.00009 0.00010 0.00019 2.52293

R8 2.56138 0.00002 0.00014 -0.00007 0.00006 2.56144

R9 2.80369 0.00000 0.00002 0.00000 0.00002 2.80371

R10 2.04142 0.00000 0.00001 0.00001 0.00001 2.04143

R11 2.53074 -0.00003 -0.00003 -0.00005 -0.00008 2.53066

R12 2.57010 0.00010 0.00013 0.00017 0.00029 2.57039

R13 2.77982 -0.00005 -0.00023 0.00001 -0.00022 2.77960

R14 2.55539 -0.00003 0.00000 -0.00010 -0.00010 2.55529

R15 3.78036 -0.00003 -0.00007 -0.00010 -0.00018 3.78019

R16 2.83028 -0.00003 -0.00015 0.00005 -0.00010 2.83017

R17 2.52274 0.00008 0.00009 0.00010 0.00019 2.52293

R18 2.56138 0.00002 0.00014 -0.00007 0.00006 2.56144

R19 2.80369 0.00000 0.00002 0.00000 0.00002 2.80371

R20 2.04142 0.00000 0.00001 0.00001 0.00001 2.04143

R21 2.52274 0.00008 0.00009 0.00010 0.00019 2.52293

R22 2.56138 0.00002 0.00014 -0.00007 0.00006 2.56144

R23 2.83028 -0.00003 -0.00015 0.00005 -0.00010 2.83017

R24 2.80369 0.00000 0.00002 0.00000 0.00002 2.80371

R25 2.77982 -0.00005 -0.00023 0.00001 -0.00022 2.77960

R26 2.04142 0.00000 0.00001 0.00001 0.00001 2.04143

R27 2.57010 0.00010 0.00013 0.00017 0.00029 2.57039

R28 2.53074 -0.00003 -0.00003 -0.00005 -0.00008 2.53066

R29 2.55539 -0.00003 0.00000 -0.00010 -0.00010 2.55529

R30 3.78036 -0.00003 -0.00007 -0.00010 -0.00018 3.78019

R31 2.52274 0.00008 0.00009 0.00010 0.00019 2.52293

R32 2.55539 -0.00003 0.00000 -0.00010 -0.00010 2.55529

R33 2.57010 0.00010 0.00013 0.00017 0.00029 2.57039

R34 3.78036 -0.00003 -0.00007 -0.00010 -0.00018 3.78019

R35 2.83028 -0.00003 -0.00015 0.00005 -0.00010 2.83017

R36 2.56138 0.00002 0.00014 -0.00007 0.00006 2.56144

R37 2.80369 0.00000 0.00002 0.00000 0.00002 2.80371

R38 2.77982 -0.00005 -0.00023 0.00001 -0.00022 2.77960

R39 2.04142 0.00000 0.00001 0.00001 0.00001 2.04143

R40 2.53074 -0.00003 -0.00003 -0.00005 -0.00008 2.53066

R41 2.06050 0.00000 0.00003 -0.00002 0.00000 2.06050

R42 2.06843 -0.00001 0.00004 -0.00005 -0.00001 2.06842

R43 2.06843 -0.00001 0.00004 -0.00005 -0.00001 2.06842

R44 2.06843 -0.00001 0.00004 -0.00005 -0.00001 2.06842

R45 2.06843 -0.00001 0.00004 -0.00005 -0.00001 2.06842

R46 2.06050 0.00000 0.00003 -0.00002 0.00000 2.06050

R47 2.06843 -0.00001 0.00004 -0.00005 -0.00001 2.06842

R48 2.06843 -0.00001 0.00004 -0.00005 -0.00001 2.06842

R49 2.06050 0.00000 0.00003 -0.00002 0.00000 2.06050

R50 2.06843 -0.00001 0.00004 -0.00005 -0.00001 2.06842

R51 2.06843 -0.00001 0.00004 -0.00005 -0.00001 2.06842

R52 2.06050 0.00000 0.00003 -0.00002 0.00000 2.06050

A1 1.89308 0.00001 0.00004 0.00001 0.00005 1.89313

A2 2.21150 -0.00002 -0.00007 -0.00005 -0.00012 2.21138

A3 2.17860 0.00002 0.00003 0.00004 0.00007 2.17867

A4 1.91062 -0.00004 -0.00008 -0.00008 -0.00016 1.91047

A5 2.19158 0.00001 0.00004 0.00001 0.00005 2.19163

A6 2.18098 0.00003 0.00004 0.00007 0.00010 2.18109

A7 1.89218 0.00003 0.00006 0.00007 0.00013 1.89231

A8 2.23228 -0.00002 -0.00004 -0.00002 -0.00006 2.23221

A9 2.15873 -0.00001 -0.00002 -0.00004 -0.00006 2.15866

A10 1.84964 0.00000 -0.00002 0.00000 -0.00003 1.84962

A11 2.15904 -0.00003 -0.00018 -0.00004 -0.00023 2.15881

A12 2.27451 0.00002 0.00021 0.00005 0.00025 2.27476

A13 1.87925 0.00000 0.00001 0.00000 0.00001 1.87926

A14 2.16991 0.00001 -0.00008 0.00006 -0.00002 2.16989

A15 2.23403 0.00000 0.00007 -0.00006 0.00001 2.23404

A16 2.17923 0.00000 0.00003 0.00000 0.00002 2.17926

A17 2.21150 -0.00002 -0.00007 -0.00005 -0.00012 2.21138

A18 2.17860 0.00002 0.00003 0.00004 0.00007 2.17867

A19 1.89308 0.00001 0.00004 0.00001 0.00005 1.89313

A20 1.91062 -0.00004 -0.00008 -0.00008 -0.00016 1.91047

A21 2.19158 0.00001 0.00004 0.00001 0.00005 2.19163

A22 2.18098 0.00003 0.00004 0.00007 0.00010 2.18109

A23 1.89218 0.00003 0.00006 0.00007 0.00013 1.89231

A24 2.23228 -0.00002 -0.00004 -0.00002 -0.00006 2.23221

A25 2.15873 -0.00001 -0.00002 -0.00004 -0.00006 2.15866

A26 1.84964 0.00000 -0.00002 0.00000 -0.00003 1.84962

A27 2.15904 -0.00003 -0.00018 -0.00004 -0.00023 2.15881

A28 2.27451 0.00002 0.00021 0.00005 0.00025 2.27476

A29 1.87925 0.00000 0.00001 0.00000 0.00001 1.87926

A30 2.16991 0.00001 -0.00008 0.00006 -0.00002 2.16989

A31 2.23403 0.00000 0.00007 -0.00006 0.00001 2.23404

A32 2.17923 0.00000 0.00003 0.00000 0.00002 2.17926

A33 1.84964 0.00000 -0.00002 0.00000 -0.00003 1.84962

A34 2.27451 0.00002 0.00021 0.00005 0.00025 2.27476

A35 2.15904 -0.00003 -0.00018 -0.00004 -0.00023 2.15881

A36 1.87925 0.00000 0.00001 0.00000 0.00001 1.87926

A37 2.23403 0.00000 0.00007 -0.00006 0.00001 2.23404

A38 2.16991 0.00001 -0.00008 0.00006 -0.00002 2.16989

A39 1.89308 0.00001 0.00004 0.00001 0.00005 1.89313

A40 2.17860 0.00002 0.00003 0.00004 0.00007 2.17867

A41 2.21150 -0.00002 -0.00007 -0.00005 -0.00012 2.21138

A42 1.91062 -0.00004 -0.00008 -0.00008 -0.00016 1.91047

A43 2.19158 0.00001 0.00004 0.00001 0.00005 2.19163

A44 2.18098 0.00003 0.00004 0.00007 0.00010 2.18109

A45 2.15873 -0.00001 -0.00002 -0.00004 -0.00006 2.15866

A46 2.23228 -0.00002 -0.00004 -0.00002 -0.00006 2.23221

A47 1.89218 0.00003 0.00006 0.00007 0.00013 1.89231

A48 2.17923 0.00000 0.00003 0.00000 0.00002 2.17926

A49 1.91062 -0.00004 -0.00008 -0.00008 -0.00016 1.91047

A50 2.18098 0.00003 0.00004 0.00007 0.00010 2.18109

A51 2.19158 0.00001 0.00004 0.00001 0.00005 2.19163

A52 2.23228 -0.00002 -0.00004 -0.00002 -0.00006 2.23221

A53 2.15873 -0.00001 -0.00002 -0.00004 -0.00006 2.15866

A54 1.89218 0.00003 0.00006 0.00007 0.00013 1.89231

A55 1.84964 0.00000 -0.00002 0.00000 -0.00003 1.84962

A56 2.15904 -0.00003 -0.00018 -0.00004 -0.00023 2.15881

A57 2.27451 0.00002 0.00021 0.00005 0.00025 2.27476

A58 1.87925 0.00000 0.00001 0.00000 0.00001 1.87926

A59 2.23403 0.00000 0.00007 -0.00006 0.00001 2.23404

A60 2.16991 0.00001 -0.00008 0.00006 -0.00002 2.16989

A61 1.89308 0.00001 0.00004 0.00001 0.00005 1.89313

A62 2.21150 -0.00002 -0.00007 -0.00005 -0.00012 2.21138

A63 2.17860 0.00002 0.00003 0.00004 0.00007 2.17867

A64 2.17923 0.00000 0.00003 0.00000 0.00002 2.17926

A65 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A66 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A67 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A68 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

A69 1.94391 0.00001 0.00009 0.00002 0.00010 1.94401

A70 1.93291 -0.00001 -0.00009 -0.00001 -0.00010 1.93281

A71 1.93291 -0.00001 -0.00009 -0.00001 -0.00010 1.93281

A72 1.89660 0.00000 -0.00002 0.00002 0.00000 1.89661

A73 1.89660 0.00000 -0.00002 0.00002 0.00000 1.89661

A74 1.85835 0.00001 0.00014 -0.00005 0.00009 1.85845

A75 1.93291 -0.00001 -0.00009 -0.00001 -0.00010 1.93281

A76 1.93291 -0.00001 -0.00009 -0.00001 -0.00010 1.93281

A77 1.94391 0.00001 0.00009 0.00002 0.00010 1.94401

A78 1.85835 0.00001 0.00014 -0.00005 0.00009 1.85845

A79 1.89660 0.00000 -0.00002 0.00002 0.00000 1.89661

A80 1.89660 0.00000 -0.00002 0.00002 0.00000 1.89661

A81 1.93291 -0.00001 -0.00009 -0.00001 -0.00010 1.93281

A82 1.93291 -0.00001 -0.00009 -0.00001 -0.00010 1.93281

A83 1.94391 0.00001 0.00009 0.00002 0.00010 1.94401

A84 1.85835 0.00001 0.00014 -0.00005 0.00009 1.85845

A85 1.89660 0.00000 -0.00002 0.00002 0.00000 1.89661

A86 1.89660 0.00000 -0.00002 0.00002 0.00000 1.89661

A87 1.93291 -0.00001 -0.00009 -0.00001 -0.00010 1.93281

A88 1.93291 -0.00001 -0.00009 -0.00001 -0.00010 1.93281

A89 1.94391 0.00001 0.00009 0.00002 0.00010 1.94401

A90 1.85835 0.00001 0.00014 -0.00005 0.00009 1.85845

A91 1.89660 0.00000 -0.00002 0.00002 0.00000 1.89661

A92 1.89660 0.00000 -0.00002 0.00002 0.00000 1.89661

A93 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A94 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A95 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A96 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D2 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D3 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D4 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D6 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D7 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D10 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D11 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D12 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D13 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D14 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D15 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D16 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D17 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D18 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D19 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D20 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D21 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D22 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D23 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D24 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D25 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D26 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D27 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D28 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D29 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D30 1.02880 0.00000 0.00003 -0.00003 -0.00001 1.02880

D31 -1.02880 0.00000 -0.00003 0.00003 0.00001 -1.02880

D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 -2.11279 0.00000 0.00003 -0.00003 -0.00001 -2.11280

D34 2.11279 0.00000 -0.00003 0.00003 0.00001 2.11280

D35 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D36 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D37 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D38 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D39 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D40 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D41 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D42 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D43 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D44 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D45 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D46 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D47 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D48 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D49 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D50 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D51 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D52 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D53 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D54 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D55 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D56 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D57 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D58 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D59 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D60 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D61 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D62 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D63 1.02880 0.00000 0.00003 -0.00003 -0.00001 1.02880

D64 -1.02880 0.00000 -0.00003 0.00003 0.00001 -1.02880

D65 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D66 -2.11279 0.00000 0.00003 -0.00003 -0.00001 -2.11280

D67 2.11279 0.00000 -0.00003 0.00003 0.00001 2.11280

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D70 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D71 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D72 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D73 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D74 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D75 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D76 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D77 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D78 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D79 -2.11279 0.00000 0.00003 -0.00003 -0.00001 -2.11280

D80 2.11279 0.00000 -0.00003 0.00003 0.00001 2.11280

D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D82 1.02880 0.00000 0.00003 -0.00003 -0.00001 1.02880

D83 -1.02880 0.00000 -0.00003 0.00003 0.00001 -1.02880

D84 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D85 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D86 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D87 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D88 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D89 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D90 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D91 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D92 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D93 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D94 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D95 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D96 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D97 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D98 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D99 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D100 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D101 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D102 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D103 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D104 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D105 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D106 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D107 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D108 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D109 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D110 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D111 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D112 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D113 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D114 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D116 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D117 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D119 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D120 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D121 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D122 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D123 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D124 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D125 1.02880 0.00000 0.00003 -0.00003 -0.00001 1.02880

D126 -1.02880 0.00000 -0.00003 0.00003 0.00001 -1.02880

D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D128 -2.11279 0.00000 0.00003 -0.00003 -0.00001 -2.11280

D129 2.11279 0.00000 -0.00003 0.00003 0.00001 2.11280

D130 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D131 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D132 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D133 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

D134 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

Item Value Threshold Converged?

Maximum Force 0.000096 0.000450 YES

RMS Force 0.000020 0.000300 YES

Maximum Displacement 0.000823 0.001800 YES

RMS Displacement 0.000215 0.001200 YES

Predicted change in Energy=-1.935777D-07

Optimization completed.

-- Stationary point found.

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! Optimized Parameters !

! (Angstroms and Degrees) !

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! Name Definition Value Derivative Info. !

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! R1 R(1,2) 1.36 -DE/DX = 0.0001 !

! R2 R(1,5) 1.471 -DE/DX = -0.0001 !

! R3 R(1,12) 1.3392 -DE/DX = 0.0 !

! R4 R(2,3) 1.3523 -DE/DX = 0.0 !

! R5 R(2,25) 2.0005 -DE/DX = 0.0 !

! R6 R(3,4) 1.4977 -DE/DX = 0.0 !

! R7 R(3,6) 1.335 -DE/DX = 0.0001 !

! R8 R(4,5) 1.3554 -DE/DX = 0.0 !

! R9 R(4,26) 1.4836 -DE/DX = 0.0 !

! R10 R(5,27) 1.0803 -DE/DX = 0.0 !

! R11 R(6,7) 1.3392 -DE/DX = 0.0 !

! R12 R(7,8) 1.36 -DE/DX = 0.0001 !

! R13 R(7,11) 1.471 -DE/DX = -0.0001 !

! R14 R(8,9) 1.3523 -DE/DX = 0.0 !

! R15 R(8,25) 2.0005 -DE/DX = 0.0 !

! R16 R(9,10) 1.4977 -DE/DX = 0.0 !

! R17 R(9,24) 1.335 -DE/DX = 0.0001 !

! R18 R(10,11) 1.3554 -DE/DX = 0.0 !

! R19 R(10,28) 1.4836 -DE/DX = 0.0 !

! R20 R(11,29) 1.0803 -DE/DX = 0.0 !

! R21 R(12,17) 1.335 -DE/DX = 0.0001 !

! R22 R(13,14) 1.3554 -DE/DX = 0.0 !

! R23 R(13,17) 1.4977 -DE/DX = 0.0 !

! R24 R(13,30) 1.4836 -DE/DX = 0.0 !

! R25 R(14,15) 1.471 -DE/DX = -0.0001 !

! R26 R(14,31) 1.0803 -DE/DX = 0.0 !

! R27 R(15,16) 1.36 -DE/DX = 0.0001 !

! R28 R(15,18) 1.3392 -DE/DX = 0.0 !

! R29 R(16,17) 1.3523 -DE/DX = 0.0 !

! R30 R(16,25) 2.0005 -DE/DX = 0.0 !

! R31 R(18,20) 1.335 -DE/DX = 0.0001 !

! R32 R(19,20) 1.3523 -DE/DX = 0.0 !

! R33 R(19,23) 1.36 -DE/DX = 0.0001 !

! R34 R(19,25) 2.0005 -DE/DX = 0.0 !

! R35 R(20,21) 1.4977 -DE/DX = 0.0 !

! R36 R(21,22) 1.3554 -DE/DX = 0.0 !

! R37 R(21,32) 1.4836 -DE/DX = 0.0 !

! R38 R(22,23) 1.471 -DE/DX = -0.0001 !

! R39 R(22,33) 1.0803 -DE/DX = 0.0 !

! R40 R(23,24) 1.3392 -DE/DX = 0.0 !

! R41 R(26,34) 1.0904 -DE/DX = 0.0 !

! R42 R(26,35) 1.0946 -DE/DX = 0.0 !

! R43 R(26,36) 1.0946 -DE/DX = 0.0 !

! R44 R(28,37) 1.0946 -DE/DX = 0.0 !

! R45 R(28,38) 1.0946 -DE/DX = 0.0 !

! R46 R(28,39) 1.0904 -DE/DX = 0.0 !

! R47 R(30,40) 1.0946 -DE/DX = 0.0 !

! R48 R(30,41) 1.0946 -DE/DX = 0.0 !

! R49 R(30,42) 1.0904 -DE/DX = 0.0 !

! R50 R(32,43) 1.0946 -DE/DX = 0.0 !

! R51 R(32,44) 1.0946 -DE/DX = 0.0 !

! R52 R(32,45) 1.0904 -DE/DX = 0.0 !

! A1 A(2,1,5) 108.4656 -DE/DX = 0.0 !

! A2 A(2,1,12) 126.7099 -DE/DX = 0.0 !

! A3 A(5,1,12) 124.8245 -DE/DX = 0.0 !

! A4 A(1,2,3) 109.4707 -DE/DX = 0.0 !

! A5 A(1,2,25) 125.5682 -DE/DX = 0.0 !

! A6 A(3,2,25) 124.9611 -DE/DX = 0.0 !

! A7 A(2,3,4) 108.4139 -DE/DX = 0.0 !

! A8 A(2,3,6) 127.9001 -DE/DX = 0.0 !

! A9 A(4,3,6) 123.686 -DE/DX = 0.0 !

! A10 A(3,4,5) 105.9768 -DE/DX = 0.0 !

! A11 A(3,4,26) 123.7036 -DE/DX = 0.0 !

! A12 A(5,4,26) 130.3196 -DE/DX = 0.0 !

! A13 A(1,5,4) 107.673 -DE/DX = 0.0 !

! A14 A(1,5,27) 124.3265 -DE/DX = 0.0 !

! A15 A(4,5,27) 128.0005 -DE/DX = 0.0 !

! A16 A(3,6,7) 124.8608 -DE/DX = 0.0 !

! A17 A(6,7,8) 126.7099 -DE/DX = 0.0 !

! A18 A(6,7,11) 124.8245 -DE/DX = 0.0 !

! A19 A(8,7,11) 108.4656 -DE/DX = 0.0 !

! A20 A(7,8,9) 109.4707 -DE/DX = 0.0 !

! A21 A(7,8,25) 125.5682 -DE/DX = 0.0 !

! A22 A(9,8,25) 124.9611 -DE/DX = 0.0 !

! A23 A(8,9,10) 108.4139 -DE/DX = 0.0 !

! A24 A(8,9,24) 127.9001 -DE/DX = 0.0 !

! A25 A(10,9,24) 123.686 -DE/DX = 0.0 !

! A26 A(9,10,11) 105.9768 -DE/DX = 0.0 !

! A27 A(9,10,28) 123.7036 -DE/DX = 0.0 !

! A28 A(11,10,28) 130.3196 -DE/DX = 0.0 !

! A29 A(7,11,10) 107.673 -DE/DX = 0.0 !

! A30 A(7,11,29) 124.3265 -DE/DX = 0.0 !

! A31 A(10,11,29) 128.0005 -DE/DX = 0.0 !

! A32 A(1,12,17) 124.8608 -DE/DX = 0.0 !

! A33 A(14,13,17) 105.9768 -DE/DX = 0.0 !

! A34 A(14,13,30) 130.3196 -DE/DX = 0.0 !

! A35 A(17,13,30) 123.7036 -DE/DX = 0.0 !

! A36 A(13,14,15) 107.673 -DE/DX = 0.0 !

! A37 A(13,14,31) 128.0005 -DE/DX = 0.0 !

! A38 A(15,14,31) 124.3265 -DE/DX = 0.0 !

! A39 A(14,15,16) 108.4656 -DE/DX = 0.0 !

! A40 A(14,15,18) 124.8245 -DE/DX = 0.0 !

! A41 A(16,15,18) 126.7099 -DE/DX = 0.0 !

! A42 A(15,16,17) 109.4707 -DE/DX = 0.0 !

! A43 A(15,16,25) 125.5682 -DE/DX = 0.0 !

! A44 A(17,16,25) 124.9611 -DE/DX = 0.0 !

! A45 A(12,17,13) 123.686 -DE/DX = 0.0 !

! A46 A(12,17,16) 127.9001 -DE/DX = 0.0 !

! A47 A(13,17,16) 108.4139 -DE/DX = 0.0 !

! A48 A(15,18,20) 124.8608 -DE/DX = 0.0 !

! A49 A(20,19,23) 109.4707 -DE/DX = 0.0 !

! A50 A(20,19,25) 124.9611 -DE/DX = 0.0 !

! A51 A(23,19,25) 125.5682 -DE/DX = 0.0 !

! A52 A(18,20,19) 127.9001 -DE/DX = 0.0 !

! A53 A(18,20,21) 123.686 -DE/DX = 0.0 !

! A54 A(19,20,21) 108.4139 -DE/DX = 0.0 !

! A55 A(20,21,22) 105.9768 -DE/DX = 0.0 !

! A56 A(20,21,32) 123.7036 -DE/DX = 0.0 !

! A57 A(22,21,32) 130.3196 -DE/DX = 0.0 !

! A58 A(21,22,23) 107.673 -DE/DX = 0.0 !

! A59 A(21,22,33) 128.0005 -DE/DX = 0.0 !

! A60 A(23,22,33) 124.3265 -DE/DX = 0.0 !

! A61 A(19,23,22) 108.4656 -DE/DX = 0.0 !

! A62 A(19,23,24) 126.7099 -DE/DX = 0.0 !

! A63 A(22,23,24) 124.8245 -DE/DX = 0.0 !

! A64 A(9,24,23) 124.8608 -DE/DX = 0.0 !

! A65 A(2,25,8) 90.0 -DE/DX = 0.0 !

! A66 A(2,25,16) 90.0 -DE/DX = 0.0 !

! A67 A(8,25,19) 90.0 -DE/DX = 0.0 !

! A68 A(16,25,19) 90.0 -DE/DX = 0.0 !

! A69 A(4,26,34) 111.3779 -DE/DX = 0.0 !

! A70 A(4,26,35) 110.7474 -DE/DX = 0.0 !

! A71 A(4,26,36) 110.7474 -DE/DX = 0.0 !

! A72 A(34,26,35) 108.6673 -DE/DX = 0.0 !

! A73 A(34,26,36) 108.6673 -DE/DX = 0.0 !

! A74 A(35,26,36) 106.4758 -DE/DX = 0.0 !

! A75 A(10,28,37) 110.7474 -DE/DX = 0.0 !

! A76 A(10,28,38) 110.7474 -DE/DX = 0.0 !

! A77 A(10,28,39) 111.3779 -DE/DX = 0.0 !

! A78 A(37,28,38) 106.4758 -DE/DX = 0.0 !

! A79 A(37,28,39) 108.6673 -DE/DX = 0.0 !

! A80 A(38,28,39) 108.6673 -DE/DX = 0.0 !

! A81 A(13,30,40) 110.7474 -DE/DX = 0.0 !

! A82 A(13,30,41) 110.7474 -DE/DX = 0.0 !

! A83 A(13,30,42) 111.3779 -DE/DX = 0.0 !

! A84 A(40,30,41) 106.4758 -DE/DX = 0.0 !

! A85 A(40,30,42) 108.6673 -DE/DX = 0.0 !

! A86 A(41,30,42) 108.6673 -DE/DX = 0.0 !

! A87 A(21,32,43) 110.7474 -DE/DX = 0.0 !

! A88 A(21,32,44) 110.7474 -DE/DX = 0.0 !

! A89 A(21,32,45) 111.3779 -DE/DX = 0.0 !

! A90 A(43,32,44) 106.4758 -DE/DX = 0.0 !

! A91 A(43,32,45) 108.6673 -DE/DX = 0.0 !

! A92 A(44,32,45) 108.6673 -DE/DX = 0.0 !

! A93 L(2,25,19,16,-1) 180.0 -DE/DX = 0.0 !

! A94 L(8,25,16,19,-1) 180.0 -DE/DX = 0.0 !

! A95 L(2,25,19,16,-2) 180.0 -DE/DX = 0.0 !

! A96 L(8,25,16,19,-2) 180.0 -DE/DX = 0.0 !

! D1 D(5,1,2,3) 0.0 -DE/DX = 0.0 !

! D2 D(5,1,2,25) 180.0 -DE/DX = 0.0 !

! D3 D(12,1,2,3) 180.0 -DE/DX = 0.0 !

! D4 D(12,1,2,25) 0.0 -DE/DX = 0.0 !

! D5 D(2,1,5,4) 0.0 -DE/DX = 0.0 !

! D6 D(2,1,5,27) 180.0 -DE/DX = 0.0 !

! D7 D(12,1,5,4) 180.0 -DE/DX = 0.0 !

! D8 D(12,1,5,27) 0.0 -DE/DX = 0.0 !

! D9 D(2,1,12,17) 0.0 -DE/DX = 0.0 !

! D10 D(5,1,12,17) 180.0 -DE/DX = 0.0 !

! D11 D(1,2,3,4) 0.0 -DE/DX = 0.0 !

! D12 D(1,2,3,6) 180.0 -DE/DX = 0.0 !

! D13 D(25,2,3,4) 180.0 -DE/DX = 0.0 !

! D14 D(25,2,3,6) 0.0 -DE/DX = 0.0 !

! D15 D(1,2,25,8) 180.0 -DE/DX = 0.0 !

! D16 D(1,2,25,16) 0.0 -DE/DX = 0.0 !

! D17 D(3,2,25,8) 0.0 -DE/DX = 0.0 !

! D18 D(3,2,25,16) 180.0 -DE/DX = 0.0 !

! D19 D(2,3,4,5) 0.0 -DE/DX = 0.0 !

! D20 D(2,3,4,26) 180.0 -DE/DX = 0.0 !

! D21 D(6,3,4,5) 180.0 -DE/DX = 0.0 !

! D22 D(6,3,4,26) 0.0 -DE/DX = 0.0 !

! D23 D(2,3,6,7) 0.0 -DE/DX = 0.0 !

! D24 D(4,3,6,7) 180.0 -DE/DX = 0.0 !

! D25 D(3,4,5,1) 0.0 -DE/DX = 0.0 !

! D26 D(3,4,5,27) 180.0 -DE/DX = 0.0 !

! D27 D(26,4,5,1) 180.0 -DE/DX = 0.0 !

! D28 D(26,4,5,27) 0.0 -DE/DX = 0.0 !

! D29 D(3,4,26,34) 180.0 -DE/DX = 0.0 !

! D30 D(3,4,26,35) 58.9461 -DE/DX = 0.0 !

! D31 D(3,4,26,36) -58.9461 -DE/DX = 0.0 !

! D32 D(5,4,26,34) 0.0 -DE/DX = 0.0 !

! D33 D(5,4,26,35) -121.0539 -DE/DX = 0.0 !

! D34 D(5,4,26,36) 121.0539 -DE/DX = 0.0 !

! D35 D(3,6,7,8) 0.0 -DE/DX = 0.0 !

! D36 D(3,6,7,11) 180.0 -DE/DX = 0.0 !

! D37 D(6,7,8,9) 180.0 -DE/DX = 0.0 !

! D38 D(6,7,8,25) 0.0 -DE/DX = 0.0 !

! D39 D(11,7,8,9) 0.0 -DE/DX = 0.0 !

! D40 D(11,7,8,25) 180.0 -DE/DX = 0.0 !

! D41 D(6,7,11,10) 180.0 -DE/DX = 0.0 !

! D42 D(6,7,11,29) 0.0 -DE/DX = 0.0 !

! D43 D(8,7,11,10) 0.0 -DE/DX = 0.0 !

! D44 D(8,7,11,29) 180.0 -DE/DX = 0.0 !

! D45 D(7,8,9,10) 0.0 -DE/DX = 0.0 !

! D46 D(7,8,9,24) 180.0 -DE/DX = 0.0 !

! D47 D(25,8,9,10) 180.0 -DE/DX = 0.0 !

! D48 D(25,8,9,24) 0.0 -DE/DX = 0.0 !

! D49 D(7,8,25,2) 0.0 -DE/DX = 0.0 !

! D50 D(7,8,25,19) 180.0 -DE/DX = 0.0 !

! D51 D(9,8,25,2) 180.0 -DE/DX = 0.0 !

! D52 D(9,8,25,19) 0.0 -DE/DX = 0.0 !

! D53 D(8,9,10,11) 0.0 -DE/DX = 0.0 !

! D54 D(8,9,10,28) 180.0 -DE/DX = 0.0 !

! D55 D(24,9,10,11) 180.0 -DE/DX = 0.0 !

! D56 D(24,9,10,28) 0.0 -DE/DX = 0.0 !

! D57 D(8,9,24,23) 0.0 -DE/DX = 0.0 !

! D58 D(10,9,24,23) 180.0 -DE/DX = 0.0 !

! D59 D(9,10,11,7) 0.0 -DE/DX = 0.0 !

! D60 D(9,10,11,29) 180.0 -DE/DX = 0.0 !

! D61 D(28,10,11,7) 180.0 -DE/DX = 0.0 !

! D62 D(28,10,11,29) 0.0 -DE/DX = 0.0 !

! D63 D(9,10,28,37) 58.9461 -DE/DX = 0.0 !

! D64 D(9,10,28,38) -58.9461 -DE/DX = 0.0 !

! D65 D(9,10,28,39) 180.0 -DE/DX = 0.0 !

! D66 D(11,10,28,37) -121.0539 -DE/DX = 0.0 !

! D67 D(11,10,28,38) 121.0539 -DE/DX = 0.0 !

! D68 D(11,10,28,39) 0.0 -DE/DX = 0.0 !

! D69 D(1,12,17,13) 180.0 -DE/DX = 0.0 !

! D70 D(1,12,17,16) 0.0 -DE/DX = 0.0 !

! D71 D(17,13,14,15) 0.0 -DE/DX = 0.0 !

! D72 D(17,13,14,31) 180.0 -DE/DX = 0.0 !

! D73 D(30,13,14,15) 180.0 -DE/DX = 0.0 !

! D74 D(30,13,14,31) 0.0 -DE/DX = 0.0 !

! D75 D(14,13,17,12) 180.0 -DE/DX = 0.0 !

! D76 D(14,13,17,16) 0.0 -DE/DX = 0.0 !

! D77 D(30,13,17,12) 0.0 -DE/DX = 0.0 !

! D78 D(30,13,17,16) 180.0 -DE/DX = 0.0 !

! D79 D(14,13,30,40) -121.0539 -DE/DX = 0.0 !

! D80 D(14,13,30,41) 121.0539 -DE/DX = 0.0 !

! D81 D(14,13,30,42) 0.0 -DE/DX = 0.0 !

! D82 D(17,13,30,40) 58.9461 -DE/DX = 0.0 !

! D83 D(17,13,30,41) -58.9461 -DE/DX = 0.0 !

! D84 D(17,13,30,42) 180.0 -DE/DX = 0.0 !

! D85 D(13,14,15,16) 0.0 -DE/DX = 0.0 !

! D86 D(13,14,15,18) 180.0 -DE/DX = 0.0 !

! D87 D(31,14,15,16) 180.0 -DE/DX = 0.0 !

! D88 D(31,14,15,18) 0.0 -DE/DX = 0.0 !

! D89 D(14,15,16,17) 0.0 -DE/DX = 0.0 !

! D90 D(14,15,16,25) 180.0 -DE/DX = 0.0 !

! D91 D(18,15,16,17) 180.0 -DE/DX = 0.0 !

! D92 D(18,15,16,25) 0.0 -DE/DX = 0.0 !

! D93 D(14,15,18,20) 180.0 -DE/DX = 0.0 !

! D94 D(16,15,18,20) 0.0 -DE/DX = 0.0 !

! D95 D(15,16,17,12) 180.0 -DE/DX = 0.0 !

! D96 D(15,16,17,13) 0.0 -DE/DX = 0.0 !

! D97 D(25,16,17,12) 0.0 -DE/DX = 0.0 !

! D98 D(25,16,17,13) 180.0 -DE/DX = 0.0 !

! D99 D(15,16,25,2) 180.0 -DE/DX = 0.0 !

! D100 D(15,16,25,19) 0.0 -DE/DX = 0.0 !

! D101 D(17,16,25,2) 0.0 -DE/DX = 0.0 !

! D102 D(17,16,25,19) 180.0 -DE/DX = 0.0 !

! D103 D(15,18,20,19) 0.0 -DE/DX = 0.0 !

! D104 D(15,18,20,21) 180.0 -DE/DX = 0.0 !

! D105 D(23,19,20,18) 180.0 -DE/DX = 0.0 !

! D106 D(23,19,20,21) 0.0 -DE/DX = 0.0 !

! D107 D(25,19,20,18) 0.0 -DE/DX = 0.0 !

! D108 D(25,19,20,21) 180.0 -DE/DX = 0.0 !

! D109 D(20,19,23,22) 0.0 -DE/DX = 0.0 !

! D110 D(20,19,23,24) 180.0 -DE/DX = 0.0 !

! D111 D(25,19,23,22) 180.0 -DE/DX = 0.0 !

! D112 D(25,19,23,24) 0.0 -DE/DX = 0.0 !

! D113 D(20,19,25,8) 180.0 -DE/DX = 0.0 !

! D114 D(20,19,25,16) 0.0 -DE/DX = 0.0 !

! D115 D(23,19,25,8) 0.0 -DE/DX = 0.0 !

! D116 D(23,19,25,16) 180.0 -DE/DX = 0.0 !

! D117 D(18,20,21,22) 180.0 -DE/DX = 0.0 !

! D118 D(18,20,21,32) 0.0 -DE/DX = 0.0 !

! D119 D(19,20,21,22) 0.0 -DE/DX = 0.0 !

! D120 D(19,20,21,32) 180.0 -DE/DX = 0.0 !

! D121 D(20,21,22,23) 0.0 -DE/DX = 0.0 !

! D122 D(20,21,22,33) 180.0 -DE/DX = 0.0 !

! D123 D(32,21,22,23) 180.0 -DE/DX = 0.0 !

! D124 D(32,21,22,33) 0.0 -DE/DX = 0.0 !

! D125 D(20,21,32,43) 58.9461 -DE/DX = 0.0 !

! D126 D(20,21,32,44) -58.9461 -DE/DX = 0.0 !

! D127 D(20,21,32,45) 180.0 -DE/DX = 0.0 !

! D128 D(22,21,32,43) -121.0539 -DE/DX = 0.0 !

! D129 D(22,21,32,44) 121.0539 -DE/DX = 0.0 !

! D130 D(22,21,32,45) 0.0 -DE/DX = 0.0 !

! D131 D(21,22,23,19) 0.0 -DE/DX = 0.0 !

! D132 D(21,22,23,24) 180.0 -DE/DX = 0.0 !

! D133 D(33,22,23,19) 180.0 -DE/DX = 0.0 !

! D134 D(33,22,23,24) 0.0 -DE/DX = 0.0 !

! D135 D(19,23,24,9) 0.0 -DE/DX = 0.0 !

! D136 D(22,23,24,9) 180.0 -DE/DX = 0.0 !

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

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Largest change from initial coordinates is atom 40 0.033 Angstoms.

Leave Link 103 at Fri Jul 5 21:14:32 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 -2.066415 -2.178693 0.000000

2 7 0 -0.745079 -1.856552 0.000000

3 6 0 -0.005184 -2.988429 0.000000

4 6 0 -0.935773 -4.161954 0.000000

5 6 0 -2.188591 -3.644629 0.000000

6 7 0 1.325250 -3.098463 0.000000

7 6 0 2.178693 -2.066415 0.000000

8 7 0 1.856552 -0.745079 0.000000

9 6 0 2.988429 -0.005184 0.000000

10 6 0 4.161954 -0.935773 0.000000

11 6 0 3.644629 -2.188591 0.000000

12 7 0 -3.098463 -1.325250 0.000000

13 6 0 -4.161954 0.935773 0.000000

14 6 0 -3.644629 2.188591 0.000000

15 6 0 -2.178693 2.066415 0.000000

16 7 0 -1.856552 0.745079 0.000000

17 6 0 -2.988429 0.005184 0.000000

18 7 0 -1.325250 3.098463 0.000000

19 7 0 0.745079 1.856552 0.000000

20 6 0 0.005184 2.988429 0.000000

21 6 0 0.935773 4.161954 0.000000

22 6 0 2.188591 3.644629 0.000000

23 6 0 2.066415 2.178693 0.000000

24 7 0 3.098463 1.325250 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -0.480197 -5.573923 0.000000

27 1 0 -3.128232 -4.177604 0.000000

28 6 0 5.573923 -0.480197 0.000000

29 1 0 4.177604 -3.128232 0.000000

30 6 0 -5.573923 0.480197 0.000000

31 1 0 -4.177604 3.128232 0.000000

32 6 0 0.480197 5.573923 0.000000

33 1 0 3.128232 4.177604 0.000000

34 1 0 -1.324446 -6.263958 0.000000

35 1 0 0.141368 -5.780804 0.876886

36 1 0 0.141368 -5.780804 -0.876886

37 1 0 5.780804 0.141368 0.876886

38 1 0 5.780804 0.141368 -0.876886

39 1 0 6.263958 -1.324446 0.000000

40 1 0 -5.780804 -0.141368 0.876886

41 1 0 -5.780804 -0.141368 -0.876886

42 1 0 -6.263958 1.324446 0.000000

43 1 0 -0.141368 5.780804 0.876886

44 1 0 -0.141368 5.780804 -0.876886

45 1 0 1.324446 6.263958 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 N 1.360038 0.000000

3 C 2.214576 1.352254 0.000000

4 C 2.282910 2.313276 1.497717 0.000000

5 C 1.471019 2.298031 2.279882 1.355425 0.000000

6 N 3.514167 2.414251 1.334977 2.498647 3.556033

7 C 4.246592 2.931294 2.370534 3.753822 4.643697

8 N 4.176711 2.829108 2.915250 4.412722 4.977004

9 C 5.502326 4.167330 4.226283 5.716476 6.328277

10 C 6.351176 4.992675 4.645260 6.032832 6.904152

11 C 5.711053 4.402248 3.736426 4.987409 6.012196

12 N 1.339212 2.412613 3.512057 3.567088 2.491463

13 C 3.753822 4.412722 5.716476 6.032832 4.987409

14 C 4.643697 4.977004 6.328277 6.904152 6.012196

15 C 4.246592 4.176711 5.502326 6.351176 5.711053

16 N 2.931294 2.829108 4.167330 4.992675 4.402248

17 C 2.370534 2.915250 4.226283 4.645260 3.736426

18 N 5.328949 4.988865 6.228389 7.270856 6.798136

19 N 4.918099 4.000963 4.902727 6.248814 6.234533

20 C 5.566927 4.902727 5.976867 7.212030 6.986423

21 C 7.015478 6.248814 7.212030 8.531714 8.408590

22 C 7.212222 6.234533 6.986423 8.408590 8.502529

23 C 6.005588 4.918099 5.566927 7.015478 7.212222

24 N 6.241280 4.989657 5.314175 6.810615 7.256214

25 Zn 3.002794 2.000481 2.988434 4.265857 4.251265

26 C 3.747489 3.726797 2.628767 1.483646 2.576972

27 H 2.263427 3.326665 3.341791 2.192515 1.080272

28 C 7.826855 6.467159 6.116998 7.478735 8.382735

29 H 6.315805 5.084287 4.185124 5.216819 6.387104

30 C 4.401399 5.364525 6.560657 6.562165 5.336166

31 H 5.711442 6.052297 7.404231 7.978489 7.058883

32 C 8.160165 7.530820 8.576099 9.838307 9.597090

33 H 8.208950 7.170325 7.821146 9.277088 9.458115

34 H 4.152097 4.445323 3.531223 2.137635 2.758193

35 H 4.314910 4.117582 2.930489 2.133035 3.280378

36 H 4.314910 4.117582 2.930489 2.133035 3.280378

37 H 8.229852 6.880971 6.636432 8.024957 8.866452

38 H 8.229852 6.880971 6.636432 8.024957 8.866452

39 H 8.374058 7.029205 6.486215 7.738706 8.765205

40 H 4.326235 5.391597 6.498652 6.356758 5.093699

41 H 4.326235 5.391597 6.498652 6.356758 5.093699

42 H 5.467298 6.369989 7.600864 7.647884 6.426532

43 H 8.235796 7.711200 8.814019 10.012915 9.684981

44 H 8.235796 7.711200 8.814019 10.012915 9.684981

45 H 9.098147 8.380072 9.347437 10.668094 10.512921

6 7 8 9 10

6 N 0.000000

7 C 1.339212 0.000000

8 N 2.412613 1.360038 0.000000

9 C 3.512057 2.214576 1.352254 0.000000

10 C 3.567088 2.282910 2.313276 1.497717 0.000000

11 C 2.491463 1.471019 2.298031 2.279882 1.355425

12 N 4.765871 5.328949 4.988865 6.228389 7.270856

13 C 6.810615 7.015478 6.248814 7.212030 8.531714

14 C 7.256214 7.212222 6.234533 6.986423 8.408590

15 C 6.241280 6.005588 4.918099 5.566927 7.015478

16 N 4.989657 4.918099 4.000963 4.902727 6.248814

17 C 5.314175 5.566927 4.902727 5.976867 7.212030

18 N 6.739959 6.241280 4.989657 5.314175 6.810615

19 N 4.988865 4.176711 2.829108 2.915250 4.412722

20 C 6.228389 5.502326 4.167330 4.226283 5.716476

21 C 7.270856 6.351176 4.992675 4.645260 6.032832

22 C 6.798136 5.711053 4.402248 3.736426 4.987409

23 C 5.328949 4.246592 2.931294 2.370534 3.753822

24 N 4.765871 3.514167 2.414251 1.334977 2.498647

25 Zn 3.369980 3.002794 2.000481 2.988434 4.265857

26 C 3.063909 4.401399 5.364525 6.560657 6.562165

27 H 4.582363 5.711442 6.052297 7.404231 7.978489

28 C 4.990646 3.747489 3.726797 2.628767 1.483646

29 H 2.852509 2.263427 3.326665 3.341791 2.192515

30 C 7.772091 8.160165 7.530820 8.576099 9.838307

31 H 8.309822 8.208950 7.170325 7.821146 9.277088

32 C 8.713461 7.826855 6.467159 6.116998 7.478735

33 H 7.496125 6.315805 5.084287 4.185124 5.216819

34 H 4.128104 5.467298 6.369989 7.600864 7.647884

35 H 3.060304 4.326235 5.391597 6.498652 6.356758

36 H 3.060304 4.326235 5.391597 6.498652 6.356758

37 H 5.578298 4.314910 4.117582 2.930489 2.133035

38 H 5.578298 4.314910 4.117582 2.930489 2.133035

39 H 5.247664 4.152097 4.445323 3.531223 2.137635

40 H 7.746570 8.235796 7.711200 8.814019 10.012915

41 H 7.746570 8.235796 7.711200 8.814019 10.012915

42 H 8.783974 9.098147 8.380072 9.347437 10.668094

43 H 9.042195 8.229852 6.880971 6.636432 8.024957

44 H 9.042195 8.229852 6.880971 6.636432 8.024957

45 H 9.362421 8.374058 7.029205 6.486215 7.738706

11 12 13 14 15

11 C 0.000000

12 N 6.798136 0.000000

13 C 8.408590 2.498647 0.000000

14 C 8.502529 3.556033 1.355425 0.000000

15 C 7.212222 3.514167 2.282910 1.471019 0.000000

16 N 6.234533 2.414251 2.313276 2.298031 1.360038

17 C 6.986423 1.334977 1.497717 2.279882 2.214576

18 N 7.256214 4.765871 3.567088 2.491463 1.339212

19 N 4.977004 4.989657 4.992675 4.402248 2.931294

20 C 6.328277 5.314175 4.645260 3.736426 2.370534

21 C 6.904152 6.810615 6.032832 4.987409 3.753822

22 C 6.012196 7.256214 6.904152 6.012196 4.643697

23 C 4.643697 6.241280 6.351176 5.711053 4.246592

24 N 3.556033 6.739959 7.270856 6.798136 5.328949

25 Zn 4.251265 3.369980 4.265857 4.251265 3.002794

26 C 5.336166 4.990646 7.478735 8.382735 7.826855

27 H 7.058883 2.852509 5.216819 6.387104 6.315805

28 C 2.576972 8.713461 9.838307 9.597090 8.160165

29 H 1.080272 7.496125 9.277088 9.458115 8.208950

30 C 9.597090 3.063909 1.483646 2.576972 3.747489

31 H 9.458115 4.582363 2.192515 1.080272 2.263427

32 C 8.382735 7.772091 6.562165 5.336166 4.401399

33 H 6.387104 8.309822 7.978489 7.058883 5.711442

34 H 6.426532 5.247664 7.738706 8.765205 8.374058

35 H 5.093699 5.578298 8.024957 8.866452 8.229852

36 H 5.093699 5.578298 8.024957 8.866452 8.229852

37 H 3.280378 9.042195 10.012915 9.684981 8.235796

38 H 3.280378 9.042195 10.012915 9.684981 8.235796

39 H 2.758193 9.362421 10.668094 10.512921 9.098147

40 H 9.684981 3.060304 2.133035 3.280378 4.314910

41 H 9.684981 3.060304 2.133035 3.280378 4.314910

42 H 10.512921 4.128104 2.137635 2.758193 4.152097

43 H 8.866452 7.746570 6.356758 5.093699 4.326235

44 H 8.866452 7.746570 6.356758 5.093699 4.326235

45 H 8.765205 8.783974 7.647884 6.426532 5.467298

16 17 18 19 20

16 N 0.000000

17 C 1.352254 0.000000

18 N 2.412613 3.512057 0.000000

19 N 2.829108 4.167330 2.414251 0.000000

20 C 2.915250 4.226283 1.334977 1.352254 0.000000

21 C 4.412722 5.716476 2.498647 2.313276 1.497717

22 C 4.977004 6.328277 3.556033 2.298031 2.279882

23 C 4.176711 5.502326 3.514167 1.360038 2.214576

24 N 4.988865 6.228389 4.765871 2.412613 3.512057

25 Zn 2.000481 2.988434 3.369980 2.000481 2.988434

26 C 6.467159 6.116998 8.713461 7.530820 8.576099

27 H 5.084287 4.185124 7.496125 7.170325 7.821146

28 C 7.530820 8.576099 7.772091 5.364525 6.560657

29 H 7.170325 7.821146 8.309822 6.052297 7.404231

30 C 3.726797 2.628767 4.990646 6.467159 6.116998

31 H 3.326665 3.341791 2.852509 5.084287 4.185124

32 C 5.364525 6.560657 3.063909 3.726797 2.628767

33 H 6.052297 7.404231 4.582363 3.326665 3.341791

34 H 7.029205 6.486215 9.362421 8.380072 9.347437

35 H 6.880971 6.636432 9.042195 7.711200 8.814019

36 H 6.880971 6.636432 9.042195 7.711200 8.814019

37 H 7.711200 8.814019 7.746570 5.391597 6.498652

38 H 7.711200 8.814019 7.746570 5.391597 6.498652

39 H 8.380072 9.347437 8.783974 6.369989 7.600864

40 H 4.117582 2.930489 5.578298 6.880971 6.636432

41 H 4.117582 2.930489 5.578298 6.880971 6.636432

42 H 4.445323 3.531223 5.247664 7.029205 6.486215

43 H 5.391597 6.498652 3.060304 4.117582 2.930489

44 H 5.391597 6.498652 3.060304 4.117582 2.930489

45 H 6.369989 7.600864 4.128104 4.445323 3.531223

21 22 23 24 25

21 C 0.000000

22 C 1.355425 0.000000

23 C 2.282910 1.471019 0.000000

24 N 3.567088 2.491463 1.339212 0.000000

25 Zn 4.265857 4.251265 3.002794 3.369980 0.000000

26 C 9.838307 9.597090 8.160165 7.772091 5.594570

27 H 9.277088 9.458115 8.208950 8.309822 5.219024

28 C 6.562165 5.336166 4.401399 3.063909 5.594570

29 H 7.978489 7.058883 5.711442 4.582363 5.219024

30 C 7.478735 8.382735 7.826855 8.713461 5.594570

31 H 5.216819 6.387104 6.315805 7.496125 5.219024

32 C 1.483646 2.576972 3.747489 4.990646 5.594570

33 H 2.192515 1.080272 2.263427 2.852509 5.219024

34 H 10.668094 10.512921 9.098147 8.783974 6.402446

35 H 10.012915 9.684981 8.235796 7.746570 5.848642

36 H 10.012915 9.684981 8.235796 7.746570 5.848642

37 H 6.356758 5.093699 4.326235 3.060304 5.848642

38 H 6.356758 5.093699 4.326235 3.060304 5.848642

39 H 7.647884 6.426532 5.467298 4.128104 6.402446

40 H 8.024957 8.866452 8.229852 9.042195 5.848642

41 H 8.024957 8.866452 8.229852 9.042195 5.848642

42 H 7.738706 8.765205 8.374058 9.362421 6.402446

43 H 2.133035 3.280378 4.314910 5.578298 5.848642

44 H 2.133035 3.280378 4.314910 5.578298 5.848642

45 H 2.137635 2.758193 4.152097 5.247664 6.402446

26 27 28 29 30

26 C 0.000000

27 H 2.993627 0.000000

28 C 7.911916 9.455069 0.000000

29 H 5.260847 7.380814 2.993627 0.000000

30 C 7.911916 5.260847 11.189139 10.397742 0.000000

31 H 9.455069 7.380814 10.397742 10.438048 2.993627

32 C 11.189139 10.397742 7.911916 9.455069 7.911916

33 H 10.397742 10.438048 5.260847 7.380814 9.455069

34 H 1.090368 2.757992 9.002188 6.332876 7.971304

35 H 1.094565 3.745594 7.640551 4.908794 8.522536

36 H 1.094565 3.745594 7.640551 4.908794 8.522536

37 H 8.522536 9.939486 1.094565 3.745594 11.393576

38 H 8.522536 9.939486 1.094565 3.745594 11.393576

39 H 7.971304 9.815994 1.090368 2.757992 11.974646

40 H 7.640551 4.908794 11.393576 10.433608 1.094565

41 H 7.640551 4.908794 11.393576 10.433608 1.094565

42 H 9.002188 6.332876 11.974646 11.351323 1.090368

43 H 11.393576 10.433608 8.522536 9.939486 7.640551

44 H 11.393576 10.433608 8.522536 9.939486 7.640551

45 H 11.974646 11.351323 7.971304 9.815994 9.002188

31 32 33 34 35

31 H 0.000000

32 C 5.260847 0.000000

33 H 7.380814 2.993627 0.000000

34 H 9.815994 11.974646 11.351323 0.000000

35 H 9.939486 11.393576 10.433608 1.775099 0.000000

36 H 9.939486 11.393576 10.433608 1.775099 1.753773

37 H 10.433608 7.640551 4.908794 9.606337 8.177736

38 H 10.433608 7.640551 4.908794 9.606337 8.363677

39 H 11.351323 9.002188 6.332876 9.054427 7.623265

40 H 3.745594 8.522536 9.939486 7.623265 8.177736

41 H 3.745594 8.522536 9.939486 7.623265 8.363677

42 H 2.757992 7.971304 9.815994 9.054427 9.606337

43 H 4.908794 1.094565 3.745594 12.134451 11.565066

44 H 4.908794 1.094565 3.745594 12.134451 11.697284

45 H 6.332876 1.090368 2.757992 12.804893 12.134451

36 37 38 39 40

36 H 0.000000

37 H 8.363677 0.000000

38 H 8.177736 1.753773 0.000000

39 H 7.623265 1.775099 1.775099 0.000000

40 H 8.363677 11.565066 11.697284 12.134451 0.000000

41 H 8.177736 11.697284 11.565066 12.134451 1.753773

42 H 9.606337 12.134451 12.134451 12.804893 1.775099

43 H 11.697284 8.177736 8.363677 9.606337 8.177736

44 H 11.565066 8.363677 8.177736 9.606337 8.363677

45 H 12.134451 7.623265 7.623265 9.054427 9.606337

41 42 43 44 45

41 H 0.000000

42 H 1.775099 0.000000

43 H 8.363677 7.623265 0.000000

44 H 8.177736 7.623265 1.753773 0.000000

45 H 9.606337 9.054427 1.775099 1.775099 0.000000

Stoichiometry C20H16N8Zn(1+,2)

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

Deg. of freedom 20

Full point group C4H NOp 8

RotChk: IX=0 Diff= 3.14D-16

Largest Abelian subgroup C2H NOp 4

Largest concise Abelian subgroup C2H NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -2.182274 2.062632 0.000000

2 7 0 -1.857841 0.741857 0.000000

3 6 0 -2.988434 0.000000 0.000000

4 6 0 -4.163571 0.928552 0.000000

5 6 0 -3.648420 2.182265 0.000000

6 7 0 -3.096160 -1.330623 0.000000

7 6 0 -2.062632 -2.182274 0.000000

8 7 0 -0.741857 -1.857841 0.000000

9 6 0 0.000000 -2.988434 0.000000

10 6 0 -0.928552 -4.163571 0.000000

11 6 0 -2.182265 -3.648420 0.000000

12 7 0 -1.330623 3.096160 0.000000

13 6 0 0.928552 4.163571 0.000000

14 6 0 2.182265 3.648420 0.000000

15 6 0 2.062632 2.182274 0.000000

16 7 0 0.741857 1.857841 0.000000

17 6 0 0.000000 2.988434 0.000000

18 7 0 3.096160 1.330623 0.000000

19 7 0 1.857841 -0.741857 0.000000

20 6 0 2.988434 0.000000 0.000000

21 6 0 4.163571 -0.928552 0.000000

22 6 0 3.648420 -2.182265 0.000000

23 6 0 2.182274 -2.062632 0.000000

24 7 0 1.330623 -3.096160 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.574748 0.470527 0.000000

27 1 0 -4.183024 3.120980 0.000000

28 6 0 -0.470527 -5.574748 0.000000

29 1 0 -3.120980 -4.183024 0.000000

30 6 0 0.470527 5.574748 0.000000

31 1 0 3.120980 4.183024 0.000000

32 6 0 5.574748 -0.470527 0.000000

33 1 0 4.183024 -3.120980 0.000000

34 1 0 -6.266246 1.313577 0.000000

35 1 0 -5.780551 -0.151397 0.876886

36 1 0 -5.780551 -0.151397 -0.876886

37 1 0 0.151397 -5.780551 0.876886

38 1 0 0.151397 -5.780551 -0.876886

39 1 0 -1.313577 -6.266246 0.000000

40 1 0 -0.151397 5.780551 0.876886

41 1 0 -0.151397 5.780551 -0.876886

42 1 0 1.313577 6.266246 0.000000

43 1 0 5.780551 0.151397 0.876886

44 1 0 5.780551 0.151397 -0.876886

45 1 0 6.266246 -1.313577 0.000000

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

Rotational constants (GHZ): 0.1830366 0.1830366 0.0917243

Leave Link 202 at Fri Jul 5 21:14:32 2019, MaxMem= 1342177280 cpu: 0.2

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

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

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

Population analysis using the SCF density.

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Orbital symmetries:

Alpha Orbitals:

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

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Beta Orbitals:

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The electronic state is 2-AU.

Alpha occ. eigenvalues -- -14.34226 -14.34226 -14.34226 -14.34225 -14.32977

Alpha occ. eigenvalues -- -14.32977 -14.32977 -14.32977 -10.28499 -10.28499

Alpha occ. eigenvalues -- -10.28499 -10.28499 -10.28381 -10.28381 -10.28381

Alpha occ. eigenvalues -- -10.28381 -10.21287 -10.21287 -10.21287 -10.21287

Alpha occ. eigenvalues -- -10.19258 -10.19258 -10.19258 -10.19258 -10.17130

Alpha occ. eigenvalues -- -10.17130 -10.17130 -10.17130 -1.03362 -1.01930

Alpha occ. eigenvalues -- -1.01930 -0.99149 -0.96932 -0.92699 -0.92699

Alpha occ. eigenvalues -- -0.89350 -0.81967 -0.81463 -0.81463 -0.81213

Alpha occ. eigenvalues -- -0.77755 -0.74051 -0.74051 -0.71953 -0.70731

Alpha occ. eigenvalues -- -0.69972 -0.69972 -0.65919 -0.63258 -0.61124

Alpha occ. eigenvalues -- -0.59685 -0.59412 -0.58855 -0.58855 -0.57368

Alpha occ. eigenvalues -- -0.57368 -0.56582 -0.56543 -0.56543 -0.56192

Alpha occ. eigenvalues -- -0.53867 -0.52552 -0.52552 -0.51765 -0.50505

Alpha occ. eigenvalues -- -0.48690 -0.46988 -0.46988 -0.45944 -0.45029

Alpha occ. eigenvalues -- -0.45029 -0.44585 -0.44389 -0.41813 -0.41707

Alpha occ. eigenvalues -- -0.41707 -0.41604 -0.41522 -0.41255 -0.40743

Alpha occ. eigenvalues -- -0.40743 -0.39670 -0.39567 -0.39248 -0.39248

Alpha occ. eigenvalues -- -0.38538 -0.38070 -0.34921 -0.34921 -0.34336

Alpha occ. eigenvalues -- -0.34336 -0.32921 -0.30187 -0.30187 -0.28442

Alpha occ. eigenvalues -- -0.28123 -0.27896 -0.27075 -0.27075 -0.26886

Alpha occ. eigenvalues -- -0.26830 -0.23632

Alpha virt. eigenvalues -- -0.13274 -0.13274 -0.06528 0.00129 0.02493

Alpha virt. eigenvalues -- 0.02493 0.02729 0.03921 0.04044 0.04044

Alpha virt. eigenvalues -- 0.04894 0.06533 0.06725 0.07433 0.07860

Alpha virt. eigenvalues -- 0.07860 0.08559 0.08856 0.09000 0.09000

Alpha virt. eigenvalues -- 0.09591 0.09591 0.09667 0.12414 0.13091

Alpha virt. eigenvalues -- 0.13133 0.13133 0.13218 0.13284 0.13284

Alpha virt. eigenvalues -- 0.13702 0.16758 0.18572 0.18940 0.19522

Alpha virt. eigenvalues -- 0.19522 0.19606 0.19762 0.19762 0.21083

Alpha virt. eigenvalues -- 0.21266 0.21519 0.21600 0.21600 0.23619

Alpha virt. eigenvalues -- 0.25841 0.26555 0.26555 0.27370 0.27407

Alpha virt. eigenvalues -- 0.27951 0.27951 0.28598 0.30631 0.30631

Alpha virt. eigenvalues -- 0.30691 0.30781 0.30866 0.30866 0.31359

Alpha virt. eigenvalues -- 0.31686 0.33751 0.34174 0.34174 0.34735

Alpha virt. eigenvalues -- 0.36194 0.36194 0.36208 0.37406 0.37507

Alpha virt. eigenvalues -- 0.37507 0.38524 0.38902 0.38902 0.39307

Alpha virt. eigenvalues -- 0.40402 0.42197 0.42197 0.42255 0.42486

Alpha virt. eigenvalues -- 0.42804 0.44428 0.45219 0.45219 0.45402

Alpha virt. eigenvalues -- 0.46787 0.47672 0.47672 0.47949 0.48011

Alpha virt. eigenvalues -- 0.48011 0.48118 0.49883 0.50470 0.50644

Alpha virt. eigenvalues -- 0.50644 0.51904 0.52740 0.53170 0.53170

Alpha virt. eigenvalues -- 0.53864 0.55059 0.55059 0.55453 0.55583

Alpha virt. eigenvalues -- 0.56550 0.56550 0.56559 0.57592 0.57676

Alpha virt. eigenvalues -- 0.57676 0.57857 0.58511 0.58511 0.58925

Alpha virt. eigenvalues -- 0.59784 0.60125 0.61405 0.61783 0.61783

Alpha virt. eigenvalues -- 0.62217 0.62217 0.62293 0.63829 0.64232

Alpha virt. eigenvalues -- 0.64232 0.66845 0.67269 0.67811 0.67920

Alpha virt. eigenvalues -- 0.67920 0.68170 0.68170 0.68503 0.69530

Alpha virt. eigenvalues -- 0.70426 0.72032 0.72349 0.72349 0.73484

Alpha virt. eigenvalues -- 0.74006 0.74778 0.74778 0.76591 0.76591

Alpha virt. eigenvalues -- 0.77899 0.78391 0.78662 0.79588 0.79588

Alpha virt. eigenvalues -- 0.80064 0.80175 0.80175 0.81273 0.81393

Alpha virt. eigenvalues -- 0.84085 0.84085 0.84109 0.86081 0.87152

Alpha virt. eigenvalues -- 0.87762 0.87762 0.88495 0.93266 0.95112

Alpha virt. eigenvalues -- 0.95112 0.96554 0.96935 0.98806 0.99083

Alpha virt. eigenvalues -- 0.99083 1.01722 1.01722 1.03453 1.03810

Alpha virt. eigenvalues -- 1.03810 1.05384 1.06730 1.06730 1.07084

Alpha virt. eigenvalues -- 1.08698 1.09416 1.11673 1.11709 1.11709

Alpha virt. eigenvalues -- 1.11908 1.12364 1.12477 1.12932 1.12932

Alpha virt. eigenvalues -- 1.12952 1.16647 1.16993 1.17709 1.17709

Alpha virt. eigenvalues -- 1.18967 1.18967 1.19180 1.22137 1.22305

Alpha virt. eigenvalues -- 1.26214 1.26390 1.27574 1.27574 1.28836

Alpha virt. eigenvalues -- 1.34360 1.34360 1.35453 1.36481 1.37389

Alpha virt. eigenvalues -- 1.38517 1.39337 1.39337 1.40476 1.40476

Alpha virt. eigenvalues -- 1.42038 1.42785 1.47715 1.48164 1.48164

Alpha virt. eigenvalues -- 1.50218 1.50248 1.50248 1.50398 1.50398

Alpha virt. eigenvalues -- 1.50562 1.50574 1.51537 1.51655 1.53659

Alpha virt. eigenvalues -- 1.53659 1.54430 1.54903 1.54903 1.55872

Alpha virt. eigenvalues -- 1.57137 1.59139 1.59251 1.59251 1.60290

Alpha virt. eigenvalues -- 1.61270 1.61416 1.61416 1.65615 1.65711

Alpha virt. eigenvalues -- 1.66756 1.66756 1.67632 1.67632 1.68523

Alpha virt. eigenvalues -- 1.69373 1.69373 1.69602 1.72571 1.73207

Alpha virt. eigenvalues -- 1.73887 1.73887 1.78532 1.78627 1.78627

Alpha virt. eigenvalues -- 1.78652 1.83592 1.84912 1.85084 1.85084

Alpha virt. eigenvalues -- 1.87150 1.88048 1.88048 1.89208 1.89377

Alpha virt. eigenvalues -- 1.91791 1.93621 1.94335 1.94624 1.94624

Alpha virt. eigenvalues -- 2.00347 2.00369 2.00486 2.00553 2.00553

Alpha virt. eigenvalues -- 2.00567 2.00663 2.00663 2.03573 2.05552

Alpha virt. eigenvalues -- 2.05943 2.07154 2.07154 2.10555 2.10555

Alpha virt. eigenvalues -- 2.13126 2.13996 2.13996 2.15539 2.15783

Alpha virt. eigenvalues -- 2.18068 2.26319 2.26830 2.27854 2.28238

Alpha virt. eigenvalues -- 2.28238 2.28795 2.31525 2.31525 2.34105

Alpha virt. eigenvalues -- 2.34272 2.34272 2.35734 2.35734 2.35766

Alpha virt. eigenvalues -- 2.36714 2.37691 2.37966 2.37966 2.38237

Alpha virt. eigenvalues -- 2.42164 2.46244 2.46524 2.46524 2.46622

Alpha virt. eigenvalues -- 2.46627 2.46627 2.47448 2.47741 2.54298

Alpha virt. eigenvalues -- 2.54350 2.54350 2.55050 2.56467 2.56467

Alpha virt. eigenvalues -- 2.57410 2.58473 2.58473 2.61355 2.62124

Alpha virt. eigenvalues -- 2.63085 2.64737 2.66163 2.68882 2.68882

Alpha virt. eigenvalues -- 2.69942 2.70997 2.70997 2.71198 2.73356

Alpha virt. eigenvalues -- 2.73356 2.74513 2.77008 2.80946 2.81634

Alpha virt. eigenvalues -- 2.81634 2.81839 2.82554 2.83036 2.83525

Alpha virt. eigenvalues -- 2.83525 2.89601 2.89601 2.91291 2.91683

Alpha virt. eigenvalues -- 2.94592 2.94819 2.94819 2.99091 3.00662

Alpha virt. eigenvalues -- 3.02430 3.02430 3.03286 3.10241 3.11028

Alpha virt. eigenvalues -- 3.12040 3.12040 3.12592 3.13099 3.13099

Alpha virt. eigenvalues -- 3.13419 3.13665 3.15259 3.15259 3.17351

Alpha virt. eigenvalues -- 3.18885 3.18885 3.19104 3.20708 3.23067

Alpha virt. eigenvalues -- 3.25362 3.26302 3.26699 3.26699 3.28533

Alpha virt. eigenvalues -- 3.28533 3.33955 3.36693 3.37513 3.37513

Alpha virt. eigenvalues -- 3.37786 3.50715 3.55223 3.55223 3.68190

Alpha virt. eigenvalues -- 3.70191 3.71002 3.71002 3.74458 3.76421

Alpha virt. eigenvalues -- 3.76583 3.76583 3.77476 3.79212 3.80013

Alpha virt. eigenvalues -- 3.80013 3.85208 3.86011 3.86011 3.86084

Alpha virt. eigenvalues -- 3.89130 4.03224 4.03224 4.03826 4.04031

Alpha virt. eigenvalues -- 4.09816 4.10641 4.10641 4.16632 4.26313

Alpha virt. eigenvalues -- 4.33578 4.33578 4.35673 4.44687 4.49420

Alpha virt. eigenvalues -- 4.59242 4.59242 4.97039 5.00483 5.00483

Alpha virt. eigenvalues -- 5.09582 5.12987 5.31099 5.31099 5.48051

Alpha virt. eigenvalues -- 7.76920 7.76920 7.88201 7.93902 8.21953

Alpha virt. eigenvalues -- 11.19162 23.41254 23.43512 23.43512 23.44809

Alpha virt. eigenvalues -- 23.66671 23.67097 23.67106 23.67106 23.76920

Alpha virt. eigenvalues -- 23.78302 23.78302 23.79795 23.83272 23.84487

Alpha virt. eigenvalues -- 23.84487 23.84781 24.11966 24.12473 24.12473

Alpha virt. eigenvalues -- 24.13183 35.54490 35.59108 35.59108 35.60369

Alpha virt. eigenvalues -- 35.65663 35.66960 35.66960 35.67373

Beta occ. eigenvalues -- -14.34371 -14.34371 -14.34371 -14.34371 -14.33075

Beta occ. eigenvalues -- -14.33075 -14.33075 -14.33075 -10.28227 -10.28227

Beta occ. eigenvalues -- -10.28227 -10.28227 -10.28110 -10.28110 -10.28110

Beta occ. eigenvalues -- -10.28110 -10.21219 -10.21219 -10.21219 -10.21219

Beta occ. eigenvalues -- -10.19282 -10.19282 -10.19282 -10.19282 -10.17131

Beta occ. eigenvalues -- -10.17131 -10.17131 -10.17131 -1.03160 -1.01728

Beta occ. eigenvalues -- -1.01728 -0.98937 -0.96840 -0.92678 -0.92678

Beta occ. eigenvalues -- -0.89524 -0.81861 -0.81385 -0.81385 -0.81143

Beta occ. eigenvalues -- -0.77184 -0.73774 -0.73774 -0.71913 -0.70591

Beta occ. eigenvalues -- -0.69750 -0.69750 -0.65633 -0.63026 -0.61072

Beta occ. eigenvalues -- -0.59585 -0.59374 -0.58706 -0.58706 -0.57389

Beta occ. eigenvalues -- -0.57389 -0.56475 -0.56382 -0.56382 -0.56160

Beta occ. eigenvalues -- -0.53748 -0.52461 -0.52461 -0.51660 -0.50431

Beta occ. eigenvalues -- -0.47951 -0.46234 -0.46234 -0.45912 -0.44994

Beta occ. eigenvalues -- -0.44994 -0.44344 -0.43951 -0.41656 -0.41522

Beta occ. eigenvalues -- -0.41503 -0.41503 -0.41483 -0.40636 -0.40636

Beta occ. eigenvalues -- -0.40585 -0.39459 -0.39205 -0.39205 -0.39189

Beta occ. eigenvalues -- -0.38487 -0.37985 -0.34917 -0.34917 -0.33593

Beta occ. eigenvalues -- -0.33593 -0.33005 -0.30280 -0.30280 -0.28556

Beta occ. eigenvalues -- -0.28033 -0.27944 -0.27744 -0.27059 -0.27059

Beta occ. eigenvalues -- -0.26813

Beta virt. eigenvalues -- -0.18531 -0.11856 -0.11856 -0.05874 0.01328

Beta virt. eigenvalues -- 0.02966 0.03338 0.03338 0.04097 0.04097

Beta virt. eigenvalues -- 0.04706 0.04904 0.06535 0.06740 0.07892

Beta virt. eigenvalues -- 0.07892 0.08200 0.08874 0.08950 0.09606

Beta virt. eigenvalues -- 0.09606 0.09720 0.09752 0.09752 0.12421

Beta virt. eigenvalues -- 0.13148 0.13148 0.13200 0.13226 0.13455

Beta virt. eigenvalues -- 0.13455 0.13874 0.17010 0.18774 0.19217

Beta virt. eigenvalues -- 0.19781 0.19781 0.19786 0.19958 0.19958

Beta virt. eigenvalues -- 0.21195 0.21343 0.21765 0.21874 0.21874

Beta virt. eigenvalues -- 0.23933 0.26144 0.26675 0.26675 0.27490

Beta virt. eigenvalues -- 0.27804 0.28175 0.28175 0.28769 0.30758

Beta virt. eigenvalues -- 0.30799 0.30799 0.30860 0.30929 0.30929

Beta virt. eigenvalues -- 0.31447 0.31780 0.33810 0.34371 0.34371

Beta virt. eigenvalues -- 0.34888 0.36326 0.36326 0.36394 0.37728

Beta virt. eigenvalues -- 0.38180 0.38180 0.38669 0.39054 0.39054

Beta virt. eigenvalues -- 0.39470 0.40856 0.42335 0.42335 0.42672

Beta virt. eigenvalues -- 0.42948 0.43314 0.44583 0.45439 0.45439

Beta virt. eigenvalues -- 0.45571 0.46922 0.47834 0.47834 0.48154

Beta virt. eigenvalues -- 0.48154 0.48220 0.48241 0.50021 0.50748

Beta virt. eigenvalues -- 0.50998 0.50998 0.52357 0.52877 0.53240

Beta virt. eigenvalues -- 0.53240 0.53924 0.55131 0.55131 0.55533

Beta virt. eigenvalues -- 0.55667 0.56632 0.56632 0.56877 0.57633

Beta virt. eigenvalues -- 0.57807 0.57807 0.57913 0.58580 0.58580

Beta virt. eigenvalues -- 0.58973 0.59855 0.60213 0.61538 0.61964

Beta virt. eigenvalues -- 0.61964 0.62338 0.62572 0.62572 0.63918

Beta virt. eigenvalues -- 0.64289 0.64289 0.67154 0.67417 0.67890

Beta virt. eigenvalues -- 0.68020 0.68020 0.68054 0.68054 0.68643

Beta virt. eigenvalues -- 0.69664 0.70437 0.72151 0.72497 0.72497

Beta virt. eigenvalues -- 0.73572 0.74204 0.74875 0.74875 0.76723

Beta virt. eigenvalues -- 0.76723 0.77881 0.78280 0.78870 0.79502

Beta virt. eigenvalues -- 0.79502 0.79877 0.80285 0.80285 0.81358

Beta virt. eigenvalues -- 0.81453 0.84175 0.84183 0.84183 0.86155

Beta virt. eigenvalues -- 0.87211 0.87833 0.87833 0.88591 0.93420

Beta virt. eigenvalues -- 0.95167 0.95167 0.96762 0.97018 0.99194

Beta virt. eigenvalues -- 0.99194 0.99223 1.02056 1.02056 1.03510

Beta virt. eigenvalues -- 1.03972 1.03972 1.05568 1.07142 1.07142

Beta virt. eigenvalues -- 1.07203 1.09060 1.09418 1.11735 1.12337

Beta virt. eigenvalues -- 1.12353 1.12353 1.12477 1.12931 1.13039

Beta virt. eigenvalues -- 1.13039 1.13508 1.17207 1.17265 1.17743

Beta virt. eigenvalues -- 1.17743 1.19368 1.19423 1.19423 1.22181

Beta virt. eigenvalues -- 1.22335 1.26296 1.26830 1.27712 1.27712

Beta virt. eigenvalues -- 1.28880 1.34849 1.34849 1.35635 1.37075

Beta virt. eigenvalues -- 1.37467 1.38971 1.39414 1.39414 1.40610

Beta virt. eigenvalues -- 1.40610 1.42285 1.42935 1.47710 1.48214

Beta virt. eigenvalues -- 1.48214 1.50294 1.50321 1.50321 1.50375

Beta virt. eigenvalues -- 1.50375 1.50508 1.50615 1.51630 1.52105

Beta virt. eigenvalues -- 1.53771 1.53771 1.54486 1.55058 1.55058

Beta virt. eigenvalues -- 1.56089 1.57367 1.59217 1.59526 1.59526

Beta virt. eigenvalues -- 1.60373 1.61475 1.61537 1.61537 1.65681

Beta virt. eigenvalues -- 1.66094 1.66922 1.66922 1.67731 1.67731

Beta virt. eigenvalues -- 1.68717 1.69718 1.69887 1.69887 1.72733

Beta virt. eigenvalues -- 1.73866 1.74054 1.74054 1.78827 1.78845

Beta virt. eigenvalues -- 1.78849 1.78849 1.83705 1.85162 1.85234

Beta virt. eigenvalues -- 1.85234 1.87256 1.88399 1.88399 1.89383

Beta virt. eigenvalues -- 1.89729 1.92076 1.93921 1.94510 1.94963

Beta virt. eigenvalues -- 1.94963 2.00506 2.00657 2.00717 2.00717

Beta virt. eigenvalues -- 2.00720 2.00786 2.01176 2.01176 2.03656

Beta virt. eigenvalues -- 2.05955 2.05971 2.07211 2.07211 2.10608

Beta virt. eigenvalues -- 2.10608 2.13250 2.14306 2.14306 2.15652

Beta virt. eigenvalues -- 2.16226 2.18220 2.26372 2.27108 2.27904

Beta virt. eigenvalues -- 2.28271 2.28271 2.28826 2.31626 2.31626

Beta virt. eigenvalues -- 2.34148 2.34332 2.34332 2.35816 2.36071

Beta virt. eigenvalues -- 2.36071 2.36748 2.37763 2.37995 2.37995

Beta virt. eigenvalues -- 2.38645 2.42208 2.46155 2.46650 2.46650

Beta virt. eigenvalues -- 2.46691 2.46691 2.46753 2.47697 2.47827

Beta virt. eigenvalues -- 2.54232 2.54237 2.54237 2.55049 2.56460

Beta virt. eigenvalues -- 2.56460 2.57854 2.58893 2.58893 2.61666

Beta virt. eigenvalues -- 2.62041 2.62963 2.65063 2.66160 2.69089

Beta virt. eigenvalues -- 2.69089 2.70119 2.70938 2.70938 2.71156

Beta virt. eigenvalues -- 2.74149 2.74149 2.75250 2.77916 2.81503

Beta virt. eigenvalues -- 2.82304 2.82304 2.82601 2.82654 2.83069

Beta virt. eigenvalues -- 2.83596 2.83596 2.89686 2.89686 2.91408

Beta virt. eigenvalues -- 2.92122 2.94658 2.95411 2.95411 2.99810

Beta virt. eigenvalues -- 3.00756 3.02517 3.02517 3.03377 3.10278

Beta virt. eigenvalues -- 3.11082 3.12106 3.12106 3.12669 3.13192

Beta virt. eigenvalues -- 3.13192 3.13516 3.13800 3.15327 3.15327

Beta virt. eigenvalues -- 3.17392 3.18944 3.18944 3.19168 3.20728

Beta virt. eigenvalues -- 3.23130 3.25417 3.26375 3.26760 3.26760

Beta virt. eigenvalues -- 3.28606 3.28606 3.34039 3.36716 3.37538

Beta virt. eigenvalues -- 3.37538 3.37817 3.50866 3.55361 3.55361

Beta virt. eigenvalues -- 3.68306 3.70321 3.71149 3.71149 3.74570

Beta virt. eigenvalues -- 3.76590 3.76718 3.76718 3.77616 3.78732

Beta virt. eigenvalues -- 3.79632 3.79632 3.84892 3.85625 3.85625

Beta virt. eigenvalues -- 3.85637 3.88814 4.03342 4.03342 4.03943

Beta virt. eigenvalues -- 4.04158 4.09810 4.10688 4.10688 4.16747

Beta virt. eigenvalues -- 4.26364 4.33742 4.33742 4.35912 4.44748

Beta virt. eigenvalues -- 4.49430 4.59267 4.59267 4.97210 5.00658

Beta virt. eigenvalues -- 5.00658 5.09779 5.13145 5.31287 5.31287

Beta virt. eigenvalues -- 5.48241 7.76902 7.76902 7.88201 7.93897

Beta virt. eigenvalues -- 8.21949 11.19152 23.41301 23.43552 23.43552

Beta virt. eigenvalues -- 23.44845 23.66691 23.67108 23.67119 23.67119

Beta virt. eigenvalues -- 23.77191 23.78591 23.78591 23.80091 23.83585

Beta virt. eigenvalues -- 23.84799 23.84799 23.85096 24.11994 24.12501

Beta virt. eigenvalues -- 24.12501 24.13212 35.54366 35.58995 35.58995

Beta virt. eigenvalues -- 35.60268 35.65512 35.66821 35.66821 35.67245

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 4.568765 0.403219 -0.128854 -0.047235 0.402264 -0.001888

2 N 0.403219 7.120889 0.389900 -0.063537 -0.092361 -0.077874

3 C -0.128854 0.389900 4.604148 0.375381 -0.064669 0.557042

4 C -0.047235 -0.063537 0.375381 5.030996 0.632645 -0.069900

5 C 0.402264 -0.092361 -0.064669 0.632645 5.081045 0.004157

6 N -0.001888 -0.077874 0.557042 -0.069900 0.004157 6.567016

7 C -0.001135 -0.005058 -0.089215 0.004496 -0.000309 0.514663

8 N 0.000720 -0.018783 -0.005858 -0.000169 -0.000203 -0.071319

9 C -0.000007 0.000616 -0.000909 0.000023 -0.000004 0.000086

10 C -0.000003 -0.000111 0.000062 0.000013 0.000000 0.003231

11 C 0.000023 0.000207 0.004124 -0.000235 0.000010 -0.040392

12 N 0.514663 -0.071319 0.000086 0.003231 -0.040392 -0.000150

13 C 0.004496 -0.000169 0.000023 0.000013 -0.000235 0.000000

14 C -0.000309 -0.000203 -0.000004 0.000000 0.000010 0.000000

15 C -0.001135 0.000720 -0.000007 -0.000003 0.000023 -0.000001

16 N -0.005058 -0.018783 0.000616 -0.000111 0.000207 -0.000004

17 C -0.089215 -0.005858 -0.000909 0.000062 0.004124 -0.000025

18 N -0.000019 -0.000004 -0.000001 0.000000 0.000000 0.000000

19 N 0.000164 -0.003650 0.000224 0.000002 0.000003 -0.000004

20 C -0.000053 0.000224 -0.000011 0.000000 0.000000 -0.000001

21 C 0.000000 0.000002 0.000000 0.000000 0.000000 0.000000

22 C 0.000000 0.000003 0.000000 0.000000 0.000000 0.000000

23 C -0.000004 0.000164 -0.000053 0.000000 0.000000 -0.000019

24 N -0.000001 -0.000004 -0.000025 0.000000 0.000000 -0.000150

25 Zn -0.015454 0.104850 -0.016767 -0.000991 -0.001118 -0.004938

26 C 0.009024 0.008228 -0.068843 0.271786 -0.052086 0.013058

27 H -0.046094 0.005535 0.009196 -0.040614 0.395502 -0.000010

28 C 0.000000 0.000000 0.000002 0.000000 0.000000 -0.000020

29 H 0.000001 0.000065 -0.000224 -0.000129 -0.000003 0.005477

30 C -0.000507 0.000059 0.000000 0.000000 -0.000046 0.000000

31 H 0.000012 0.000001 0.000000 0.000000 0.000000 0.000000

32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

33 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

34 H 0.000203 -0.000232 0.006189 -0.039530 -0.005559 0.000056

35 H -0.000186 0.000409 -0.005251 -0.042909 -0.000326 0.003632

36 H -0.000186 0.000409 -0.005251 -0.042909 -0.000326 0.003632

37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000007

38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000007

39 H 0.000000 0.000000 0.000001 0.000000 0.000000 -0.000009

40 H -0.000045 0.000013 0.000000 0.000000 -0.000020 0.000000

41 H -0.000045 0.000013 0.000000 0.000000 -0.000020 0.000000

42 H 0.000038 0.000000 0.000000 0.000000 -0.000001 0.000000

43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 8 9 10 11 12

1 C -0.001135 0.000720 -0.000007 -0.000003 0.000023 0.514663

2 N -0.005058 -0.018783 0.000616 -0.000111 0.000207 -0.071319

3 C -0.089215 -0.005858 -0.000909 0.000062 0.004124 0.000086

4 C 0.004496 -0.000169 0.000023 0.000013 -0.000235 0.003231

5 C -0.000309 -0.000203 -0.000004 0.000000 0.000010 -0.040392

6 N 0.514663 -0.071319 0.000086 0.003231 -0.040392 -0.000150

7 C 4.568765 0.403219 -0.128854 -0.047235 0.402264 -0.000019

8 N 0.403219 7.120889 0.389900 -0.063537 -0.092361 -0.000004

9 C -0.128854 0.389900 4.604148 0.375381 -0.064669 -0.000001

10 C -0.047235 -0.063537 0.375381 5.030996 0.632645 0.000000

11 C 0.402264 -0.092361 -0.064669 0.632645 5.081045 0.000000

12 N -0.000019 -0.000004 -0.000001 0.000000 0.000000 6.567016

13 C 0.000000 0.000002 0.000000 0.000000 0.000000 -0.069900

14 C 0.000000 0.000003 0.000000 0.000000 0.000000 0.004157

15 C -0.000004 0.000164 -0.000053 0.000000 0.000000 -0.001888

16 N 0.000164 -0.003650 0.000224 0.000002 0.000003 -0.077874

17 C -0.000053 0.000224 -0.000011 0.000000 0.000000 0.557042

18 N -0.000001 -0.000004 -0.000025 0.000000 0.000000 -0.000150

19 N 0.000720 -0.018783 -0.005858 -0.000169 -0.000203 -0.000004

20 C -0.000007 0.000616 -0.000909 0.000023 -0.000004 -0.000025

21 C -0.000003 -0.000111 0.000062 0.000013 0.000000 0.000000

22 C 0.000023 0.000207 0.004124 -0.000235 0.000010 0.000000

23 C -0.001135 -0.005058 -0.089215 0.004496 -0.000309 -0.000001

24 N -0.001888 -0.077874 0.557042 -0.069900 0.004157 0.000000

25 Zn -0.015454 0.104850 -0.016767 -0.000991 -0.001118 -0.004938

26 C -0.000507 0.000059 0.000000 0.000000 -0.000046 -0.000020

27 H 0.000012 0.000001 0.000000 0.000000 0.000000 0.005477

28 C 0.009024 0.008228 -0.068843 0.271786 -0.052086 0.000000

29 H -0.046094 0.005535 0.009196 -0.040614 0.395502 0.000000

30 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.013058

31 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000010

32 C 0.000000 0.000000 0.000002 0.000000 0.000000 0.000000

33 H 0.000001 0.000065 -0.000224 -0.000129 -0.000003 0.000000

34 H 0.000038 0.000000 0.000000 0.000000 -0.000001 -0.000009

35 H -0.000045 0.000013 0.000000 0.000000 -0.000020 0.000007

36 H -0.000045 0.000013 0.000000 0.000000 -0.000020 0.000007

37 H -0.000186 0.000409 -0.005251 -0.042909 -0.000326 0.000000

38 H -0.000186 0.000409 -0.005251 -0.042909 -0.000326 0.000000

39 H 0.000203 -0.000232 0.006189 -0.039530 -0.005559 0.000000

40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.003632

41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.003632

42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000056

43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

45 H 0.000000 0.000000 0.000001 0.000000 0.000000 0.000000

13 14 15 16 17 18

1 C 0.004496 -0.000309 -0.001135 -0.005058 -0.089215 -0.000019

2 N -0.000169 -0.000203 0.000720 -0.018783 -0.005858 -0.000004

3 C 0.000023 -0.000004 -0.000007 0.000616 -0.000909 -0.000001

4 C 0.000013 0.000000 -0.000003 -0.000111 0.000062 0.000000

5 C -0.000235 0.000010 0.000023 0.000207 0.004124 0.000000

6 N 0.000000 0.000000 -0.000001 -0.000004 -0.000025 0.000000

7 C 0.000000 0.000000 -0.000004 0.000164 -0.000053 -0.000001

8 N 0.000002 0.000003 0.000164 -0.003650 0.000224 -0.000004

9 C 0.000000 0.000000 -0.000053 0.000224 -0.000011 -0.000025

10 C 0.000000 0.000000 0.000000 0.000002 0.000000 0.000000

11 C 0.000000 0.000000 0.000000 0.000003 0.000000 0.000000

12 N -0.069900 0.004157 -0.001888 -0.077874 0.557042 -0.000150

13 C 5.030996 0.632645 -0.047235 -0.063537 0.375381 0.003231

14 C 0.632645 5.081045 0.402264 -0.092361 -0.064669 -0.040392

15 C -0.047235 0.402264 4.568765 0.403219 -0.128854 0.514663

16 N -0.063537 -0.092361 0.403219 7.120889 0.389900 -0.071319

17 C 0.375381 -0.064669 -0.128854 0.389900 4.604148 0.000086

18 N 0.003231 -0.040392 0.514663 -0.071319 0.000086 6.567016

19 N -0.000111 0.000207 -0.005058 -0.018783 0.000616 -0.077874

20 C 0.000062 0.004124 -0.089215 -0.005858 -0.000909 0.557042

21 C 0.000013 -0.000235 0.004496 -0.000169 0.000023 -0.069900

22 C 0.000000 0.000010 -0.000309 -0.000203 -0.000004 0.004157

23 C -0.000003 0.000023 -0.001135 0.000720 -0.000007 -0.001888

24 N 0.000000 0.000000 -0.000019 -0.000004 -0.000001 -0.000150

25 Zn -0.000991 -0.001118 -0.015454 0.104850 -0.016767 -0.004938

26 C 0.000000 0.000000 0.000000 0.000000 0.000002 0.000000

27 H -0.000129 -0.000003 0.000001 0.000065 -0.000224 0.000000

28 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

29 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

30 C 0.271786 -0.052086 0.009024 0.008228 -0.068843 -0.000020

31 H -0.040614 0.395502 -0.046094 0.005535 0.009196 0.005477

32 C 0.000000 -0.000046 -0.000507 0.000059 0.000000 0.013058

33 H 0.000000 0.000000 0.000012 0.000001 0.000000 -0.000010

34 H 0.000000 0.000000 0.000000 0.000000 0.000001 0.000000

35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

40 H -0.042909 -0.000326 -0.000186 0.000409 -0.005251 0.000007

41 H -0.042909 -0.000326 -0.000186 0.000409 -0.005251 0.000007

42 H -0.039530 -0.005559 0.000203 -0.000232 0.006189 -0.000009

43 H 0.000000 -0.000020 -0.000045 0.000013 0.000000 0.003632

44 H 0.000000 -0.000020 -0.000045 0.000013 0.000000 0.003632

45 H 0.000000 -0.000001 0.000038 0.000000 0.000000 0.000056

19 20 21 22 23 24

1 C 0.000164 -0.000053 0.000000 0.000000 -0.000004 -0.000001

2 N -0.003650 0.000224 0.000002 0.000003 0.000164 -0.000004

3 C 0.000224 -0.000011 0.000000 0.000000 -0.000053 -0.000025

4 C 0.000002 0.000000 0.000000 0.000000 0.000000 0.000000

5 C 0.000003 0.000000 0.000000 0.000000 0.000000 0.000000

6 N -0.000004 -0.000001 0.000000 0.000000 -0.000019 -0.000150

7 C 0.000720 -0.000007 -0.000003 0.000023 -0.001135 -0.001888

8 N -0.018783 0.000616 -0.000111 0.000207 -0.005058 -0.077874

9 C -0.005858 -0.000909 0.000062 0.004124 -0.089215 0.557042

10 C -0.000169 0.000023 0.000013 -0.000235 0.004496 -0.069900

11 C -0.000203 -0.000004 0.000000 0.000010 -0.000309 0.004157

12 N -0.000004 -0.000025 0.000000 0.000000 -0.000001 0.000000

13 C -0.000111 0.000062 0.000013 0.000000 -0.000003 0.000000

14 C 0.000207 0.004124 -0.000235 0.000010 0.000023 0.000000

15 C -0.005058 -0.089215 0.004496 -0.000309 -0.001135 -0.000019

16 N -0.018783 -0.005858 -0.000169 -0.000203 0.000720 -0.000004

17 C 0.000616 -0.000909 0.000023 -0.000004 -0.000007 -0.000001

18 N -0.077874 0.557042 -0.069900 0.004157 -0.001888 -0.000150

19 N 7.120889 0.389900 -0.063537 -0.092361 0.403219 -0.071319

20 C 0.389900 4.604148 0.375381 -0.064669 -0.128854 0.000086

21 C -0.063537 0.375381 5.030996 0.632645 -0.047235 0.003231

22 C -0.092361 -0.064669 0.632645 5.081045 0.402264 -0.040392

23 C 0.403219 -0.128854 -0.047235 0.402264 4.568765 0.514663

24 N -0.071319 0.000086 0.003231 -0.040392 0.514663 6.567016

25 Zn 0.104850 -0.016767 -0.000991 -0.001118 -0.015454 -0.004938

26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

28 C 0.000059 0.000000 0.000000 -0.000046 -0.000507 0.013058

29 H 0.000001 0.000000 0.000000 0.000000 0.000012 -0.000010

30 C 0.000000 0.000002 0.000000 0.000000 0.000000 0.000000

31 H 0.000065 -0.000224 -0.000129 -0.000003 0.000001 0.000000

32 C 0.008228 -0.068843 0.271786 -0.052086 0.009024 -0.000020

33 H 0.005535 0.009196 -0.040614 0.395502 -0.046094 0.005477

34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 H 0.000013 0.000000 0.000000 -0.000020 -0.000045 0.003632

38 H 0.000013 0.000000 0.000000 -0.000020 -0.000045 0.003632

39 H 0.000000 0.000000 0.000000 -0.000001 0.000038 0.000056

40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

42 H 0.000000 0.000001 0.000000 0.000000 0.000000 0.000000

43 H 0.000409 -0.005251 -0.042909 -0.000326 -0.000186 0.000007

44 H 0.000409 -0.005251 -0.042909 -0.000326 -0.000186 0.000007

45 H -0.000232 0.006189 -0.039530 -0.005559 0.000203 -0.000009

25 26 27 28 29 30

1 C -0.015454 0.009024 -0.046094 0.000000 0.000001 -0.000507

2 N 0.104850 0.008228 0.005535 0.000000 0.000065 0.000059

3 C -0.016767 -0.068843 0.009196 0.000002 -0.000224 0.000000

4 C -0.000991 0.271786 -0.040614 0.000000 -0.000129 0.000000

5 C -0.001118 -0.052086 0.395502 0.000000 -0.000003 -0.000046

6 N -0.004938 0.013058 -0.000010 -0.000020 0.005477 0.000000

7 C -0.015454 -0.000507 0.000012 0.009024 -0.046094 0.000000

8 N 0.104850 0.000059 0.000001 0.008228 0.005535 0.000000

9 C -0.016767 0.000000 0.000000 -0.068843 0.009196 0.000000

10 C -0.000991 0.000000 0.000000 0.271786 -0.040614 0.000000

11 C -0.001118 -0.000046 0.000000 -0.052086 0.395502 0.000000

12 N -0.004938 -0.000020 0.005477 0.000000 0.000000 0.013058

13 C -0.000991 0.000000 -0.000129 0.000000 0.000000 0.271786

14 C -0.001118 0.000000 -0.000003 0.000000 0.000000 -0.052086

15 C -0.015454 0.000000 0.000001 0.000000 0.000000 0.009024

16 N 0.104850 0.000000 0.000065 0.000000 0.000000 0.008228

17 C -0.016767 0.000002 -0.000224 0.000000 0.000000 -0.068843

18 N -0.004938 0.000000 0.000000 0.000000 0.000000 -0.000020

19 N 0.104850 0.000000 0.000000 0.000059 0.000001 0.000000

20 C -0.016767 0.000000 0.000000 0.000000 0.000000 0.000002

21 C -0.000991 0.000000 0.000000 0.000000 0.000000 0.000000

22 C -0.001118 0.000000 0.000000 -0.000046 0.000000 0.000000

23 C -0.015454 0.000000 0.000000 -0.000507 0.000012 0.000000

24 N -0.004938 0.000000 0.000000 0.013058 -0.000010 0.000000

25 Zn 10.188336 0.000411 0.000025 0.000411 0.000025 0.000411

26 C 0.000411 5.357168 -0.004283 0.000000 0.000058 0.000000

27 H 0.000025 -0.004283 0.426033 0.000000 0.000000 0.000058

28 C 0.000411 0.000000 0.000000 5.357168 -0.004283 0.000000

29 H 0.000025 0.000058 0.000000 -0.004283 0.426033 0.000000

30 C 0.000411 0.000000 0.000058 0.000000 0.000000 5.357168

31 H 0.000025 0.000000 0.000000 0.000000 0.000000 -0.004283

32 C 0.000411 0.000000 0.000000 0.000000 0.000000 0.000000

33 H 0.000025 0.000000 0.000000 0.000058 0.000000 0.000000

34 H 0.000051 0.388481 0.001240 0.000000 0.000000 0.000000

35 H 0.000075 0.386967 -0.000100 0.000000 0.000032 0.000000

36 H 0.000075 0.386967 -0.000100 0.000000 0.000032 0.000000

37 H 0.000075 0.000000 0.000000 0.386967 -0.000100 0.000000

38 H 0.000075 0.000000 0.000000 0.386967 -0.000100 0.000000

39 H 0.000051 0.000000 0.000000 0.388481 0.001240 0.000000

40 H 0.000075 0.000000 0.000032 0.000000 0.000000 0.386967

41 H 0.000075 0.000000 0.000032 0.000000 0.000000 0.386967

42 H 0.000051 0.000000 0.000000 0.000000 0.000000 0.388481

43 H 0.000075 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000075 0.000000 0.000000 0.000000 0.000000 0.000000

45 H 0.000051 0.000000 0.000000 0.000000 0.000000 0.000000

31 32 33 34 35 36

1 C 0.000012 0.000000 0.000000 0.000203 -0.000186 -0.000186

2 N 0.000001 0.000000 0.000000 -0.000232 0.000409 0.000409

3 C 0.000000 0.000000 0.000000 0.006189 -0.005251 -0.005251

4 C 0.000000 0.000000 0.000000 -0.039530 -0.042909 -0.042909

5 C 0.000000 0.000000 0.000000 -0.005559 -0.000326 -0.000326

6 N 0.000000 0.000000 0.000000 0.000056 0.003632 0.003632

7 C 0.000000 0.000000 0.000001 0.000038 -0.000045 -0.000045

8 N 0.000000 0.000000 0.000065 0.000000 0.000013 0.000013

9 C 0.000000 0.000002 -0.000224 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 -0.000129 0.000000 0.000000 0.000000

11 C 0.000000 0.000000 -0.000003 -0.000001 -0.000020 -0.000020

12 N -0.000010 0.000000 0.000000 -0.000009 0.000007 0.000007

13 C -0.040614 0.000000 0.000000 0.000000 0.000000 0.000000

14 C 0.395502 -0.000046 0.000000 0.000000 0.000000 0.000000

15 C -0.046094 -0.000507 0.000012 0.000000 0.000000 0.000000

16 N 0.005535 0.000059 0.000001 0.000000 0.000000 0.000000

17 C 0.009196 0.000000 0.000000 0.000001 0.000000 0.000000

18 N 0.005477 0.013058 -0.000010 0.000000 0.000000 0.000000

19 N 0.000065 0.008228 0.005535 0.000000 0.000000 0.000000

20 C -0.000224 -0.068843 0.009196 0.000000 0.000000 0.000000

21 C -0.000129 0.271786 -0.040614 0.000000 0.000000 0.000000

22 C -0.000003 -0.052086 0.395502 0.000000 0.000000 0.000000

23 C 0.000001 0.009024 -0.046094 0.000000 0.000000 0.000000

24 N 0.000000 -0.000020 0.005477 0.000000 0.000000 0.000000

25 Zn 0.000025 0.000411 0.000025 0.000051 0.000075 0.000075

26 C 0.000000 0.000000 0.000000 0.388481 0.386967 0.386967

27 H 0.000000 0.000000 0.000000 0.001240 -0.000100 -0.000100

28 C 0.000000 0.000000 0.000058 0.000000 0.000000 0.000000

29 H 0.000000 0.000000 0.000000 0.000000 0.000032 0.000032

30 C -0.004283 0.000000 0.000000 0.000000 0.000000 0.000000

31 H 0.426033 0.000058 0.000000 0.000000 0.000000 0.000000

32 C 0.000058 5.357168 -0.004283 0.000000 0.000000 0.000000

33 H 0.000000 -0.004283 0.426033 0.000000 0.000000 0.000000

34 H 0.000000 0.000000 0.000000 0.446962 -0.023873 -0.023873

35 H 0.000000 0.000000 0.000000 -0.023873 0.457354 -0.027507

36 H 0.000000 0.000000 0.000000 -0.023873 -0.027507 0.457354

37 H 0.000000 0.000000 0.000032 0.000000 0.000000 0.000000

38 H 0.000000 0.000000 0.000032 0.000000 0.000000 0.000000

39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

40 H -0.000100 0.000000 0.000000 0.000000 0.000000 0.000000

41 H -0.000100 0.000000 0.000000 0.000000 0.000000 0.000000

42 H 0.001240 0.000000 0.000000 0.000000 0.000000 0.000000

43 H 0.000032 0.386967 -0.000100 0.000000 0.000000 0.000000

44 H 0.000032 0.386967 -0.000100 0.000000 0.000000 0.000000

45 H 0.000000 0.388481 0.001240 0.000000 0.000000 0.000000

37 38 39 40 41 42

1 C 0.000000 0.000000 0.000000 -0.000045 -0.000045 0.000038

2 N 0.000000 0.000000 0.000000 0.000013 0.000013 0.000000

3 C 0.000000 0.000000 0.000001 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 C 0.000000 0.000000 0.000000 -0.000020 -0.000020 -0.000001

6 N 0.000007 0.000007 -0.000009 0.000000 0.000000 0.000000

7 C -0.000186 -0.000186 0.000203 0.000000 0.000000 0.000000

8 N 0.000409 0.000409 -0.000232 0.000000 0.000000 0.000000

9 C -0.005251 -0.005251 0.006189 0.000000 0.000000 0.000000

10 C -0.042909 -0.042909 -0.039530 0.000000 0.000000 0.000000

11 C -0.000326 -0.000326 -0.005559 0.000000 0.000000 0.000000

12 N 0.000000 0.000000 0.000000 0.003632 0.003632 0.000056

13 C 0.000000 0.000000 0.000000 -0.042909 -0.042909 -0.039530

14 C 0.000000 0.000000 0.000000 -0.000326 -0.000326 -0.005559

15 C 0.000000 0.000000 0.000000 -0.000186 -0.000186 0.000203

16 N 0.000000 0.000000 0.000000 0.000409 0.000409 -0.000232

17 C 0.000000 0.000000 0.000000 -0.005251 -0.005251 0.006189

18 N 0.000000 0.000000 0.000000 0.000007 0.000007 -0.000009

19 N 0.000013 0.000013 0.000000 0.000000 0.000000 0.000000

20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000001

21 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

22 C -0.000020 -0.000020 -0.000001 0.000000 0.000000 0.000000

23 C -0.000045 -0.000045 0.000038 0.000000 0.000000 0.000000

24 N 0.003632 0.003632 0.000056 0.000000 0.000000 0.000000

25 Zn 0.000075 0.000075 0.000051 0.000075 0.000075 0.000051

26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000 0.000032 0.000032 0.000000

28 C 0.386967 0.386967 0.388481 0.000000 0.000000 0.000000

29 H -0.000100 -0.000100 0.001240 0.000000 0.000000 0.000000

30 C 0.000000 0.000000 0.000000 0.386967 0.386967 0.388481

31 H 0.000000 0.000000 0.000000 -0.000100 -0.000100 0.001240

32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

33 H 0.000032 0.000032 0.000000 0.000000 0.000000 0.000000

34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 H 0.457354 -0.027507 -0.023873 0.000000 0.000000 0.000000

38 H -0.027507 0.457354 -0.023873 0.000000 0.000000 0.000000

39 H -0.023873 -0.023873 0.446962 0.000000 0.000000 0.000000

40 H 0.000000 0.000000 0.000000 0.457354 -0.027507 -0.023873

41 H 0.000000 0.000000 0.000000 -0.027507 0.457354 -0.023873

42 H 0.000000 0.000000 0.000000 -0.023873 -0.023873 0.446962

43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

43 44 45

1 C 0.000000 0.000000 0.000000

2 N 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000

5 C 0.000000 0.000000 0.000000

6 N 0.000000 0.000000 0.000000

7 C 0.000000 0.000000 0.000000

8 N 0.000000 0.000000 0.000000

9 C 0.000000 0.000000 0.000001

10 C 0.000000 0.000000 0.000000

11 C 0.000000 0.000000 0.000000

12 N 0.000000 0.000000 0.000000

13 C 0.000000 0.000000 0.000000

14 C -0.000020 -0.000020 -0.000001

15 C -0.000045 -0.000045 0.000038

16 N 0.000013 0.000013 0.000000

17 C 0.000000 0.000000 0.000000

18 N 0.003632 0.003632 0.000056

19 N 0.000409 0.000409 -0.000232

20 C -0.005251 -0.005251 0.006189

21 C -0.042909 -0.042909 -0.039530

22 C -0.000326 -0.000326 -0.005559

23 C -0.000186 -0.000186 0.000203

24 N 0.000007 0.000007 -0.000009

25 Zn 0.000075 0.000075 0.000051

26 C 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000

28 C 0.000000 0.000000 0.000000

29 H 0.000000 0.000000 0.000000

30 C 0.000000 0.000000 0.000000

31 H 0.000032 0.000032 0.000000

32 C 0.386967 0.386967 0.388481

33 H -0.000100 -0.000100 0.001240

34 H 0.000000 0.000000 0.000000

35 H 0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000

37 H 0.000000 0.000000 0.000000

38 H 0.000000 0.000000 0.000000

39 H 0.000000 0.000000 0.000000

40 H 0.000000 0.000000 0.000000

41 H 0.000000 0.000000 0.000000

42 H 0.000000 0.000000 0.000000

43 H 0.457354 -0.027507 -0.023873

44 H -0.027507 0.457354 -0.023873

45 H -0.023873 -0.023873 0.446962

Atomic-Atomic Spin Densities.

1 2 3 4 5 6

1 C 0.186572 0.004047 -0.012472 -0.008705 0.012937 0.000169

2 N 0.004047 -0.058325 -0.001696 -0.001549 0.000340 0.001073

3 C -0.012472 -0.001696 0.187465 0.021020 -0.005928 -0.000109

4 C -0.008705 -0.001549 0.021020 0.052292 -0.008087 -0.000676

5 C 0.012937 0.000340 -0.005928 -0.008087 -0.019601 -0.000079

6 N 0.000169 0.001073 -0.000109 -0.000676 -0.000079 -0.082611

7 C 0.000185 0.000026 -0.011385 -0.000417 0.000033 0.002345

8 N 0.000033 0.000221 -0.000327 -0.000014 0.000000 0.000690

9 C -0.000007 0.000021 0.000200 0.000002 0.000000 0.000077

10 C 0.000000 -0.000002 0.000058 0.000000 0.000000 0.000019

11 C 0.000001 -0.000003 -0.000286 0.000009 0.000000 0.000204

12 N 0.002345 0.000690 0.000077 0.000019 0.000204 0.000002

13 C -0.000417 -0.000014 0.000002 0.000000 0.000009 0.000000

14 C 0.000033 0.000000 0.000000 0.000000 0.000000 0.000000

15 C 0.000185 0.000033 -0.000007 0.000000 0.000001 0.000000

16 N 0.000026 0.000221 0.000021 -0.000002 -0.000003 0.000000

17 C -0.011385 -0.000327 0.000200 0.000058 -0.000286 0.000000

18 N 0.000000 -0.000001 0.000000 0.000000 0.000000 0.000000

19 N 0.000001 0.000013 -0.000001 0.000000 0.000000 -0.000001

20 C -0.000007 -0.000001 0.000002 0.000000 0.000000 0.000000

21 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

22 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

23 C 0.000002 0.000001 -0.000007 0.000000 0.000000 0.000000

24 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000002

25 Zn 0.000254 0.001164 -0.000481 -0.000055 0.000014 -0.000107

26 C 0.000003 0.000007 -0.001251 -0.003629 0.001244 0.000322

27 H 0.000042 -0.000020 -0.000085 0.000331 0.000337 -0.000002

28 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000001

29 H 0.000000 0.000001 -0.000005 0.000000 0.000000 0.000082

30 C 0.000035 0.000000 0.000000 0.000000 0.000001 0.000000

31 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

33 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

34 H 0.000011 0.000000 0.000033 -0.000175 0.000008 -0.000001

35 H 0.000026 0.000008 -0.000462 -0.001159 0.000076 0.000021

36 H 0.000026 0.000008 -0.000462 -0.001159 0.000076 0.000021

37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

40 H 0.000028 0.000000 0.000000 0.000000 0.000002 0.000000

41 H 0.000028 0.000000 0.000000 0.000000 0.000002 0.000000

42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 8 9 10 11 12

1 C 0.000185 0.000033 -0.000007 0.000000 0.000001 0.002345

2 N 0.000026 0.000221 0.000021 -0.000002 -0.000003 0.000690

3 C -0.011385 -0.000327 0.000200 0.000058 -0.000286 0.000077

4 C -0.000417 -0.000014 0.000002 0.000000 0.000009 0.000019

5 C 0.000033 0.000000 0.000000 0.000000 0.000000 0.000204

6 N 0.002345 0.000690 0.000077 0.000019 0.000204 0.000002

7 C 0.186572 0.004047 -0.012472 -0.008705 0.012937 0.000000

8 N 0.004047 -0.058325 -0.001696 -0.001549 0.000340 -0.000001

9 C -0.012472 -0.001696 0.187465 0.021020 -0.005928 0.000000

10 C -0.008705 -0.001549 0.021020 0.052292 -0.008087 0.000000

11 C 0.012937 0.000340 -0.005928 -0.008087 -0.019601 0.000000

12 N 0.000000 -0.000001 0.000000 0.000000 0.000000 -0.082611

13 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000676

14 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000079

15 C 0.000002 0.000001 -0.000007 0.000000 0.000000 0.000169

16 N 0.000001 0.000013 -0.000001 0.000000 0.000000 0.001073

17 C -0.000007 -0.000001 0.000002 0.000000 0.000000 -0.000109

18 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000002

19 N 0.000033 0.000221 -0.000327 -0.000014 0.000000 0.000000

20 C -0.000007 0.000021 0.000200 0.000002 0.000000 0.000000

21 C 0.000000 -0.000002 0.000058 0.000000 0.000000 0.000000

22 C 0.000001 -0.000003 -0.000286 0.000009 0.000000 0.000000

23 C 0.000185 0.000026 -0.011385 -0.000417 0.000033 0.000000

24 N 0.000169 0.001073 -0.000109 -0.000676 -0.000079 0.000000

25 Zn 0.000254 0.001164 -0.000481 -0.000055 0.000014 -0.000107

26 C 0.000035 0.000000 0.000000 0.000000 0.000001 0.000001

27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000082

28 C 0.000003 0.000007 -0.001251 -0.003629 0.001244 0.000000

29 H 0.000042 -0.000020 -0.000085 0.000331 0.000337 0.000000

30 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000322

31 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

33 H 0.000000 0.000001 -0.000005 0.000000 0.000000 0.000000

34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 H 0.000028 0.000000 0.000000 0.000000 0.000002 0.000000

36 H 0.000028 0.000000 0.000000 0.000000 0.000002 0.000000

37 H 0.000026 0.000008 -0.000462 -0.001159 0.000076 0.000000

38 H 0.000026 0.000008 -0.000462 -0.001159 0.000076 0.000000

39 H 0.000011 0.000000 0.000033 -0.000175 0.000008 0.000000

40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000021

41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000021

42 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000001

43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

13 14 15 16 17 18

1 C -0.000417 0.000033 0.000185 0.000026 -0.011385 0.000000

2 N -0.000014 0.000000 0.000033 0.000221 -0.000327 -0.000001

3 C 0.000002 0.000000 -0.000007 0.000021 0.000200 0.000000

4 C 0.000000 0.000000 0.000000 -0.000002 0.000058 0.000000

5 C 0.000009 0.000000 0.000001 -0.000003 -0.000286 0.000000

6 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 C 0.000000 0.000000 0.000002 0.000001 -0.000007 0.000000

8 N 0.000000 0.000000 0.000001 0.000013 -0.000001 0.000000

9 C 0.000000 0.000000 -0.000007 -0.000001 0.000002 0.000000

10 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

11 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

12 N -0.000676 -0.000079 0.000169 0.001073 -0.000109 0.000002

13 C 0.052292 -0.008087 -0.008705 -0.001549 0.021020 0.000019

14 C -0.008087 -0.019601 0.012937 0.000340 -0.005928 0.000204

15 C -0.008705 0.012937 0.186572 0.004047 -0.012472 0.002345

16 N -0.001549 0.000340 0.004047 -0.058325 -0.001696 0.000690

17 C 0.021020 -0.005928 -0.012472 -0.001696 0.187465 0.000077

18 N 0.000019 0.000204 0.002345 0.000690 0.000077 -0.082611

19 N -0.000002 -0.000003 0.000026 0.000221 0.000021 0.001073

20 C 0.000058 -0.000286 -0.011385 -0.000327 0.000200 -0.000109

21 C 0.000000 0.000009 -0.000417 -0.000014 0.000002 -0.000676

22 C 0.000000 0.000000 0.000033 0.000000 0.000000 -0.000079

23 C 0.000000 0.000001 0.000185 0.000033 -0.000007 0.000169

24 N 0.000000 0.000000 0.000000 -0.000001 0.000000 0.000002

25 Zn -0.000055 0.000014 0.000254 0.001164 -0.000481 -0.000107

26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000 0.000001 -0.000005 0.000000

28 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

29 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

30 C -0.003629 0.001244 0.000003 0.000007 -0.001251 0.000001

31 H 0.000331 0.000337 0.000042 -0.000020 -0.000085 0.000082

32 C 0.000000 0.000001 0.000035 0.000000 0.000000 0.000322

33 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

40 H -0.001159 0.000076 0.000026 0.000008 -0.000462 0.000000

41 H -0.001159 0.000076 0.000026 0.000008 -0.000462 0.000000

42 H -0.000175 0.000008 0.000011 0.000000 0.000033 0.000000

43 H 0.000000 0.000002 0.000028 0.000000 0.000000 0.000021

44 H 0.000000 0.000002 0.000028 0.000000 0.000000 0.000021

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000001

19 20 21 22 23 24

1 C 0.000001 -0.000007 0.000000 0.000000 0.000002 0.000000

2 N 0.000013 -0.000001 0.000000 0.000000 0.000001 0.000000

3 C -0.000001 0.000002 0.000000 0.000000 -0.000007 0.000000

4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

6 N -0.000001 0.000000 0.000000 0.000000 0.000000 0.000002

7 C 0.000033 -0.000007 0.000000 0.000001 0.000185 0.000169

8 N 0.000221 0.000021 -0.000002 -0.000003 0.000026 0.001073

9 C -0.000327 0.000200 0.000058 -0.000286 -0.011385 -0.000109

10 C -0.000014 0.000002 0.000000 0.000009 -0.000417 -0.000676

11 C 0.000000 0.000000 0.000000 0.000000 0.000033 -0.000079

12 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

13 C -0.000002 0.000058 0.000000 0.000000 0.000000 0.000000

14 C -0.000003 -0.000286 0.000009 0.000000 0.000001 0.000000

15 C 0.000026 -0.011385 -0.000417 0.000033 0.000185 0.000000

16 N 0.000221 -0.000327 -0.000014 0.000000 0.000033 -0.000001

17 C 0.000021 0.000200 0.000002 0.000000 -0.000007 0.000000

18 N 0.001073 -0.000109 -0.000676 -0.000079 0.000169 0.000002

19 N -0.058325 -0.001696 -0.001549 0.000340 0.004047 0.000690

20 C -0.001696 0.187465 0.021020 -0.005928 -0.012472 0.000077

21 C -0.001549 0.021020 0.052292 -0.008087 -0.008705 0.000019

22 C 0.000340 -0.005928 -0.008087 -0.019601 0.012937 0.000204

23 C 0.004047 -0.012472 -0.008705 0.012937 0.186572 0.002345

24 N 0.000690 0.000077 0.000019 0.000204 0.002345 -0.082611

25 Zn 0.001164 -0.000481 -0.000055 0.000014 0.000254 -0.000107

26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

28 C 0.000000 0.000000 0.000000 0.000001 0.000035 0.000322

29 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

30 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

31 H 0.000001 -0.000005 0.000000 0.000000 0.000000 0.000000

32 C 0.000007 -0.001251 -0.003629 0.001244 0.000003 0.000001

33 H -0.000020 -0.000085 0.000331 0.000337 0.000042 0.000082

34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 H 0.000000 0.000000 0.000000 0.000002 0.000028 0.000021

38 H 0.000000 0.000000 0.000000 0.000002 0.000028 0.000021

39 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000001

40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

43 H 0.000008 -0.000462 -0.001159 0.000076 0.000026 0.000000

44 H 0.000008 -0.000462 -0.001159 0.000076 0.000026 0.000000

45 H 0.000000 0.000033 -0.000175 0.000008 0.000011 0.000000

25 26 27 28 29 30

1 C 0.000254 0.000003 0.000042 0.000000 0.000000 0.000035

2 N 0.001164 0.000007 -0.000020 0.000000 0.000001 0.000000

3 C -0.000481 -0.001251 -0.000085 0.000000 -0.000005 0.000000

4 C -0.000055 -0.003629 0.000331 0.000000 0.000000 0.000000

5 C 0.000014 0.001244 0.000337 0.000000 0.000000 0.000001

6 N -0.000107 0.000322 -0.000002 0.000001 0.000082 0.000000

7 C 0.000254 0.000035 0.000000 0.000003 0.000042 0.000000

8 N 0.001164 0.000000 0.000000 0.000007 -0.000020 0.000000

9 C -0.000481 0.000000 0.000000 -0.001251 -0.000085 0.000000

10 C -0.000055 0.000000 0.000000 -0.003629 0.000331 0.000000

11 C 0.000014 0.000001 0.000000 0.001244 0.000337 0.000000

12 N -0.000107 0.000001 0.000082 0.000000 0.000000 0.000322

13 C -0.000055 0.000000 0.000000 0.000000 0.000000 -0.003629

14 C 0.000014 0.000000 0.000000 0.000000 0.000000 0.001244

15 C 0.000254 0.000000 0.000000 0.000000 0.000000 0.000003

16 N 0.001164 0.000000 0.000001 0.000000 0.000000 0.000007

17 C -0.000481 0.000000 -0.000005 0.000000 0.000000 -0.001251

18 N -0.000107 0.000000 0.000000 0.000000 0.000000 0.000001

19 N 0.001164 0.000000 0.000000 0.000000 0.000000 0.000000

20 C -0.000481 0.000000 0.000000 0.000000 0.000000 0.000000

21 C -0.000055 0.000000 0.000000 0.000000 0.000000 0.000000

22 C 0.000014 0.000000 0.000000 0.000001 0.000000 0.000000

23 C 0.000254 0.000000 0.000000 0.000035 0.000000 0.000000

24 N -0.000107 0.000000 0.000000 0.000322 -0.000002 0.000000

25 Zn -0.000493 0.000000 0.000000 0.000000 0.000000 0.000000

26 C 0.000000 -0.002651 0.000125 0.000000 0.000000 0.000000

27 H 0.000000 0.000125 -0.000588 0.000000 0.000000 0.000000

28 C 0.000000 0.000000 0.000000 -0.002651 0.000125 0.000000

29 H 0.000000 0.000000 0.000000 0.000125 -0.000588 0.000000

30 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.002651

31 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000125

32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

33 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

34 H 0.000002 0.000265 -0.000037 0.000000 0.000000 0.000000

35 H 0.000000 0.001674 0.000001 0.000000 0.000000 0.000000

36 H 0.000000 0.001674 0.000001 0.000000 0.000000 0.000000

37 H 0.000000 0.000000 0.000000 0.001674 0.000001 0.000000

38 H 0.000000 0.000000 0.000000 0.001674 0.000001 0.000000

39 H 0.000002 0.000000 0.000000 0.000265 -0.000037 0.000000

40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.001674

41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.001674

42 H 0.000002 0.000000 0.000000 0.000000 0.000000 0.000265

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 0.000002 0.000000 0.000000 0.000000 0.000000 0.000000

31 32 33 34 35 36

1 C 0.000000 0.000000 0.000000 0.000011 0.000026 0.000026

2 N 0.000000 0.000000 0.000000 0.000000 0.000008 0.000008

3 C 0.000000 0.000000 0.000000 0.000033 -0.000462 -0.000462

4 C 0.000000 0.000000 0.000000 -0.000175 -0.001159 -0.001159

5 C 0.000000 0.000000 0.000000 0.000008 0.000076 0.000076

6 N 0.000000 0.000000 0.000000 -0.000001 0.000021 0.000021

7 C 0.000000 0.000000 0.000000 0.000000 0.000028 0.000028

8 N 0.000000 0.000000 0.000001 0.000000 0.000000 0.000000

9 C 0.000000 0.000000 -0.000005 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

11 C 0.000000 0.000000 0.000000 0.000000 0.000002 0.000002

12 N -0.000002 0.000000 0.000000 0.000000 0.000000 0.000000

13 C 0.000331 0.000000 0.000000 0.000000 0.000000 0.000000

14 C 0.000337 0.000001 0.000000 0.000000 0.000000 0.000000

15 C 0.000042 0.000035 0.000000 0.000000 0.000000 0.000000

16 N -0.000020 0.000000 0.000000 0.000000 0.000000 0.000000

17 C -0.000085 0.000000 0.000000 0.000000 0.000000 0.000000

18 N 0.000082 0.000322 -0.000002 0.000000 0.000000 0.000000

19 N 0.000001 0.000007 -0.000020 0.000000 0.000000 0.000000

20 C -0.000005 -0.001251 -0.000085 0.000000 0.000000 0.000000

21 C 0.000000 -0.003629 0.000331 0.000000 0.000000 0.000000

22 C 0.000000 0.001244 0.000337 0.000000 0.000000 0.000000

23 C 0.000000 0.000003 0.000042 0.000000 0.000000 0.000000

24 N 0.000000 0.000001 0.000082 0.000000 0.000000 0.000000

25 Zn 0.000000 0.000000 0.000000 0.000002 0.000000 0.000000

26 C 0.000000 0.000000 0.000000 0.000265 0.001674 0.001674

27 H 0.000000 0.000000 0.000000 -0.000037 0.000001 0.000001

28 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

29 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

30 C 0.000125 0.000000 0.000000 0.000000 0.000000 0.000000

31 H -0.000588 0.000000 0.000000 0.000000 0.000000 0.000000

32 C 0.000000 -0.002651 0.000125 0.000000 0.000000 0.000000

33 H 0.000000 0.000125 -0.000588 0.000000 0.000000 0.000000

34 H 0.000000 0.000000 0.000000 -0.000398 -0.000002 -0.000002

35 H 0.000000 0.000000 0.000000 -0.000002 0.003991 -0.000830

36 H 0.000000 0.000000 0.000000 -0.000002 -0.000830 0.003991

37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

40 H 0.000001 0.000000 0.000000 0.000000 0.000000 0.000000

41 H 0.000001 0.000000 0.000000 0.000000 0.000000 0.000000

42 H -0.000037 0.000000 0.000000 0.000000 0.000000 0.000000

43 H 0.000000 0.001674 0.000001 0.000000 0.000000 0.000000

44 H 0.000000 0.001674 0.000001 0.000000 0.000000 0.000000

45 H 0.000000 0.000265 -0.000037 0.000000 0.000000 0.000000

37 38 39 40 41 42

1 C 0.000000 0.000000 0.000000 0.000028 0.000028 0.000000

2 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 C 0.000000 0.000000 0.000000 0.000002 0.000002 0.000000

6 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

7 C 0.000026 0.000026 0.000011 0.000000 0.000000 0.000000

8 N 0.000008 0.000008 0.000000 0.000000 0.000000 0.000000

9 C -0.000462 -0.000462 0.000033 0.000000 0.000000 0.000000

10 C -0.001159 -0.001159 -0.000175 0.000000 0.000000 0.000000

11 C 0.000076 0.000076 0.000008 0.000000 0.000000 0.000000

12 N 0.000000 0.000000 0.000000 0.000021 0.000021 -0.000001

13 C 0.000000 0.000000 0.000000 -0.001159 -0.001159 -0.000175

14 C 0.000000 0.000000 0.000000 0.000076 0.000076 0.000008

15 C 0.000000 0.000000 0.000000 0.000026 0.000026 0.000011

16 N 0.000000 0.000000 0.000000 0.000008 0.000008 0.000000

17 C 0.000000 0.000000 0.000000 -0.000462 -0.000462 0.000033

18 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

19 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

21 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

22 C 0.000002 0.000002 0.000000 0.000000 0.000000 0.000000

23 C 0.000028 0.000028 0.000000 0.000000 0.000000 0.000000

24 N 0.000021 0.000021 -0.000001 0.000000 0.000000 0.000000

25 Zn 0.000000 0.000000 0.000002 0.000000 0.000000 0.000002

26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

28 C 0.001674 0.001674 0.000265 0.000000 0.000000 0.000000

29 H 0.000001 0.000001 -0.000037 0.000000 0.000000 0.000000

30 C 0.000000 0.000000 0.000000 0.001674 0.001674 0.000265

31 H 0.000000 0.000000 0.000000 0.000001 0.000001 -0.000037

32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

33 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 H 0.003991 -0.000830 -0.000002 0.000000 0.000000 0.000000

38 H -0.000830 0.003991 -0.000002 0.000000 0.000000 0.000000

39 H -0.000002 -0.000002 -0.000398 0.000000 0.000000 0.000000

40 H 0.000000 0.000000 0.000000 0.003991 -0.000830 -0.000002

41 H 0.000000 0.000000 0.000000 -0.000830 0.003991 -0.000002

42 H 0.000000 0.000000 0.000000 -0.000002 -0.000002 -0.000398

43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

43 44 45

1 C 0.000000 0.000000 0.000000

2 N 0.000000 0.000000 0.000000

3 C 0.000000 0.000000 0.000000

4 C 0.000000 0.000000 0.000000

5 C 0.000000 0.000000 0.000000

6 N 0.000000 0.000000 0.000000

7 C 0.000000 0.000000 0.000000

8 N 0.000000 0.000000 0.000000

9 C 0.000000 0.000000 0.000000

10 C 0.000000 0.000000 0.000000

11 C 0.000000 0.000000 0.000000

12 N 0.000000 0.000000 0.000000

13 C 0.000000 0.000000 0.000000

14 C 0.000002 0.000002 0.000000

15 C 0.000028 0.000028 0.000000

16 N 0.000000 0.000000 0.000000

17 C 0.000000 0.000000 0.000000

18 N 0.000021 0.000021 -0.000001

19 N 0.000008 0.000008 0.000000

20 C -0.000462 -0.000462 0.000033

21 C -0.001159 -0.001159 -0.000175

22 C 0.000076 0.000076 0.000008

23 C 0.000026 0.000026 0.000011

24 N 0.000000 0.000000 0.000000

25 Zn 0.000000 0.000000 0.000002

26 C 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000000

28 C 0.000000 0.000000 0.000000

29 H 0.000000 0.000000 0.000000

30 C 0.000000 0.000000 0.000000

31 H 0.000000 0.000000 0.000000

32 C 0.001674 0.001674 0.000265

33 H 0.000001 0.000001 -0.000037

34 H 0.000000 0.000000 0.000000

35 H 0.000000 0.000000 0.000000

36 H 0.000000 0.000000 0.000000

37 H 0.000000 0.000000 0.000000

38 H 0.000000 0.000000 0.000000

39 H 0.000000 0.000000 0.000000

40 H 0.000000 0.000000 0.000000

41 H 0.000000 0.000000 0.000000

42 H 0.000000 0.000000 0.000000

43 H 0.003991 -0.000830 -0.000002

44 H -0.000830 0.003991 -0.000002

45 H -0.000002 -0.000002 -0.000398

Mulliken charges and spin densities:

1 2

1 C 0.433843 0.173993

2 N -0.677583 -0.054062

3 C 0.439856 0.174112

4 C 0.029623 0.048102

5 C -0.262311 -0.018704

6 N -0.405360 -0.078558

7 C 0.433843 0.173993

8 N -0.677583 -0.054062

9 C 0.439856 0.174112

10 C 0.029623 0.048102

11 C -0.262311 -0.018704

12 N -0.405360 -0.078558

13 C 0.029623 0.048102

14 C -0.262311 -0.018704

15 C 0.433843 0.173993

16 N -0.677583 -0.054062

17 C 0.439856 0.174112

18 N -0.405360 -0.078558

19 N -0.677583 -0.054062

20 C 0.439856 0.174112

21 C 0.029623 0.048102

22 C -0.262311 -0.018704

23 C 0.433843 0.173993

24 N -0.405360 -0.078558

25 Zn 1.546788 0.002669

26 C -0.696424 -0.002180

27 H 0.248348 0.000182

28 C -0.696424 -0.002180

29 H 0.248348 0.000182

30 C -0.696424 -0.002180

31 H 0.248348 0.000182

32 C -0.696424 -0.002180

33 H 0.248348 0.000182

34 H 0.249855 -0.000296

35 H 0.251728 0.003372

36 H 0.251728 0.003372

37 H 0.251728 0.003372

38 H 0.251728 0.003372

39 H 0.249855 -0.000296

40 H 0.251728 0.003372

41 H 0.251728 0.003372

42 H 0.249855 -0.000296

43 H 0.251728 0.003372

44 H 0.251728 0.003372

45 H 0.249855 -0.000296

Sum of Mulliken charges = 1.00000 1.00000

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

1 2

1 C 0.433843 0.173993

2 N -0.677583 -0.054062

3 C 0.439856 0.174112

4 C 0.029623 0.048102

5 C -0.013963 -0.018522

6 N -0.405360 -0.078558

7 C 0.433843 0.173993

8 N -0.677583 -0.054062

9 C 0.439856 0.174112

10 C 0.029623 0.048102

11 C -0.013963 -0.018522

12 N -0.405360 -0.078558

13 C 0.029623 0.048102

14 C -0.013963 -0.018522

15 C 0.433843 0.173993

16 N -0.677583 -0.054062

17 C 0.439856 0.174112

18 N -0.405360 -0.078558

19 N -0.677583 -0.054062

20 C 0.439856 0.174112

21 C 0.029623 0.048102

22 C -0.013963 -0.018522

23 C 0.433843 0.173993

24 N -0.405360 -0.078558

25 Zn 1.546788 0.002669

26 C 0.056888 0.004269

28 C 0.056888 0.004269

30 C 0.056888 0.004269

32 C 0.056888 0.004269

Electronic spatial extent (au): <R\*\*2>= 11120.7464

Charge= 1.0000 electrons

Dipole moment (field-independent basis, Debye):

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

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

XX= -120.7059 YY= -120.7059 ZZ= -167.3012

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XX= 15.5318 YY= 15.5318 ZZ= -31.0636

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

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

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

YYZ= 0.0000 XYZ= 0.0000

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

XXXX= -6205.4855 YYYY= -6205.4855 ZZZZ= -197.4556 XXXY= -311.7629

XXXZ= 0.0000 YYYX= 311.7629 YYYZ= 0.0000 ZZZX= 0.0000

ZZZY= 0.0000 XXYY= -2259.0663 XXZZ= -1318.2789 YYZZ= -1318.2789

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 2.766571019833D+03 E-N=-8.556975833456D+03 KE= 1.320598028643D+03

Symmetry AG KE= 6.514027370571D+02

Symmetry BG KE= 6.561836078981D+01

Symmetry AU KE= 2.129681930232D+01

Symmetry BU KE= 5.822801114940D+02

Isotropic Fermi Contact Couplings

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

1 C(13) 0.01423 15.99742 5.70828 5.33616

2 N(14) -0.00856 -2.76423 -0.98635 -0.92205

3 C(13) 0.01289 14.48747 5.16949 4.83250

4 C(13) -0.00061 -0.69099 -0.24656 -0.23049

5 C(13) -0.00590 -6.63232 -2.36658 -2.21230

6 N(14) -0.01198 -3.86977 -1.38083 -1.29082

7 C(13) 0.01423 15.99742 5.70828 5.33616

8 N(14) -0.00856 -2.76423 -0.98635 -0.92205

9 C(13) 0.01289 14.48747 5.16949 4.83250

10 C(13) -0.00061 -0.69099 -0.24656 -0.23049

11 C(13) -0.00590 -6.63232 -2.36658 -2.21230

12 N(14) -0.01198 -3.86977 -1.38083 -1.29082

13 C(13) -0.00061 -0.69099 -0.24656 -0.23049

14 C(13) -0.00590 -6.63232 -2.36658 -2.21230

15 C(13) 0.01423 15.99742 5.70828 5.33616

16 N(14) -0.00856 -2.76423 -0.98635 -0.92205

17 C(13) 0.01289 14.48747 5.16949 4.83250

18 N(14) -0.01198 -3.86977 -1.38083 -1.29082

19 N(14) -0.00856 -2.76423 -0.98635 -0.92205

20 C(13) 0.01289 14.48747 5.16949 4.83250

21 C(13) -0.00061 -0.69099 -0.24656 -0.23049

22 C(13) -0.00590 -6.63232 -2.36658 -2.21230

23 C(13) 0.01423 15.99742 5.70828 5.33616

24 N(14) -0.01198 -3.86977 -1.38083 -1.29082

25 Zn(67) 0.00000 0.00000 0.00000 0.00000

26 C(13) -0.00201 -2.26473 -0.80811 -0.75543

27 H(1) -0.00005 -0.22891 -0.08168 -0.07636

28 C(13) -0.00201 -2.26473 -0.80811 -0.75543

29 H(1) -0.00005 -0.22891 -0.08168 -0.07636

30 C(13) -0.00201 -2.26473 -0.80811 -0.75543

31 H(1) -0.00005 -0.22891 -0.08168 -0.07636

32 C(13) -0.00201 -2.26473 -0.80811 -0.75543

33 H(1) -0.00005 -0.22891 -0.08168 -0.07636

34 H(1) -0.00010 -0.44657 -0.15935 -0.14896

35 H(1) 0.00213 9.53262 3.40148 3.17974

36 H(1) 0.00213 9.53262 3.40148 3.17974

37 H(1) 0.00213 9.53262 3.40148 3.17974

38 H(1) 0.00213 9.53262 3.40148 3.17974

39 H(1) -0.00010 -0.44657 -0.15935 -0.14896

40 H(1) 0.00213 9.53262 3.40148 3.17974

41 H(1) 0.00213 9.53262 3.40148 3.17974

42 H(1) -0.00010 -0.44657 -0.15935 -0.14896

43 H(1) 0.00213 9.53262 3.40148 3.17974

44 H(1) 0.00213 9.53262 3.40148 3.17974

45 H(1) -0.00010 -0.44657 -0.15935 -0.14896

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

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

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

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

1 Atom -0.104371 -0.109217 0.213589

2 Atom 0.044839 0.046658 -0.091497

3 Atom -0.107200 -0.108935 0.216135

4 Atom -0.029822 -0.035403 0.065224

5 Atom 0.003736 0.005238 -0.008974

6 Atom 0.064339 0.075328 -0.139666

7 Atom -0.109217 -0.104371 0.213589

8 Atom 0.046658 0.044839 -0.091497

9 Atom -0.108935 -0.107200 0.216135

10 Atom -0.035403 -0.029822 0.065224

11 Atom 0.005238 0.003736 -0.008974

12 Atom 0.075328 0.064339 -0.139666

13 Atom -0.035403 -0.029822 0.065224

14 Atom 0.005238 0.003736 -0.008974

15 Atom -0.109217 -0.104371 0.213589

16 Atom 0.046658 0.044839 -0.091497

17 Atom -0.108935 -0.107200 0.216135

18 Atom 0.064339 0.075328 -0.139666

19 Atom 0.044839 0.046658 -0.091497

20 Atom -0.107200 -0.108935 0.216135

21 Atom -0.029822 -0.035403 0.065224

22 Atom 0.003736 0.005238 -0.008974

23 Atom -0.104371 -0.109217 0.213589

24 Atom 0.075328 0.064339 -0.139666

25 Atom 0.003569 0.003569 -0.007137

26 Atom 0.000695 -0.004231 0.003536

27 Atom 0.001925 0.000030 -0.001955

28 Atom -0.004231 0.000695 0.003536

29 Atom 0.000030 0.001925 -0.001955

30 Atom -0.004231 0.000695 0.003536

31 Atom 0.000030 0.001925 -0.001955

32 Atom 0.000695 -0.004231 0.003536

33 Atom 0.001925 0.000030 -0.001955

34 Atom 0.001813 -0.000715 -0.001097

35 Atom 0.001952 -0.000839 -0.001113

36 Atom 0.001952 -0.000839 -0.001113

37 Atom -0.000839 0.001952 -0.001113

38 Atom -0.000839 0.001952 -0.001113

39 Atom -0.000715 0.001813 -0.001097

40 Atom -0.000839 0.001952 -0.001113

41 Atom -0.000839 0.001952 -0.001113

42 Atom -0.000715 0.001813 -0.001097

43 Atom 0.001952 -0.000839 -0.001113

44 Atom 0.001952 -0.000839 -0.001113

45 Atom 0.001813 -0.000715 -0.001097

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

XY XZ YZ

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

1 Atom -0.000174 0.000000 0.000000

2 Atom 0.001555 0.000000 0.000000

3 Atom -0.004051 0.000000 0.000000

4 Atom -0.000543 0.000000 0.000000

5 Atom -0.001395 0.000000 0.000000

6 Atom -0.005715 0.000000 0.000000

7 Atom 0.000174 0.000000 0.000000

8 Atom -0.001555 0.000000 0.000000

9 Atom 0.004051 0.000000 0.000000

10 Atom 0.000543 0.000000 0.000000

11 Atom 0.001395 0.000000 0.000000

12 Atom 0.005715 0.000000 0.000000

13 Atom 0.000543 0.000000 0.000000

14 Atom 0.001395 0.000000 0.000000

15 Atom 0.000174 0.000000 0.000000

16 Atom -0.001555 0.000000 0.000000

17 Atom 0.004051 0.000000 0.000000

18 Atom -0.005715 0.000000 0.000000

19 Atom 0.001555 0.000000 0.000000

20 Atom -0.004051 0.000000 0.000000

21 Atom -0.000543 0.000000 0.000000

22 Atom -0.001395 0.000000 0.000000

23 Atom -0.000174 0.000000 0.000000

24 Atom 0.005715 0.000000 0.000000

25 Atom 0.000000 0.000000 0.000000

26 Atom -0.000289 0.000000 0.000000

27 Atom -0.002116 0.000000 0.000000

28 Atom 0.000289 0.000000 0.000000

29 Atom 0.002116 0.000000 0.000000

30 Atom 0.000289 0.000000 0.000000

31 Atom 0.002116 0.000000 0.000000

32 Atom -0.000289 0.000000 0.000000

33 Atom -0.002116 0.000000 0.000000

34 Atom -0.000965 0.000000 0.000000

35 Atom 0.000827 -0.001044 -0.000875

36 Atom 0.000827 0.001044 0.000875

37 Atom -0.000827 0.000875 -0.001044

38 Atom -0.000827 -0.000875 0.001044

39 Atom 0.000965 0.000000 0.000000

40 Atom -0.000827 -0.000875 0.001044

41 Atom -0.000827 0.000875 -0.001044

42 Atom 0.000965 0.000000 0.000000

43 Atom 0.000827 0.001044 0.000875

44 Atom 0.000827 -0.001044 -0.000875

45 Atom -0.000965 0.000000 0.000000

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

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Anisotropic Spin Dipole Couplings in Principal Axis System

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

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

Baa -0.1092 -14.657 -5.230 -4.889 0.0359 0.9994 0.0000

1 C(13) Bbb -0.1044 -14.005 -4.997 -4.671 0.9994 -0.0359 0.0000

Bcc 0.2136 28.662 10.227 9.560 0.0000 0.0000 1.0000

Baa -0.0915 -3.529 -1.259 -1.177 0.0000 0.0000 1.0000

2 N(14) Bbb 0.0439 1.695 0.605 0.565 0.8675 -0.4975 0.0000

Bcc 0.0476 1.834 0.654 0.612 0.4975 0.8675 0.0000

Baa -0.1122 -15.058 -5.373 -5.023 0.6287 0.7776 0.0000

3 C(13) Bbb -0.1039 -13.946 -4.976 -4.652 0.7776 -0.6287 0.0000

Bcc 0.2161 29.003 10.349 9.674 0.0000 0.0000 1.0000

Baa -0.0355 -4.758 -1.698 -1.587 0.0960 0.9954 0.0000

4 C(13) Bbb -0.0298 -3.995 -1.425 -1.333 0.9954 -0.0960 0.0000

Bcc 0.0652 8.752 3.123 2.920 0.0000 0.0000 1.0000

Baa -0.0090 -1.204 -0.430 -0.402 0.0000 0.0000 1.0000

5 C(13) Bbb 0.0029 0.389 0.139 0.130 0.8584 0.5129 0.0000

Bcc 0.0061 0.815 0.291 0.272 -0.5129 0.8584 0.0000

Baa -0.1397 -5.387 -1.922 -1.797 0.0000 0.0000 1.0000

6 N(14) Bbb 0.0619 2.388 0.852 0.796 0.9201 0.3917 0.0000

Bcc 0.0778 2.999 1.070 1.000 -0.3917 0.9201 0.0000

Baa -0.1092 -14.657 -5.230 -4.889 0.9994 -0.0359 0.0000

7 C(13) Bbb -0.1044 -14.005 -4.997 -4.671 0.0359 0.9994 0.0000

Bcc 0.2136 28.662 10.227 9.560 0.0000 0.0000 1.0000

Baa -0.0915 -3.529 -1.259 -1.177 0.0000 0.0000 1.0000

8 N(14) Bbb 0.0439 1.695 0.605 0.565 0.4975 0.8675 0.0000

Bcc 0.0476 1.834 0.654 0.612 0.8675 -0.4975 0.0000

Baa -0.1122 -15.058 -5.373 -5.023 0.7776 -0.6287 0.0000

9 C(13) Bbb -0.1039 -13.946 -4.976 -4.652 0.6287 0.7776 0.0000

Bcc 0.2161 29.003 10.349 9.674 0.0000 0.0000 1.0000

Baa -0.0355 -4.758 -1.698 -1.587 0.9954 -0.0960 0.0000

10 C(13) Bbb -0.0298 -3.995 -1.425 -1.333 0.0960 0.9954 0.0000

Bcc 0.0652 8.752 3.123 2.920 0.0000 0.0000 1.0000

Baa -0.0090 -1.204 -0.430 -0.402 0.0000 0.0000 1.0000

11 C(13) Bbb 0.0029 0.389 0.139 0.130 -0.5129 0.8584 0.0000

Bcc 0.0061 0.815 0.291 0.272 0.8584 0.5129 0.0000

Baa -0.1397 -5.387 -1.922 -1.797 0.0000 0.0000 1.0000

12 N(14) Bbb 0.0619 2.388 0.852 0.796 -0.3917 0.9201 0.0000

Bcc 0.0778 2.999 1.070 1.000 0.9201 0.3917 0.0000

Baa -0.0355 -4.758 -1.698 -1.587 0.9954 -0.0960 0.0000

13 C(13) Bbb -0.0298 -3.995 -1.425 -1.333 0.0960 0.9954 0.0000

Bcc 0.0652 8.752 3.123 2.920 0.0000 0.0000 1.0000

Baa -0.0090 -1.204 -0.430 -0.402 0.0000 0.0000 1.0000

14 C(13) Bbb 0.0029 0.389 0.139 0.130 -0.5129 0.8584 0.0000

Bcc 0.0061 0.815 0.291 0.272 0.8584 0.5129 0.0000

Baa -0.1092 -14.657 -5.230 -4.889 0.9994 -0.0359 0.0000

15 C(13) Bbb -0.1044 -14.005 -4.997 -4.671 0.0359 0.9994 0.0000

Bcc 0.2136 28.662 10.227 9.560 0.0000 0.0000 1.0000

Baa -0.0915 -3.529 -1.259 -1.177 0.0000 0.0000 1.0000

16 N(14) Bbb 0.0439 1.695 0.605 0.565 0.4975 0.8675 0.0000

Bcc 0.0476 1.834 0.654 0.612 0.8675 -0.4975 0.0000

Baa -0.1122 -15.058 -5.373 -5.023 0.7776 -0.6287 0.0000

17 C(13) Bbb -0.1039 -13.946 -4.976 -4.652 0.6287 0.7776 0.0000

Bcc 0.2161 29.003 10.349 9.674 0.0000 0.0000 1.0000

Baa -0.1397 -5.387 -1.922 -1.797 0.0000 0.0000 1.0000

18 N(14) Bbb 0.0619 2.388 0.852 0.796 0.9201 0.3917 0.0000

Bcc 0.0778 2.999 1.070 1.000 -0.3917 0.9201 0.0000

Baa -0.0915 -3.529 -1.259 -1.177 0.0000 0.0000 1.0000

19 N(14) Bbb 0.0439 1.695 0.605 0.565 0.8675 -0.4975 0.0000

Bcc 0.0476 1.834 0.654 0.612 0.4975 0.8675 0.0000

Baa -0.1122 -15.058 -5.373 -5.023 0.6287 0.7776 0.0000

20 C(13) Bbb -0.1039 -13.946 -4.976 -4.652 0.7776 -0.6287 0.0000

Bcc 0.2161 29.003 10.349 9.674 0.0000 0.0000 1.0000

Baa -0.0355 -4.758 -1.698 -1.587 0.0960 0.9954 0.0000

21 C(13) Bbb -0.0298 -3.995 -1.425 -1.333 0.9954 -0.0960 0.0000

Bcc 0.0652 8.752 3.123 2.920 0.0000 0.0000 1.0000

Baa -0.0090 -1.204 -0.430 -0.402 0.0000 0.0000 1.0000

22 C(13) Bbb 0.0029 0.389 0.139 0.130 0.8584 0.5129 0.0000

Bcc 0.0061 0.815 0.291 0.272 -0.5129 0.8584 0.0000

Baa -0.1092 -14.657 -5.230 -4.889 0.0359 0.9994 0.0000

23 C(13) Bbb -0.1044 -14.005 -4.997 -4.671 0.9994 -0.0359 0.0000

Bcc 0.2136 28.662 10.227 9.560 0.0000 0.0000 1.0000

Baa -0.1397 -5.387 -1.922 -1.797 0.0000 0.0000 1.0000

24 N(14) Bbb 0.0619 2.388 0.852 0.796 -0.3917 0.9201 0.0000

Bcc 0.0778 2.999 1.070 1.000 0.9201 0.3917 0.0000

Baa -0.0071 -0.239 -0.085 -0.080 0.0000 0.0000 1.0000

25 Zn(67) Bbb 0.0036 0.119 0.043 0.040 1.0000 -0.0029 0.0000

Bcc 0.0036 0.119 0.043 0.040 0.0029 1.0000 0.0000

Baa -0.0042 -0.570 -0.203 -0.190 0.0584 0.9983 0.0000

26 C(13) Bbb 0.0007 0.096 0.034 0.032 0.9983 -0.0584 0.0000

Bcc 0.0035 0.474 0.169 0.158 0.0000 0.0000 1.0000

Baa -0.0020 -1.043 -0.372 -0.348 0.0000 0.0000 1.0000

27 H(1) Bbb -0.0013 -0.716 -0.255 -0.239 0.5438 0.8392 0.0000

Bcc 0.0033 1.759 0.627 0.587 0.8392 -0.5438 0.0000

Baa -0.0042 -0.570 -0.203 -0.190 0.9983 -0.0584 0.0000

28 C(13) Bbb 0.0007 0.096 0.034 0.032 0.0584 0.9983 0.0000

Bcc 0.0035 0.474 0.169 0.158 0.0000 0.0000 1.0000

Baa -0.0020 -1.043 -0.372 -0.348 0.0000 0.0000 1.0000

29 H(1) Bbb -0.0013 -0.716 -0.255 -0.239 0.8392 -0.5438 0.0000

Bcc 0.0033 1.759 0.627 0.587 0.5438 0.8392 0.0000

Baa -0.0042 -0.570 -0.203 -0.190 0.9983 -0.0584 0.0000

30 C(13) Bbb 0.0007 0.096 0.034 0.032 0.0584 0.9983 0.0000

Bcc 0.0035 0.474 0.169 0.158 0.0000 0.0000 1.0000

Baa -0.0020 -1.043 -0.372 -0.348 0.0000 0.0000 1.0000

31 H(1) Bbb -0.0013 -0.716 -0.255 -0.239 0.8392 -0.5438 0.0000

Bcc 0.0033 1.759 0.627 0.587 0.5438 0.8392 0.0000

Baa -0.0042 -0.570 -0.203 -0.190 0.0584 0.9983 0.0000

32 C(13) Bbb 0.0007 0.096 0.034 0.032 0.9983 -0.0584 0.0000

Bcc 0.0035 0.474 0.169 0.158 0.0000 0.0000 1.0000

Baa -0.0020 -1.043 -0.372 -0.348 0.0000 0.0000 1.0000

33 H(1) Bbb -0.0013 -0.716 -0.255 -0.239 0.5438 0.8392 0.0000

Bcc 0.0033 1.759 0.627 0.587 0.8392 -0.5438 0.0000

Baa -0.0011 -0.585 -0.209 -0.195 0.0000 0.0000 1.0000

34 H(1) Bbb -0.0010 -0.556 -0.198 -0.185 0.3202 0.9473 0.0000

Bcc 0.0021 1.141 0.407 0.381 0.9473 -0.3202 0.0000

Baa -0.0019 -1.005 -0.359 -0.335 0.0880 0.5976 0.7969

35 H(1) Bbb -0.0007 -0.383 -0.137 -0.128 -0.4304 0.7443 -0.5106

Bcc 0.0026 1.388 0.495 0.463 0.8984 0.2980 -0.3227

Baa -0.0019 -1.005 -0.359 -0.335 -0.0880 -0.5976 0.7969

36 H(1) Bbb -0.0007 -0.383 -0.137 -0.128 -0.4304 0.7443 0.5106

Bcc 0.0026 1.388 0.495 0.463 0.8984 0.2980 0.3227

Baa -0.0019 -1.005 -0.359 -0.335 -0.5976 0.0880 0.7969

37 H(1) Bbb -0.0007 -0.383 -0.137 -0.128 0.7443 0.4304 0.5106

Bcc 0.0026 1.388 0.495 0.463 -0.2980 0.8984 -0.3227

Baa -0.0019 -1.005 -0.359 -0.335 0.5976 -0.0880 0.7969

38 H(1) Bbb -0.0007 -0.383 -0.137 -0.128 0.7443 0.4304 -0.5106

Bcc 0.0026 1.388 0.495 0.463 -0.2980 0.8984 0.3227

Baa -0.0011 -0.585 -0.209 -0.195 0.0000 0.0000 1.0000

39 H(1) Bbb -0.0010 -0.556 -0.198 -0.185 0.9473 -0.3202 0.0000

Bcc 0.0021 1.141 0.407 0.381 0.3202 0.9473 0.0000

Baa -0.0019 -1.005 -0.359 -0.335 0.5976 -0.0880 0.7969

40 H(1) Bbb -0.0007 -0.383 -0.137 -0.128 0.7443 0.4304 -0.5106

Bcc 0.0026 1.388 0.495 0.463 -0.2980 0.8984 0.3227

Baa -0.0019 -1.005 -0.359 -0.335 -0.5976 0.0880 0.7969

41 H(1) Bbb -0.0007 -0.383 -0.137 -0.128 0.7443 0.4304 0.5106

Bcc 0.0026 1.388 0.495 0.463 -0.2980 0.8984 -0.3227

Baa -0.0011 -0.585 -0.209 -0.195 0.0000 0.0000 1.0000

42 H(1) Bbb -0.0010 -0.556 -0.198 -0.185 0.9473 -0.3202 0.0000

Bcc 0.0021 1.141 0.407 0.381 0.3202 0.9473 0.0000

Baa -0.0019 -1.005 -0.359 -0.335 -0.0880 -0.5976 0.7969

43 H(1) Bbb -0.0007 -0.383 -0.137 -0.128 -0.4304 0.7443 0.5106

Bcc 0.0026 1.388 0.495 0.463 0.8984 0.2980 0.3227

Baa -0.0019 -1.005 -0.359 -0.335 0.0880 0.5976 0.7969

44 H(1) Bbb -0.0007 -0.383 -0.137 -0.128 -0.4304 0.7443 -0.5106

Bcc 0.0026 1.388 0.495 0.463 0.8984 0.2980 -0.3227

Baa -0.0011 -0.585 -0.209 -0.195 0.0000 0.0000 1.0000

45 H(1) Bbb -0.0010 -0.556 -0.198 -0.185 0.3202 0.9473 0.0000

Bcc 0.0021 1.141 0.407 0.381 0.9473 -0.3202 0.0000

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

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Fri Jul 5 21:14:33 2019, MaxMem= 1342177280 cpu: 16.8

(Enter /apps/gaussian/g09d01/g09/l9999.exe)

1\1\GINC-K241\FOpt\UB3LYP\GenECP\C20H16N8Zn1(1+,2)\Z5105842\05-Jul-201

9\0\\#p opt b3lyp/genecp scrf=(solvent=dmso,smd) empiricaldispersion=g

d3bj\\ZntAzPcation\\1,2\C,-2.0664148636,-2.178692856,0.\N,-0.745078814

6,-1.8565515165,0.\C,-0.0051842407,-2.9884292162,0.\C,-0.9357731084,-4

.1619541754,0.\C,-2.1885905894,-3.644629236,0.\N,1.3252498579,-3.09846

33064,0.\C,2.178692856,-2.0664148636,0.\N,1.8565515165,-0.7450788146,0

.\C,2.9884292162,-0.0051842407,0.\C,4.1619541754,-0.9357731084,0.\C,3.

644629236,-2.1885905894,0.\N,-3.0984633064,-1.3252498579,0.\C,-4.16195

41754,0.9357731084,0.\C,-3.644629236,2.1885905894,0.\C,-2.178692856,2.

0664148636,0.\N,-1.8565515165,0.7450788146,0.\C,-2.9884292162,0.005184

2407,0.\N,-1.3252498579,3.0984633064,0.\N,0.7450788146,1.8565515165,0.

\C,0.0051842407,2.9884292162,0.\C,0.9357731084,4.1619541754,0.\C,2.188

5905894,3.644629236,0.\C,2.0664148636,2.178692856,0.\N,3.0984633064,1.

3252498579,0.\Zn,0.,0.,0.\C,-0.48019691,-5.5739233198,0.\H,-3.12823233

04,-4.1776035649,0.\C,5.5739233198,-0.48019691,0.\H,4.1776035649,-3.12

82323304,0.\C,-5.5739233198,0.48019691,0.\H,-4.1776035649,3.1282323304

,0.\C,0.48019691,5.5739233198,0.\H,3.1282323304,4.1776035649,0.\H,-1.3

244455274,-6.2639575518,0.\H,0.1413683654,-5.78080446,0.876886323\H,0.

1413683654,-5.78080446,-0.876886323\H,5.78080446,0.1413683654,0.876886

323\H,5.78080446,0.1413683654,-0.876886323\H,6.2639575518,-1.324445527

4,0.\H,-5.78080446,-0.1413683654,0.876886323\H,-5.78080446,-0.14136836

54,-0.876886323\H,-6.2639575518,1.3244455274,0.\H,-0.1413683654,5.7808

0446,0.876886323\H,-0.1413683654,5.78080446,-0.876886323\H,1.324445527

4,6.2639575518,0.\\Version=ES64L-G09RevD.01\State=2-AU\HF=-1275.699501

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e=0.,0.,0.\Quadrupole=11.5475089,11.5475089,-23.0950178,0.,0.,0.\PG=C0

4H [O(Zn1),SGH(C20H8N8),X(H8)]\\@

THE NUMBERS ARE MEANINGLESS, BUT THE TRENDS ARE IMPORTANT.

-- LARRY BURGGRAF

Job cpu time: 0 days 1 hours 27 minutes 43.7 seconds.

File lengths (MBytes): RWF= 700 Int= 0 D2E= 0 Chk= 35 Scr= 2

Normal termination of Gaussian 09 at Fri Jul 5 21:14:34 2019.