Entering Gaussian System, Link 0=g09

Input=ZnTSPsimanion.com

Output=ZnTSPsimanion.log

Initial command:

/home/kira/g09/l1.exe "/home/kira/g09/scratch/Gau-5515.inp" -scrdir="/home/kira/g09/scratch/"

Entering Link 1 = /home/kira/g09/l1.exe PID= 5522.

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Cite this work as:

Gaussian 09, Revision E.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-G09RevE.01 30-Nov-2015

30-Jul-2019

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

%nprocshared=16

Will use up to 16 processors via shared memory.

%mem=32GB

%chk=ZnTSPsimanion.chk

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

#p opt=calcall b3lyp/genecp scrf=(solvent=dmso,smd) empiricaldispersio

n=gd3bj

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

1/10=4,14=-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=2,72=21,74=-5,124=41,140=1/1,2,3;

4//1;

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

8/6=4,10=90,11=11/1;

11/6=1,8=1,9=11,15=111,16=1/1,2,10;

10/6=1/2;

6/7=2,8=2,9=2,10=2,18=1,28=1/1;

7/10=1,25=1/1,2,3,16;

1/10=4,14=-1,18=20,19=15,26=3/3(3);

2/9=110/2;

7/8=1,9=1,25=1,44=-1/16;

99//99;

2/9=110/2;

3/5=7,6=1,11=2,16=1,17=8,25=1,30=1,70=32205,71=2,72=21,74=-5,82=7,124=41,140=1/1,2,3;

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

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

8/6=4,10=90,11=11/1;

11/6=1,8=1,9=11,15=111,16=1/1,2,10;

10/6=1/2;

7/10=1,25=1/1,2,3,16;

1/10=4,14=-1,18=20,19=15,26=3/3(-8);

2/9=110/2;

6/7=2,8=2,9=2,10=2,18=1,19=2,28=1/1;

7/8=1,9=1,25=1,44=-1/16;

99//99;

Leave Link 1 at Tue Jul 30 19:37:54 2019, MaxMem= 4294967296 cpu: 0.9

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

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ZnTSPsimanion

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

Symbolic Z-matrix:

Charge = -1 Multiplicity = 2

C -4.28512 0.67918 -0.0289

C -2.89702 1.10836 -0.00931

N -2.0872 0. 0.00248

C -2.89702 -1.10836 -0.00931

C -4.28512 -0.67918 -0.0289

C -2.46729 -2.44445 -0.01134

C -1.10583 -2.90629 -0.01024

N 0. -2.09397 0.00694

C 1.10583 -2.90629 -0.01024

C 0.69172 -4.27095 -0.03823

C -0.69172 -4.27095 -0.03823

C -2.46729 2.44445 -0.01134

C -1.10583 2.90629 -0.01024

C -0.69172 4.27095 -0.03823

C 0.69172 4.27095 -0.03823

C 1.10583 2.90629 -0.01024

N 0. 2.09397 0.00694

C 2.46729 2.44445 -0.01134

C 2.89702 1.10836 -0.00931

C 4.28512 0.67918 -0.0289

C 4.28512 -0.67918 -0.0289

C 2.89702 -1.10836 -0.00931

N 2.0872 0. 0.00248

H -5.14186 1.33703 -0.0444

H -5.14186 -1.33703 -0.0444

H 1.34642 -5.13014 -0.05969

H -1.34642 -5.13014 -0.05969

H -1.34642 5.13014 -0.05969

H 1.34642 5.13014 -0.05969

H 5.14186 1.33703 -0.0444

H 5.14186 -1.33703 -0.0444

Zn 0. 0. 0.14529

C 2.46729 -2.44445 -0.01134

C 3.47489 -3.45093 -0.02511

C -3.47489 3.45093 -0.02511

C 4.31487 -4.31951 -0.03829

C -4.31487 4.31951 -0.03829

C -3.47489 -3.45093 -0.02511

C -4.31487 -4.31951 -0.03829

C 3.47489 3.45093 -0.02511

C 4.31487 4.31951 -0.03829

H 5.06065 5.08224 -0.0501

H 5.06065 -5.08224 -0.0501

H -5.06065 -5.08224 -0.0501

H -5.06065 5.08224 -0.0501

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

NMic= 0 NMicF= 0.

Isotopes and Nuclear Properties:

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

in nuclear magnetons)

Atom 1 2 3 4 5 6 7 8 9 10

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

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

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

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

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

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

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

Atom 11 12 13 14 15 16 17 18 19 20

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

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

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

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

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

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

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

Atom 21 22 23 24 25 26 27 28 29 30

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

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

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

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

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

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

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

Atom 31 32 33 34 35 36 37 38 39 40

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

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

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

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

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

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

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

Atom 41 42 43 44 45

IAtWgt= 12 1 1 1 1

AtmWgt= 12.0000000 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 0 1 1 1 1

AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 0.0000000 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 6.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Leave Link 101 at Tue Jul 30 19:37:54 2019, MaxMem= 4294967296 cpu: 7.1

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Initialization pass.

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

! Initial Parameters !

! (Angstroms and Degrees) !

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

! Name Definition Value Derivative Info. !

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

! R1 R(1,2) 1.4531 calculate D2E/DX2 analytically !

! R2 R(1,5) 1.3584 calculate D2E/DX2 analytically !

! R3 R(1,24) 1.0803 calculate D2E/DX2 analytically !

! R4 R(2,3) 1.3727 calculate D2E/DX2 analytically !

! R5 R(2,12) 1.4035 calculate D2E/DX2 analytically !

! R6 R(3,4) 1.3727 calculate D2E/DX2 analytically !

! R7 R(3,32) 2.0921 calculate D2E/DX2 analytically !

! R8 R(4,5) 1.4531 calculate D2E/DX2 analytically !

! R9 R(4,6) 1.4035 calculate D2E/DX2 analytically !

! R10 R(5,25) 1.0803 calculate D2E/DX2 analytically !

! R11 R(6,7) 1.4377 calculate D2E/DX2 analytically !

! R12 R(6,38) 1.4242 calculate D2E/DX2 analytically !

! R13 R(7,8) 1.3722 calculate D2E/DX2 analytically !

! R14 R(7,11) 1.4264 calculate D2E/DX2 analytically !

! R15 R(8,9) 1.3722 calculate D2E/DX2 analytically !

! R16 R(8,32) 2.0985 calculate D2E/DX2 analytically !

! R17 R(9,10) 1.4264 calculate D2E/DX2 analytically !

! R18 R(9,33) 1.4377 calculate D2E/DX2 analytically !

! R19 R(10,11) 1.3834 calculate D2E/DX2 analytically !

! R20 R(10,26) 1.0804 calculate D2E/DX2 analytically !

! R21 R(11,27) 1.0804 calculate D2E/DX2 analytically !

! R22 R(12,13) 1.4377 calculate D2E/DX2 analytically !

! R23 R(12,35) 1.4242 calculate D2E/DX2 analytically !

! R24 R(13,14) 1.4264 calculate D2E/DX2 analytically !

! R25 R(13,17) 1.3722 calculate D2E/DX2 analytically !

! R26 R(14,15) 1.3834 calculate D2E/DX2 analytically !

! R27 R(14,28) 1.0804 calculate D2E/DX2 analytically !

! R28 R(15,16) 1.4264 calculate D2E/DX2 analytically !

! R29 R(15,29) 1.0804 calculate D2E/DX2 analytically !

! R30 R(16,17) 1.3722 calculate D2E/DX2 analytically !

! R31 R(16,18) 1.4377 calculate D2E/DX2 analytically !

! R32 R(17,32) 2.0985 calculate D2E/DX2 analytically !

! R33 R(18,19) 1.4035 calculate D2E/DX2 analytically !

! R34 R(18,40) 1.4242 calculate D2E/DX2 analytically !

! R35 R(19,20) 1.4531 calculate D2E/DX2 analytically !

! R36 R(19,23) 1.3727 calculate D2E/DX2 analytically !

! R37 R(20,21) 1.3584 calculate D2E/DX2 analytically !

! R38 R(20,30) 1.0803 calculate D2E/DX2 analytically !

! R39 R(21,22) 1.4531 calculate D2E/DX2 analytically !

! R40 R(21,31) 1.0803 calculate D2E/DX2 analytically !

! R41 R(22,23) 1.3727 calculate D2E/DX2 analytically !

! R42 R(22,33) 1.4035 calculate D2E/DX2 analytically !

! R43 R(23,32) 2.0921 calculate D2E/DX2 analytically !

! R44 R(33,34) 1.4242 calculate D2E/DX2 analytically !

! R45 R(34,36) 1.2084 calculate D2E/DX2 analytically !

! R46 R(35,37) 1.2084 calculate D2E/DX2 analytically !

! R47 R(36,43) 1.0668 calculate D2E/DX2 analytically !

! R48 R(37,45) 1.0668 calculate D2E/DX2 analytically !

! R49 R(38,39) 1.2084 calculate D2E/DX2 analytically !

! R50 R(39,44) 1.0668 calculate D2E/DX2 analytically !

! R51 R(40,41) 1.2084 calculate D2E/DX2 analytically !

! R52 R(41,42) 1.0668 calculate D2E/DX2 analytically !

! A1 A(2,1,5) 107.1794 calculate D2E/DX2 analytically !

! A2 A(2,1,24) 125.3057 calculate D2E/DX2 analytically !

! A3 A(5,1,24) 127.5145 calculate D2E/DX2 analytically !

! A4 A(1,2,3) 108.9772 calculate D2E/DX2 analytically !

! A5 A(1,2,12) 125.0057 calculate D2E/DX2 analytically !

! A6 A(3,2,12) 126.0158 calculate D2E/DX2 analytically !

! A7 A(2,3,4) 107.6867 calculate D2E/DX2 analytically !

! A8 A(2,3,32) 126.0961 calculate D2E/DX2 analytically !

! A9 A(4,3,32) 126.0961 calculate D2E/DX2 analytically !

! A10 A(3,4,5) 108.9772 calculate D2E/DX2 analytically !

! A11 A(3,4,6) 126.0158 calculate D2E/DX2 analytically !

! A12 A(5,4,6) 125.0057 calculate D2E/DX2 analytically !

! A13 A(1,5,4) 107.1794 calculate D2E/DX2 analytically !

! A14 A(1,5,25) 127.5145 calculate D2E/DX2 analytically !

! A15 A(4,5,25) 125.3057 calculate D2E/DX2 analytically !

! A16 A(4,6,7) 126.5677 calculate D2E/DX2 analytically !

! A17 A(4,6,38) 117.1377 calculate D2E/DX2 analytically !

! A18 A(7,6,38) 116.2931 calculate D2E/DX2 analytically !

! A19 A(6,7,8) 124.9591 calculate D2E/DX2 analytically !

! A20 A(6,7,11) 125.6095 calculate D2E/DX2 analytically !

! A21 A(8,7,11) 109.4293 calculate D2E/DX2 analytically !

! A22 A(7,8,9) 107.3872 calculate D2E/DX2 analytically !

! A23 A(7,8,32) 126.2641 calculate D2E/DX2 analytically !

! A24 A(9,8,32) 126.2641 calculate D2E/DX2 analytically !

! A25 A(8,9,10) 109.4293 calculate D2E/DX2 analytically !

! A26 A(8,9,33) 124.9591 calculate D2E/DX2 analytically !

! A27 A(10,9,33) 125.6095 calculate D2E/DX2 analytically !

! A28 A(9,10,11) 106.877 calculate D2E/DX2 analytically !

! A29 A(9,10,26) 125.824 calculate D2E/DX2 analytically !

! A30 A(11,10,26) 127.2984 calculate D2E/DX2 analytically !

! A31 A(7,11,10) 106.877 calculate D2E/DX2 analytically !

! A32 A(7,11,27) 125.824 calculate D2E/DX2 analytically !

! A33 A(10,11,27) 127.2984 calculate D2E/DX2 analytically !

! A34 A(2,12,13) 126.5677 calculate D2E/DX2 analytically !

! A35 A(2,12,35) 117.1377 calculate D2E/DX2 analytically !

! A36 A(13,12,35) 116.2931 calculate D2E/DX2 analytically !

! A37 A(12,13,14) 125.6095 calculate D2E/DX2 analytically !

! A38 A(12,13,17) 124.9591 calculate D2E/DX2 analytically !

! A39 A(14,13,17) 109.4293 calculate D2E/DX2 analytically !

! A40 A(13,14,15) 106.877 calculate D2E/DX2 analytically !

! A41 A(13,14,28) 125.824 calculate D2E/DX2 analytically !

! A42 A(15,14,28) 127.2984 calculate D2E/DX2 analytically !

! A43 A(14,15,16) 106.877 calculate D2E/DX2 analytically !

! A44 A(14,15,29) 127.2984 calculate D2E/DX2 analytically !

! A45 A(16,15,29) 125.824 calculate D2E/DX2 analytically !

! A46 A(15,16,17) 109.4293 calculate D2E/DX2 analytically !

! A47 A(15,16,18) 125.6095 calculate D2E/DX2 analytically !

! A48 A(17,16,18) 124.9591 calculate D2E/DX2 analytically !

! A49 A(13,17,16) 107.3872 calculate D2E/DX2 analytically !

! A50 A(13,17,32) 126.2641 calculate D2E/DX2 analytically !

! A51 A(16,17,32) 126.2641 calculate D2E/DX2 analytically !

! A52 A(16,18,19) 126.5677 calculate D2E/DX2 analytically !

! A53 A(16,18,40) 116.2931 calculate D2E/DX2 analytically !

! A54 A(19,18,40) 117.1377 calculate D2E/DX2 analytically !

! A55 A(18,19,20) 125.0057 calculate D2E/DX2 analytically !

! A56 A(18,19,23) 126.0158 calculate D2E/DX2 analytically !

! A57 A(20,19,23) 108.9772 calculate D2E/DX2 analytically !

! A58 A(19,20,21) 107.1794 calculate D2E/DX2 analytically !

! A59 A(19,20,30) 125.3057 calculate D2E/DX2 analytically !

! A60 A(21,20,30) 127.5145 calculate D2E/DX2 analytically !

! A61 A(20,21,22) 107.1794 calculate D2E/DX2 analytically !

! A62 A(20,21,31) 127.5145 calculate D2E/DX2 analytically !

! A63 A(22,21,31) 125.3057 calculate D2E/DX2 analytically !

! A64 A(21,22,23) 108.9772 calculate D2E/DX2 analytically !

! A65 A(21,22,33) 125.0057 calculate D2E/DX2 analytically !

! A66 A(23,22,33) 126.0158 calculate D2E/DX2 analytically !

! A67 A(19,23,22) 107.6867 calculate D2E/DX2 analytically !

! A68 A(19,23,32) 126.0961 calculate D2E/DX2 analytically !

! A69 A(22,23,32) 126.0961 calculate D2E/DX2 analytically !

! A70 A(3,32,8) 89.7421 calculate D2E/DX2 analytically !

! A71 A(3,32,17) 89.7421 calculate D2E/DX2 analytically !

! A72 A(8,32,23) 89.7421 calculate D2E/DX2 analytically !

! A73 A(17,32,23) 89.7421 calculate D2E/DX2 analytically !

! A74 A(9,33,22) 126.5677 calculate D2E/DX2 analytically !

! A75 A(9,33,34) 116.2931 calculate D2E/DX2 analytically !

! A76 A(22,33,34) 117.1377 calculate D2E/DX2 analytically !

! A77 L(3,32,23,17,-1) 179.4843 calculate D2E/DX2 analytically !

! A78 L(8,32,17,23,-1) 179.4843 calculate D2E/DX2 analytically !

! A79 L(33,34,36,26,-1) 179.0082 calculate D2E/DX2 analytically !

! A80 L(12,35,37,24,-1) 180.9903 calculate D2E/DX2 analytically !

! A81 L(34,36,43,26,-1) 180.3145 calculate D2E/DX2 analytically !

! A82 L(35,37,45,28,-1) 180.3145 calculate D2E/DX2 analytically !

! A83 L(6,38,39,25,-1) 180.9903 calculate D2E/DX2 analytically !

! A84 L(38,39,44,27,-1) 180.3145 calculate D2E/DX2 analytically !

! A85 L(18,40,41,29,-1) 179.0082 calculate D2E/DX2 analytically !

! A86 L(40,41,42,29,-1) 180.3145 calculate D2E/DX2 analytically !

! A87 L(3,32,23,17,-2) 187.8116 calculate D2E/DX2 analytically !

! A88 L(8,32,17,23,-2) 172.4574 calculate D2E/DX2 analytically !

! A89 L(33,34,36,26,-2) 179.9426 calculate D2E/DX2 analytically !

! A90 L(12,35,37,24,-2) 180.08 calculate D2E/DX2 analytically !

! A91 L(34,36,43,26,-2) 179.9841 calculate D2E/DX2 analytically !

! A92 L(35,37,45,28,-2) 179.9841 calculate D2E/DX2 analytically !

! A93 L(6,38,39,25,-2) 179.92 calculate D2E/DX2 analytically !

! A94 L(38,39,44,27,-2) 180.0159 calculate D2E/DX2 analytically !

! A95 L(18,40,41,29,-2) 180.0574 calculate D2E/DX2 analytically !

! A96 L(40,41,42,29,-2) 180.0159 calculate D2E/DX2 analytically !

! D1 D(5,1,2,3) -0.0156 calculate D2E/DX2 analytically !

! D2 D(5,1,2,12) 179.5962 calculate D2E/DX2 analytically !

! D3 D(24,1,2,3) -179.794 calculate D2E/DX2 analytically !

! D4 D(24,1,2,12) -0.1822 calculate D2E/DX2 analytically !

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

! D6 D(2,1,5,25) -179.772 calculate D2E/DX2 analytically !

! D7 D(24,1,5,4) 179.772 calculate D2E/DX2 analytically !

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

! D9 D(1,2,3,4) 0.0252 calculate D2E/DX2 analytically !

! D10 D(1,2,3,32) -176.1612 calculate D2E/DX2 analytically !

! D11 D(12,2,3,4) -179.5817 calculate D2E/DX2 analytically !

! D12 D(12,2,3,32) 4.2319 calculate D2E/DX2 analytically !

! D13 D(1,2,12,13) -179.1151 calculate D2E/DX2 analytically !

! D14 D(1,2,12,35) 0.4216 calculate D2E/DX2 analytically !

! D15 D(3,2,12,13) 0.4311 calculate D2E/DX2 analytically !

! D16 D(3,2,12,35) 179.9678 calculate D2E/DX2 analytically !

! D17 D(2,3,4,5) -0.0252 calculate D2E/DX2 analytically !

! D18 D(2,3,4,6) 179.5817 calculate D2E/DX2 analytically !

! D19 D(32,3,4,5) 176.1612 calculate D2E/DX2 analytically !

! D20 D(32,3,4,6) -4.2319 calculate D2E/DX2 analytically !

! D21 D(2,3,32,8) -178.4776 calculate D2E/DX2 analytically !

! D22 D(2,3,32,17) -6.0202 calculate D2E/DX2 analytically !

! D23 D(4,3,32,8) 6.0202 calculate D2E/DX2 analytically !

! D24 D(4,3,32,17) 178.4776 calculate D2E/DX2 analytically !

! D25 D(3,4,5,1) 0.0156 calculate D2E/DX2 analytically !

! D26 D(3,4,5,25) 179.794 calculate D2E/DX2 analytically !

! D27 D(6,4,5,1) -179.5962 calculate D2E/DX2 analytically !

! D28 D(6,4,5,25) 0.1822 calculate D2E/DX2 analytically !

! D29 D(3,4,6,7) -0.4311 calculate D2E/DX2 analytically !

! D30 D(3,4,6,38) -179.9678 calculate D2E/DX2 analytically !

! D31 D(5,4,6,7) 179.1151 calculate D2E/DX2 analytically !

! D32 D(5,4,6,38) -0.4216 calculate D2E/DX2 analytically !

! D33 D(4,6,7,8) 0.7082 calculate D2E/DX2 analytically !

! D34 D(4,6,7,11) -178.7215 calculate D2E/DX2 analytically !

! D35 D(38,6,7,8) -179.7517 calculate D2E/DX2 analytically !

! D36 D(38,6,7,11) 0.8186 calculate D2E/DX2 analytically !

! D37 D(6,7,8,9) -179.4715 calculate D2E/DX2 analytically !

! D38 D(6,7,8,32) 3.7149 calculate D2E/DX2 analytically !

! D39 D(11,7,8,9) 0.0369 calculate D2E/DX2 analytically !

! D40 D(11,7,8,32) -176.7767 calculate D2E/DX2 analytically !

! D41 D(6,7,11,10) 179.4816 calculate D2E/DX2 analytically !

! D42 D(6,7,11,27) -0.2675 calculate D2E/DX2 analytically !

! D43 D(8,7,11,10) -0.0228 calculate D2E/DX2 analytically !

! D44 D(8,7,11,27) -179.7719 calculate D2E/DX2 analytically !

! D45 D(7,8,9,10) -0.0369 calculate D2E/DX2 analytically !

! D46 D(7,8,9,33) 179.4715 calculate D2E/DX2 analytically !

! D47 D(32,8,9,10) 176.7767 calculate D2E/DX2 analytically !

! D48 D(32,8,9,33) -3.7149 calculate D2E/DX2 analytically !

! D49 D(7,8,32,3) -5.7918 calculate D2E/DX2 analytically !

! D50 D(7,8,32,23) -177.9802 calculate D2E/DX2 analytically !

! D51 D(9,8,32,3) 177.9802 calculate D2E/DX2 analytically !

! D52 D(9,8,32,23) 5.7918 calculate D2E/DX2 analytically !

! D53 D(8,9,10,11) 0.0228 calculate D2E/DX2 analytically !

! D54 D(8,9,10,26) 179.7719 calculate D2E/DX2 analytically !

! D55 D(33,9,10,11) -179.4816 calculate D2E/DX2 analytically !

! D56 D(33,9,10,26) 0.2675 calculate D2E/DX2 analytically !

! D57 D(8,9,33,22) -0.7082 calculate D2E/DX2 analytically !

! D58 D(8,9,33,34) 179.7517 calculate D2E/DX2 analytically !

! D59 D(10,9,33,22) 178.7215 calculate D2E/DX2 analytically !

! D60 D(10,9,33,34) -0.8186 calculate D2E/DX2 analytically !

! D61 D(9,10,11,7) 0.0 calculate D2E/DX2 analytically !

! D62 D(9,10,11,27) 179.7443 calculate D2E/DX2 analytically !

! D63 D(26,10,11,7) -179.7443 calculate D2E/DX2 analytically !

! D64 D(26,10,11,27) 0.0 calculate D2E/DX2 analytically !

! D65 D(2,12,13,14) 178.7215 calculate D2E/DX2 analytically !

! D66 D(2,12,13,17) -0.7082 calculate D2E/DX2 analytically !

! D67 D(35,12,13,14) -0.8186 calculate D2E/DX2 analytically !

! D68 D(35,12,13,17) 179.7517 calculate D2E/DX2 analytically !

! D69 D(12,13,14,15) -179.4816 calculate D2E/DX2 analytically !

! D70 D(12,13,14,28) 0.2675 calculate D2E/DX2 analytically !

! D71 D(17,13,14,15) 0.0228 calculate D2E/DX2 analytically !

! D72 D(17,13,14,28) 179.7719 calculate D2E/DX2 analytically !

! D73 D(12,13,17,16) 179.4715 calculate D2E/DX2 analytically !

! D74 D(12,13,17,32) -3.7149 calculate D2E/DX2 analytically !

! D75 D(14,13,17,16) -0.0369 calculate D2E/DX2 analytically !

! D76 D(14,13,17,32) 176.7767 calculate D2E/DX2 analytically !

! D77 D(13,14,15,16) 0.0 calculate D2E/DX2 analytically !

! D78 D(13,14,15,29) 179.7443 calculate D2E/DX2 analytically !

! D79 D(28,14,15,16) -179.7443 calculate D2E/DX2 analytically !

! D80 D(28,14,15,29) 0.0 calculate D2E/DX2 analytically !

! D81 D(14,15,16,17) -0.0228 calculate D2E/DX2 analytically !

! D82 D(14,15,16,18) 179.4816 calculate D2E/DX2 analytically !

! D83 D(29,15,16,17) -179.7719 calculate D2E/DX2 analytically !

! D84 D(29,15,16,18) -0.2675 calculate D2E/DX2 analytically !

! D85 D(15,16,17,13) 0.0369 calculate D2E/DX2 analytically !

! D86 D(15,16,17,32) -176.7767 calculate D2E/DX2 analytically !

! D87 D(18,16,17,13) -179.4715 calculate D2E/DX2 analytically !

! D88 D(18,16,17,32) 3.7149 calculate D2E/DX2 analytically !

! D89 D(15,16,18,19) -178.7215 calculate D2E/DX2 analytically !

! D90 D(15,16,18,40) 0.8186 calculate D2E/DX2 analytically !

! D91 D(17,16,18,19) 0.7082 calculate D2E/DX2 analytically !

! D92 D(17,16,18,40) -179.7517 calculate D2E/DX2 analytically !

! D93 D(13,17,32,3) 5.7918 calculate D2E/DX2 analytically !

! D94 D(13,17,32,23) 177.9802 calculate D2E/DX2 analytically !

! D95 D(16,17,32,3) -177.9802 calculate D2E/DX2 analytically !

! D96 D(16,17,32,23) -5.7918 calculate D2E/DX2 analytically !

! D97 D(16,18,19,20) 179.1151 calculate D2E/DX2 analytically !

! D98 D(16,18,19,23) -0.4311 calculate D2E/DX2 analytically !

! D99 D(40,18,19,20) -0.4216 calculate D2E/DX2 analytically !

! D100 D(40,18,19,23) -179.9678 calculate D2E/DX2 analytically !

! D101 D(18,19,20,21) -179.5962 calculate D2E/DX2 analytically !

! D102 D(18,19,20,30) 0.1822 calculate D2E/DX2 analytically !

! D103 D(23,19,20,21) 0.0156 calculate D2E/DX2 analytically !

! D104 D(23,19,20,30) 179.794 calculate D2E/DX2 analytically !

! D105 D(18,19,23,22) 179.5817 calculate D2E/DX2 analytically !

! D106 D(18,19,23,32) -4.2319 calculate D2E/DX2 analytically !

! D107 D(20,19,23,22) -0.0252 calculate D2E/DX2 analytically !

! D108 D(20,19,23,32) 176.1612 calculate D2E/DX2 analytically !

! D109 D(19,20,21,22) 0.0 calculate D2E/DX2 analytically !

! D110 D(19,20,21,31) 179.772 calculate D2E/DX2 analytically !

! D111 D(30,20,21,22) -179.772 calculate D2E/DX2 analytically !

! D112 D(30,20,21,31) 0.0 calculate D2E/DX2 analytically !

! D113 D(20,21,22,23) -0.0156 calculate D2E/DX2 analytically !

! D114 D(20,21,22,33) 179.5962 calculate D2E/DX2 analytically !

! D115 D(31,21,22,23) -179.794 calculate D2E/DX2 analytically !

! D116 D(31,21,22,33) -0.1822 calculate D2E/DX2 analytically !

! D117 D(21,22,23,19) 0.0252 calculate D2E/DX2 analytically !

! D118 D(21,22,23,32) -176.1612 calculate D2E/DX2 analytically !

! D119 D(33,22,23,19) -179.5817 calculate D2E/DX2 analytically !

! D120 D(33,22,23,32) 4.2319 calculate D2E/DX2 analytically !

! D121 D(21,22,33,9) -179.1151 calculate D2E/DX2 analytically !

! D122 D(21,22,33,34) 0.4216 calculate D2E/DX2 analytically !

! D123 D(23,22,33,9) 0.4311 calculate D2E/DX2 analytically !

! D124 D(23,22,33,34) 179.9678 calculate D2E/DX2 analytically !

! D125 D(19,23,32,8) 178.4776 calculate D2E/DX2 analytically !

! D126 D(19,23,32,17) 6.0202 calculate D2E/DX2 analytically !

! D127 D(22,23,32,8) -6.0202 calculate D2E/DX2 analytically !

! D128 D(22,23,32,17) -178.4776 calculate D2E/DX2 analytically !

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

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

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Jul 30 19:37:54 2019, MaxMem= 4294967296 cpu: 0.3

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -4.285118 0.679179 -0.028897

2 6 0 -2.897023 1.108362 -0.009305

3 7 0 -2.087198 0.000000 0.002478

4 6 0 -2.897023 -1.108362 -0.009305

5 6 0 -4.285118 -0.679179 -0.028897

6 6 0 -2.467286 -2.444453 -0.011342

7 6 0 -1.105827 -2.906291 -0.010238

8 7 0 0.000000 -2.093972 0.006940

9 6 0 1.105827 -2.906291 -0.010238

10 6 0 0.691724 -4.270946 -0.038229

11 6 0 -0.691724 -4.270946 -0.038229

12 6 0 -2.467286 2.444453 -0.011342

13 6 0 -1.105827 2.906291 -0.010238

14 6 0 -0.691724 4.270946 -0.038229

15 6 0 0.691724 4.270946 -0.038229

16 6 0 1.105827 2.906291 -0.010238

17 7 0 0.000000 2.093972 0.006940

18 6 0 2.467286 2.444453 -0.011342

19 6 0 2.897023 1.108362 -0.009305

20 6 0 4.285118 0.679179 -0.028897

21 6 0 4.285118 -0.679179 -0.028897

22 6 0 2.897023 -1.108362 -0.009305

23 7 0 2.087198 0.000000 0.002478

24 1 0 -5.141862 1.337033 -0.044399

25 1 0 -5.141862 -1.337033 -0.044399

26 1 0 1.346423 -5.130142 -0.059689

27 1 0 -1.346423 -5.130142 -0.059689

28 1 0 -1.346423 5.130142 -0.059689

29 1 0 1.346423 5.130142 -0.059689

30 1 0 5.141862 1.337033 -0.044399

31 1 0 5.141862 -1.337033 -0.044399

32 30 0 0.000000 0.000000 0.145291

33 6 0 2.467286 -2.444453 -0.011342

34 6 0 3.474889 -3.450929 -0.025111

35 6 0 -3.474889 3.450929 -0.025111

36 6 0 4.314871 -4.319507 -0.038288

37 6 0 -4.314871 4.319507 -0.038288

38 6 0 -3.474889 -3.450929 -0.025111

39 6 0 -4.314871 -4.319507 -0.038288

40 6 0 3.474889 3.450929 -0.025111

41 6 0 4.314871 4.319507 -0.038288

42 1 0 5.060646 5.082244 -0.050098

43 1 0 5.060646 -5.082244 -0.050098

44 1 0 -5.060646 -5.082244 -0.050098

45 1 0 -5.060646 5.082244 -0.050098

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.453062 0.000000

3 N 2.300679 1.372743 0.000000

4 C 2.263294 2.216725 1.372743 0.000000

5 C 1.358359 2.263294 2.300679 1.453062 0.000000

6 C 3.614125 3.578711 2.473865 1.403501 2.533972

7 C 4.792060 4.396115 3.067536 2.537899 3.881786

8 N 5.104301 4.318327 2.956541 3.060136 4.512778

9 C 6.474430 5.669238 4.317650 4.388093 5.832895

10 C 7.019457 6.466598 5.095590 4.783500 6.137575

11 C 6.116887 5.813874 4.493326 3.855660 5.080685

12 C 2.533972 1.403501 2.473865 3.578711 3.614125

13 C 3.881786 2.537899 3.067536 4.396115 4.792060

14 C 5.080685 3.855660 4.493326 5.813874 6.116887

15 C 6.137575 4.783500 5.095590 6.466598 7.019457

16 C 5.832895 4.388093 4.317650 5.669238 6.474430

17 N 4.512778 3.060136 2.956541 4.318327 5.104301

18 C 6.979360 5.528196 5.169030 6.434152 7.439916

19 C 7.194980 5.794046 5.105983 6.203615 7.401273

20 C 8.570237 7.194980 6.408485 7.401273 8.677217

21 C 8.677217 7.401273 6.408485 7.194980 8.570237

22 C 7.401273 6.203615 5.105983 5.794046 7.194980

23 N 6.408485 5.105983 4.174396 5.105983 6.408485

24 H 1.080287 2.256728 3.334790 3.319712 2.190745

25 H 2.190745 3.319712 3.334790 2.256728 1.080287

26 H 8.090947 7.545085 6.173490 5.846716 7.178181

27 H 6.510384 6.428518 5.183722 4.310640 5.333662

28 H 5.333662 4.310640 5.183722 6.428518 6.510384

29 H 7.178181 5.846716 6.173490 7.545085 8.090947

30 H 9.449919 8.042213 7.351813 8.402670 9.640192

31 H 9.640192 8.402670 7.351813 8.042213 9.449919

32 Zn 4.342104 3.105658 2.092078 3.105658 4.342104

33 C 7.439916 6.434152 5.169030 5.528196 6.979360

34 C 8.790650 7.835091 6.545723 6.788898 8.240165

35 C 2.887746 2.412840 3.719591 4.595793 4.208833

36 C 9.947199 9.026296 7.723101 7.894536 9.338731

37 C 3.640461 3.510354 4.860281 5.610071 4.998784

38 C 4.208833 4.595793 3.719591 2.412840 2.887746

39 C 4.998784 5.610071 4.860281 3.510354 3.640461

40 C 8.240165 6.788898 6.545723 7.835091 8.790650

41 C 9.338731 7.894536 7.723101 9.026296 9.947199

42 H 10.331057 8.894824 8.770612 10.082151 10.978969

43 H 10.978969 10.082151 8.770612 8.894824 10.331057

44 H 5.813423 6.557937 5.888409 4.524894 4.470891

45 H 4.470891 4.524894 5.888409 6.557937 5.813423

6 7 8 9 10

6 C 0.000000

7 C 1.437660 0.000000

8 N 2.492122 1.372229 0.000000

9 C 3.602837 2.211654 1.372229 0.000000

10 C 3.649129 2.257045 2.284674 1.426376 0.000000

11 C 2.547434 1.426376 2.284674 2.257045 1.383447

12 C 4.888906 5.521235 5.165766 6.434097 7.421364

13 C 5.521235 5.812582 5.121111 6.219126 7.398966

14 C 6.946216 7.189227 6.402554 7.398966 8.653198

15 C 7.421364 7.398966 6.402554 7.189227 8.541891

16 C 6.434097 6.219126 5.121111 5.812582 7.189227

17 N 5.165766 5.121111 4.187944 5.121111 6.402554

18 C 6.946323 6.434097 5.165766 5.521235 6.946216

19 C 6.434152 5.669238 4.318327 4.396115 5.813874

20 C 7.439916 6.474430 5.104301 4.792060 6.116887

21 C 6.979360 5.832895 4.512778 3.881786 5.080685

22 C 5.528196 4.388093 3.060136 2.537899 3.855660

23 N 5.169030 4.317650 2.956541 3.067536 4.493326

24 H 4.631855 5.856325 6.181680 7.552522 8.091982

25 H 2.894965 4.330509 5.197531 6.441844 6.529824

26 H 4.664723 3.310814 3.321991 2.237375 1.080422

27 H 2.910601 2.237375 3.321991 3.310814 2.211950

28 H 7.657230 8.040186 7.348818 8.402395 9.619509

29 H 8.480637 8.402395 7.348818 8.040186 9.423882

30 H 8.497050 7.552522 6.181680 5.856325 7.159133

31 H 7.689382 6.441844 5.197531 4.330509 5.330254

32 Zn 3.476692 3.113450 2.098538 3.113450 4.330489

33 C 4.934572 3.602837 2.492122 1.437660 2.547434

34 C 6.026826 4.613005 3.730578 2.430906 2.901484

35 C 5.980884 6.784314 6.543837 7.835651 8.774291

36 C 7.036633 5.601958 4.855220 3.506555 3.623473

37 C 7.011808 7.906384 7.729998 9.033101 9.942930

38 C 1.424236 2.430906 3.730578 4.613005 4.246559

39 C 2.632513 3.506555 4.855220 5.601958 5.006830

40 C 8.370494 7.835651 6.543837 6.784314 8.208138

41 C 9.578598 9.033101 7.729998 7.906384 9.323255

42 H 10.645301 10.091763 8.781313 8.913970 10.323264

43 H 7.976792 6.539247 5.877343 4.514084 4.443628

44 H 3.699319 4.514084 5.877343 6.539247 5.809312

45 H 7.961041 8.913970 8.781313 10.091763 10.980530

11 12 13 14 15

11 C 0.000000

12 C 6.946216 0.000000

13 C 7.189227 1.437660 0.000000

14 C 8.541891 2.547434 1.426376 0.000000

15 C 8.653198 3.649129 2.257045 1.383447 0.000000

16 C 7.398966 3.602837 2.211654 2.257045 1.426376

17 N 6.402554 2.492122 1.372229 2.284674 2.284674

18 C 7.421364 4.934572 3.602837 3.649129 2.547434

19 C 6.466598 5.528196 4.388093 4.783500 3.855660

20 C 7.019457 6.979360 5.832895 6.137575 5.080685

21 C 6.137575 7.439916 6.474430 7.019457 6.116887

22 C 4.783500 6.434152 5.669238 6.466598 5.813874

23 N 5.095590 5.169030 4.317650 5.095590 4.493326

24 H 7.159133 2.894965 4.330509 5.330254 6.529824

25 H 5.330254 4.631855 5.856325 7.159133 8.091982

26 H 2.211950 8.480637 8.402395 9.619509 9.423882

27 H 1.080422 7.657230 8.040186 9.423882 9.619509

28 H 9.423882 2.910601 2.237375 1.080422 2.211950

29 H 9.619509 4.664723 3.310814 2.211950 1.080422

30 H 8.091982 7.689382 6.441844 6.529824 5.330254

31 H 6.529824 8.497050 7.552522 8.091982 7.159133

32 Zn 4.330489 3.476692 3.113450 4.330489 4.330489

33 C 3.649129 6.946323 6.434097 7.421364 6.946216

34 C 4.246559 8.370494 7.835651 8.774291 8.208138

35 C 8.208138 1.424236 2.430906 2.901484 4.246559

36 C 5.006830 9.578598 9.033101 9.942930 9.323255

37 C 9.323255 2.632513 3.506555 3.623473 5.006830

38 C 2.901484 5.980884 6.784314 8.208138 8.774291

39 C 3.623473 7.011808 7.906384 9.323255 9.942930

40 C 8.774291 6.026826 4.613005 4.246559 2.901484

41 C 9.942930 7.036633 5.601958 5.006830 3.623473

42 H 10.980530 7.976792 6.539247 5.809312 4.443628

43 H 5.809312 10.645301 10.091763 10.980530 10.323264

44 H 4.443628 7.961041 8.913970 10.323264 10.980530

45 H 10.323264 3.699319 4.514084 4.443628 5.809312

16 17 18 19 20

16 C 0.000000

17 N 1.372229 0.000000

18 C 1.437660 2.492122 0.000000

19 C 2.537899 3.060136 1.403501 0.000000

20 C 3.881786 4.512778 2.533972 1.453062 0.000000

21 C 4.792060 5.104301 3.614125 2.263294 1.358359

22 C 4.396115 4.318327 3.578711 2.216725 2.263294

23 N 3.067536 2.956541 2.473865 1.372743 2.300679

24 H 6.441844 5.197531 7.689382 8.042213 9.449919

25 H 7.552522 6.181680 8.497050 8.402670 9.640192

26 H 8.040186 7.348818 7.657230 6.428518 6.510384

27 H 8.402395 7.348818 8.480637 7.545085 8.090947

28 H 3.310814 3.321991 4.664723 5.846716 7.178181

29 H 2.237375 3.321991 2.910601 4.310640 5.333662

30 H 4.330509 5.197531 2.894965 2.256728 1.080287

31 H 5.856325 6.181680 4.631855 3.319712 2.190745

32 Zn 3.113450 2.098538 3.476692 3.105658 4.342104

33 C 5.521235 5.165766 4.888906 3.578711 3.614125

34 C 6.784314 6.543837 5.980884 4.595793 4.208833

35 C 4.613005 3.730578 6.026826 6.788898 8.240165

36 C 7.906384 7.729998 7.011808 5.610071 4.998784

37 C 5.601958 4.855220 7.036633 7.894536 9.338731

38 C 7.835651 6.543837 8.370494 7.835091 8.790650

39 C 9.033101 7.729998 9.578598 9.026296 9.947199

40 C 2.430906 3.730578 1.424236 2.412840 2.887746

41 C 3.506555 4.855220 2.632513 3.510354 3.640461

42 H 4.514084 5.877343 3.699319 4.524894 4.470891

43 H 8.913970 8.781313 7.961041 6.557937 5.813423

44 H 10.091763 8.781313 10.645301 10.082151 10.978969

45 H 6.539247 5.877343 7.976792 8.894824 10.331057

21 22 23 24 25

21 C 0.000000

22 C 1.453062 0.000000

23 N 2.300679 1.372743 0.000000

24 H 9.640192 8.402670 7.351813 0.000000

25 H 9.449919 8.042213 7.351813 2.674066 0.000000

26 H 5.333662 4.310640 5.183722 9.160918 7.515700

27 H 7.178181 5.846716 6.173490 7.498663 5.365936

28 H 8.090947 7.545085 6.173490 5.365936 7.498663

29 H 6.510384 6.428518 5.183722 7.515700 9.160918

30 H 2.190745 3.319712 3.334790 10.283723 10.625704

31 H 1.080287 2.256728 3.334790 10.625704 10.283723

32 Zn 4.342104 3.105658 2.092078 5.316237 5.316237

33 C 2.533972 1.403501 2.473865 8.497050 7.689382

34 C 2.887746 2.412840 3.719591 9.857654 8.872278

35 C 8.790650 7.835091 6.545723 2.692160 5.069886

36 C 3.640461 3.510354 4.860281 11.019359 9.915895

37 C 9.947199 9.026296 7.723101 3.095013 5.716677

38 C 8.240165 6.788898 6.545723 5.069886 2.692160

39 C 9.338731 7.894536 7.723101 5.716677 3.095013

40 C 4.208833 4.595793 3.719591 8.872278 9.857654

41 C 4.998784 5.610071 4.860281 9.915895 11.019359

42 H 5.813423 6.557937 5.888409 10.868201 12.053975

43 H 4.470891 4.524894 5.888409 12.053975 10.868201

44 H 10.331057 8.894824 8.770612 6.419793 3.746095

45 H 10.978969 10.082151 8.770612 3.746095 6.419793

26 27 28 29 30

26 H 0.000000

27 H 2.692846 0.000000

28 H 10.607774 10.260285 0.000000

29 H 10.260285 10.607774 2.692846 0.000000

30 H 7.498663 9.160918 7.515700 5.365936 0.000000

31 H 5.365936 7.515700 9.160918 7.498663 2.674066

32 Zn 5.307846 5.307846 5.307846 5.307846 5.316237

33 C 2.910601 4.664723 8.480637 7.657230 4.631855

34 C 2.711332 5.105488 9.842816 8.841173 5.069886

35 C 9.842816 8.841173 2.711332 5.105488 8.872278

36 C 3.077218 5.719076 11.015743 9.904949 5.716677

37 C 11.015743 9.904949 3.077218 5.719076 9.915895

38 C 5.105488 2.711332 8.841173 9.842816 9.857654

39 C 5.719076 3.077218 9.904949 11.015743 11.019359

40 C 8.841173 9.842816 5.105488 2.711332 2.692160

41 C 9.904949 11.015743 5.719076 3.077218 3.095013

42 H 10.866847 12.055847 6.407256 3.714544 3.746095

43 H 3.714544 6.407256 12.055847 10.866847 6.419793

44 H 6.407256 3.714544 10.866847 12.055847 12.053975

45 H 12.055847 10.866847 3.714544 6.407256 10.868201

31 32 33 34 35

31 H 0.000000

32 Zn 5.316237 0.000000

33 C 2.894965 3.476692 0.000000

34 C 2.692160 4.900286 1.424236 0.000000

35 C 9.857654 4.900286 8.370494 9.794644 0.000000

36 C 3.095013 6.108187 2.632513 1.208376 11.002736

37 C 11.019359 6.108187 9.578598 11.002736 1.208376

38 C 8.872278 4.900286 6.026826 6.949779 6.901857

39 C 9.915895 6.108187 7.036633 7.838046 7.815716

40 C 5.069886 4.900286 5.980884 6.901857 6.949779

41 C 5.716677 6.108187 7.011808 7.815716 7.838046

42 H 6.419793 7.174783 7.961041 8.679302 8.690062

43 H 3.746095 7.174783 3.699319 2.275179 12.069425

44 H 10.868201 7.174783 7.976792 8.690062 8.679302

45 H 12.053975 7.174783 10.645301 12.069425 2.275179

36 37 38 39 40

36 C 0.000000

37 C 12.210856 0.000000

38 C 7.838046 7.815716 0.000000

39 C 8.629742 8.639014 1.208376 0.000000

40 C 7.815716 7.838046 9.794644 11.002736 0.000000

41 C 8.639014 8.629742 11.002736 12.210856 1.208376

42 H 9.431290 9.406499 12.069425 13.277552 2.275179

43 H 1.066812 13.277552 8.690062 9.406499 8.679302

44 H 9.406499 9.431290 2.275179 1.066812 12.069425

45 H 13.277552 1.066812 8.679302 9.431290 8.690062

41 42 43 44 45

41 C 0.000000

42 H 1.066812 0.000000

43 H 9.431290 10.164487 0.000000

44 H 13.277552 14.344245 10.121293 0.000000

45 H 9.406499 10.121293 14.344245 10.164487 0.000000

Stoichiometry C28H12N4Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C28H12)]

Deg. of freedom 34

Full point group C2V NOp 4

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.679179 4.285118 -0.028897

2 6 0 1.108362 2.897023 -0.009305

3 7 0 0.000000 2.087198 0.002478

4 6 0 -1.108362 2.897023 -0.009305

5 6 0 -0.679179 4.285118 -0.028897

6 6 0 -2.444453 2.467286 -0.011342

7 6 0 -2.906291 1.105827 -0.010238

8 7 0 -2.093972 0.000000 0.006940

9 6 0 -2.906291 -1.105827 -0.010238

10 6 0 -4.270946 -0.691724 -0.038229

11 6 0 -4.270946 0.691724 -0.038229

12 6 0 2.444453 2.467286 -0.011342

13 6 0 2.906291 1.105827 -0.010238

14 6 0 4.270946 0.691724 -0.038229

15 6 0 4.270946 -0.691724 -0.038229

16 6 0 2.906291 -1.105827 -0.010238

17 7 0 2.093972 -0.000000 0.006940

18 6 0 2.444453 -2.467286 -0.011342

19 6 0 1.108362 -2.897023 -0.009305

20 6 0 0.679179 -4.285118 -0.028897

21 6 0 -0.679179 -4.285118 -0.028897

22 6 0 -1.108362 -2.897023 -0.009305

23 7 0 -0.000000 -2.087198 0.002478

24 1 0 1.337033 5.141862 -0.044399

25 1 0 -1.337033 5.141862 -0.044399

26 1 0 -5.130142 -1.346423 -0.059689

27 1 0 -5.130142 1.346423 -0.059689

28 1 0 5.130142 1.346423 -0.059689

29 1 0 5.130142 -1.346423 -0.059689

30 1 0 1.337033 -5.141862 -0.044399

31 1 0 -1.337033 -5.141862 -0.044399

32 30 0 0.000000 0.000000 0.145291

33 6 0 -2.444453 -2.467286 -0.011342

34 6 0 -3.450929 -3.474889 -0.025111

35 6 0 3.450929 3.474889 -0.025111

36 6 0 -4.319507 -4.314871 -0.038288

37 6 0 4.319507 4.314871 -0.038288

38 6 0 -3.450929 3.474889 -0.025111

39 6 0 -4.319507 4.314871 -0.038288

40 6 0 3.450929 -3.474889 -0.025111

41 6 0 4.319507 -4.314871 -0.038288

42 1 0 5.082244 -5.060646 -0.050098

43 1 0 -5.082244 -5.060646 -0.050098

44 1 0 -5.082244 5.060646 -0.050098

45 1 0 5.082244 5.060646 -0.050098

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

Rotational constants (GHZ): 0.1461487 0.1455538 0.0729592

Leave Link 202 at Tue Jul 30 19:37:54 2019, MaxMem= 4294967296 cpu: 0.2

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

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

Centers: 32

S 1 1.00

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

S 1 1.00

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

S 1 1.00

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

P 1 1.00

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

P 1 1.00

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

D 3 1.00

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

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

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

D 1 1.00

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

D 1 1.00

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

\*\*\*\*

Centers: 24 25 26 27 28 29 30 31 42 43

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

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

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

Centers: 3 8 17 23

6-311G\*

\*\*\*\*

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

Pseudopotential Parameters

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

Center Atomic Valence Angular Power

Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

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

1 6

No pseudopotential on this center.

2 6

No pseudopotential on this center.

3 7

No pseudopotential on this center.

4 6

No pseudopotential on this center.

5 6

No pseudopotential on this center.

6 6

No pseudopotential on this center.

7 6

No pseudopotential on this center.

8 7

No pseudopotential on this center.

9 6

No pseudopotential on this center.

10 6

No pseudopotential on this center.

11 6

No pseudopotential on this center.

12 6

No pseudopotential on this center.

13 6

No pseudopotential on this center.

14 6

No pseudopotential on this center.

15 6

No pseudopotential on this center.

16 6

No pseudopotential on this center.

17 7

No pseudopotential on this center.

18 6

No pseudopotential on this center.

19 6

No pseudopotential on this center.

20 6

No pseudopotential on this center.

21 6

No pseudopotential on this center.

22 6

No pseudopotential on this center.

23 7

No pseudopotential on this center.

24 1

No pseudopotential on this center.

25 1

No pseudopotential on this center.

26 1

No pseudopotential on this center.

27 1

No pseudopotential on this center.

28 1

No pseudopotential on this center.

29 1

No pseudopotential on this center.

30 1

No pseudopotential on this center.

31 1

No pseudopotential on this center.

32 30 12

F and up

1 386.7379660 -18.00000000 0.00000000

2 72.8587359 -124.35274030 0.00000000

2 15.9066170 -30.66018220 0.00000000

2 4.3502340 -10.63589890 0.00000000

2 1.2842199 -0.76836230 0.00000000

S - F

0 19.0867858 3.00000000 0.00000000

1 5.0231080 22.52342250 0.00000000

2 1.2701744 48.44659420 0.00000000

2 1.0671287 -44.55601190 0.00000000

2 0.9264190 12.99839580 0.00000000

P - F

0 43.4927750 5.00000000 0.00000000

1 20.8692669 20.74355890 0.00000000

2 21.7118378 90.30271580 0.00000000

2 6.3616915 74.66103160 0.00000000

2 1.2291195 9.88944240 0.00000000

D - F

2 13.5851800 -4.84903590 0.00000000

2 9.8373050 3.69133790 0.00000000

2 0.8373113 -0.50373190 0.00000000

33 6

No pseudopotential on this center.

34 6

No pseudopotential on this center.

35 6

No pseudopotential on this center.

36 6

No pseudopotential on this center.

37 6

No pseudopotential on this center.

38 6

No pseudopotential on this center.

39 6

No pseudopotential on this center.

40 6

No pseudopotential on this center.

41 6

No pseudopotential on this center.

42 1

No pseudopotential on this center.

43 1

No pseudopotential on this center.

44 1

No pseudopotential on this center.

45 1

No pseudopotential on this center.

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

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

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

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

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

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

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

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

111 alpha electrons 110 beta electrons

nuclear repulsion energy 3054.0433289654 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= 13 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= -0.1304045554 Hartrees.

Nuclear repulsion after empirical dispersion term = 3053.9129244100 Hartrees.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

2nd derivatives : Analytical E(r).r(xy)/FMM algorithm (CHGder, D2EAlg=3).

Cavity 2nd derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3886

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.37D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 104

GePol: Fraction of low-weight points (<1% of avg) = 2.68%

GePol: Cavity surface area = 416.072 Ang\*\*2

GePol: Cavity volume = 420.616 Ang\*\*3

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

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

PCM non-electrostatic energy = 0.0083769318 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3053.9213013417 Hartrees.

Leave Link 301 at Tue Jul 30 19:37:55 2019, MaxMem= 4294967296 cpu: 3.0

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16185 LenP2D= 44720.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.45D-05 NBF= 172 148 158 158

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

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Tue Jul 30 19:37:55 2019, MaxMem= 4294967296 cpu: 12.2

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Jul 30 19:37:55 2019, MaxMem= 4294967296 cpu: 1.4

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

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1359.66986507023

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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

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The electronic state of the initial guess is 2-B2.

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

Leave Link 401 at Tue Jul 30 19:37:57 2019, MaxMem= 4294967296 cpu: 27.5

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1387497 IEndB= 1387497 NGot= 4294967296 MDV= 4294047352

LenX= 4294047352 LenY= 4293596440

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= 650000000 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= 45302988.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.77D-15 for 3866.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.53D-15 for 1368 1239.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.22D-15 for 3866.

Iteration 1 A^-1\*A deviation from orthogonality is 1.05D-14 for 1053 1003.

E= -1358.38857345787

DIIS: error= 8.46D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1358.38857345787 IErMin= 1 ErrMin= 8.46D-02

ErrMax= 8.46D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.04D+00 BMatP= 4.04D+00

IDIUse=3 WtCom= 1.54D-01 WtEn= 8.46D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.028 Goal= None Shift= 0.000

Gap= 0.092 Goal= None Shift= 0.000

GapD= 0.028 DampG=0.250 DampE=0.250 DampFc=0.1250 IDamp=-1.

Damping current iteration by 1.25D-01

RMSDP=2.90D-03 MaxDP=1.24D-01 OVMax= 1.69D-01

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.60D-04 CP: 9.95D-01

E= -1358.55067254594 Delta-E= -0.162099088070 Rises=F Damp=T

DIIS: error= 6.07D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1358.55067254594 IErMin= 2 ErrMin= 6.07D-02

ErrMax= 6.07D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.36D+00 BMatP= 4.04D+00

IDIUse=3 WtCom= 3.93D-01 WtEn= 6.07D-01

Coeff-Com: -0.301D+01 0.401D+01

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

Coeff: -0.118D+01 0.218D+01

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.68D-03 MaxDP=6.97D-02 DE=-1.62D-01 OVMax= 4.92D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 9.96D-04 CP: 9.59D-01 3.00D+00

E= -1359.05706741020 Delta-E= -0.506394864257 Rises=F Damp=F

DIIS: error= 3.71D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.05706741020 IErMin= 3 ErrMin= 3.71D-02

ErrMax= 3.71D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.22D-01 BMatP= 2.36D+00

IDIUse=3 WtCom= 6.29D-01 WtEn= 3.71D-01

Coeff-Com: 0.146D+01-0.143D+01 0.974D+00

Coeff-En: 0.134D-01 0.000D+00 0.987D+00

Coeff: 0.921D+00-0.900D+00 0.979D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=8.36D-04 MaxDP=3.94D-02 DE=-5.06D-01 OVMax= 4.83D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.51D-04 CP: 9.68D-01 3.00D+00 3.73D-01

E= -1359.16350764279 Delta-E= -0.106440232594 Rises=F Damp=F

DIIS: error= 1.53D-02 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.16350764279 IErMin= 4 ErrMin= 1.53D-02

ErrMax= 1.53D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.60D-02 BMatP= 6.22D-01

IDIUse=3 WtCom= 8.47D-01 WtEn= 1.53D-01

Coeff-Com: -0.186D+00 0.252D+00 0.263D+00 0.671D+00

Coeff-En: 0.000D+00 0.000D+00 0.397D-01 0.960D+00

Coeff: -0.158D+00 0.213D+00 0.229D+00 0.715D+00

Gap= 0.037 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=2.54D-04 MaxDP=1.10D-02 DE=-1.06D-01 OVMax= 2.32D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 9.13D-05 CP: 9.66D-01 3.00D+00 5.30D-01 6.78D-01

E= -1359.18044681068 Delta-E= -0.016939167896 Rises=F Damp=F

DIIS: error= 2.20D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.18044681068 IErMin= 5 ErrMin= 2.20D-03

ErrMax= 2.20D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.49D-03 BMatP= 9.60D-02

IDIUse=3 WtCom= 9.78D-01 WtEn= 2.20D-02

Coeff-Com: -0.185D+00 0.218D+00 0.985D-01 0.455D+00 0.414D+00

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

Coeff: -0.181D+00 0.213D+00 0.963D-01 0.445D+00 0.427D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=5.91D-05 MaxDP=2.47D-03 DE=-1.69D-02 OVMax= 8.38D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.32D-05 CP: 9.66D-01 3.00D+00 5.25D-01 7.42D-01 5.52D-01

E= -1359.18190185079 Delta-E= -0.001455040107 Rises=F Damp=F

DIIS: error= 4.88D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.18190185079 IErMin= 6 ErrMin= 4.88D-04

ErrMax= 4.88D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.38D-04 BMatP= 6.49D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.88D-03

Coeff-Com: -0.738D-01 0.844D-01 0.246D-01 0.151D+00 0.202D+00 0.611D+00

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

Coeff: -0.734D-01 0.840D-01 0.244D-01 0.151D+00 0.201D+00 0.613D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=9.23D-06 MaxDP=3.28D-04 DE=-1.46D-03 OVMax= 1.85D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 7.60D-06 CP: 9.66D-01 3.00D+00 5.27D-01 7.42D-01 5.67D-01

CP: 7.94D-01

E= -1359.18193143053 Delta-E= -0.000029579737 Rises=F Damp=F

DIIS: error= 1.00D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.18193143053 IErMin= 7 ErrMin= 1.00D-04

ErrMax= 1.00D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.48D-05 BMatP= 1.38D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.00D-03

Coeff-Com: -0.243D-01 0.273D-01 0.311D-02 0.364D-01 0.630D-01 0.297D+00

Coeff-Com: 0.598D+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: -0.242D-01 0.272D-01 0.311D-02 0.364D-01 0.630D-01 0.296D+00

Coeff: 0.598D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=3.51D-06 MaxDP=1.56D-04 DE=-2.96D-05 OVMax= 1.06D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 3.37D-06 CP: 9.66D-01 3.00D+00 5.27D-01 7.42D-01 5.75D-01

CP: 8.20D-01 9.95D-01

E= -1359.18193630067 Delta-E= -0.000004870139 Rises=F Damp=F

DIIS: error= 5.00D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.18193630067 IErMin= 8 ErrMin= 5.00D-05

ErrMax= 5.00D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.09D-06 BMatP= 1.48D-05

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

Coeff-Com: 0.167D-01-0.194D-01-0.525D-02-0.324D-01-0.367D-01-0.732D-01

Coeff-Com: 0.245D+00 0.905D+00

Coeff: 0.167D-01-0.194D-01-0.525D-02-0.324D-01-0.367D-01-0.732D-01

Coeff: 0.245D+00 0.905D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=2.81D-06 MaxDP=1.69D-04 DE=-4.87D-06 OVMax= 8.78D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.78D-06 CP: 9.66D-01 3.00D+00 5.27D-01 7.42D-01 5.80D-01

CP: 8.63D-01 1.23D+00 1.15D+00

E= -1359.18193841176 Delta-E= -0.000002111095 Rises=F Damp=F

DIIS: error= 3.75D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1359.18193841176 IErMin= 9 ErrMin= 3.75D-05

ErrMax= 3.75D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-06 BMatP= 3.09D-06

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

Coeff-Com: 0.157D-01-0.180D-01-0.365D-02-0.270D-01-0.348D-01-0.102D+00

Coeff-Com: 0.255D-03 0.517D+00 0.653D+00

Coeff: 0.157D-01-0.180D-01-0.365D-02-0.270D-01-0.348D-01-0.102D+00

Coeff: 0.255D-03 0.517D+00 0.653D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.39D-06 MaxDP=9.20D-05 DE=-2.11D-06 OVMax= 4.09D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 8.89D-07 CP: 9.66D-01 3.00D+00 5.27D-01 7.42D-01 5.84D-01

CP: 8.80D-01 1.28D+00 1.35D+00 1.20D+00

E= -1359.18193894215 Delta-E= -0.000000530392 Rises=F Damp=F

DIIS: error= 1.93D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1359.18193894215 IErMin=10 ErrMin= 1.93D-05

ErrMax= 1.93D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.90D-07 BMatP= 1.10D-06

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

Coeff-Com: 0.778D-03-0.804D-03 0.104D-03-0.169D-03-0.204D-02-0.196D-01

Coeff-Com: -0.112D+00-0.602D-01 0.373D+00 0.820D+00

Coeff: 0.778D-03-0.804D-03 0.104D-03-0.169D-03-0.204D-02-0.196D-01

Coeff: -0.112D+00-0.602D-01 0.373D+00 0.820D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=8.56D-07 MaxDP=4.30D-05 DE=-5.30D-07 OVMax= 2.60D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 4.51D-07 CP: 9.66D-01 3.00D+00 5.27D-01 7.42D-01 5.83D-01

CP: 8.86D-01 1.33D+00 1.47D+00 1.47D+00 9.84D-01

E= -1359.18193910540 Delta-E= -0.000000163247 Rises=F Damp=F

DIIS: error= 5.92D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1359.18193910540 IErMin=11 ErrMin= 5.92D-06

ErrMax= 5.92D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.51D-08 BMatP= 2.90D-07

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

Coeff-Com: -0.158D-02 0.185D-02 0.323D-03 0.262D-02 0.266D-02 0.215D-02

Coeff-Com: -0.433D-01-0.730D-01 0.563D-01 0.331D+00 0.721D+00

Coeff: -0.158D-02 0.185D-02 0.323D-03 0.262D-02 0.266D-02 0.215D-02

Coeff: -0.433D-01-0.730D-01 0.563D-01 0.331D+00 0.721D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=2.79D-07 MaxDP=1.52D-05 DE=-1.63D-07 OVMax= 9.09D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.02D-07 CP: 9.66D-01 3.00D+00 5.27D-01 7.42D-01 5.84D-01

CP: 8.86D-01 1.33D+00 1.49D+00 1.52D+00 1.12D+00

CP: 1.15D+00

E= -1359.18193912624 Delta-E= -0.000000020836 Rises=F Damp=F

DIIS: error= 3.67D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1359.18193912624 IErMin=12 ErrMin= 3.67D-06

ErrMax= 3.67D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.54D-08 BMatP= 3.51D-08

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

Coeff-Com: -0.109D-02 0.124D-02 0.118D-03 0.135D-02 0.193D-02 0.640D-02

Coeff-Com: 0.137D-01-0.203D-01-0.956D-01-0.659D-01 0.440D+00 0.718D+00

Coeff: -0.109D-02 0.124D-02 0.118D-03 0.135D-02 0.193D-02 0.640D-02

Coeff: 0.137D-01-0.203D-01-0.956D-01-0.659D-01 0.440D+00 0.718D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.76D-07 MaxDP=8.34D-06 DE=-2.08D-08 OVMax= 4.18D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.20D-07 CP: 9.66D-01 3.00D+00 5.27D-01 7.42D-01 5.84D-01

CP: 8.86D-01 1.33D+00 1.50D+00 1.55D+00 1.16D+00

CP: 1.37D+00 1.16D+00

E= -1359.18193913583 Delta-E= -0.000000009597 Rises=F Damp=F

DIIS: error= 1.45D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1359.18193913583 IErMin=13 ErrMin= 1.45D-06

ErrMax= 1.45D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.21D-09 BMatP= 1.54D-08

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

Coeff-Com: 0.154D-03-0.191D-03 0.486D-05-0.165D-03 0.154D-04 0.130D-02

Coeff-Com: 0.159D-01 0.768D-02-0.385D-01-0.947D-01-0.849D-01 0.149D+00

Coeff-Com: 0.104D+01

Coeff: 0.154D-03-0.191D-03 0.486D-05-0.165D-03 0.154D-04 0.130D-02

Coeff: 0.159D-01 0.768D-02-0.385D-01-0.947D-01-0.849D-01 0.149D+00

Coeff: 0.104D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.18D-07 MaxDP=5.61D-06 DE=-9.60D-09 OVMax= 2.39D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 6.36D-08 CP: 9.66D-01 3.00D+00 5.27D-01 7.42D-01 5.84D-01

CP: 8.86D-01 1.34D+00 1.50D+00 1.57D+00 1.20D+00

CP: 1.51D+00 1.43D+00 1.24D+00

E= -1359.18193913839 Delta-E= -0.000000002559 Rises=F Damp=F

DIIS: error= 7.36D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1359.18193913839 IErMin=14 ErrMin= 7.36D-07

ErrMax= 7.36D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.00D-10 BMatP= 2.21D-09

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

Coeff-Com: 0.369D-03-0.430D-03-0.238D-04-0.426D-03-0.449D-03-0.688D-03

Coeff-Com: 0.553D-02 0.886D-02 0.237D-02-0.388D-01-0.152D+00-0.924D-01

Coeff-Com: 0.574D+00 0.694D+00

Coeff: 0.369D-03-0.430D-03-0.238D-04-0.426D-03-0.449D-03-0.688D-03

Coeff: 0.553D-02 0.886D-02 0.237D-02-0.388D-01-0.152D+00-0.924D-01

Coeff: 0.574D+00 0.694D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=5.01D-08 MaxDP=2.38D-06 DE=-2.56D-09 OVMax= 9.92D-06

Cycle 15 Pass 1 IDiag 1:

RMSU= 2.51D-08 CP: 9.66D-01 3.00D+00 5.27D-01 7.42D-01 5.84D-01

CP: 8.86D-01 1.34D+00 1.50D+00 1.57D+00 1.21D+00

CP: 1.56D+00 1.51D+00 1.46D+00 1.03D+00

E= -1359.18193913890 Delta-E= -0.000000000507 Rises=F Damp=F

DIIS: error= 3.57D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1359.18193913890 IErMin=15 ErrMin= 3.57D-07

ErrMax= 3.57D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.90D-11 BMatP= 9.00D-10

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

Coeff-Com: -0.960D-05 0.122D-04-0.130D-04-0.260D-04-0.497D-04-0.397D-04

Coeff-Com: -0.103D-02 0.124D-02 0.470D-02-0.353D-03-0.178D-01-0.226D-01

Coeff-Com: -0.531D-01 0.172D+00 0.917D+00

Coeff: -0.960D-05 0.122D-04-0.130D-04-0.260D-04-0.497D-04-0.397D-04

Coeff: -0.103D-02 0.124D-02 0.470D-02-0.353D-03-0.178D-01-0.226D-01

Coeff: -0.531D-01 0.172D+00 0.917D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.71D-08 MaxDP=7.82D-07 DE=-5.07D-10 OVMax= 3.73D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.07D-08 CP: 9.66D-01 3.00D+00 5.27D-01 7.42D-01 5.84D-01

CP: 8.86D-01 1.34D+00 1.50D+00 1.57D+00 1.21D+00

CP: 1.57D+00 1.54D+00 1.50D+00 1.15D+00 1.12D+00

E= -1359.18193913893 Delta-E= -0.000000000029 Rises=F Damp=F

DIIS: error= 1.66D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1359.18193913893 IErMin=16 ErrMin= 1.66D-07

ErrMax= 1.66D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.81D-11 BMatP= 9.90D-11

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

Coeff-Com: -0.250D-04 0.301D-04-0.897D-05-0.287D-05-0.279D-04-0.938D-04

Coeff-Com: -0.132D-02 0.202D-03 0.350D-02 0.410D-02 0.279D-02-0.613D-02

Coeff-Com: -0.901D-01 0.276D-01 0.550D+00 0.510D+00

Coeff: -0.250D-04 0.301D-04-0.897D-05-0.287D-05-0.279D-04-0.938D-04

Coeff: -0.132D-02 0.202D-03 0.350D-02 0.410D-02 0.279D-02-0.613D-02

Coeff: -0.901D-01 0.276D-01 0.550D+00 0.510D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=6.10D-09 MaxDP=2.89D-07 DE=-2.91D-11 OVMax= 1.49D-06

Error on total polarization charges = 0.06720

SCF Done: E(UB3LYP) = -1359.18193914 A.U. after 16 cycles

NFock= 16 Conv=0.61D-08 -V/T= 1.9682

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7630 S= 0.5065

<L.S>= 0.000000000000E+00

KE= 1.403885104174D+03 PE=-9.377468724805D+03 EE= 3.560480380150D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.26

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7630, after 0.7501

Leave Link 502 at Tue Jul 30 19:39:31 2019, MaxMem= 4294967296 cpu: 1459.4

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 636

NBasis= 636 NAE= 111 NBE= 110 NFC= 0 NFV= 0

NROrb= 636 NOA= 111 NOB= 110 NVA= 525 NVB= 526

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.13698093D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.38377542D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.13684683D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.88637072D-01

Leave Link 801 at Tue Jul 30 19:39:31 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 45.

Will process 46 centers per pass.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16185 LenP2D= 44720.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 11 by ecpmxn.

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

Leave Link 1101 at Tue Jul 30 19:39:35 2019, MaxMem= 4294967296 cpu: 56.7

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Tue Jul 30 19:39:35 2019, MaxMem= 4294967296 cpu: 1.5

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 45.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966832.

G2DrvN: will do 46 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

G2PCM: DoFxE=T DoFxN=T DoGrad=T DoDP/DQ/DG/TGxP=FFFF NFrqRd= 0 IEInf=0 SqF1=F DoCFld=F IF1Alg=4.

GePol: Maximum number of non-zero 1st derivatives = 256

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Tue Jul 30 19:41:54 2019, MaxMem= 4294967296 cpu: 2225.8

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=111111111111111111111111111111111111111111111

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Using symmetry in CPHF.

Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.

Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.

NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 4294965570 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 0.

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

IRaf= 650000000 NMat= 42 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

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

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

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

NMat0= 42 NMatS0= 42 NMatT0= 0 NMatD0= 42 NMtDS0= 0 NMtDT0= 0

Integrals replicated using symmetry in FoFCou.

There are 42 degrees of freedom in the 1st order CPHF. IDoFFX=4 NUNeed= 42.

42 vectors produced by pass 0 Test12= 2.77D-13 2.38D-09 XBig12= 8.01D+03 5.90D+01.

AX will form 42 AO Fock derivatives at one time.

42 vectors produced by pass 1 Test12= 2.77D-13 2.38D-09 XBig12= 1.07D+03 6.82D+00.

42 vectors produced by pass 2 Test12= 2.77D-13 2.38D-09 XBig12= 2.78D+02 5.61D+00.

42 vectors produced by pass 3 Test12= 2.77D-13 2.38D-09 XBig12= 6.51D+01 1.68D+00.

42 vectors produced by pass 4 Test12= 2.77D-13 2.38D-09 XBig12= 4.89D+00 4.09D-01.

42 vectors produced by pass 5 Test12= 2.77D-13 2.38D-09 XBig12= 1.60D-01 3.82D-02.

42 vectors produced by pass 6 Test12= 2.77D-13 2.38D-09 XBig12= 5.40D-03 6.50D-03.

42 vectors produced by pass 7 Test12= 2.77D-13 2.38D-09 XBig12= 1.35D-04 1.04D-03.

38 vectors produced by pass 8 Test12= 2.77D-13 2.38D-09 XBig12= 2.37D-06 1.24D-04.

21 vectors produced by pass 9 Test12= 2.77D-13 2.38D-09 XBig12= 3.17D-08 1.58D-05.

5 vectors produced by pass 10 Test12= 2.77D-13 2.38D-09 XBig12= 3.96D-10 1.63D-06.

2 vectors produced by pass 11 Test12= 2.77D-13 2.38D-09 XBig12= 5.39D-12 1.68D-07.

2 vectors produced by pass 12 Test12= 2.77D-13 2.38D-09 XBig12= 7.17D-14 2.11D-08.

1 vectors produced by pass 13 Test12= 2.77D-13 2.38D-09 XBig12= 1.90D-15 2.44D-09.

InvSVY: IOpt=1 It= 1 EMax= 9.95D-14

Solved reduced A of dimension 405 with 42 vectors.

FullF1: Do perturbations 1 to 42.

Isotropic polarizability for W= 0.000000 1003.72 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Tue Jul 30 21:22:18 2019, MaxMem= 4294967296 cpu: 96390.4

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

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

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

Population analysis using the SCF density.

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

Orbital symmetries:

Alpha Orbitals:

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

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

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(B2)

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The electronic state is 2-B2.

Alpha occ. eigenvalues -- -14.29462 -14.29462 -14.29399 -14.29398 -10.20536

Alpha occ. eigenvalues -- -10.20535 -10.20535 -10.20535 -10.19586 -10.19586

Alpha occ. eigenvalues -- -10.19586 -10.19586 -10.19503 -10.19503 -10.19503

Alpha occ. eigenvalues -- -10.19503 -10.17460 -10.17460 -10.17460 -10.17460

Alpha occ. eigenvalues -- -10.16584 -10.16584 -10.16515 -10.16515 -10.16032

Alpha occ. eigenvalues -- -10.16032 -10.16032 -10.16032 -10.15201 -10.15201

Alpha occ. eigenvalues -- -10.15144 -10.15144 -0.95528 -0.94908 -0.94391

Alpha occ. eigenvalues -- -0.93723 -0.83355 -0.81557 -0.81263 -0.79562

Alpha occ. eigenvalues -- -0.76310 -0.76171 -0.75349 -0.74929 -0.74191

Alpha occ. eigenvalues -- -0.73458 -0.73425 -0.71646 -0.71312 -0.66472

Alpha occ. eigenvalues -- -0.65777 -0.61250 -0.58815 -0.58175 -0.57713

Alpha occ. eigenvalues -- -0.57320 -0.56604 -0.55901 -0.54888 -0.54840

Alpha occ. eigenvalues -- -0.54553 -0.54092 -0.53984 -0.53848 -0.53435

Alpha occ. eigenvalues -- -0.51845 -0.51258 -0.51252 -0.50799 -0.50183

Alpha occ. eigenvalues -- -0.50102 -0.49102 -0.47994 -0.44141 -0.43307

Alpha occ. eigenvalues -- -0.43304 -0.42826 -0.41645 -0.41518 -0.41492

Alpha occ. eigenvalues -- -0.41147 -0.39929 -0.39736 -0.38741 -0.38490

Alpha occ. eigenvalues -- -0.37225 -0.37161 -0.36786 -0.36685 -0.36323

Alpha occ. eigenvalues -- -0.36270 -0.33153 -0.32943 -0.31477 -0.30965

Alpha occ. eigenvalues -- -0.30683 -0.28648 -0.28298 -0.28261 -0.27936

Alpha occ. eigenvalues -- -0.26616 -0.26001 -0.25718 -0.25668 -0.25226

Alpha occ. eigenvalues -- -0.24254 -0.23917 -0.23532 -0.20382 -0.19186

Alpha occ. eigenvalues -- -0.12977

Alpha virt. eigenvalues -- -0.09139 -0.05389 0.03009 0.03714 0.03954

Alpha virt. eigenvalues -- 0.04091 0.04403 0.04470 0.04622 0.04984

Alpha virt. eigenvalues -- 0.05067 0.05353 0.06038 0.06058 0.06133

Alpha virt. eigenvalues -- 0.06182 0.06257 0.07599 0.08233 0.08777

Alpha virt. eigenvalues -- 0.08820 0.08847 0.10091 0.10190 0.10298

Alpha virt. eigenvalues -- 0.10369 0.11886 0.12842 0.13024 0.14039

Alpha virt. eigenvalues -- 0.15140 0.16764 0.17472 0.17473 0.17578

Alpha virt. eigenvalues -- 0.18276 0.19413 0.20222 0.21038 0.23007

Alpha virt. eigenvalues -- 0.23961 0.24441 0.24877 0.25117 0.25484

Alpha virt. eigenvalues -- 0.25637 0.25772 0.26750 0.26831 0.27486

Alpha virt. eigenvalues -- 0.27658 0.27786 0.29027 0.30704 0.31109

Alpha virt. eigenvalues -- 0.31888 0.32184 0.33338 0.33507 0.33959

Alpha virt. eigenvalues -- 0.36191 0.36210 0.36326 0.36403 0.36557

Alpha virt. eigenvalues -- 0.36945 0.37114 0.37277 0.37314 0.37623

Alpha virt. eigenvalues -- 0.37687 0.39133 0.39508 0.40329 0.40859

Alpha virt. eigenvalues -- 0.41273 0.41294 0.41731 0.42151 0.42282

Alpha virt. eigenvalues -- 0.42601 0.43273 0.43400 0.44130 0.44374

Alpha virt. eigenvalues -- 0.44866 0.45077 0.45104 0.45527 0.45971

Alpha virt. eigenvalues -- 0.46351 0.46791 0.48188 0.48438 0.48727

Alpha virt. eigenvalues -- 0.49129 0.49642 0.49761 0.50224 0.50432

Alpha virt. eigenvalues -- 0.51838 0.52123 0.52354 0.52551 0.52756

Alpha virt. eigenvalues -- 0.53050 0.53258 0.53360 0.55763 0.57101

Alpha virt. eigenvalues -- 0.57278 0.57917 0.58040 0.58339 0.58339

Alpha virt. eigenvalues -- 0.58388 0.58652 0.58754 0.59426 0.59653

Alpha virt. eigenvalues -- 0.61924 0.62838 0.63075 0.63311 0.63403

Alpha virt. eigenvalues -- 0.63642 0.63966 0.64373 0.64774 0.64788

Alpha virt. eigenvalues -- 0.65563 0.65649 0.65955 0.66208 0.66348

Alpha virt. eigenvalues -- 0.69187 0.69294 0.69805 0.69884 0.71171

Alpha virt. eigenvalues -- 0.71203 0.71342 0.71445 0.72645 0.72676

Alpha virt. eigenvalues -- 0.74590 0.74724 0.75062 0.75356 0.75359

Alpha virt. eigenvalues -- 0.75817 0.75851 0.76335 0.76371 0.76551

Alpha virt. eigenvalues -- 0.78130 0.78768 0.79876 0.82244 0.82280

Alpha virt. eigenvalues -- 0.82873 0.82903 0.84100 0.85054 0.85496

Alpha virt. eigenvalues -- 0.86550 0.86741 0.87083 0.89325 0.90857

Alpha virt. eigenvalues -- 0.91365 0.92053 0.92266 0.93550 0.93655

Alpha virt. eigenvalues -- 0.95744 0.96348 0.97184 0.97815 0.98484

Alpha virt. eigenvalues -- 0.98735 1.00452 1.01702 1.01849 1.01940

Alpha virt. eigenvalues -- 1.02217 1.02640 1.02917 1.03013 1.05416

Alpha virt. eigenvalues -- 1.06699 1.07113 1.07195 1.07432 1.08355

Alpha virt. eigenvalues -- 1.08768 1.09884 1.09954 1.12580 1.13288

Alpha virt. eigenvalues -- 1.13397 1.13544 1.13754 1.14090 1.14212

Alpha virt. eigenvalues -- 1.14870 1.14985 1.15230 1.16084 1.16781

Alpha virt. eigenvalues -- 1.17528 1.17798 1.18417 1.18562 1.19409

Alpha virt. eigenvalues -- 1.20048 1.20131 1.20263 1.20392 1.22128

Alpha virt. eigenvalues -- 1.22370 1.22412 1.22623 1.23115 1.25020

Alpha virt. eigenvalues -- 1.25803 1.26033 1.26068 1.26732 1.26779

Alpha virt. eigenvalues -- 1.28892 1.29333 1.29571 1.30577 1.32889

Alpha virt. eigenvalues -- 1.33118 1.34816 1.35059 1.35451 1.38350

Alpha virt. eigenvalues -- 1.43882 1.44317 1.44550 1.48879 1.49146

Alpha virt. eigenvalues -- 1.49665 1.49769 1.50591 1.53350 1.53573

Alpha virt. eigenvalues -- 1.53756 1.56077 1.56081 1.56245 1.56274

Alpha virt. eigenvalues -- 1.56317 1.56322 1.58422 1.58840 1.59614

Alpha virt. eigenvalues -- 1.59770 1.59893 1.60173 1.60564 1.60670

Alpha virt. eigenvalues -- 1.62204 1.62336 1.62612 1.63670 1.63929

Alpha virt. eigenvalues -- 1.64516 1.66043 1.66049 1.66452 1.67003

Alpha virt. eigenvalues -- 1.67086 1.68095 1.71288 1.71354 1.73178

Alpha virt. eigenvalues -- 1.74181 1.74913 1.76862 1.77882 1.77981

Alpha virt. eigenvalues -- 1.78006 1.80096 1.80466 1.80669 1.81064

Alpha virt. eigenvalues -- 1.81224 1.81559 1.82094 1.82233 1.84798

Alpha virt. eigenvalues -- 1.85713 1.87291 1.87475 1.88978 1.89839

Alpha virt. eigenvalues -- 1.89863 1.89939 1.89954 1.91131 1.91222

Alpha virt. eigenvalues -- 1.91593 1.91966 1.94345 1.95539 1.95685

Alpha virt. eigenvalues -- 1.95713 1.95989 1.96197 1.96945 1.97464

Alpha virt. eigenvalues -- 1.98403 1.98528 2.00480 2.00861 2.02225

Alpha virt. eigenvalues -- 2.04251 2.04587 2.05254 2.05612 2.05995

Alpha virt. eigenvalues -- 2.10328 2.11048 2.12992 2.13261 2.15127

Alpha virt. eigenvalues -- 2.19182 2.20890 2.27296 2.28234 2.28813

Alpha virt. eigenvalues -- 2.29302 2.29724 2.32642 2.32667 2.34651

Alpha virt. eigenvalues -- 2.34912 2.35744 2.37140 2.37388 2.37540

Alpha virt. eigenvalues -- 2.38161 2.38552 2.41602 2.41671 2.41828

Alpha virt. eigenvalues -- 2.42006 2.42307 2.42731 2.44566 2.46796

Alpha virt. eigenvalues -- 2.49451 2.49465 2.50437 2.50848 2.53335

Alpha virt. eigenvalues -- 2.54500 2.55015 2.55073 2.57230 2.57593

Alpha virt. eigenvalues -- 2.58156 2.58549 2.58972 2.59154 2.59275

Alpha virt. eigenvalues -- 2.61048 2.61569 2.62962 2.63808 2.63857

Alpha virt. eigenvalues -- 2.65623 2.65951 2.66014 2.67925 2.68543

Alpha virt. eigenvalues -- 2.72248 2.72392 2.74800 2.77985 2.79023

Alpha virt. eigenvalues -- 2.79398 2.81424 2.82157 2.83774 2.84264

Alpha virt. eigenvalues -- 2.84537 2.85717 2.88089 2.88537 2.89499

Alpha virt. eigenvalues -- 2.89523 2.89536 2.89554 2.92958 2.96455

Alpha virt. eigenvalues -- 2.96556 2.97047 2.97262 2.97439 2.98523

Alpha virt. eigenvalues -- 2.98746 2.99766 2.99860 3.00743 3.01754

Alpha virt. eigenvalues -- 3.02827 3.03758 3.05293 3.05378 3.05781

Alpha virt. eigenvalues -- 3.05972 3.06751 3.06989 3.08426 3.09299

Alpha virt. eigenvalues -- 3.09505 3.09777 3.10450 3.18078 3.18665

Alpha virt. eigenvalues -- 3.19806 3.20193 3.20544 3.22095 3.22447

Alpha virt. eigenvalues -- 3.24467 3.26697 3.26748 3.27598 3.29437

Alpha virt. eigenvalues -- 3.31411 3.31631 3.32154 3.32184 3.33602

Alpha virt. eigenvalues -- 3.33645 3.35153 3.36365 3.37036 3.38888

Alpha virt. eigenvalues -- 3.39162 3.46125 3.49606 3.53086 3.53254

Alpha virt. eigenvalues -- 3.54083 3.57508 3.58053 3.58514 3.59344

Alpha virt. eigenvalues -- 3.60743 3.64437 3.66632 3.66637 3.82612

Alpha virt. eigenvalues -- 3.83005 3.83416 3.85212 3.86932 3.87104

Alpha virt. eigenvalues -- 3.87294 3.91130 3.93788 3.95784 3.97938

Alpha virt. eigenvalues -- 4.01324 4.12973 4.21673 4.22349 4.33787

Alpha virt. eigenvalues -- 4.34502 4.48253 4.52904 4.53321 4.62607

Alpha virt. eigenvalues -- 4.66983 4.67110 4.67459 5.15494 5.20185

Alpha virt. eigenvalues -- 5.20426 5.32433 7.79080 7.79275 7.88085

Alpha virt. eigenvalues -- 7.93858 8.13956 11.11966 23.28015 23.33234

Alpha virt. eigenvalues -- 23.33519 23.36288 23.53152 23.55358 23.58505

Alpha virt. eigenvalues -- 23.59508 23.76347 23.77980 23.79023 23.81054

Alpha virt. eigenvalues -- 23.89970 23.91084 23.97517 23.98024 24.02482

Alpha virt. eigenvalues -- 24.02773 24.04870 24.04987 24.11603 24.11607

Alpha virt. eigenvalues -- 24.14905 24.15119 24.94461 24.94516 24.94827

Alpha virt. eigenvalues -- 24.94838 35.63666 35.65164 35.66442 35.66452

Beta occ. eigenvalues -- -14.29444 -14.29444 -14.29302 -14.29301 -10.20571

Beta occ. eigenvalues -- -10.20571 -10.20571 -10.20571 -10.19447 -10.19447

Beta occ. eigenvalues -- -10.19447 -10.19446 -10.19385 -10.19385 -10.19385

Beta occ. eigenvalues -- -10.19385 -10.17492 -10.17492 -10.17492 -10.17492

Beta occ. eigenvalues -- -10.16590 -10.16590 -10.16521 -10.16521 -10.15966

Beta occ. eigenvalues -- -10.15966 -10.15966 -10.15966 -10.15105 -10.15105

Beta occ. eigenvalues -- -10.15048 -10.15048 -0.95376 -0.94767 -0.94225

Beta occ. eigenvalues -- -0.93573 -0.83102 -0.81350 -0.80998 -0.79364

Beta occ. eigenvalues -- -0.76226 -0.76092 -0.75170 -0.74721 -0.74099

Beta occ. eigenvalues -- -0.73349 -0.73260 -0.71440 -0.71100 -0.66065

Beta occ. eigenvalues -- -0.65725 -0.61048 -0.58686 -0.58081 -0.57677

Beta occ. eigenvalues -- -0.57163 -0.56560 -0.55880 -0.54850 -0.54840

Beta occ. eigenvalues -- -0.54545 -0.53977 -0.53898 -0.53712 -0.53336

Beta occ. eigenvalues -- -0.51791 -0.51194 -0.51184 -0.50700 -0.50102

Beta occ. eigenvalues -- -0.50014 -0.49040 -0.47904 -0.44037 -0.43214

Beta occ. eigenvalues -- -0.43213 -0.42379 -0.41552 -0.41437 -0.41192

Beta occ. eigenvalues -- -0.40521 -0.39875 -0.39680 -0.38425 -0.38285

Beta occ. eigenvalues -- -0.37146 -0.37022 -0.36703 -0.36654 -0.36210

Beta occ. eigenvalues -- -0.35720 -0.32665 -0.32501 -0.31133 -0.30831

Beta occ. eigenvalues -- -0.30655 -0.28619 -0.28263 -0.28227 -0.27900

Beta occ. eigenvalues -- -0.26200 -0.25537 -0.25315 -0.25278 -0.25135

Beta occ. eigenvalues -- -0.23489 -0.23461 -0.23218 -0.19403 -0.17996

Beta virt. eigenvalues -- -0.09132 -0.08967 -0.04204 0.03095 0.03748

Beta virt. eigenvalues -- 0.03990 0.04118 0.04646 0.04725 0.05021

Beta virt. eigenvalues -- 0.05221 0.05372 0.05437 0.06094 0.06223

Beta virt. eigenvalues -- 0.06240 0.06569 0.06953 0.08126 0.08255

Beta virt. eigenvalues -- 0.08801 0.08851 0.08879 0.10108 0.10204

Beta virt. eigenvalues -- 0.10333 0.10408 0.11911 0.12846 0.13086

Beta virt. eigenvalues -- 0.14074 0.15530 0.16820 0.18084 0.18124

Beta virt. eigenvalues -- 0.18143 0.18374 0.19461 0.20292 0.21141

Beta virt. eigenvalues -- 0.23281 0.24123 0.24546 0.24951 0.25177

Beta virt. eigenvalues -- 0.25563 0.25688 0.25861 0.26819 0.26957

Beta virt. eigenvalues -- 0.27632 0.27776 0.27912 0.29105 0.30893

Beta virt. eigenvalues -- 0.31190 0.31971 0.32262 0.33397 0.33558

Beta virt. eigenvalues -- 0.34025 0.36369 0.36376 0.36534 0.36550

Beta virt. eigenvalues -- 0.36733 0.37125 0.37173 0.37367 0.37517

Beta virt. eigenvalues -- 0.37660 0.37844 0.39248 0.39657 0.40471

Beta virt. eigenvalues -- 0.41033 0.41312 0.41526 0.41971 0.42256

Beta virt. eigenvalues -- 0.42574 0.42740 0.43425 0.43511 0.44229

Beta virt. eigenvalues -- 0.44572 0.45024 0.45232 0.45301 0.45614

Beta virt. eigenvalues -- 0.46240 0.46488 0.46915 0.48306 0.48689

Beta virt. eigenvalues -- 0.48924 0.49310 0.49920 0.49939 0.50335

Beta virt. eigenvalues -- 0.50533 0.51973 0.52182 0.52536 0.52624

Beta virt. eigenvalues -- 0.52980 0.53173 0.53335 0.53426 0.55932

Beta virt. eigenvalues -- 0.57241 0.57387 0.58024 0.58144 0.58414

Beta virt. eigenvalues -- 0.58505 0.58660 0.58729 0.58856 0.59551

Beta virt. eigenvalues -- 0.59698 0.62008 0.62856 0.63277 0.63476

Beta virt. eigenvalues -- 0.63479 0.63697 0.63987 0.64451 0.64858

Beta virt. eigenvalues -- 0.64866 0.65655 0.65688 0.66043 0.66365

Beta virt. eigenvalues -- 0.66393 0.69201 0.69415 0.69823 0.69957

Beta virt. eigenvalues -- 0.71268 0.71287 0.71521 0.71716 0.72737

Beta virt. eigenvalues -- 0.72748 0.74641 0.75081 0.75114 0.75415

Beta virt. eigenvalues -- 0.75419 0.75909 0.75935 0.76449 0.76458

Beta virt. eigenvalues -- 0.76642 0.78191 0.78989 0.80221 0.82302

Beta virt. eigenvalues -- 0.82369 0.82939 0.82940 0.84200 0.85098

Beta virt. eigenvalues -- 0.85627 0.86637 0.86782 0.87263 0.89417

Beta virt. eigenvalues -- 0.90944 0.91415 0.92194 0.92380 0.93652

Beta virt. eigenvalues -- 0.93700 0.95812 0.96481 0.97244 0.98097

Beta virt. eigenvalues -- 0.98694 0.98757 1.00545 1.01842 1.02092

Beta virt. eigenvalues -- 1.02288 1.02327 1.02680 1.02991 1.03156

Beta virt. eigenvalues -- 1.05472 1.07005 1.07288 1.07355 1.07636

Beta virt. eigenvalues -- 1.08689 1.09034 1.10019 1.10159 1.12702

Beta virt. eigenvalues -- 1.13367 1.13443 1.13844 1.13898 1.14190

Beta virt. eigenvalues -- 1.14322 1.15012 1.15170 1.15433 1.16219

Beta virt. eigenvalues -- 1.16870 1.17601 1.18005 1.18539 1.18785

Beta virt. eigenvalues -- 1.19555 1.20166 1.20176 1.20477 1.20530

Beta virt. eigenvalues -- 1.22228 1.22456 1.22536 1.22885 1.23193

Beta virt. eigenvalues -- 1.25054 1.25954 1.26111 1.26172 1.26820

Beta virt. eigenvalues -- 1.26923 1.29018 1.29445 1.29819 1.30759

Beta virt. eigenvalues -- 1.33157 1.33301 1.34943 1.35193 1.35575

Beta virt. eigenvalues -- 1.38410 1.43998 1.44431 1.44628 1.49024

Beta virt. eigenvalues -- 1.49340 1.49929 1.49967 1.50847 1.53506

Beta virt. eigenvalues -- 1.53638 1.53819 1.56121 1.56180 1.56376

Beta virt. eigenvalues -- 1.56407 1.56445 1.56445 1.58712 1.58898

Beta virt. eigenvalues -- 1.59737 1.59878 1.60000 1.60317 1.60766

Beta virt. eigenvalues -- 1.60803 1.62269 1.62459 1.62762 1.63803

Beta virt. eigenvalues -- 1.64013 1.64852 1.66126 1.66161 1.66491

Beta virt. eigenvalues -- 1.67034 1.67264 1.68311 1.71318 1.71498

Beta virt. eigenvalues -- 1.73280 1.74344 1.75006 1.77100 1.77970

Beta virt. eigenvalues -- 1.78050 1.78126 1.80397 1.80694 1.80712

Beta virt. eigenvalues -- 1.81119 1.81509 1.81655 1.82199 1.82332

Beta virt. eigenvalues -- 1.84826 1.85962 1.87370 1.87686 1.89169

Beta virt. eigenvalues -- 1.89992 1.90128 1.90161 1.90307 1.91313

Beta virt. eigenvalues -- 1.91416 1.91764 1.92187 1.94623 1.95771

Beta virt. eigenvalues -- 1.95909 1.96041 1.96140 1.96378 1.97156

Beta virt. eigenvalues -- 1.97731 1.98550 1.98583 2.00562 2.00909

Beta virt. eigenvalues -- 2.02488 2.04412 2.04801 2.05475 2.05732

Beta virt. eigenvalues -- 2.06474 2.10426 2.11117 2.13030 2.13598

Beta virt. eigenvalues -- 2.15154 2.19306 2.20952 2.27601 2.28543

Beta virt. eigenvalues -- 2.28906 2.29317 2.29949 2.32888 2.32922

Beta virt. eigenvalues -- 2.34896 2.35006 2.35783 2.37388 2.37468

Beta virt. eigenvalues -- 2.37771 2.38522 2.38589 2.41620 2.41683

Beta virt. eigenvalues -- 2.41865 2.42032 2.42446 2.42810 2.44656

Beta virt. eigenvalues -- 2.47098 2.49486 2.49626 2.50502 2.50978

Beta virt. eigenvalues -- 2.53622 2.54764 2.55290 2.55321 2.57337

Beta virt. eigenvalues -- 2.57931 2.58255 2.58783 2.59099 2.59186

Beta virt. eigenvalues -- 2.59654 2.61121 2.61741 2.63019 2.64048

Beta virt. eigenvalues -- 2.64182 2.65632 2.65987 2.66308 2.68166

Beta virt. eigenvalues -- 2.68718 2.72304 2.72437 2.74873 2.78247

Beta virt. eigenvalues -- 2.79236 2.79599 2.81606 2.82391 2.83977

Beta virt. eigenvalues -- 2.84311 2.84921 2.86087 2.88129 2.88591

Beta virt. eigenvalues -- 2.89634 2.89640 2.89653 2.89664 2.93013

Beta virt. eigenvalues -- 2.96658 2.96727 2.97118 2.97323 2.97983

Beta virt. eigenvalues -- 2.98741 2.99093 2.99758 2.99844 3.00766

Beta virt. eigenvalues -- 3.02103 3.02887 3.03771 3.05725 3.05836

Beta virt. eigenvalues -- 3.05915 3.06051 3.06805 3.07064 3.08497

Beta virt. eigenvalues -- 3.09578 3.09823 3.09836 3.10502 3.18091

Beta virt. eigenvalues -- 3.18697 3.19832 3.20243 3.20624 3.22124

Beta virt. eigenvalues -- 3.22479 3.24556 3.26788 3.26810 3.27651

Beta virt. eigenvalues -- 3.29502 3.31491 3.31676 3.32197 3.32241

Beta virt. eigenvalues -- 3.33672 3.33689 3.35222 3.36395 3.37125

Beta virt. eigenvalues -- 3.38993 3.39199 3.46212 3.49682 3.53138

Beta virt. eigenvalues -- 3.53294 3.54130 3.57510 3.58115 3.58519

Beta virt. eigenvalues -- 3.59507 3.60879 3.64513 3.66684 3.66720

Beta virt. eigenvalues -- 3.82754 3.83109 3.83516 3.85270 3.87026

Beta virt. eigenvalues -- 3.87491 3.87564 3.91410 3.93890 3.95926

Beta virt. eigenvalues -- 3.98059 4.01448 4.13138 4.21832 4.22523

Beta virt. eigenvalues -- 4.33944 4.34641 4.48331 4.52953 4.53550

Beta virt. eigenvalues -- 4.62737 4.67168 4.67171 4.67636 5.15597

Beta virt. eigenvalues -- 5.20297 5.20521 5.32543 7.79080 7.79300

Beta virt. eigenvalues -- 7.88084 7.93860 8.13960 11.11975 23.28058

Beta virt. eigenvalues -- 23.33268 23.33559 23.36323 23.53184 23.55360

Beta virt. eigenvalues -- 23.58614 23.59584 23.76423 23.78067 23.79083

Beta virt. eigenvalues -- 23.81125 23.90063 23.91180 23.97620 23.98133

Beta virt. eigenvalues -- 24.02568 24.02870 24.04933 24.05057 24.11716

Beta virt. eigenvalues -- 24.11717 24.14899 24.15116 24.94474 24.94529

Beta virt. eigenvalues -- 24.94840 24.94851 35.63714 35.65238 35.66406

Beta virt. eigenvalues -- 35.66610

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 5.170049 0.393438 -0.076760 -0.066269 0.541997 0.012800

2 C 0.393438 4.886870 0.431485 -0.142859 -0.066269 -0.000721

3 N -0.076760 0.431485 6.977840 0.431485 -0.076760 -0.028564

4 C -0.066269 -0.142859 0.431485 4.886870 0.393438 0.428978

5 C 0.541997 -0.066269 -0.076760 0.393438 5.170049 -0.073316

6 C 0.012800 -0.000721 -0.028564 0.428978 -0.073316 5.253993

7 C -0.001130 -0.000397 -0.016136 -0.107086 0.012604 0.389185

8 N 0.000053 0.000343 -0.013940 -0.018992 -0.000335 -0.021511

9 C -0.000005 0.000004 0.000257 -0.000274 0.000042 0.000226

10 C 0.000001 -0.000005 0.000044 -0.001205 -0.000005 0.014171

11 C -0.000006 0.000047 -0.000255 0.013687 -0.000175 -0.078359

12 C -0.073316 0.428978 -0.028564 -0.000721 0.012800 -0.002150

13 C 0.012604 -0.107086 -0.016136 -0.000397 -0.001130 0.000179

14 C -0.000175 0.013687 -0.000255 0.000047 -0.000006 0.000001

15 C -0.000005 -0.001205 0.000044 -0.000005 0.000001 -0.000000

16 C 0.000042 -0.000274 0.000257 0.000004 -0.000005 0.000002

17 N -0.000335 -0.018992 -0.013940 0.000343 0.000053 -0.000152

18 C 0.000001 0.000196 -0.000144 0.000001 -0.000000 0.000002

19 C -0.000000 -0.000060 0.000158 -0.000004 0.000000 0.000001

20 C -0.000000 -0.000000 0.000001 0.000000 0.000000 -0.000000

21 C 0.000000 0.000000 0.000001 -0.000000 -0.000000 0.000001

22 C 0.000000 -0.000004 0.000158 -0.000060 -0.000000 0.000196

23 N 0.000001 0.000158 -0.001633 0.000158 0.000001 -0.000144

24 H 0.387522 -0.038768 0.005410 0.005824 -0.034594 -0.000200

25 H -0.034594 0.005824 0.005410 -0.038768 0.387522 -0.005590

26 H 0.000000 0.000000 0.000002 0.000010 0.000000 -0.000195

27 H -0.000000 0.000001 0.000000 -0.000043 0.000004 -0.005605

28 H 0.000004 -0.000043 0.000000 0.000001 -0.000000 0.000000

29 H 0.000000 0.000010 0.000002 0.000000 0.000000 0.000000

30 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

31 H 0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.000000

32 Zn 0.002530 -0.014489 0.134943 -0.014489 0.002530 -0.011576

33 C -0.000000 0.000001 -0.000144 0.000196 0.000001 -0.002119

34 C -0.000000 0.000000 -0.000000 0.000002 0.000000 -0.000048

35 C -0.015042 -0.078372 0.003864 -0.000516 0.002592 -0.000054

36 C -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000002

37 C -0.000230 -0.005901 -0.000051 -0.000049 0.000356 -0.000002

38 C 0.002592 -0.000516 0.003864 -0.078372 -0.015042 0.547807

39 C 0.000356 -0.000049 -0.000051 -0.005901 -0.000230 -0.109539

40 C 0.000000 0.000002 -0.000000 0.000000 -0.000000 0.000000

41 C 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

42 H 0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000

43 H -0.000000 0.000000 0.000000 0.000000 0.000000 -0.000000

44 H 0.000002 -0.000000 0.000001 -0.000077 0.000100 0.001954

45 H 0.000100 -0.000077 0.000001 -0.000000 0.000002 -0.000000

7 8 9 10 11 12

1 C -0.001130 0.000053 -0.000005 0.000001 -0.000006 -0.073316

2 C -0.000397 0.000343 0.000004 -0.000005 0.000047 0.428978

3 N -0.016136 -0.013940 0.000257 0.000044 -0.000255 -0.028564

4 C -0.107086 -0.018992 -0.000274 -0.001205 0.013687 -0.000721

5 C 0.012604 -0.000335 0.000042 -0.000005 -0.000175 0.012800

6 C 0.389185 -0.021511 0.000226 0.014171 -0.078359 -0.002150

7 C 4.898828 0.438861 -0.153496 -0.072310 0.445207 0.000179

8 N 0.438861 6.946834 0.438861 -0.083928 -0.083928 -0.000152

9 C -0.153496 0.438861 4.898828 0.445207 -0.072310 0.000002

10 C -0.072310 -0.083928 0.445207 5.217685 0.495966 -0.000000

11 C 0.445207 -0.083928 -0.072310 0.495966 5.217685 0.000001

12 C 0.000179 -0.000152 0.000002 -0.000000 0.000001 5.253993

13 C -0.000051 0.000147 -0.000005 0.000000 -0.000000 0.389185

14 C -0.000000 0.000002 0.000000 0.000000 -0.000000 -0.078359

15 C 0.000000 0.000002 -0.000000 -0.000000 0.000000 0.014171

16 C -0.000005 0.000147 -0.000051 -0.000000 0.000000 0.000226

17 N 0.000147 -0.001488 0.000147 0.000002 0.000002 -0.021511

18 C 0.000002 -0.000152 0.000179 0.000001 -0.000000 -0.002119

19 C 0.000004 0.000343 -0.000397 0.000047 -0.000005 0.000196

20 C -0.000005 0.000053 -0.001130 -0.000006 0.000001 0.000001

21 C 0.000042 -0.000335 0.012604 -0.000175 -0.000005 -0.000000

22 C -0.000274 -0.018992 -0.107086 0.013687 -0.001205 0.000001

23 N 0.000257 -0.013940 -0.016136 -0.000255 0.000044 -0.000144

24 H 0.000008 0.000002 0.000000 0.000000 0.000000 -0.005590

25 H 0.000003 -0.000002 0.000001 -0.000000 0.000002 -0.000200

26 H 0.005522 0.005887 -0.040361 0.389919 -0.035952 0.000000

27 H -0.040361 0.005887 0.005522 -0.035952 0.389919 0.000000

28 H -0.000000 0.000000 -0.000000 0.000000 -0.000000 -0.005605

29 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000195

30 H 0.000000 0.000002 0.000008 0.000000 0.000000 0.000000

31 H 0.000001 -0.000002 0.000003 0.000002 -0.000000 0.000000

32 Zn -0.013929 0.136849 -0.013929 0.002345 0.002345 -0.011576

33 C 0.000226 -0.021511 0.389185 -0.078359 0.014171 0.000002

34 C -0.000432 0.003961 -0.075406 -0.016249 0.002399 0.000000

35 C 0.000002 -0.000000 0.000000 -0.000000 0.000000 0.547807

36 C -0.000050 -0.000054 -0.004850 -0.000409 0.000314 0.000000

37 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.109539

38 C -0.075406 0.003961 -0.000432 0.002399 -0.016249 -0.000054

39 C -0.004850 -0.000054 -0.000050 0.000314 -0.000409 -0.000002

40 C 0.000000 -0.000000 0.000002 0.000000 -0.000000 -0.000048

41 C -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000002

42 H 0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

43 H -0.000000 0.000001 -0.000010 0.000088 0.000001 0.000000

44 H -0.000010 0.000001 -0.000000 0.000001 0.000088 -0.000000

45 H 0.000000 0.000000 0.000000 -0.000000 0.000000 0.001954

13 14 15 16 17 18

1 C 0.012604 -0.000175 -0.000005 0.000042 -0.000335 0.000001

2 C -0.107086 0.013687 -0.001205 -0.000274 -0.018992 0.000196

3 N -0.016136 -0.000255 0.000044 0.000257 -0.013940 -0.000144

4 C -0.000397 0.000047 -0.000005 0.000004 0.000343 0.000001

5 C -0.001130 -0.000006 0.000001 -0.000005 0.000053 -0.000000

6 C 0.000179 0.000001 -0.000000 0.000002 -0.000152 0.000002

7 C -0.000051 -0.000000 0.000000 -0.000005 0.000147 0.000002

8 N 0.000147 0.000002 0.000002 0.000147 -0.001488 -0.000152

9 C -0.000005 0.000000 -0.000000 -0.000051 0.000147 0.000179

10 C 0.000000 0.000000 -0.000000 -0.000000 0.000002 0.000001

11 C -0.000000 -0.000000 0.000000 0.000000 0.000002 -0.000000

12 C 0.389185 -0.078359 0.014171 0.000226 -0.021511 -0.002119

13 C 4.898828 0.445207 -0.072310 -0.153496 0.438861 0.000226

14 C 0.445207 5.217685 0.495966 -0.072310 -0.083928 0.014171

15 C -0.072310 0.495966 5.217685 0.445207 -0.083928 -0.078359

16 C -0.153496 -0.072310 0.445207 4.898828 0.438861 0.389185

17 N 0.438861 -0.083928 -0.083928 0.438861 6.946834 -0.021511

18 C 0.000226 0.014171 -0.078359 0.389185 -0.021511 5.253993

19 C -0.000274 -0.001205 0.013687 -0.107086 -0.018992 0.428978

20 C 0.000042 -0.000005 -0.000175 0.012604 -0.000335 -0.073316

21 C -0.000005 0.000001 -0.000006 -0.001130 0.000053 0.012800

22 C 0.000004 -0.000005 0.000047 -0.000397 0.000343 -0.000721

23 N 0.000257 0.000044 -0.000255 -0.016136 -0.013940 -0.028564

24 H 0.000003 0.000002 -0.000000 0.000001 -0.000002 0.000000

25 H 0.000008 0.000000 0.000000 0.000000 0.000002 0.000000

26 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

27 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

28 H -0.040361 0.389919 -0.035952 0.005522 0.005887 -0.000195

29 H 0.005522 -0.035952 0.389919 -0.040361 0.005887 -0.005605

30 H 0.000001 -0.000000 0.000002 0.000003 -0.000002 -0.005590

31 H 0.000000 0.000000 0.000000 0.000008 0.000002 -0.000200

32 Zn -0.013929 0.002345 0.002345 -0.013929 0.136849 -0.011576

33 C 0.000002 -0.000000 0.000001 0.000179 -0.000152 -0.002150

34 C 0.000000 -0.000000 0.000000 0.000002 -0.000000 -0.000054

35 C -0.075406 -0.016249 0.002399 -0.000432 0.003961 -0.000048

36 C -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000002

37 C -0.004850 -0.000409 0.000314 -0.000050 -0.000054 -0.000002

38 C 0.000002 0.000000 -0.000000 0.000000 -0.000000 0.000000

39 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

40 C -0.000432 0.002399 -0.016249 -0.075406 0.003961 0.547807

41 C -0.000050 0.000314 -0.000409 -0.004850 -0.000054 -0.109539

42 H -0.000000 0.000001 0.000088 -0.000010 0.000001 0.001954

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 -0.000010 0.000088 0.000001 -0.000000 0.000001 -0.000000

19 20 21 22 23 24

1 C -0.000000 -0.000000 0.000000 0.000000 0.000001 0.387522

2 C -0.000060 -0.000000 0.000000 -0.000004 0.000158 -0.038768

3 N 0.000158 0.000001 0.000001 0.000158 -0.001633 0.005410

4 C -0.000004 0.000000 -0.000000 -0.000060 0.000158 0.005824

5 C 0.000000 0.000000 -0.000000 -0.000000 0.000001 -0.034594

6 C 0.000001 -0.000000 0.000001 0.000196 -0.000144 -0.000200

7 C 0.000004 -0.000005 0.000042 -0.000274 0.000257 0.000008

8 N 0.000343 0.000053 -0.000335 -0.018992 -0.013940 0.000002

9 C -0.000397 -0.001130 0.012604 -0.107086 -0.016136 0.000000

10 C 0.000047 -0.000006 -0.000175 0.013687 -0.000255 0.000000

11 C -0.000005 0.000001 -0.000005 -0.001205 0.000044 0.000000

12 C 0.000196 0.000001 -0.000000 0.000001 -0.000144 -0.005590

13 C -0.000274 0.000042 -0.000005 0.000004 0.000257 0.000003

14 C -0.001205 -0.000005 0.000001 -0.000005 0.000044 0.000002

15 C 0.013687 -0.000175 -0.000006 0.000047 -0.000255 -0.000000

16 C -0.107086 0.012604 -0.001130 -0.000397 -0.016136 0.000001

17 N -0.018992 -0.000335 0.000053 0.000343 -0.013940 -0.000002

18 C 0.428978 -0.073316 0.012800 -0.000721 -0.028564 0.000000

19 C 4.886870 0.393438 -0.066269 -0.142859 0.431485 -0.000000

20 C 0.393438 5.170049 0.541997 -0.066269 -0.076760 -0.000000

21 C -0.066269 0.541997 5.170049 0.393438 -0.076760 0.000000

22 C -0.142859 -0.066269 0.393438 4.886870 0.431485 -0.000000

23 N 0.431485 -0.076760 -0.076760 0.431485 6.977840 0.000000

24 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.440097

25 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.002321

26 H 0.000001 -0.000000 0.000004 -0.000043 0.000000 -0.000000

27 H 0.000000 0.000000 0.000000 0.000010 0.000002 -0.000000

28 H 0.000010 0.000000 0.000000 0.000000 0.000002 -0.000008

29 H -0.000043 0.000004 -0.000000 0.000001 0.000000 -0.000000

30 H -0.038768 0.387522 -0.034594 0.005824 0.005410 -0.000000

31 H 0.005824 -0.034594 0.387522 -0.038768 0.005410 -0.000000

32 Zn -0.014489 0.002530 0.002530 -0.014489 0.134943 -0.000441

33 C -0.000721 0.012800 -0.073316 0.428978 -0.028564 0.000000

34 C -0.000516 0.002592 -0.015042 -0.078372 0.003864 -0.000000

35 C 0.000002 0.000000 -0.000000 0.000000 -0.000000 0.007430

36 C -0.000049 0.000356 -0.000230 -0.005901 -0.000051 -0.000000

37 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.004081

38 C 0.000000 -0.000000 0.000000 0.000002 -0.000000 -0.000086

39 C -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000008

40 C -0.078372 -0.015042 0.002592 -0.000516 0.003864 -0.000000

41 C -0.005901 -0.000230 0.000356 -0.000049 -0.000051 -0.000000

42 H -0.000077 0.000100 0.000002 -0.000000 0.000001 -0.000000

43 H -0.000000 0.000002 0.000100 -0.000077 0.000001 -0.000000

44 H 0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000

45 H 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000074

25 26 27 28 29 30

1 C -0.034594 0.000000 -0.000000 0.000004 0.000000 -0.000000

2 C 0.005824 0.000000 0.000001 -0.000043 0.000010 -0.000000

3 N 0.005410 0.000002 0.000000 0.000000 0.000002 0.000000

4 C -0.038768 0.000010 -0.000043 0.000001 0.000000 -0.000000

5 C 0.387522 0.000000 0.000004 -0.000000 0.000000 0.000000

6 C -0.005590 -0.000195 -0.005605 0.000000 0.000000 0.000000

7 C 0.000003 0.005522 -0.040361 -0.000000 -0.000000 0.000000

8 N -0.000002 0.005887 0.005887 0.000000 0.000000 0.000002

9 C 0.000001 -0.040361 0.005522 -0.000000 -0.000000 0.000008

10 C -0.000000 0.389919 -0.035952 0.000000 -0.000000 0.000000

11 C 0.000002 -0.035952 0.389919 -0.000000 0.000000 0.000000

12 C -0.000200 0.000000 0.000000 -0.005605 -0.000195 0.000000

13 C 0.000008 -0.000000 -0.000000 -0.040361 0.005522 0.000001

14 C 0.000000 0.000000 -0.000000 0.389919 -0.035952 -0.000000

15 C 0.000000 -0.000000 0.000000 -0.035952 0.389919 0.000002

16 C 0.000000 -0.000000 -0.000000 0.005522 -0.040361 0.000003

17 N 0.000002 0.000000 0.000000 0.005887 0.005887 -0.000002

18 C 0.000000 0.000000 0.000000 -0.000195 -0.005605 -0.005590

19 C -0.000000 0.000001 0.000000 0.000010 -0.000043 -0.038768

20 C 0.000000 -0.000000 0.000000 0.000000 0.000004 0.387522

21 C -0.000000 0.000004 0.000000 0.000000 -0.000000 -0.034594

22 C -0.000000 -0.000043 0.000010 0.000000 0.000001 0.005824

23 N 0.000000 0.000000 0.000002 0.000002 0.000000 0.005410

24 H -0.002321 -0.000000 -0.000000 -0.000008 -0.000000 -0.000000

25 H 0.440097 -0.000000 -0.000008 -0.000000 -0.000000 -0.000000

26 H -0.000000 0.454390 -0.001957 -0.000000 -0.000000 -0.000000

27 H -0.000008 -0.001957 0.454390 -0.000000 -0.000000 -0.000000

28 H -0.000000 -0.000000 -0.000000 0.454390 -0.001957 -0.000000

29 H -0.000000 -0.000000 -0.000000 -0.001957 0.454390 -0.000008

30 H -0.000000 -0.000000 -0.000000 -0.000000 -0.000008 0.440097

31 H -0.000000 -0.000008 -0.000000 -0.000000 -0.000000 -0.002321

32 Zn -0.000441 -0.000485 -0.000485 -0.000485 -0.000485 -0.000441

33 C 0.000000 -0.005605 -0.000195 0.000000 0.000000 -0.000200

34 C -0.000000 0.006978 -0.000088 -0.000000 -0.000000 -0.000086

35 C -0.000086 -0.000000 -0.000000 0.006978 -0.000088 -0.000000

36 C -0.000000 0.003745 -0.000010 -0.000000 -0.000000 -0.000008

37 C -0.000008 -0.000000 -0.000000 0.003745 -0.000010 -0.000000

38 C 0.007430 -0.000088 0.006978 -0.000000 -0.000000 -0.000000

39 C 0.004081 -0.000010 0.003745 -0.000000 -0.000000 -0.000000

40 C -0.000000 -0.000000 -0.000000 -0.000088 0.006978 0.007430

41 C -0.000000 -0.000000 -0.000000 -0.000010 0.003745 0.004081

42 H -0.000000 -0.000000 -0.000000 -0.000000 0.000062 0.000074

43 H -0.000000 0.000062 -0.000000 -0.000000 -0.000000 -0.000000

44 H 0.000074 -0.000000 0.000062 -0.000000 -0.000000 -0.000000

45 H -0.000000 -0.000000 -0.000000 0.000062 -0.000000 -0.000000

31 32 33 34 35 36

1 C 0.000000 0.002530 -0.000000 -0.000000 -0.015042 -0.000000

2 C -0.000000 -0.014489 0.000001 0.000000 -0.078372 -0.000000

3 N 0.000000 0.134943 -0.000144 -0.000000 0.003864 0.000000

4 C -0.000000 -0.014489 0.000196 0.000002 -0.000516 0.000000

5 C -0.000000 0.002530 0.000001 0.000000 0.002592 0.000000

6 C 0.000000 -0.011576 -0.002119 -0.000048 -0.000054 -0.000002

7 C 0.000001 -0.013929 0.000226 -0.000432 0.000002 -0.000050

8 N -0.000002 0.136849 -0.021511 0.003961 -0.000000 -0.000054

9 C 0.000003 -0.013929 0.389185 -0.075406 0.000000 -0.004850

10 C 0.000002 0.002345 -0.078359 -0.016249 -0.000000 -0.000409

11 C -0.000000 0.002345 0.014171 0.002399 0.000000 0.000314

12 C 0.000000 -0.011576 0.000002 0.000000 0.547807 0.000000

13 C 0.000000 -0.013929 0.000002 0.000000 -0.075406 -0.000000

14 C 0.000000 0.002345 -0.000000 -0.000000 -0.016249 -0.000000

15 C 0.000000 0.002345 0.000001 0.000000 0.002399 0.000000

16 C 0.000008 -0.013929 0.000179 0.000002 -0.000432 0.000000

17 N 0.000002 0.136849 -0.000152 -0.000000 0.003961 0.000000

18 C -0.000200 -0.011576 -0.002150 -0.000054 -0.000048 -0.000002

19 C 0.005824 -0.014489 -0.000721 -0.000516 0.000002 -0.000049

20 C -0.034594 0.002530 0.012800 0.002592 0.000000 0.000356

21 C 0.387522 0.002530 -0.073316 -0.015042 -0.000000 -0.000230

22 C -0.038768 -0.014489 0.428978 -0.078372 0.000000 -0.005901

23 N 0.005410 0.134943 -0.028564 0.003864 -0.000000 -0.000051

24 H -0.000000 -0.000441 0.000000 -0.000000 0.007430 -0.000000

25 H -0.000000 -0.000441 0.000000 -0.000000 -0.000086 -0.000000

26 H -0.000008 -0.000485 -0.005605 0.006978 -0.000000 0.003745

27 H -0.000000 -0.000485 -0.000195 -0.000088 -0.000000 -0.000010

28 H -0.000000 -0.000485 0.000000 -0.000000 0.006978 -0.000000

29 H -0.000000 -0.000485 0.000000 -0.000000 -0.000088 -0.000000

30 H -0.002321 -0.000441 -0.000200 -0.000086 -0.000000 -0.000008

31 H 0.440097 -0.000441 -0.005590 0.007430 -0.000000 0.004081

32 Zn -0.000441 10.249478 -0.011576 -0.000844 -0.000844 -0.000060

33 C -0.005590 -0.011576 5.253993 0.547807 0.000000 -0.109539

34 C 0.007430 -0.000844 0.547807 4.808441 0.000000 0.851266

35 C -0.000000 -0.000844 0.000000 0.000000 4.808441 0.000000

36 C 0.004081 -0.000060 -0.109539 0.851266 0.000000 5.228233

37 C -0.000000 -0.000060 0.000000 0.000000 0.851266 0.000000

38 C -0.000000 -0.000844 -0.000048 -0.000001 -0.000001 -0.000000

39 C -0.000000 -0.000060 -0.000002 -0.000000 -0.000000 -0.000000

40 C -0.000086 -0.000844 -0.000054 -0.000001 -0.000001 -0.000000

41 C -0.000008 -0.000060 -0.000002 -0.000000 -0.000000 -0.000000

42 H -0.000000 -0.000004 -0.000000 -0.000000 -0.000000 0.000000

43 H 0.000074 -0.000004 0.001954 -0.019758 0.000000 0.372480

44 H -0.000000 -0.000004 -0.000000 -0.000000 -0.000000 0.000000

45 H -0.000000 -0.000004 0.000000 0.000000 -0.019758 0.000000

37 38 39 40 41 42

1 C -0.000230 0.002592 0.000356 0.000000 0.000000 0.000000

2 C -0.005901 -0.000516 -0.000049 0.000002 0.000000 0.000000

3 N -0.000051 0.003864 -0.000051 -0.000000 0.000000 0.000000

4 C -0.000049 -0.078372 -0.005901 0.000000 -0.000000 0.000000

5 C 0.000356 -0.015042 -0.000230 -0.000000 -0.000000 -0.000000

6 C -0.000002 0.547807 -0.109539 0.000000 0.000000 0.000000

7 C 0.000000 -0.075406 -0.004850 0.000000 -0.000000 0.000000

8 N 0.000000 0.003961 -0.000054 -0.000000 0.000000 0.000000

9 C -0.000000 -0.000432 -0.000050 0.000002 0.000000 0.000000

10 C -0.000000 0.002399 0.000314 0.000000 0.000000 0.000000

11 C 0.000000 -0.016249 -0.000409 -0.000000 -0.000000 -0.000000

12 C -0.109539 -0.000054 -0.000002 -0.000048 -0.000002 -0.000000

13 C -0.004850 0.000002 0.000000 -0.000432 -0.000050 -0.000000

14 C -0.000409 0.000000 0.000000 0.002399 0.000314 0.000001

15 C 0.000314 -0.000000 -0.000000 -0.016249 -0.000409 0.000088

16 C -0.000050 0.000000 -0.000000 -0.075406 -0.004850 -0.000010

17 N -0.000054 -0.000000 0.000000 0.003961 -0.000054 0.000001

18 C -0.000002 0.000000 0.000000 0.547807 -0.109539 0.001954

19 C 0.000000 0.000000 -0.000000 -0.078372 -0.005901 -0.000077

20 C 0.000000 -0.000000 -0.000000 -0.015042 -0.000230 0.000100

21 C -0.000000 0.000000 0.000000 0.002592 0.000356 0.000002

22 C -0.000000 0.000002 0.000000 -0.000516 -0.000049 -0.000000

23 N 0.000000 -0.000000 0.000000 0.003864 -0.000051 0.000001

24 H 0.004081 -0.000086 -0.000008 -0.000000 -0.000000 -0.000000

25 H -0.000008 0.007430 0.004081 -0.000000 -0.000000 -0.000000

26 H -0.000000 -0.000088 -0.000010 -0.000000 -0.000000 -0.000000

27 H -0.000000 0.006978 0.003745 -0.000000 -0.000000 -0.000000

28 H 0.003745 -0.000000 -0.000000 -0.000088 -0.000010 -0.000000

29 H -0.000010 -0.000000 -0.000000 0.006978 0.003745 0.000062

30 H -0.000000 -0.000000 -0.000000 0.007430 0.004081 0.000074

31 H -0.000000 -0.000000 -0.000000 -0.000086 -0.000008 -0.000000

32 Zn -0.000060 -0.000844 -0.000060 -0.000844 -0.000060 -0.000004

33 C 0.000000 -0.000048 -0.000002 -0.000054 -0.000002 -0.000000

34 C 0.000000 -0.000001 -0.000000 -0.000001 -0.000000 -0.000000

35 C 0.851266 -0.000001 -0.000000 -0.000001 -0.000000 -0.000000

36 C 0.000000 -0.000000 -0.000000 -0.000000 -0.000000 0.000000

37 C 5.228233 -0.000000 -0.000000 -0.000000 -0.000000 0.000000

38 C -0.000000 4.808441 0.851266 0.000000 0.000000 0.000000

39 C -0.000000 0.851266 5.228233 0.000000 0.000000 0.000000

40 C -0.000000 0.000000 0.000000 4.808441 0.851266 -0.019758

41 C -0.000000 0.000000 0.000000 0.851266 5.228233 0.372480

42 H 0.000000 0.000000 0.000000 -0.019758 0.372480 0.355024

43 H 0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

44 H 0.000000 -0.019758 0.372480 0.000000 0.000000 0.000000

45 H 0.372480 -0.000000 0.000000 -0.000000 0.000000 0.000000

43 44 45

1 C -0.000000 0.000002 0.000100

2 C 0.000000 -0.000000 -0.000077

3 N 0.000000 0.000001 0.000001

4 C 0.000000 -0.000077 -0.000000

5 C 0.000000 0.000100 0.000002

6 C -0.000000 0.001954 -0.000000

7 C -0.000000 -0.000010 0.000000

8 N 0.000001 0.000001 0.000000

9 C -0.000010 -0.000000 0.000000

10 C 0.000088 0.000001 -0.000000

11 C 0.000001 0.000088 0.000000

12 C 0.000000 -0.000000 0.001954

13 C 0.000000 0.000000 -0.000010

14 C -0.000000 0.000000 0.000088

15 C 0.000000 -0.000000 0.000001

16 C 0.000000 0.000000 -0.000000

17 N 0.000000 0.000000 0.000001

18 C -0.000000 0.000000 -0.000000

19 C -0.000000 0.000000 0.000000

20 C 0.000002 -0.000000 0.000000

21 C 0.000100 0.000000 -0.000000

22 C -0.000077 0.000000 0.000000

23 N 0.000001 0.000000 0.000000

24 H -0.000000 -0.000000 0.000074

25 H -0.000000 0.000074 -0.000000

26 H 0.000062 -0.000000 -0.000000

27 H -0.000000 0.000062 -0.000000

28 H -0.000000 -0.000000 0.000062

29 H -0.000000 -0.000000 -0.000000

30 H -0.000000 -0.000000 -0.000000

31 H 0.000074 -0.000000 -0.000000

32 Zn -0.000004 -0.000004 -0.000004

33 C 0.001954 -0.000000 0.000000

34 C -0.019758 -0.000000 0.000000

35 C 0.000000 -0.000000 -0.019758

36 C 0.372480 0.000000 0.000000

37 C 0.000000 0.000000 0.372480

38 C -0.000000 -0.019758 -0.000000

39 C 0.000000 0.372480 0.000000

40 C -0.000000 0.000000 -0.000000

41 C 0.000000 0.000000 0.000000

42 H 0.000000 0.000000 0.000000

43 H 0.355024 0.000000 0.000000

44 H 0.000000 0.355024 0.000000

45 H 0.000000 0.000000 0.355024

Atomic-Atomic Spin Densities.

1 2 3 4 5 6

1 C -0.006945 -0.005441 0.002072 0.000415 0.008257 -0.000637

2 C -0.005441 -0.028881 -0.012103 0.004075 0.000415 0.000630

3 N 0.002072 -0.012103 0.104215 -0.012103 0.002072 -0.005460

4 C 0.000415 0.004075 -0.012103 -0.028881 -0.005441 0.022807

5 C 0.008257 0.000415 0.002072 -0.005441 -0.006945 -0.001041

6 C -0.000637 0.000630 -0.005460 0.022807 -0.001041 0.114174

7 C 0.000017 -0.000067 0.001876 -0.002924 0.000283 -0.037978

8 N 0.000000 0.000005 -0.000039 0.000332 -0.000001 0.000393

9 C -0.000000 0.000002 -0.000086 0.000078 -0.000000 0.000786

10 C -0.000000 0.000000 -0.000011 0.000041 -0.000001 0.000894

11 C 0.000000 -0.000002 0.000059 -0.000691 0.000013 -0.007477

12 C -0.001041 0.022807 -0.005460 0.000630 -0.000637 0.000099

13 C 0.000283 -0.002924 0.001876 -0.000067 0.000017 -0.000008

14 C 0.000013 -0.000691 0.000059 -0.000002 0.000000 -0.000000

15 C -0.000001 0.000041 -0.000011 0.000000 -0.000000 0.000000

16 C -0.000000 0.000078 -0.000086 0.000002 -0.000000 0.000000

17 N -0.000001 0.000332 -0.000039 0.000005 0.000000 0.000000

18 C 0.000000 -0.000009 0.000011 -0.000000 0.000000 -0.000000

19 C 0.000000 0.000001 0.000001 -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 0.000000 -0.000000 0.000001 0.000001 0.000000 -0.000009

23 N -0.000000 0.000001 -0.000040 0.000001 -0.000000 0.000011

24 H -0.000215 0.000226 -0.000006 -0.000044 0.000128 -0.000008

25 H 0.000128 -0.000044 -0.000006 0.000226 -0.000215 0.000021

26 H 0.000000 -0.000000 -0.000000 -0.000001 -0.000000 0.000003

27 H -0.000000 0.000000 -0.000000 0.000013 0.000000 0.000307

28 H 0.000000 0.000013 -0.000000 0.000000 -0.000000 0.000000

29 H -0.000000 -0.000001 -0.000000 -0.000000 0.000000 -0.000000

30 H 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000

31 H 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000

32 Zn 0.000017 0.000015 -0.001851 0.000015 0.000017 0.000065

33 C 0.000000 -0.000000 0.000011 -0.000009 0.000000 -0.000027

34 C 0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

35 C 0.000099 -0.000685 -0.000049 0.000015 -0.000076 0.000002

36 C -0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

37 C 0.000204 -0.000586 0.000016 0.000000 0.000001 0.000000

38 C -0.000076 0.000015 -0.000049 -0.000685 0.000099 0.004883

39 C 0.000001 0.000000 0.000016 -0.000586 0.000204 -0.002987

40 C 0.000000 -0.000000 0.000000 -0.000000 0.000000 -0.000000

41 C -0.000000 -0.000000 -0.000000 0.000000 -0.000000 0.000000

42 H 0.000000 -0.000000 0.000000 -0.000000 -0.000000 -0.000000

43 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 -0.000000

44 H -0.000000 0.000000 0.000000 -0.000005 0.000001 -0.000006

45 H 0.000001 -0.000005 0.000000 0.000000 -0.000000 0.000000

7 8 9 10 11 12

1 C 0.000017 0.000000 -0.000000 -0.000000 0.000000 -0.001041

2 C -0.000067 0.000005 0.000002 0.000000 -0.000002 0.022807

3 N 0.001876 -0.000039 -0.000086 -0.000011 0.000059 -0.005460

4 C -0.002924 0.000332 0.000078 0.000041 -0.000691 0.000630

5 C 0.000283 -0.000001 -0.000000 -0.000001 0.000013 -0.000637

6 C -0.037978 0.000393 0.000786 0.000894 -0.007477 0.000099

7 C 0.100889 0.002656 -0.011675 -0.011101 0.032579 -0.000008

8 N 0.002656 -0.029978 0.002656 -0.000283 -0.000283 0.000000

9 C -0.011675 0.002656 0.100889 0.032579 -0.011101 0.000000

10 C -0.011101 -0.000283 0.032579 0.083878 -0.034279 0.000000

11 C 0.032579 -0.000283 -0.011101 -0.034279 0.083878 -0.000000

12 C -0.000008 0.000000 0.000000 0.000000 -0.000000 0.114174

13 C 0.000002 0.000001 -0.000001 -0.000000 0.000000 -0.037978

14 C 0.000000 -0.000000 -0.000000 -0.000000 0.000000 -0.007477

15 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 0.000894

16 C -0.000001 0.000001 0.000002 0.000000 -0.000000 0.000786

17 N 0.000001 -0.000007 0.000001 -0.000000 -0.000000 0.000393

18 C 0.000000 0.000000 -0.000008 -0.000000 0.000000 -0.000027

19 C 0.000002 0.000005 -0.000067 -0.000002 0.000000 -0.000009

20 C -0.000000 0.000000 0.000017 0.000000 -0.000000 0.000000

21 C -0.000000 -0.000001 0.000283 0.000013 -0.000001 0.000000

22 C 0.000078 0.000332 -0.002924 -0.000691 0.000041 -0.000000

23 N -0.000086 -0.000039 0.001876 0.000059 -0.000011 0.000011

24 H 0.000000 -0.000000 -0.000000 0.000000 -0.000000 0.000021

25 H -0.000004 0.000000 0.000000 -0.000000 0.000000 -0.000008

26 H 0.000024 -0.000029 -0.000483 0.000203 0.000152 -0.000000

27 H -0.000483 -0.000029 0.000024 0.000152 0.000203 0.000000

28 H -0.000000 0.000000 0.000000 0.000000 -0.000000 0.000307

29 H 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000003

30 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

31 H 0.000000 0.000000 -0.000004 0.000000 -0.000000 0.000000

32 Zn 0.000259 0.000062 0.000259 -0.000036 -0.000036 0.000065

33 C 0.000786 0.000393 -0.037978 -0.007477 0.000894 -0.000000

34 C -0.000020 -0.000085 0.000205 0.000129 0.000075 -0.000000

35 C -0.000000 0.000000 0.000000 0.000000 -0.000000 0.004883

36 C -0.000006 -0.000000 0.001128 0.000623 -0.000023 0.000000

37 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.002987

38 C 0.000205 -0.000085 -0.000020 0.000075 0.000129 0.000002

39 C 0.001128 -0.000000 -0.000006 -0.000023 0.000623 0.000000

40 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

41 C -0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000

42 H 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

43 H -0.000000 -0.000000 0.000002 0.000000 0.000000 -0.000000

44 H 0.000002 -0.000000 -0.000000 0.000000 0.000000 0.000000

45 H -0.000000 0.000000 0.000000 -0.000000 -0.000000 -0.000006

13 14 15 16 17 18

1 C 0.000283 0.000013 -0.000001 -0.000000 -0.000001 0.000000

2 C -0.002924 -0.000691 0.000041 0.000078 0.000332 -0.000009

3 N 0.001876 0.000059 -0.000011 -0.000086 -0.000039 0.000011

4 C -0.000067 -0.000002 0.000000 0.000002 0.000005 -0.000000

5 C 0.000017 0.000000 -0.000000 -0.000000 0.000000 0.000000

6 C -0.000008 -0.000000 0.000000 0.000000 0.000000 -0.000000

7 C 0.000002 0.000000 -0.000000 -0.000001 0.000001 0.000000

8 N 0.000001 -0.000000 -0.000000 0.000001 -0.000007 0.000000

9 C -0.000001 -0.000000 0.000000 0.000002 0.000001 -0.000008

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 C -0.037978 -0.007477 0.000894 0.000786 0.000393 -0.000027

13 C 0.100889 0.032579 -0.011101 -0.011675 0.002656 0.000786

14 C 0.032579 0.083878 -0.034279 -0.011101 -0.000283 0.000894

15 C -0.011101 -0.034279 0.083878 0.032579 -0.000283 -0.007477

16 C -0.011675 -0.011101 0.032579 0.100889 0.002656 -0.037978

17 N 0.002656 -0.000283 -0.000283 0.002656 -0.029978 0.000393

18 C 0.000786 0.000894 -0.007477 -0.037978 0.000393 0.114174

19 C 0.000078 0.000041 -0.000691 -0.002924 0.000332 0.022807

20 C -0.000000 -0.000001 0.000013 0.000283 -0.000001 -0.001041

21 C -0.000000 -0.000000 0.000000 0.000017 0.000000 -0.000637

22 C 0.000002 0.000000 -0.000002 -0.000067 0.000005 0.000630

23 N -0.000086 -0.000011 0.000059 0.001876 -0.000039 -0.005460

24 H -0.000004 0.000000 -0.000000 0.000000 0.000000 0.000000

25 H 0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.000000

26 H 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

27 H -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000

28 H -0.000483 0.000203 0.000152 0.000024 -0.000029 0.000003

29 H 0.000024 0.000152 0.000203 -0.000483 -0.000029 0.000307

30 H 0.000000 -0.000000 0.000000 -0.000004 0.000000 0.000021

31 H -0.000000 0.000000 -0.000000 0.000000 -0.000000 -0.000008

32 Zn 0.000259 -0.000036 -0.000036 0.000259 0.000062 0.000065

33 C 0.000000 0.000000 -0.000000 -0.000008 0.000000 0.000099

34 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000002

35 C 0.000205 0.000129 0.000075 -0.000020 -0.000085 0.000000

36 C -0.000000 -0.000000 0.000000 0.000000 0.000000 0.000000

37 C 0.001128 0.000623 -0.000023 -0.000006 -0.000000 0.000000

38 C -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000

39 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

40 C -0.000020 0.000075 0.000129 0.000205 -0.000085 0.004883

41 C -0.000006 -0.000023 0.000623 0.001128 -0.000000 -0.002987

42 H -0.000000 0.000000 0.000000 0.000002 -0.000000 -0.000006

43 H 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000000

44 H -0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

45 H 0.000002 0.000000 0.000000 -0.000000 -0.000000 -0.000000

19 20 21 22 23 24

1 C 0.000000 -0.000000 -0.000000 0.000000 -0.000000 -0.000215

2 C 0.000001 0.000000 0.000000 -0.000000 0.000001 0.000226

3 N 0.000001 -0.000000 -0.000000 0.000001 -0.000040 -0.000006

4 C -0.000000 0.000000 0.000000 0.000001 0.000001 -0.000044

5 C 0.000000 -0.000000 -0.000000 0.000000 -0.000000 0.000128

6 C -0.000000 0.000000 0.000000 -0.000009 0.000011 -0.000008

7 C 0.000002 -0.000000 -0.000000 0.000078 -0.000086 0.000000

8 N 0.000005 0.000000 -0.000001 0.000332 -0.000039 -0.000000

9 C -0.000067 0.000017 0.000283 -0.002924 0.001876 -0.000000

10 C -0.000002 0.000000 0.000013 -0.000691 0.000059 0.000000

11 C 0.000000 -0.000000 -0.000001 0.000041 -0.000011 -0.000000

12 C -0.000009 0.000000 0.000000 -0.000000 0.000011 0.000021

13 C 0.000078 -0.000000 -0.000000 0.000002 -0.000086 -0.000004

14 C 0.000041 -0.000001 -0.000000 0.000000 -0.000011 0.000000

15 C -0.000691 0.000013 0.000000 -0.000002 0.000059 -0.000000

16 C -0.002924 0.000283 0.000017 -0.000067 0.001876 0.000000

17 N 0.000332 -0.000001 0.000000 0.000005 -0.000039 0.000000

18 C 0.022807 -0.001041 -0.000637 0.000630 -0.005460 0.000000

19 C -0.028881 -0.005441 0.000415 0.004075 -0.012103 0.000000

20 C -0.005441 -0.006945 0.008257 0.000415 0.002072 0.000000

21 C 0.000415 0.008257 -0.006945 -0.005441 0.002072 0.000000

22 C 0.004075 0.000415 -0.005441 -0.028881 -0.012103 0.000000

23 N -0.012103 0.002072 0.002072 -0.012103 0.104215 -0.000000

24 H 0.000000 0.000000 0.000000 0.000000 -0.000000 0.000175

25 H 0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000007

26 H 0.000000 -0.000000 0.000000 0.000013 -0.000000 0.000000

27 H -0.000000 0.000000 -0.000000 -0.000001 -0.000000 0.000000

28 H -0.000001 -0.000000 0.000000 -0.000000 -0.000000 0.000000

29 H 0.000013 0.000000 -0.000000 0.000000 -0.000000 -0.000000

30 H 0.000226 -0.000215 0.000128 -0.000044 -0.000006 0.000000

31 H -0.000044 0.000128 -0.000215 0.000226 -0.000006 0.000000

32 Zn 0.000015 0.000017 0.000017 0.000015 -0.001851 0.000000

33 C 0.000630 -0.000637 -0.001041 0.022807 -0.005460 0.000000

34 C 0.000015 -0.000076 0.000099 -0.000685 -0.000049 0.000000

35 C -0.000000 0.000000 0.000000 -0.000000 0.000000 0.000017

36 C 0.000000 0.000001 0.000204 -0.000586 0.000016 0.000000

37 C -0.000000 -0.000000 -0.000000 0.000000 -0.000000 0.000067

38 C -0.000000 0.000000 0.000000 -0.000000 0.000000 -0.000000

39 C 0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000

40 C -0.000685 0.000099 -0.000076 0.000015 -0.000049 0.000000

41 C -0.000586 0.000204 0.000001 0.000000 0.000016 0.000000

42 H -0.000005 0.000001 -0.000000 0.000000 0.000000 0.000000

43 H 0.000000 -0.000000 0.000001 -0.000005 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 0.000002

25 26 27 28 29 30

1 C 0.000128 0.000000 -0.000000 0.000000 -0.000000 0.000000

2 C -0.000044 -0.000000 0.000000 0.000013 -0.000001 0.000000

3 N -0.000006 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000

4 C 0.000226 -0.000001 0.000013 0.000000 -0.000000 0.000000

5 C -0.000215 -0.000000 0.000000 -0.000000 0.000000 0.000000

6 C 0.000021 0.000003 0.000307 0.000000 -0.000000 0.000000

7 C -0.000004 0.000024 -0.000483 -0.000000 0.000000 -0.000000

8 N 0.000000 -0.000029 -0.000029 0.000000 0.000000 -0.000000

9 C 0.000000 -0.000483 0.000024 0.000000 -0.000000 0.000000

10 C -0.000000 0.000203 0.000152 0.000000 -0.000000 -0.000000

11 C 0.000000 0.000152 0.000203 -0.000000 0.000000 0.000000

12 C -0.000008 -0.000000 0.000000 0.000307 0.000003 0.000000

13 C 0.000000 0.000000 -0.000000 -0.000483 0.000024 0.000000

14 C -0.000000 0.000000 -0.000000 0.000203 0.000152 -0.000000

15 C 0.000000 -0.000000 0.000000 0.000152 0.000203 0.000000

16 C -0.000000 -0.000000 0.000000 0.000024 -0.000483 -0.000004

17 N -0.000000 0.000000 0.000000 -0.000029 -0.000029 0.000000

18 C 0.000000 0.000000 -0.000000 0.000003 0.000307 0.000021

19 C 0.000000 0.000000 -0.000000 -0.000001 0.000013 0.000226

20 C 0.000000 -0.000000 0.000000 -0.000000 0.000000 -0.000215

21 C 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000128

22 C 0.000000 0.000013 -0.000001 -0.000000 0.000000 -0.000044

23 N -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000006

24 H -0.000007 0.000000 0.000000 0.000000 -0.000000 0.000000

25 H 0.000175 -0.000000 0.000000 0.000000 0.000000 0.000000

26 H -0.000000 -0.004247 0.000076 0.000000 -0.000000 0.000000

27 H 0.000000 0.000076 -0.004247 -0.000000 0.000000 0.000000

28 H 0.000000 0.000000 -0.000000 -0.004247 0.000076 -0.000000

29 H 0.000000 -0.000000 0.000000 0.000076 -0.004247 0.000000

30 H 0.000000 0.000000 0.000000 -0.000000 0.000000 0.000175

31 H 0.000000 0.000000 -0.000000 0.000000 0.000000 -0.000007

32 Zn 0.000000 -0.000003 -0.000003 -0.000003 -0.000003 0.000000

33 C 0.000000 0.000307 0.000003 -0.000000 0.000000 -0.000008

34 C 0.000000 -0.000206 0.000003 -0.000000 -0.000000 -0.000000

35 C -0.000000 -0.000000 -0.000000 -0.000206 0.000003 0.000000

36 C 0.000000 -0.000147 0.000000 -0.000000 -0.000000 -0.000000

37 C -0.000000 -0.000000 -0.000000 -0.000147 0.000000 0.000000

38 C 0.000017 0.000003 -0.000206 -0.000000 -0.000000 0.000000

39 C 0.000067 0.000000 -0.000147 -0.000000 -0.000000 0.000000

40 C 0.000000 -0.000000 -0.000000 0.000003 -0.000206 0.000017

41 C 0.000000 -0.000000 -0.000000 0.000000 -0.000147 0.000067

42 H 0.000000 -0.000000 -0.000000 0.000000 -0.000006 0.000002

43 H 0.000000 -0.000006 0.000000 -0.000000 -0.000000 -0.000000

44 H 0.000002 0.000000 -0.000006 -0.000000 -0.000000 0.000000

45 H -0.000000 -0.000000 -0.000000 -0.000006 0.000000 0.000000

31 32 33 34 35 36

1 C 0.000000 0.000017 0.000000 0.000000 0.000099 -0.000000

2 C 0.000000 0.000015 -0.000000 -0.000000 -0.000685 0.000000

3 N -0.000000 -0.001851 0.000011 0.000000 -0.000049 -0.000000

4 C 0.000000 0.000015 -0.000009 -0.000000 0.000015 -0.000000

5 C 0.000000 0.000017 0.000000 0.000000 -0.000076 -0.000000

6 C 0.000000 0.000065 -0.000027 0.000000 0.000002 0.000000

7 C 0.000000 0.000259 0.000786 -0.000020 -0.000000 -0.000006

8 N 0.000000 0.000062 0.000393 -0.000085 0.000000 -0.000000

9 C -0.000004 0.000259 -0.037978 0.000205 0.000000 0.001128

10 C 0.000000 -0.000036 -0.007477 0.000129 0.000000 0.000623

11 C -0.000000 -0.000036 0.000894 0.000075 -0.000000 -0.000023

12 C 0.000000 0.000065 -0.000000 -0.000000 0.004883 0.000000

13 C -0.000000 0.000259 0.000000 0.000000 0.000205 -0.000000

14 C 0.000000 -0.000036 0.000000 0.000000 0.000129 -0.000000

15 C -0.000000 -0.000036 -0.000000 -0.000000 0.000075 0.000000

16 C 0.000000 0.000259 -0.000008 -0.000000 -0.000020 0.000000

17 N -0.000000 0.000062 0.000000 0.000000 -0.000085 0.000000

18 C -0.000008 0.000065 0.000099 0.000002 0.000000 0.000000

19 C -0.000044 0.000015 0.000630 0.000015 -0.000000 0.000000

20 C 0.000128 0.000017 -0.000637 -0.000076 0.000000 0.000001

21 C -0.000215 0.000017 -0.001041 0.000099 0.000000 0.000204

22 C 0.000226 0.000015 0.022807 -0.000685 -0.000000 -0.000586

23 N -0.000006 -0.001851 -0.005460 -0.000049 0.000000 0.000016

24 H 0.000000 0.000000 0.000000 0.000000 0.000017 0.000000

25 H 0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000

26 H 0.000000 -0.000003 0.000307 -0.000206 -0.000000 -0.000147

27 H -0.000000 -0.000003 0.000003 0.000003 -0.000000 0.000000

28 H 0.000000 -0.000003 -0.000000 -0.000000 -0.000206 -0.000000

29 H 0.000000 -0.000003 0.000000 -0.000000 0.000003 -0.000000

30 H -0.000007 0.000000 -0.000008 -0.000000 0.000000 -0.000000

31 H 0.000175 0.000000 0.000021 0.000017 0.000000 0.000067

32 Zn 0.000000 -0.001588 0.000065 -0.000018 -0.000018 -0.000004

33 C 0.000021 0.000065 0.114174 0.004883 -0.000000 -0.002987

34 C 0.000017 -0.000018 0.004883 -0.029770 0.000000 -0.001024

35 C 0.000000 -0.000018 -0.000000 0.000000 -0.029770 0.000000

36 C 0.000067 -0.000004 -0.002987 -0.001024 0.000000 0.056570

37 C 0.000000 -0.000004 0.000000 0.000000 -0.001024 -0.000000

38 C 0.000000 -0.000018 0.000000 0.000000 0.000000 0.000000

39 C 0.000000 -0.000004 0.000000 0.000000 0.000000 -0.000000

40 C -0.000000 -0.000018 0.000002 0.000000 0.000000 0.000000

41 C -0.000000 -0.000004 0.000000 0.000000 0.000000 0.000000

42 H -0.000000 -0.000000 0.000000 0.000000 0.000000 0.000000

43 H 0.000002 -0.000000 -0.000006 -0.000234 -0.000000 -0.000242

44 H 0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000000

45 H 0.000000 -0.000000 -0.000000 -0.000000 -0.000234 -0.000000

37 38 39 40 41 42

1 C 0.000204 -0.000076 0.000001 0.000000 -0.000000 0.000000

2 C -0.000586 0.000015 0.000000 -0.000000 -0.000000 -0.000000

3 N 0.000016 -0.000049 0.000016 0.000000 -0.000000 0.000000

4 C 0.000000 -0.000685 -0.000586 -0.000000 0.000000 -0.000000

5 C 0.000001 0.000099 0.000204 0.000000 -0.000000 -0.000000

6 C 0.000000 0.004883 -0.002987 -0.000000 0.000000 -0.000000

7 C 0.000000 0.000205 0.001128 0.000000 -0.000000 0.000000

8 N 0.000000 -0.000085 -0.000000 0.000000 0.000000 0.000000

9 C -0.000000 -0.000020 -0.000006 -0.000000 0.000000 -0.000000

10 C -0.000000 0.000075 -0.000023 -0.000000 0.000000 -0.000000

11 C 0.000000 0.000129 0.000623 0.000000 -0.000000 -0.000000

12 C -0.002987 0.000002 0.000000 0.000000 0.000000 -0.000000

13 C 0.001128 -0.000000 0.000000 -0.000020 -0.000006 -0.000000

14 C 0.000623 -0.000000 0.000000 0.000075 -0.000023 0.000000

15 C -0.000023 0.000000 -0.000000 0.000129 0.000623 0.000000

16 C -0.000006 0.000000 -0.000000 0.000205 0.001128 0.000002

17 N -0.000000 0.000000 0.000000 -0.000085 -0.000000 -0.000000

18 C 0.000000 -0.000000 0.000000 0.004883 -0.002987 -0.000006

19 C -0.000000 -0.000000 0.000000 -0.000685 -0.000586 -0.000005

20 C -0.000000 0.000000 -0.000000 0.000099 0.000204 0.000001

21 C -0.000000 0.000000 -0.000000 -0.000076 0.000001 -0.000000

22 C 0.000000 -0.000000 -0.000000 0.000015 0.000000 0.000000

23 N -0.000000 0.000000 -0.000000 -0.000049 0.000016 0.000000

24 H 0.000067 -0.000000 -0.000000 0.000000 0.000000 0.000000

25 H -0.000000 0.000017 0.000067 0.000000 0.000000 0.000000

26 H -0.000000 0.000003 0.000000 -0.000000 -0.000000 -0.000000

27 H -0.000000 -0.000206 -0.000147 -0.000000 -0.000000 -0.000000

28 H -0.000147 -0.000000 -0.000000 0.000003 0.000000 0.000000

29 H 0.000000 -0.000000 -0.000000 -0.000206 -0.000147 -0.000006

30 H 0.000000 0.000000 0.000000 0.000017 0.000067 0.000002

31 H 0.000000 0.000000 0.000000 -0.000000 -0.000000 -0.000000

32 Zn -0.000004 -0.000018 -0.000004 -0.000018 -0.000004 -0.000000

33 C 0.000000 0.000000 0.000000 0.000002 0.000000 0.000000

34 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 C -0.001024 0.000000 0.000000 0.000000 0.000000 0.000000

36 C -0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000

37 C 0.056570 0.000000 0.000000 0.000000 -0.000000 0.000000

38 C 0.000000 -0.029770 -0.001024 0.000000 0.000000 -0.000000

39 C 0.000000 -0.001024 0.056570 0.000000 -0.000000 -0.000000

40 C 0.000000 0.000000 0.000000 -0.029770 -0.001024 -0.000234

41 C -0.000000 0.000000 -0.000000 -0.001024 0.056570 -0.000242

42 H 0.000000 -0.000000 -0.000000 -0.000234 -0.000242 -0.001799

43 H -0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 -0.000234 -0.000242 -0.000000 -0.000000 -0.000000

45 H -0.000242 0.000000 0.000000 0.000000 0.000000 -0.000000

43 44 45

1 C -0.000000 -0.000000 0.000001

2 C -0.000000 0.000000 -0.000005

3 N 0.000000 0.000000 0.000000

4 C -0.000000 -0.000005 0.000000

5 C 0.000000 0.000001 -0.000000

6 C -0.000000 -0.000006 0.000000

7 C -0.000000 0.000002 -0.000000

8 N -0.000000 -0.000000 0.000000

9 C 0.000002 -0.000000 0.000000

10 C 0.000000 0.000000 -0.000000

11 C 0.000000 0.000000 -0.000000

12 C -0.000000 0.000000 -0.000006

13 C 0.000000 -0.000000 0.000002

14 C -0.000000 -0.000000 0.000000

15 C -0.000000 -0.000000 0.000000

16 C -0.000000 0.000000 -0.000000

17 N 0.000000 0.000000 -0.000000

18 C 0.000000 -0.000000 -0.000000

19 C 0.000000 -0.000000 -0.000000

20 C -0.000000 -0.000000 0.000000

21 C 0.000001 0.000000 -0.000000

22 C -0.000005 -0.000000 -0.000000

23 N 0.000000 0.000000 0.000000

24 H 0.000000 -0.000000 0.000002

25 H 0.000000 0.000002 -0.000000

26 H -0.000006 0.000000 -0.000000

27 H 0.000000 -0.000006 -0.000000

28 H -0.000000 -0.000000 -0.000006

29 H -0.000000 -0.000000 0.000000

30 H -0.000000 0.000000 0.000000

31 H 0.000002 0.000000 0.000000

32 Zn -0.000000 -0.000000 -0.000000

33 C -0.000006 -0.000000 -0.000000

34 C -0.000234 0.000000 -0.000000

35 C -0.000000 0.000000 -0.000234

36 C -0.000242 0.000000 -0.000000

37 C -0.000000 0.000000 -0.000242

38 C 0.000000 -0.000234 0.000000

39 C 0.000000 -0.000242 0.000000

40 C 0.000000 -0.000000 0.000000

41 C 0.000000 -0.000000 0.000000

42 H 0.000000 -0.000000 -0.000000

43 H -0.001799 -0.000000 -0.000000

44 H -0.000000 -0.001799 0.000000

45 H -0.000000 0.000000 -0.001799

Mulliken charges and spin densities:

1 2

1 C -0.256226 -0.002850

2 C 0.315042 -0.022783

3 N -0.721893 0.074888

4 C 0.315042 -0.022783

5 C -0.256226 -0.002850

6 C -0.309650 0.089439

7 C 0.294849 0.076437

8 N -0.702881 -0.024022

9 C 0.294849 0.076437

10 C -0.293020 0.064743

11 C -0.293020 0.064743

12 C -0.309650 0.089439

13 C 0.294849 0.076437

14 C -0.293020 0.064743

15 C -0.293020 0.064743

16 C 0.294849 0.076437

17 N -0.702881 -0.024022

18 C -0.309650 0.089439

19 C 0.315042 -0.022783

20 C -0.256226 -0.002850

21 C -0.256226 -0.002850

22 C 0.315042 -0.022783

23 N -0.721893 0.074888

24 H 0.231565 0.000353

25 H 0.231565 0.000353

26 H 0.218185 -0.004339

27 H 0.218185 -0.004339

28 H 0.218185 -0.004339

29 H 0.218185 -0.004339

30 H 0.231565 0.000353

31 H 0.231565 0.000353

32 Zn 1.354749 -0.003988

33 C -0.309650 0.089439

34 C -0.027846 -0.026739

35 C -0.027846 -0.026739

36 C -0.339261 0.053590

37 C -0.339261 0.053590

38 C -0.027846 -0.026739

39 C -0.339261 0.053590

40 C -0.027846 -0.026739

41 C -0.339261 0.053590

42 H 0.290062 -0.002287

43 H 0.290062 -0.002287

44 H 0.290062 -0.002287

45 H 0.290062 -0.002287

Sum of Mulliken charges = -1.00000 1.00000

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

1 2

1 C -0.024661 -0.002497

2 C 0.315042 -0.022783

3 N -0.721893 0.074888

4 C 0.315042 -0.022783

5 C -0.024661 -0.002497

6 C -0.309650 0.089439

7 C 0.294849 0.076437

8 N -0.702881 -0.024022

9 C 0.294849 0.076437

10 C -0.074835 0.060404

11 C -0.074835 0.060404

12 C -0.309650 0.089439

13 C 0.294849 0.076437

14 C -0.074835 0.060404

15 C -0.074835 0.060404

16 C 0.294849 0.076437

17 N -0.702881 -0.024022

18 C -0.309650 0.089439

19 C 0.315042 -0.022783

20 C -0.024661 -0.002497

21 C -0.024661 -0.002497

22 C 0.315042 -0.022783

23 N -0.721893 0.074888

32 Zn 1.354749 -0.003988

33 C -0.309650 0.089439

34 C -0.027846 -0.026739

35 C -0.027846 -0.026739

36 C -0.049199 0.051302

37 C -0.049199 0.051302

38 C -0.027846 -0.026739

39 C -0.049199 0.051302

40 C -0.027846 -0.026739

41 C -0.049199 0.051302

APT charges:

1

1 C 0.167785

2 C 0.443051

3 N -1.295350

4 C 0.443052

5 C 0.167782

6 C -0.235667

7 C -0.477097

8 N -0.595094

9 C -0.477097

10 C 0.259635

11 C 0.259636

12 C -0.235668

13 C -0.477096

14 C 0.259636

15 C 0.259636

16 C -0.477097

17 N -0.595093

18 C -0.235665

19 C 0.443049

20 C 0.167783

21 C 0.167784

22 C 0.443052

23 N -1.295351

24 H 0.080374

25 H 0.080373

26 H 0.070634

27 H 0.070634

28 H 0.070634

29 H 0.070634

30 H 0.080373

31 H 0.080373

32 Zn 1.355236

33 C -0.235667

34 C 0.746414

35 C 0.746415

36 C -1.023467

37 C -1.023468

38 C 0.746414

39 C -1.023468

40 C 0.746415

41 C -1.023470

42 H 0.324754

43 H 0.324752

44 H 0.324753

45 H 0.324752

Sum of APT charges = -1.00000

APT charges with hydrogens summed into heavy atoms:

1

1 C 0.248159

2 C 0.443051

3 N -1.295350

4 C 0.443052

5 C 0.248155

6 C -0.235667

7 C -0.477097

8 N -0.595094

9 C -0.477097

10 C 0.330270

11 C 0.330270

12 C -0.235668

13 C -0.477096

14 C 0.330270

15 C 0.330270

16 C -0.477097

17 N -0.595093

18 C -0.235665

19 C 0.443049

20 C 0.248156

21 C 0.248157

22 C 0.443052

23 N -1.295351

32 Zn 1.355236

33 C -0.235667

34 C 0.746414

35 C 0.746415

36 C -0.698714

37 C -0.698716

38 C 0.746414

39 C -0.698715

40 C 0.746415

41 C -0.698716

Electronic spatial extent (au): <R\*\*2>= 13596.6638

Charge= -1.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -0.0000 Y= 0.0000 Z= 0.8107 Tot= 0.8107

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

XX= -218.0649 YY= -199.7777 ZZ= -205.3072

XY= -0.0000 XZ= -0.0000 YZ= -0.0000

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

XX= -10.3483 YY= 7.9389 ZZ= 2.4094

XY= -0.0000 XZ= -0.0000 YZ= -0.0000

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

XXX= -0.0000 YYY= 0.0000 ZZZ= 9.9256 XYY= 0.0000

XXY= -0.0000 XXZ= -1.1771 XZZ= -0.0000 YZZ= -0.0000

YYZ= -1.0632 XYZ= 0.0000

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

XXXX= -9142.7500 YYYY= -8801.1079 ZZZZ= -234.9788 XXXY= -0.0000

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

ZZZY= 0.0000 XXYY= -2380.8485 XXZZ= -1864.2372 YYZZ= -1851.3844

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= -0.0000

N-N= 3.053921301342D+03 E-N=-9.377468698844D+03 KE= 1.403885104174D+03

Symmetry A1 KE= 4.231360060618D+02

Symmetry A2 KE= 2.909086728330D+02

Symmetry B1 KE= 3.441849714194D+02

Symmetry B2 KE= 3.456554538600D+02

Exact polarizability:1648.084 0.0001175.732 -0.000 0.000 187.338

Approx polarizability:1778.016 -0.0001188.031 0.000 -0.000 220.189

Isotropic Fermi Contact Couplings

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

1 C(13) -0.00009 -0.10627 -0.03792 -0.03545

2 C(13) -0.00637 -7.16144 -2.55538 -2.38880

3 N(14) 0.00894 2.88855 1.03071 0.96352

4 C(13) -0.00637 -7.16144 -2.55538 -2.38880

5 C(13) -0.00009 -0.10627 -0.03792 -0.03545

6 C(13) 0.00372 4.18387 1.49291 1.39559

7 C(13) 0.00077 0.86042 0.30702 0.28700

8 N(14) -0.00564 -1.82241 -0.65028 -0.60789

9 C(13) 0.00077 0.86042 0.30702 0.28700

10 C(13) -0.00002 -0.02476 -0.00883 -0.00826

11 C(13) -0.00002 -0.02476 -0.00883 -0.00826

12 C(13) 0.00372 4.18387 1.49291 1.39559

13 C(13) 0.00077 0.86042 0.30702 0.28700

14 C(13) -0.00002 -0.02476 -0.00883 -0.00826

15 C(13) -0.00002 -0.02476 -0.00883 -0.00826

16 C(13) 0.00077 0.86042 0.30702 0.28700

17 N(14) -0.00564 -1.82241 -0.65028 -0.60789

18 C(13) 0.00372 4.18387 1.49291 1.39559

19 C(13) -0.00637 -7.16144 -2.55538 -2.38880

20 C(13) -0.00009 -0.10627 -0.03792 -0.03545

21 C(13) -0.00009 -0.10627 -0.03792 -0.03545

22 C(13) -0.00637 -7.16144 -2.55538 -2.38880

23 N(14) 0.00894 2.88855 1.03071 0.96352

24 H(1) 0.00008 0.35921 0.12817 0.11982

25 H(1) 0.00008 0.35921 0.12817 0.11982

26 H(1) -0.00122 -5.45049 -1.94487 -1.81809

27 H(1) -0.00122 -5.45049 -1.94487 -1.81809

28 H(1) -0.00122 -5.45049 -1.94487 -1.81809

29 H(1) -0.00122 -5.45049 -1.94487 -1.81809

30 H(1) 0.00008 0.35921 0.12817 0.11982

31 H(1) 0.00008 0.35921 0.12817 0.11982

32 Zn(67) 0.00000 0.00000 0.00000 0.00000

33 C(13) 0.00372 4.18387 1.49291 1.39559

34 C(13) -0.00673 -7.56160 -2.69817 -2.52228

35 C(13) -0.00673 -7.56160 -2.69817 -2.52228

36 C(13) 0.00270 3.03305 1.08227 1.01172

37 C(13) 0.00270 3.03305 1.08227 1.01172

38 C(13) -0.00673 -7.56160 -2.69817 -2.52228

39 C(13) 0.00270 3.03305 1.08227 1.01172

40 C(13) -0.00673 -7.56160 -2.69817 -2.52228

41 C(13) 0.00270 3.03305 1.08227 1.01172

42 H(1) -0.00087 -3.87932 -1.38424 -1.29400

43 H(1) -0.00087 -3.87932 -1.38424 -1.29400

44 H(1) -0.00087 -3.87932 -1.38424 -1.29400

45 H(1) -0.00087 -3.87932 -1.38424 -1.29400

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

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

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

1 Atom 0.003376 0.003794 -0.007170

2 Atom 0.015244 0.006388 -0.021632

3 Atom -0.086579 -0.090721 0.177300

4 Atom 0.015244 0.006388 -0.021632

5 Atom 0.003376 0.003794 -0.007170

6 Atom -0.060409 -0.059370 0.119779

7 Atom -0.050663 -0.050732 0.101395

8 Atom 0.019858 0.019939 -0.039798

9 Atom -0.050663 -0.050732 0.101395

10 Atom -0.042675 -0.043212 0.085888

11 Atom -0.042675 -0.043212 0.085888

12 Atom -0.060409 -0.059370 0.119779

13 Atom -0.050663 -0.050732 0.101395

14 Atom -0.042675 -0.043212 0.085888

15 Atom -0.042675 -0.043212 0.085888

16 Atom -0.050663 -0.050732 0.101395

17 Atom 0.019858 0.019939 -0.039798

18 Atom -0.060409 -0.059370 0.119779

19 Atom 0.015244 0.006388 -0.021632

20 Atom 0.003376 0.003794 -0.007170

21 Atom 0.003376 0.003794 -0.007170

22 Atom 0.015244 0.006388 -0.021632

23 Atom -0.086579 -0.090721 0.177300

24 Atom 0.000408 0.000722 -0.001130

25 Atom 0.000408 0.000722 -0.001130

26 Atom 0.004674 -0.002453 -0.002221

27 Atom 0.004674 -0.002453 -0.002221

28 Atom 0.004674 -0.002453 -0.002221

29 Atom 0.004674 -0.002453 -0.002221

30 Atom 0.000408 0.000722 -0.001130

31 Atom 0.000408 0.000722 -0.001130

32 Atom -0.008704 0.008234 0.000470

33 Atom -0.060409 -0.059370 0.119779

34 Atom 0.007117 0.007907 -0.015024

35 Atom 0.007117 0.007907 -0.015024

36 Atom -0.025299 -0.023978 0.049278

37 Atom -0.025299 -0.023978 0.049278

38 Atom 0.007117 0.007907 -0.015024

39 Atom -0.025299 -0.023978 0.049278

40 Atom 0.007117 0.007907 -0.015024

41 Atom -0.025299 -0.023978 0.049278

42 Atom 0.000161 0.000609 -0.000770

43 Atom 0.000161 0.000609 -0.000770

44 Atom 0.000161 0.000609 -0.000770

45 Atom 0.000161 0.000609 -0.000770

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XY XZ YZ

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

1 Atom -0.000569 -0.000164 0.000087

2 Atom 0.000959 -0.000311 0.000026

3 Atom -0.000000 0.000000 0.008287

4 Atom -0.000959 0.000311 0.000026

5 Atom 0.000569 0.000164 0.000087

6 Atom 0.001461 -0.001620 0.000851

7 Atom 0.003266 -0.002510 0.000882

8 Atom 0.000000 0.001917 0.000000

9 Atom -0.003266 -0.002510 -0.000882

10 Atom 0.000277 -0.003600 -0.000009

11 Atom -0.000277 -0.003600 0.000009

12 Atom -0.001461 0.001620 0.000851

13 Atom -0.003266 0.002510 0.000882

14 Atom 0.000277 0.003600 0.000009

15 Atom -0.000277 0.003600 -0.000009

16 Atom 0.003266 0.002510 -0.000882

17 Atom -0.000000 -0.001917 0.000000

18 Atom 0.001461 0.001620 -0.000851

19 Atom -0.000959 -0.000311 -0.000026

20 Atom 0.000569 -0.000164 -0.000087

21 Atom -0.000569 0.000164 -0.000087

22 Atom 0.000959 0.000311 -0.000026

23 Atom 0.000000 0.000000 -0.008287

24 Atom -0.000709 0.000002 -0.000001

25 Atom 0.000709 -0.000002 -0.000001

26 Atom 0.006018 0.000147 0.000140

27 Atom -0.006018 0.000147 -0.000140

28 Atom 0.006018 -0.000147 -0.000140

29 Atom -0.006018 -0.000147 0.000140

30 Atom 0.000709 0.000002 0.000001

31 Atom -0.000709 -0.000002 0.000001

32 Atom -0.000000 -0.000000 0.000000

33 Atom -0.001461 -0.001620 -0.000851

34 Atom 0.008859 0.000168 0.000316

35 Atom 0.008859 -0.000168 -0.000316

36 Atom -0.002760 -0.000338 -0.000847

37 Atom -0.002760 0.000338 0.000847

38 Atom -0.008859 0.000168 -0.000316

39 Atom 0.002760 -0.000338 0.000847

40 Atom -0.008859 -0.000168 0.000316

41 Atom 0.002760 0.000338 -0.000847

42 Atom -0.003903 -0.000044 0.000026

43 Atom 0.003903 0.000044 0.000026

44 Atom -0.003903 0.000044 -0.000026

45 Atom 0.003903 -0.000044 -0.000026

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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 -0.0072 -0.963 -0.343 -0.321 0.0152 -0.0071 0.9999

1 C(13) Bbb 0.0030 0.400 0.143 0.133 0.8192 0.5734 -0.0083

Bcc 0.0042 0.563 0.201 0.188 -0.5733 0.8192 0.0145

Baa -0.0216 -2.903 -1.036 -0.968 0.0085 -0.0012 1.0000

2 C(13) Bbb 0.0063 0.843 0.301 0.281 -0.1064 0.9943 0.0021

Bcc 0.0153 2.060 0.735 0.687 0.9943 0.1064 -0.0083

Baa -0.0910 -3.509 -1.252 -1.170 0.0000 0.9995 -0.0309

3 N(14) Bbb -0.0866 -3.339 -1.191 -1.114 1.0000 -0.0000 0.0000

Bcc 0.1776 6.848 2.444 2.284 0.0000 0.0309 0.9995

Baa -0.0216 -2.903 -1.036 -0.968 -0.0085 -0.0012 1.0000

4 C(13) Bbb 0.0063 0.843 0.301 0.281 0.1064 0.9943 0.0021

Bcc 0.0153 2.060 0.735 0.687 0.9943 -0.1064 0.0083

Baa -0.0072 -0.963 -0.343 -0.321 -0.0152 -0.0071 0.9999

5 C(13) Bbb 0.0030 0.400 0.143 0.133 0.8192 -0.5734 0.0083

Bcc 0.0042 0.563 0.201 0.188 0.5733 0.8192 0.0145

Baa -0.0615 -8.247 -2.943 -2.751 0.8174 -0.5760 0.0100

6 C(13) Bbb -0.0583 -7.829 -2.793 -2.611 0.5760 0.8174 0.0013

Bcc 0.1198 16.076 5.736 5.362 -0.0090 0.0047 0.9999

Baa -0.0540 -7.246 -2.586 -2.417 -0.7052 0.7089 -0.0154

7 C(13) Bbb -0.0474 -6.366 -2.272 -2.123 0.7088 0.7053 0.0078

Bcc 0.1014 13.612 4.857 4.541 -0.0164 0.0054 0.9999

Baa -0.0399 -1.537 -0.549 -0.513 -0.0321 -0.0000 0.9995

8 N(14) Bbb 0.0199 0.768 0.274 0.256 0.9995 0.0000 0.0321

Bcc 0.0199 0.769 0.274 0.257 -0.0000 1.0000 -0.0000

Baa -0.0540 -7.246 -2.586 -2.417 0.7052 0.7089 0.0154

9 C(13) Bbb -0.0474 -6.366 -2.272 -2.123 0.7088 -0.7053 0.0078

Bcc 0.1014 13.612 4.857 4.541 -0.0164 -0.0054 0.9999

Baa -0.0433 -5.817 -2.076 -1.940 -0.4359 0.8999 -0.0121

10 C(13) Bbb -0.0426 -5.722 -2.042 -1.909 0.8995 0.4361 0.0252

Bcc 0.0860 11.539 4.117 3.849 -0.0280 -0.0001 0.9996

Baa -0.0433 -5.817 -2.076 -1.940 0.4359 0.8999 0.0121

11 C(13) Bbb -0.0426 -5.722 -2.042 -1.909 0.8995 -0.4361 0.0252

Bcc 0.0860 11.539 4.117 3.849 -0.0280 0.0001 0.9996

Baa -0.0615 -8.247 -2.943 -2.751 0.8174 0.5760 -0.0100

12 C(13) Bbb -0.0583 -7.829 -2.793 -2.611 -0.5760 0.8174 0.0013

Bcc 0.1198 16.076 5.736 5.362 0.0090 0.0047 0.9999

Baa -0.0540 -7.246 -2.586 -2.417 0.7052 0.7089 -0.0154

13 C(13) Bbb -0.0474 -6.366 -2.272 -2.123 0.7088 -0.7053 -0.0078

Bcc 0.1014 13.612 4.857 4.541 0.0164 0.0054 0.9999

Baa -0.0433 -5.817 -2.076 -1.940 -0.4359 0.8999 0.0121

14 C(13) Bbb -0.0426 -5.722 -2.042 -1.909 0.8995 0.4361 -0.0252

Bcc 0.0860 11.539 4.117 3.849 0.0280 0.0001 0.9996

Baa -0.0433 -5.817 -2.076 -1.940 0.4359 0.8999 -0.0121

15 C(13) Bbb -0.0426 -5.722 -2.042 -1.909 0.8995 -0.4361 -0.0252

Bcc 0.0860 11.539 4.117 3.849 0.0280 -0.0001 0.9996

Baa -0.0540 -7.246 -2.586 -2.417 -0.7052 0.7089 0.0154

16 C(13) Bbb -0.0474 -6.366 -2.272 -2.123 0.7088 0.7053 -0.0078

Bcc 0.1014 13.612 4.857 4.541 0.0164 -0.0054 0.9999

Baa -0.0399 -1.537 -0.549 -0.513 0.0321 0.0000 0.9995

17 N(14) Bbb 0.0199 0.768 0.274 0.256 0.9995 0.0000 -0.0321

Bcc 0.0199 0.769 0.274 0.257 -0.0000 1.0000 0.0000

Baa -0.0615 -8.247 -2.943 -2.751 0.8174 -0.5760 -0.0100

18 C(13) Bbb -0.0583 -7.829 -2.793 -2.611 0.5760 0.8174 -0.0013

Bcc 0.1198 16.076 5.736 5.362 0.0090 -0.0047 0.9999

Baa -0.0216 -2.903 -1.036 -0.968 0.0085 0.0012 1.0000

19 C(13) Bbb 0.0063 0.843 0.301 0.281 0.1064 0.9943 -0.0021

Bcc 0.0153 2.060 0.735 0.687 0.9943 -0.1064 -0.0083

Baa -0.0072 -0.963 -0.343 -0.321 0.0152 0.0071 0.9999

20 C(13) Bbb 0.0030 0.400 0.143 0.133 0.8192 -0.5734 -0.0083

Bcc 0.0042 0.563 0.201 0.188 0.5733 0.8192 -0.0145

Baa -0.0072 -0.963 -0.343 -0.321 -0.0152 0.0071 0.9999

21 C(13) Bbb 0.0030 0.400 0.143 0.133 0.8192 0.5734 0.0083

Bcc 0.0042 0.563 0.201 0.188 -0.5733 0.8192 -0.0145

Baa -0.0216 -2.903 -1.036 -0.968 -0.0085 0.0012 1.0000

22 C(13) Bbb 0.0063 0.843 0.301 0.281 -0.1064 0.9943 -0.0021

Bcc 0.0153 2.060 0.735 0.687 0.9943 0.1064 0.0083

Baa -0.0910 -3.509 -1.252 -1.170 -0.0000 0.9995 0.0309

23 N(14) Bbb -0.0866 -3.339 -1.191 -1.114 1.0000 0.0000 0.0000

Bcc 0.1776 6.848 2.444 2.284 0.0000 -0.0309 0.9995

Baa -0.0011 -0.603 -0.215 -0.201 -0.0015 0.0002 1.0000

24 H(1) Bbb -0.0002 -0.086 -0.031 -0.029 0.7798 0.6260 0.0011

Bcc 0.0013 0.689 0.246 0.230 -0.6260 0.7798 -0.0011

Baa -0.0011 -0.603 -0.215 -0.201 0.0015 0.0002 1.0000

25 H(1) Bbb -0.0002 -0.086 -0.031 -0.029 0.7798 -0.6260 -0.0011

Bcc 0.0013 0.689 0.246 0.230 0.6260 0.7798 -0.0011

Baa -0.0059 -3.140 -1.120 -1.047 -0.4950 0.8688 -0.0134

26 H(1) Bbb -0.0022 -1.187 -0.423 -0.396 -0.0232 0.0022 0.9997

Bcc 0.0081 4.326 1.544 1.443 0.8686 0.4952 0.0190

Baa -0.0059 -3.140 -1.120 -1.047 0.4950 0.8688 0.0134

27 H(1) Bbb -0.0022 -1.187 -0.423 -0.396 -0.0232 -0.0022 0.9997

Bcc 0.0081 4.326 1.544 1.443 0.8686 -0.4952 0.0190

Baa -0.0059 -3.140 -1.120 -1.047 -0.4950 0.8688 0.0134

28 H(1) Bbb -0.0022 -1.187 -0.423 -0.396 0.0232 -0.0022 0.9997

Bcc 0.0081 4.326 1.544 1.443 0.8686 0.4952 -0.0190

Baa -0.0059 -3.140 -1.120 -1.047 0.4950 0.8688 -0.0134

29 H(1) Bbb -0.0022 -1.187 -0.423 -0.396 0.0232 0.0022 0.9997

Bcc 0.0081 4.326 1.544 1.443 0.8686 -0.4952 -0.0190

Baa -0.0011 -0.603 -0.215 -0.201 -0.0015 -0.0002 1.0000

30 H(1) Bbb -0.0002 -0.086 -0.031 -0.029 0.7798 -0.6260 0.0011

Bcc 0.0013 0.689 0.246 0.230 0.6260 0.7798 0.0011

Baa -0.0011 -0.603 -0.215 -0.201 0.0015 -0.0002 1.0000

31 H(1) Bbb -0.0002 -0.086 -0.031 -0.029 0.7798 0.6260 -0.0011

Bcc 0.0013 0.689 0.246 0.230 -0.6260 0.7798 0.0011

Baa -0.0087 -0.291 -0.104 -0.097 1.0000 0.0000 0.0000

32 Zn(67) Bbb 0.0005 0.016 0.006 0.005 -0.0000 -0.0000 1.0000

Bcc 0.0082 0.275 0.098 0.092 -0.0000 1.0000 0.0000

Baa -0.0615 -8.247 -2.943 -2.751 0.8174 0.5760 0.0100

33 C(13) Bbb -0.0583 -7.829 -2.793 -2.611 -0.5760 0.8174 -0.0013

Bcc 0.1198 16.076 5.736 5.362 -0.0090 -0.0047 0.9999

Baa -0.0150 -2.017 -0.720 -0.673 -0.0025 -0.0128 0.9999

34 C(13) Bbb -0.0014 -0.182 -0.065 -0.061 0.7228 -0.6911 -0.0071

Bcc 0.0164 2.199 0.784 0.733 0.6911 0.7227 0.0110

Baa -0.0150 -2.017 -0.720 -0.673 0.0025 0.0128 0.9999

35 C(13) Bbb -0.0014 -0.182 -0.065 -0.061 0.7228 -0.6911 0.0071

Bcc 0.0164 2.199 0.784 0.733 0.6911 0.7227 -0.0110

Baa -0.0275 -3.688 -1.316 -1.230 0.7845 0.6200 0.0103

36 C(13) Bbb -0.0218 -2.926 -1.044 -0.976 -0.6201 0.7845 0.0064

Bcc 0.0493 6.614 2.360 2.206 -0.0041 -0.0114 0.9999

Baa -0.0275 -3.688 -1.316 -1.230 0.7845 0.6200 -0.0103

37 C(13) Bbb -0.0218 -2.926 -1.044 -0.976 -0.6201 0.7845 -0.0064

Bcc 0.0493 6.614 2.360 2.206 0.0041 0.0114 0.9999

Baa -0.0150 -2.017 -0.720 -0.673 -0.0025 0.0128 0.9999

38 C(13) Bbb -0.0014 -0.182 -0.065 -0.061 0.7228 0.6911 -0.0071

Bcc 0.0164 2.199 0.784 0.733 -0.6911 0.7227 -0.0110

Baa -0.0275 -3.688 -1.316 -1.230 0.7845 -0.6200 0.0103

39 C(13) Bbb -0.0218 -2.926 -1.044 -0.976 0.6201 0.7845 -0.0064

Bcc 0.0493 6.614 2.360 2.206 -0.0041 0.0114 0.9999

Baa -0.0150 -2.017 -0.720 -0.673 0.0025 -0.0128 0.9999

40 C(13) Bbb -0.0014 -0.182 -0.065 -0.061 0.7228 0.6911 0.0071

Bcc 0.0164 2.199 0.784 0.733 -0.6911 0.7227 0.0110

Baa -0.0275 -3.688 -1.316 -1.230 0.7845 -0.6200 -0.0103

41 C(13) Bbb -0.0218 -2.926 -1.044 -0.976 0.6201 0.7845 0.0064

Bcc 0.0493 6.614 2.360 2.206 0.0041 -0.0114 0.9999

Baa -0.0035 -1.880 -0.671 -0.627 0.7271 0.6865 0.0051

42 H(1) Bbb -0.0008 -0.411 -0.147 -0.137 0.0029 -0.0105 0.9999

Bcc 0.0043 2.292 0.818 0.764 -0.6865 0.7271 0.0096

Baa -0.0035 -1.880 -0.671 -0.627 0.7271 -0.6865 -0.0051

43 H(1) Bbb -0.0008 -0.411 -0.147 -0.137 -0.0029 -0.0105 0.9999

Bcc 0.0043 2.292 0.818 0.764 0.6865 0.7271 0.0096

Baa -0.0035 -1.880 -0.671 -0.627 0.7271 0.6865 -0.0051

44 H(1) Bbb -0.0008 -0.411 -0.147 -0.137 -0.0029 0.0105 0.9999

Bcc 0.0043 2.292 0.818 0.764 -0.6865 0.7271 -0.0096

Baa -0.0035 -1.880 -0.671 -0.627 0.7271 -0.6865 0.0051

45 H(1) Bbb -0.0008 -0.411 -0.147 -0.137 0.0029 0.0105 0.9999

Bcc 0.0043 2.292 0.818 0.764 0.6865 0.7271 -0.0096

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

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Tue Jul 30 21:22:21 2019, MaxMem= 4294967296 cpu: 31.7

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16185 LenP2D= 44720.

LDataN: DoStor=T MaxTD1= 7 Len= 274

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 256

Leave Link 701 at Tue Jul 30 21:22:56 2019, MaxMem= 4294967296 cpu: 560.4

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

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

Leave Link 702 at Tue Jul 30 21:22:56 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

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

wScrn= 0.000000 ICntrl= 100127 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Tue Jul 30 21:25:33 2019, MaxMem= 4294967296 cpu: 2520.8

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

Dipole = 7.95891131D-14-1.93178806D-13 3.18960568D-01

Polarizability= 1.64808366D+03 2.66730482D-05 1.17573184D+03

-6.98404304D-06 3.39488307D-06 1.87338127D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000005031 0.000081879 -0.000000555

2 6 0.000010228 0.000039971 0.000001570

3 7 -0.000073518 -0.000000000 0.000086774

4 6 0.000010228 -0.000039971 0.000001570

5 6 -0.000005031 -0.000081879 -0.000000555

6 6 -0.000054347 0.000032056 0.000000900

7 6 0.000006226 0.000028899 0.000000063

8 7 0.000000000 -0.000059711 0.000126250

9 6 -0.000006226 0.000028899 0.000000063

10 6 -0.000001608 -0.000045957 -0.000001131

11 6 0.000001608 -0.000045957 -0.000001131

12 6 -0.000054347 -0.000032056 0.000000900

13 6 0.000006226 -0.000028899 0.000000063

14 6 0.000001608 0.000045957 -0.000001131

15 6 -0.000001608 0.000045957 -0.000001131

16 6 -0.000006226 -0.000028899 0.000000063

17 7 0.000000000 0.000059711 0.000126250

18 6 0.000054347 -0.000032056 0.000000900

19 6 -0.000010228 0.000039971 0.000001570

20 6 0.000005031 0.000081879 -0.000000555

21 6 0.000005031 -0.000081879 -0.000000555

22 6 -0.000010228 -0.000039971 0.000001570

23 7 0.000073518 -0.000000000 0.000086774

24 1 0.000001546 0.000001886 0.000000106

25 1 0.000001546 -0.000001886 0.000000106

26 1 0.000000717 0.000001178 0.000000328

27 1 -0.000000717 0.000001178 0.000000328

28 1 -0.000000717 -0.000001178 0.000000328

29 1 0.000000717 -0.000001178 0.000000328

30 1 -0.000001546 0.000001886 0.000000106

31 1 -0.000001546 -0.000001886 0.000000106

32 30 0.000000000 0.000000000 -0.000429889

33 6 0.000054347 0.000032056 0.000000900

34 6 -0.000008182 0.000000326 -0.000002568

35 6 0.000008182 -0.000000326 -0.000002568

36 6 0.000004335 -0.000005211 0.000001206

37 6 -0.000004335 0.000005211 0.000001206

38 6 0.000008182 0.000000326 -0.000002568

39 6 -0.000004335 -0.000005211 0.000001206

40 6 -0.000008182 -0.000000326 -0.000002568

41 6 0.000004335 0.000005211 0.000001206

42 1 0.000001291 -0.000001265 0.000001043

43 1 0.000001291 0.000001265 0.000001043

44 1 -0.000001291 0.000001265 0.000001043

45 1 -0.000001291 -0.000001265 0.000001043

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

Cartesian Forces: Max 0.000429889 RMS 0.000048062

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

Leave Link 716 at Tue Jul 30 21:25:33 2019, MaxMem= 4294967296 cpu: 1.2

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000102822 RMS 0.000022748

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 = .22748D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Second derivative matrix not updated -- analytic derivatives used.

ITU= 0

Eigenvalues --- -0.00090 0.00162 0.00235 0.00247 0.00323

Eigenvalues --- 0.00706 0.00828 0.00866 0.00890 0.01065

Eigenvalues --- 0.01118 0.01139 0.01230 0.01239 0.01264

Eigenvalues --- 0.01286 0.01486 0.01521 0.01532 0.01624

Eigenvalues --- 0.01633 0.01728 0.01945 0.01961 0.01978

Eigenvalues --- 0.02021 0.02114 0.02120 0.02133 0.02150

Eigenvalues --- 0.02843 0.02994 0.03191 0.03510 0.03991

Eigenvalues --- 0.04098 0.04144 0.04147 0.04158 0.04164

Eigenvalues --- 0.04303 0.04351 0.04799 0.04954 0.07455

Eigenvalues --- 0.08291 0.08318 0.08518 0.08521 0.09101

Eigenvalues --- 0.09109 0.09248 0.09250 0.09275 0.09614

Eigenvalues --- 0.09631 0.09640 0.09664 0.10407 0.10410

Eigenvalues --- 0.10443 0.10513 0.12452 0.12941 0.13026

Eigenvalues --- 0.13149 0.14805 0.16897 0.16930 0.19237

Eigenvalues --- 0.19868 0.19997 0.20114 0.20353 0.20639

Eigenvalues --- 0.20644 0.20804 0.21691 0.21899 0.21959

Eigenvalues --- 0.22036 0.25990 0.26265 0.27699 0.28036

Eigenvalues --- 0.28085 0.29435 0.30071 0.31773 0.32518

Eigenvalues --- 0.32738 0.32961 0.33568 0.35620 0.35694

Eigenvalues --- 0.35858 0.36104 0.36467 0.37030 0.37104

Eigenvalues --- 0.37163 0.37324 0.37402 0.37567 0.37769

Eigenvalues --- 0.38093 0.38315 0.38847 0.39197 0.40235

Eigenvalues --- 0.40238 0.40240 0.40242 0.41381 0.41521

Eigenvalues --- 0.42147 0.42651 0.45540 0.46304 0.46597

Eigenvalues --- 0.46870 0.50227 0.50245 0.52698 0.53113

Eigenvalues --- 1.03394 1.04139 1.04471 1.04703

Eigenvalue 1 is -9.03D-04 should be greater than 0.000000 Eigenvector:

A88 A87 D126 D127 D22

1 0.30581 -0.29208 -0.22954 0.22949 0.22943

D23 D96 D93 D52 D49

1 -0.22938 0.22282 -0.22277 -0.22272 0.22267

RFO step: Lambda=-9.79140540D-04 EMin=-9.03314491D-04

I= 1 Eig= -9.03D-04 Dot1= 1.63D-04

I= 1 Stepn= 6.00D-01 RXN= 6.00D-01 EDone=F

Mixed 1 eigenvectors in step. Raw Step.Grad= 1.63D-04.

RFO eigenvector is Hessian eigenvector with negative curvature.

Taking step of 6.00D-01 in eigenvector direction(s). Step.Grad= -9.34D-07.

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.03578038 RMS(Int)= 0.00260362

Iteration 2 RMS(Cart)= 0.00357491 RMS(Int)= 0.00191338

Iteration 3 RMS(Cart)= 0.00000282 RMS(Int)= 0.00191338

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00191338

ITry= 1 IFail=0 DXMaxC= 4.39D-01 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 9.69D-03 for atom 37.

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

(Linear) (Quad) (Total)

R1 2.74589 0.00000 0.00000 0.00170 0.00110 2.74699

R2 2.56693 0.00009 0.00000 0.00146 -0.00295 2.56397

R3 2.04145 -0.00000 0.00000 0.00007 0.00007 2.04152

R4 2.59411 0.00002 0.00000 -0.00293 -0.00248 2.59163

R5 2.65223 -0.00001 0.00000 0.00404 0.00143 2.65366

R6 2.59411 0.00002 0.00000 -0.00292 -0.00248 2.59163

R7 3.95345 0.00006 0.00000 0.00201 0.00368 3.95713

R8 2.74589 0.00000 0.00000 0.00170 0.00110 2.74699

R9 2.65223 -0.00001 0.00000 0.00404 0.00143 2.65366

R10 2.04145 -0.00000 0.00000 0.00007 0.00007 2.04152

R11 2.71678 0.00005 0.00000 0.00478 0.00015 2.71694

R12 2.69142 0.00000 0.00000 0.00017 0.00060 2.69202

R13 2.59314 0.00001 0.00000 -0.00272 -0.00054 2.59259

R14 2.69546 0.00005 0.00000 0.00159 0.00177 2.69723

R15 2.59314 0.00001 0.00000 -0.00273 -0.00054 2.59259

R16 3.96566 0.00004 0.00000 0.00050 0.00235 3.96801

R17 2.69546 0.00005 0.00000 0.00159 0.00177 2.69723

R18 2.71678 0.00005 0.00000 0.00477 0.00015 2.71694

R19 2.61434 0.00002 0.00000 0.00146 -0.00304 2.61129

R20 2.04170 -0.00000 0.00000 0.00007 0.00007 2.04177

R21 2.04170 -0.00000 0.00000 0.00007 0.00007 2.04177

R22 2.71678 0.00005 0.00000 0.00477 0.00015 2.71694

R23 2.69142 0.00000 0.00000 0.00017 0.00060 2.69202

R24 2.69546 0.00005 0.00000 0.00159 0.00177 2.69723

R25 2.59314 0.00002 0.00000 -0.00271 -0.00054 2.59259

R26 2.61434 0.00002 0.00000 0.00145 -0.00304 2.61129

R27 2.04170 -0.00000 0.00000 0.00007 0.00007 2.04177

R28 2.69546 0.00005 0.00000 0.00159 0.00177 2.69723

R29 2.04170 -0.00000 0.00000 0.00007 0.00007 2.04177

R30 2.59314 0.00001 0.00000 -0.00272 -0.00054 2.59259

R31 2.71678 0.00005 0.00000 0.00476 0.00015 2.71694

R32 3.96566 0.00005 0.00000 0.00066 0.00235 3.96801

R33 2.65223 -0.00001 0.00000 0.00403 0.00143 2.65366

R34 2.69142 0.00000 0.00000 0.00017 0.00060 2.69202

R35 2.74589 0.00000 0.00000 0.00170 0.00110 2.74699

R36 2.59411 0.00002 0.00000 -0.00292 -0.00248 2.59163

R37 2.56693 0.00009 0.00000 0.00146 -0.00295 2.56397

R38 2.04145 -0.00000 0.00000 0.00007 0.00007 2.04152

R39 2.74589 0.00000 0.00000 0.00171 0.00110 2.74699

R40 2.04145 -0.00000 0.00000 0.00007 0.00007 2.04152

R41 2.59411 0.00002 0.00000 -0.00291 -0.00248 2.59163

R42 2.65223 -0.00001 0.00000 0.00404 0.00143 2.65366

R43 3.95345 0.00006 0.00000 0.00217 0.00368 3.95713

R44 2.69142 0.00000 0.00000 0.00017 0.00060 2.69202

R45 2.28350 0.00001 0.00000 0.00001 0.00001 2.28351

R46 2.28350 0.00001 0.00000 0.00001 0.00001 2.28351

R47 2.01598 -0.00000 0.00000 0.00002 0.00034 2.01632

R48 2.01598 -0.00000 0.00000 0.00002 0.00034 2.01632

R49 2.28350 0.00001 0.00000 0.00001 0.00001 2.28351

R50 2.01598 -0.00000 0.00000 0.00002 0.00034 2.01632

R51 2.28350 0.00001 0.00000 0.00001 0.00001 2.28351

R52 2.01598 -0.00000 0.00000 0.00002 0.00034 2.01632

A1 1.87063 -0.00000 0.00000 0.00110 0.00073 1.87136

A2 2.18700 -0.00000 0.00000 0.00045 0.00065 2.18765

A3 2.22555 0.00000 0.00000 -0.00153 -0.00138 2.22417

A4 1.90201 -0.00001 0.00000 -0.00533 -0.00255 1.89946

A5 2.18176 -0.00000 0.00000 0.00500 0.00279 2.18455

A6 2.19939 0.00001 0.00000 0.00041 -0.00024 2.19915

A7 1.87949 0.00002 0.00000 0.00847 0.00362 1.88311

A8 2.20079 -0.00001 0.00000 -0.00173 -0.00078 2.20001

A9 2.20079 -0.00001 0.00000 -0.00181 -0.00078 2.20001

A10 1.90201 -0.00001 0.00000 -0.00533 -0.00255 1.89946

A11 2.19939 0.00001 0.00000 0.00043 -0.00024 2.19915

A12 2.18176 -0.00000 0.00000 0.00499 0.00279 2.18455

A13 1.87063 -0.00000 0.00000 0.00110 0.00073 1.87136

A14 2.22555 0.00000 0.00000 -0.00153 -0.00138 2.22417

A15 2.18700 -0.00000 0.00000 0.00045 0.00065 2.18765

A16 2.20902 0.00001 0.00000 0.00717 0.00389 2.21291

A17 2.04444 -0.00000 0.00000 -0.00338 -0.00061 2.04383

A18 2.02970 -0.00001 0.00000 -0.00370 -0.00326 2.02644

A19 2.18095 0.00000 0.00000 0.00041 0.00023 2.18118

A20 2.19230 0.00001 0.00000 0.00482 0.00343 2.19573

A21 1.90990 -0.00001 0.00000 -0.00516 -0.00362 1.90628

A22 1.87426 0.00002 0.00000 0.00811 0.00426 1.87852

A23 2.20372 -0.00001 0.00000 -0.00203 -0.00151 2.20222

A24 2.20372 -0.00001 0.00000 -0.00196 -0.00151 2.20222

A25 1.90990 -0.00001 0.00000 -0.00515 -0.00362 1.90628

A26 2.18095 0.00000 0.00000 0.00039 0.00023 2.18118

A27 2.19230 0.00001 0.00000 0.00483 0.00343 2.19573

A28 1.86536 0.00000 0.00000 0.00110 0.00149 1.86684

A29 2.19604 -0.00000 0.00000 0.00048 -0.00005 2.19599

A30 2.22178 0.00000 0.00000 -0.00156 -0.00142 2.22035

A31 1.86536 0.00000 0.00000 0.00110 0.00149 1.86684

A32 2.19604 -0.00000 0.00000 0.00048 -0.00005 2.19599

A33 2.22178 0.00000 0.00000 -0.00156 -0.00142 2.22035

A34 2.20902 0.00001 0.00000 0.00716 0.00389 2.21291

A35 2.04444 -0.00000 0.00000 -0.00338 -0.00061 2.04383

A36 2.02970 -0.00001 0.00000 -0.00370 -0.00326 2.02644

A37 2.19230 0.00000 0.00000 0.00481 0.00343 2.19573

A38 2.18095 0.00000 0.00000 0.00042 0.00023 2.18118

A39 1.90990 -0.00001 0.00000 -0.00515 -0.00362 1.90628

A40 1.86536 0.00000 0.00000 0.00110 0.00149 1.86684

A41 2.19604 -0.00000 0.00000 0.00048 -0.00005 2.19599

A42 2.22178 0.00000 0.00000 -0.00156 -0.00142 2.22035

A43 1.86536 0.00000 0.00000 0.00110 0.00149 1.86684

A44 2.22178 0.00000 0.00000 -0.00156 -0.00142 2.22035

A45 2.19604 -0.00000 0.00000 0.00048 -0.00005 2.19599

A46 1.90990 -0.00001 0.00000 -0.00515 -0.00362 1.90628

A47 2.19230 0.00000 0.00000 0.00482 0.00343 2.19573

A48 2.18095 0.00000 0.00000 0.00040 0.00023 2.18118

A49 1.87426 0.00002 0.00000 0.00809 0.00426 1.87852

A50 2.20372 -0.00001 0.00000 -0.00202 -0.00151 2.20222

A51 2.20372 -0.00001 0.00000 -0.00195 -0.00151 2.20222

A52 2.20902 0.00001 0.00000 0.00715 0.00389 2.21291

A53 2.02970 -0.00001 0.00000 -0.00369 -0.00326 2.02644

A54 2.04444 0.00000 0.00000 -0.00338 -0.00061 2.04383

A55 2.18176 -0.00000 0.00000 0.00498 0.00279 2.18455

A56 2.19939 0.00001 0.00000 0.00042 -0.00024 2.19915

A57 1.90201 -0.00001 0.00000 -0.00532 -0.00255 1.89946

A58 1.87063 -0.00000 0.00000 0.00110 0.00073 1.87136

A59 2.18700 -0.00000 0.00000 0.00045 0.00065 2.18765

A60 2.22555 0.00000 0.00000 -0.00153 -0.00138 2.22417

A61 1.87063 -0.00000 0.00000 0.00110 0.00073 1.87136

A62 2.22555 0.00000 0.00000 -0.00153 -0.00138 2.22417

A63 2.18700 -0.00000 0.00000 0.00045 0.00065 2.18765

A64 1.90201 -0.00001 0.00000 -0.00533 -0.00255 1.89946

A65 2.18176 -0.00000 0.00000 0.00497 0.00279 2.18455

A66 2.19939 0.00001 0.00000 0.00044 -0.00024 2.19915

A67 1.87949 0.00002 0.00000 0.00845 0.00362 1.88311

A68 2.20079 -0.00001 0.00000 -0.00172 -0.00078 2.20001

A69 2.20079 -0.00001 0.00000 -0.00180 -0.00078 2.20001

A70 1.56630 0.00001 0.00000 0.01215 0.00400 1.57029

A71 1.56630 0.00001 0.00000 0.01209 0.00400 1.57029

A72 1.56630 0.00001 0.00000 0.01209 0.00400 1.57029

A73 1.56630 0.00001 0.00000 0.01203 0.00400 1.57029

A74 2.20902 0.00001 0.00000 0.00716 0.00389 2.21291

A75 2.02970 -0.00001 0.00000 -0.00370 -0.00326 2.02644

A76 2.04444 -0.00000 0.00000 -0.00338 -0.00061 2.04383

A77 3.13259 0.00001 0.00000 0.02413 0.00799 3.14058

A78 3.13259 0.00001 0.00000 0.02413 0.00799 3.14058

A79 3.12428 0.00001 0.00000 -0.00052 -0.00034 3.12394

A80 3.15888 -0.00001 0.00000 0.00058 0.00037 3.15924

A81 3.14708 0.00000 0.00000 0.00006 0.00335 3.15043

A82 3.14708 0.00000 0.00000 0.00006 0.00335 3.15043

A83 3.15888 -0.00001 0.00000 0.00059 0.00037 3.15924

A84 3.14708 0.00000 0.00000 0.00006 0.00335 3.15043

A85 3.12428 0.00001 0.00000 -0.00052 -0.00034 3.12394

A86 3.14708 0.00000 0.00000 0.00006 0.00335 3.15043

A87 3.27793 -0.00009 0.00000 -0.17525 -0.17519 3.10274

A88 3.00995 0.00010 0.00000 0.18348 0.18353 3.19348

A89 3.14059 0.00001 0.00000 0.00131 0.00130 3.14189

A90 3.14299 -0.00001 0.00000 -0.00186 -0.00187 3.14112

A91 3.14132 0.00000 0.00000 0.00014 0.00008 3.14140

A92 3.14132 0.00000 0.00000 0.00015 0.00008 3.14140

A93 3.14020 0.00001 0.00000 0.00187 0.00187 3.14206

A94 3.14187 -0.00000 0.00000 -0.00015 -0.00008 3.14179

A95 3.14259 -0.00001 0.00000 -0.00130 -0.00130 3.14129

A96 3.14187 -0.00000 0.00000 -0.00014 -0.00008 3.14179

D1 -0.00027 0.00001 0.00000 0.00299 0.00287 0.00259

D2 3.13455 0.00002 0.00000 0.01543 0.01523 -3.13341

D3 -3.13800 0.00000 0.00000 -0.00358 -0.00361 3.14158

D4 -0.00318 0.00001 0.00000 0.00886 0.00876 0.00558

D5 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D6 -3.13761 -0.00001 0.00000 -0.00676 -0.00666 3.13891

D7 3.13761 0.00001 0.00000 0.00676 0.00666 -3.13891

D8 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00044 -0.00002 0.00000 -0.00483 -0.00465 -0.00421

D10 -3.07459 -0.00002 0.00000 -0.08236 -0.08224 3.12635

D11 -3.13429 -0.00003 0.00000 -0.01746 -0.01716 3.13173

D12 0.07386 -0.00003 0.00000 -0.09499 -0.09475 -0.02089

D13 -3.12615 -0.00003 0.00000 -0.02758 -0.02728 3.12976

D14 0.00736 -0.00000 0.00000 -0.01449 -0.01442 -0.00706

D15 0.00752 -0.00002 0.00000 -0.01304 -0.01282 -0.00529

D16 3.14103 0.00001 0.00000 0.00005 0.00005 3.14108

D17 -0.00044 0.00002 0.00000 0.00483 0.00465 0.00421

D18 3.13429 0.00003 0.00000 0.01746 0.01716 -3.13173

D19 3.07459 0.00002 0.00000 0.08236 0.08224 -3.12635

D20 -0.07386 0.00003 0.00000 0.09499 0.09475 0.02089

D21 -3.11502 -0.00005 0.00000 -0.04582 -0.04602 3.12214

D22 -0.10507 0.00005 0.00000 0.13766 0.13751 0.03243

D23 0.10507 -0.00005 0.00000 -0.13763 -0.13751 -0.03243

D24 3.11502 0.00005 0.00000 0.04585 0.04602 -3.12214

D25 0.00027 -0.00001 0.00000 -0.00298 -0.00287 -0.00259

D26 3.13800 -0.00000 0.00000 0.00358 0.00361 -3.14158

D27 -3.13455 -0.00002 0.00000 -0.01543 -0.01523 3.13341

D28 0.00318 -0.00001 0.00000 -0.00886 -0.00876 -0.00558

D29 -0.00752 0.00002 0.00000 0.01303 0.01282 0.00529

D30 -3.14103 -0.00001 0.00000 -0.00008 -0.00005 -3.14108

D31 3.12615 0.00003 0.00000 0.02757 0.02728 -3.12976

D32 -0.00736 0.00000 0.00000 0.01445 0.01442 0.00706

D33 0.01236 -0.00002 0.00000 -0.01794 -0.01776 -0.00540

D34 -3.11928 -0.00003 0.00000 -0.02848 -0.02824 3.13567

D35 -3.13726 0.00000 0.00000 -0.00492 -0.00499 3.14093

D36 0.01429 -0.00000 0.00000 -0.01547 -0.01548 -0.00119

D37 -3.13237 -0.00002 0.00000 -0.00825 -0.00795 -3.14032

D38 0.06484 -0.00003 0.00000 -0.08570 -0.08549 -0.02065

D39 0.00064 -0.00001 0.00000 0.00089 0.00108 0.00173

D40 -3.08534 -0.00002 0.00000 -0.07656 -0.07645 3.12140

D41 3.13254 0.00001 0.00000 0.00863 0.00844 3.14099

D42 -0.00467 0.00001 0.00000 0.00383 0.00374 -0.00093

D43 -0.00040 0.00001 0.00000 -0.00055 -0.00067 -0.00106

D44 -3.13761 0.00000 0.00000 -0.00535 -0.00537 3.14020

D45 -0.00064 0.00001 0.00000 -0.00089 -0.00108 -0.00173

D46 3.13237 0.00002 0.00000 0.00824 0.00795 3.14032

D47 3.08534 0.00002 0.00000 0.07656 0.07645 -3.12140

D48 -0.06484 0.00003 0.00000 0.08569 0.08549 0.02065

D49 -0.10109 0.00005 0.00000 0.13360 0.13345 0.03237

D50 -3.10634 -0.00004 0.00000 -0.04164 -0.04174 3.13510

D51 3.10634 0.00004 0.00000 0.04161 0.04174 -3.13510

D52 0.10109 -0.00005 0.00000 -0.13363 -0.13345 -0.03237

D53 0.00040 -0.00001 0.00000 0.00055 0.00067 0.00106

D54 3.13761 -0.00000 0.00000 0.00535 0.00537 -3.14020

D55 -3.13254 -0.00001 0.00000 -0.00863 -0.00844 -3.14099

D56 0.00467 -0.00001 0.00000 -0.00383 -0.00374 0.00093

D57 -0.01236 0.00002 0.00000 0.01796 0.01776 0.00540

D58 3.13726 -0.00000 0.00000 0.00497 0.00499 -3.14093

D59 3.11928 0.00003 0.00000 0.02850 0.02824 -3.13567

D60 -0.01429 0.00000 0.00000 0.01551 0.01548 0.00119

D61 -0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D62 3.13713 0.00001 0.00000 0.00490 0.00479 -3.14126

D63 -3.13713 -0.00001 0.00000 -0.00490 -0.00479 3.14126

D64 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D65 3.11928 0.00003 0.00000 0.02844 0.02824 -3.13567

D66 -0.01236 0.00002 0.00000 0.01792 0.01776 0.00540

D67 -0.01429 0.00000 0.00000 0.01545 0.01548 0.00119

D68 3.13726 -0.00000 0.00000 0.00493 0.00499 -3.14093

D69 -3.13254 -0.00001 0.00000 -0.00861 -0.00844 -3.14099

D70 0.00467 -0.00001 0.00000 -0.00381 -0.00374 0.00093

D71 0.00040 -0.00001 0.00000 0.00056 0.00067 0.00106

D72 3.13761 -0.00000 0.00000 0.00535 0.00537 -3.14020

D73 3.13237 0.00002 0.00000 0.00822 0.00795 3.14032

D74 -0.06484 0.00003 0.00000 0.08576 0.08549 0.02065

D75 -0.00064 0.00001 0.00000 -0.00090 -0.00108 -0.00173

D76 3.08534 0.00002 0.00000 0.07664 0.07645 -3.12140

D77 -0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D78 3.13713 0.00001 0.00000 0.00489 0.00479 -3.14126

D79 -3.13713 -0.00001 0.00000 -0.00489 -0.00479 3.14126

D80 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D81 -0.00040 0.00001 0.00000 -0.00055 -0.00067 -0.00106

D82 3.13254 0.00001 0.00000 0.00860 0.00844 3.14099

D83 -3.13761 0.00000 0.00000 -0.00535 -0.00537 3.14020

D84 -0.00467 0.00001 0.00000 0.00381 0.00374 -0.00093

D85 0.00064 -0.00001 0.00000 0.00090 0.00108 0.00173

D86 -3.08534 -0.00002 0.00000 -0.07664 -0.07645 3.12140

D87 -3.13237 -0.00002 0.00000 -0.00821 -0.00795 -3.14032

D88 0.06484 -0.00003 0.00000 -0.08575 -0.08549 -0.02065

D89 -3.11928 -0.00003 0.00000 -0.02846 -0.02824 3.13567

D90 0.01429 -0.00000 0.00000 -0.01549 -0.01548 -0.00119

D91 0.01236 -0.00002 0.00000 -0.01795 -0.01776 -0.00540

D92 -3.13726 0.00000 0.00000 -0.00497 -0.00499 3.14093

D93 0.10109 -0.00005 0.00000 -0.13366 -0.13345 -0.03237

D94 3.10634 0.00004 0.00000 0.04159 0.04174 -3.13510

D95 -3.10634 -0.00004 0.00000 -0.04156 -0.04174 3.13510

D96 -0.10109 0.00005 0.00000 0.13369 0.13345 0.03237

D97 3.12615 0.00003 0.00000 0.02754 0.02728 -3.12976

D98 -0.00752 0.00002 0.00000 0.01303 0.01282 0.00529

D99 -0.00736 0.00000 0.00000 0.01448 0.01442 0.00706

D100 -3.14103 -0.00001 0.00000 -0.00004 -0.00005 -3.14108

D101 -3.13455 -0.00002 0.00000 -0.01540 -0.01523 3.13341

D102 0.00318 -0.00001 0.00000 -0.00884 -0.00876 -0.00558

D103 0.00027 -0.00001 0.00000 -0.00297 -0.00287 -0.00259

D104 3.13800 -0.00000 0.00000 0.00359 0.00361 -3.14158

D105 3.13429 0.00003 0.00000 0.01742 0.01716 -3.13173

D106 -0.07386 0.00003 0.00000 0.09505 0.09475 0.02089

D107 -0.00044 0.00002 0.00000 0.00481 0.00465 0.00421

D108 3.07459 0.00002 0.00000 0.08245 0.08224 -3.12635

D109 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D110 3.13761 0.00001 0.00000 0.00675 0.00666 -3.13891

D111 -3.13761 -0.00001 0.00000 -0.00675 -0.00666 3.13891

D112 -0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D113 -0.00027 0.00001 0.00000 0.00297 0.00287 0.00259

D114 3.13455 0.00002 0.00000 0.01540 0.01523 -3.13341

D115 -3.13800 0.00000 0.00000 -0.00359 -0.00361 3.14158

D116 -0.00318 0.00001 0.00000 0.00884 0.00876 0.00558

D117 0.00044 -0.00002 0.00000 -0.00481 -0.00465 -0.00421

D118 -3.07459 -0.00002 0.00000 -0.08245 -0.08224 3.12635

D119 -3.13429 -0.00003 0.00000 -0.01742 -0.01716 3.13173

D120 0.07386 -0.00003 0.00000 -0.09506 -0.09475 -0.02089

D121 -3.12615 -0.00003 0.00000 -0.02753 -0.02728 3.12976

D122 0.00736 -0.00000 0.00000 -0.01444 -0.01442 -0.00706

D123 0.00752 -0.00002 0.00000 -0.01302 -0.01282 -0.00529

D124 3.14103 0.00001 0.00000 0.00007 0.00005 3.14108

D125 3.11502 0.00005 0.00000 0.04576 0.04602 -3.12214

D126 0.10507 -0.00005 0.00000 -0.13772 -0.13751 -0.03243

D127 -0.10507 0.00005 0.00000 0.13770 0.13751 0.03243

D128 -3.11502 -0.00005 0.00000 -0.04579 -0.04602 3.12214

Item Value Threshold Converged?

Maximum Force 0.000103 0.000450 YES

RMS Force 0.000023 0.000300 YES

Maximum Displacement 0.439463 0.001800 NO

RMS Displacement 0.034893 0.001200 NO

Predicted change in Energy=-2.963095D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Jul 30 21:25:34 2019, MaxMem= 4294967296 cpu: 1.5

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -4.289160 0.678398 -0.029272

2 6 0 -2.900715 1.108766 -0.038081

3 7 0 -2.093630 0.000000 -0.046569

4 6 0 -2.900715 -1.108766 -0.038081

5 6 0 -4.289160 -0.678398 -0.029272

6 6 0 -2.468007 -2.444676 -0.031427

7 6 0 -1.107324 -2.909016 -0.026098

8 7 0 -0.000000 -2.099072 -0.032785

9 6 0 1.107324 -2.909016 -0.026098

10 6 0 0.690918 -4.274169 -0.012502

11 6 0 -0.690918 -4.274169 -0.012502

12 6 0 -2.468007 2.444676 -0.031427

13 6 0 -1.107324 2.909016 -0.026098

14 6 0 -0.690918 4.274169 -0.012502

15 6 0 0.690918 4.274169 -0.012502

16 6 0 1.107324 2.909016 -0.026098

17 7 0 0.000000 2.099072 -0.032785

18 6 0 2.468007 2.444676 -0.031427

19 6 0 2.900715 1.108766 -0.038081

20 6 0 4.289160 0.678398 -0.029272

21 6 0 4.289160 -0.678398 -0.029272

22 6 0 2.900715 -1.108766 -0.038081

23 7 0 2.093630 -0.000000 -0.046569

24 1 0 -5.146944 1.335094 -0.021528

25 1 0 -5.146944 -1.335094 -0.021528

26 1 0 1.344416 -5.134550 -0.003647

27 1 0 -1.344416 -5.134550 -0.003647

28 1 0 -1.344416 5.134550 -0.003647

29 1 0 1.344416 5.134550 -0.003647

30 1 0 5.146944 1.335094 -0.021528

31 1 0 5.146944 -1.335094 -0.021528

32 30 0 0.000000 0.000000 -0.087263

33 6 0 2.468007 -2.444676 -0.031427

34 6 0 3.474441 -3.452837 -0.023669

35 6 0 -3.474441 3.452837 -0.023669

36 6 0 4.312921 -4.322945 -0.016554

37 6 0 -4.312921 4.322945 -0.016554

38 6 0 -3.474441 -3.452837 -0.023669

39 6 0 -4.312921 -4.322945 -0.016554

40 6 0 3.474441 3.452837 -0.023669

41 6 0 4.312921 4.322945 -0.016554

42 1 0 5.060055 5.084670 -0.010531

43 1 0 5.060055 -5.084670 -0.010531

44 1 0 -5.060055 -5.084670 -0.010531

45 1 0 -5.060055 5.084670 -0.010531

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.453642 0.000000

3 N 2.298016 1.371430 0.000000

4 C 2.263143 2.217533 1.371430 0.000000

5 C 1.356796 2.263143 2.298016 1.453642 0.000000

6 C 3.615273 3.579698 2.473223 1.404256 2.536995

7 C 4.795168 4.399883 3.071741 2.541121 3.885840

8 N 5.109916 4.324858 2.964722 3.065107 4.518321

9 C 6.480092 5.675129 4.325378 4.393793 5.839324

10 C 7.023488 6.471204 5.101313 4.787510 6.142559

11 C 6.121727 5.818921 4.498586 3.860522 5.086963

12 C 2.536995 1.404256 2.473223 3.579698 3.615273

13 C 3.885840 2.541121 3.071741 4.399883 4.795168

14 C 5.086963 3.860522 4.498586 5.818921 6.121727

15 C 6.142559 4.787510 5.101313 6.471204 7.023488

16 C 5.839324 4.393793 4.325378 5.675129 6.480092

17 N 4.518321 3.065107 2.964722 4.324858 5.109916

18 C 6.984200 5.532438 5.175442 6.438180 7.443984

19 C 7.202749 5.801429 5.115947 6.210800 7.408666

20 C 8.578320 7.202749 6.418764 7.408666 8.684957

21 C 8.684957 7.408666 6.418764 7.202749 8.578320

22 C 7.408666 6.210800 5.115947 5.801429 7.202749

23 N 6.418764 5.115947 4.187260 5.115947 6.418764

24 H 1.080325 2.257663 3.332541 3.319378 2.188607

25 H 2.188607 3.319378 3.332541 2.257663 1.080325

26 H 8.094949 7.549922 6.179450 5.850577 7.182975

27 H 6.516329 6.434458 5.189101 4.316270 5.341298

28 H 5.341298 4.316270 5.189101 6.434458 6.516329

29 H 7.182975 5.850577 6.179450 7.549922 8.094949

30 H 9.458930 8.050857 7.362677 8.410561 9.648537

31 H 9.648537 8.410561 7.362677 8.050857 9.458930

32 Zn 4.342866 3.105789 2.094025 3.105789 4.342866

33 C 7.443984 6.438180 5.175442 5.532438 6.984200

34 C 8.794352 7.839071 6.551795 6.792458 8.244455

35 C 2.891594 2.413304 3.718770 4.597564 4.210808

36 C 9.950346 9.029977 7.728690 7.897338 9.342306

37 C 3.644647 3.510803 4.859425 5.612333 5.001416

38 C 4.210808 4.597564 3.718770 2.413304 2.891594

39 C 5.001416 5.612333 4.859425 3.510803 3.644647

40 C 8.244455 6.792458 6.551795 7.839071 8.794352

41 C 9.342306 7.897338 7.728690 9.029977 9.950346

42 H 10.335541 8.898450 8.776695 10.086291 10.982765

43 H 10.982765 10.086291 8.776695 8.898450 10.335541

44 H 5.814428 6.559128 5.886836 4.524524 4.473238

45 H 4.473238 4.524524 5.886836 6.559128 5.814428

6 7 8 9 10

6 C 0.000000

7 C 1.437740 0.000000

8 N 2.492088 1.371940 0.000000

9 C 3.605361 2.214647 1.371940 0.000000

10 C 3.650508 2.257765 2.282285 1.427312 0.000000

11 C 2.550577 1.427312 2.282285 2.257765 1.381837

12 C 4.889353 5.523903 5.170755 6.437782 7.424422

13 C 5.523903 5.818032 5.129050 6.225284 7.404864

14 C 6.949912 7.195257 6.410615 7.404864 8.659304

15 C 7.424422 7.404864 6.410615 7.195257 8.548338

16 C 6.437782 6.225284 5.129050 5.818032 7.195257

17 N 5.170755 5.129050 4.198144 5.129050 6.410615

18 C 6.947661 6.437782 5.170755 5.523903 6.949912

19 C 6.438180 5.675129 4.324858 4.399883 5.818921

20 C 7.443984 6.480092 5.109916 4.795168 6.121727

21 C 6.984200 5.839324 4.518321 3.885840 5.086963

22 C 5.532438 4.393793 3.065107 2.541121 3.860522

23 N 5.175442 4.325378 2.964722 3.071741 4.498586

24 H 4.632868 5.859268 6.187459 7.558330 8.095958

25 H 2.899651 4.335410 5.203347 6.449272 6.535968

26 H 4.665914 3.311273 3.320004 2.238240 1.080459

27 H 2.915244 2.238240 3.320004 3.311273 2.209733

28 H 7.662108 8.047091 7.357553 8.408953 9.626352

29 H 8.484103 8.408953 7.357553 8.047091 9.431390

30 H 8.501425 7.558330 6.187459 5.859268 7.163803

31 H 7.695371 6.449272 5.203347 4.335410 5.338015

32 Zn 3.474279 3.113243 2.099779 3.113243 4.330298

33 C 4.936013 3.605361 2.492088 1.437740 2.550577

34 C 6.027365 4.613926 3.728874 2.428784 2.902190

35 C 5.982778 6.787962 6.549467 7.840010 8.778210

36 C 7.036270 5.601637 4.852542 3.503590 3.622333

37 C 7.014601 7.910576 7.735881 9.037721 9.947301

38 C 1.424555 2.428784 3.728874 4.613926 4.245577

39 C 2.632836 3.503590 4.852542 5.601637 5.004079

40 C 8.372180 7.840010 6.549467 6.787962 8.213084

41 C 9.580287 9.037721 7.735881 7.910576 9.328949

42 H 10.647216 10.096327 8.786967 8.917586 10.328466

43 H 7.977576 6.539899 5.875240 4.511961 4.443678

44 H 3.699827 4.511961 5.875240 6.539899 5.807806

45 H 7.963052 8.917586 8.786967 10.096327 10.984606

11 12 13 14 15

11 C 0.000000

12 C 6.949912 0.000000

13 C 7.195257 1.437740 0.000000

14 C 8.548338 2.550577 1.427312 0.000000

15 C 8.659304 3.650508 2.257765 1.381837 0.000000

16 C 7.404864 3.605361 2.214647 2.257765 1.427312

17 N 6.410615 2.492088 1.371940 2.282285 2.282285

18 C 7.424422 4.936013 3.605361 3.650508 2.550577

19 C 6.471204 5.532438 4.393793 4.787510 3.860522

20 C 7.023488 6.984200 5.839324 6.142559 5.086963

21 C 6.142559 7.443984 6.480092 7.023488 6.121727

22 C 4.787510 6.438180 5.675129 6.471204 5.818921

23 N 5.101313 5.175442 4.325378 5.101313 4.498586

24 H 7.163803 2.899651 4.335410 5.338015 6.535968

25 H 5.338015 4.632868 5.859268 7.163803 8.095958

26 H 2.209733 8.484103 8.408953 9.626352 9.431390

27 H 1.080459 7.662108 8.047091 9.431390 9.626352

28 H 9.431390 2.915244 2.238240 1.080459 2.209733

29 H 9.626352 4.665914 3.311273 2.209733 1.080459

30 H 8.095958 7.695371 6.449272 6.535968 5.338015

31 H 6.535968 8.501425 7.558330 8.095958 7.163803

32 Zn 4.330298 3.474279 3.113243 4.330298 4.330298

33 C 3.650508 6.947661 6.437782 7.424422 6.949912

34 C 4.245577 8.372180 7.840010 8.778210 8.213084

35 C 8.213084 1.424555 2.428784 2.902190 4.245577

36 C 5.004079 9.580287 9.037721 9.947301 9.328949

37 C 9.328949 2.632836 3.503590 3.622333 5.004079

38 C 2.902190 5.982778 6.787962 8.213084 8.778210

39 C 3.622333 7.014601 7.910576 9.328949 9.947301

40 C 8.778210 6.027365 4.613926 4.245577 2.902190

41 C 9.947301 7.036270 5.601637 5.004079 3.622333

42 H 10.984606 7.977576 6.539899 5.807806 4.443678

43 H 5.807806 10.647216 10.096327 10.984606 10.328466

44 H 4.443678 7.963052 8.917586 10.328466 10.984606

45 H 10.328466 3.699827 4.511961 4.443678 5.807806

16 17 18 19 20

16 C 0.000000

17 N 1.371940 0.000000

18 C 1.437740 2.492088 0.000000

19 C 2.541121 3.065107 1.404256 0.000000

20 C 3.885840 4.518321 2.536995 1.453642 0.000000

21 C 4.795168 5.109916 3.615273 2.263143 1.356796

22 C 4.399883 4.324858 3.579698 2.217533 2.263143

23 N 3.071741 2.964722 2.473223 1.371430 2.298016

24 H 6.449272 5.203347 7.695371 8.050857 9.458930

25 H 7.558330 6.187459 8.501425 8.410561 9.648537

26 H 8.047091 7.357553 7.662108 6.434458 6.516329

27 H 8.408953 7.357553 8.484103 7.549922 8.094949

28 H 3.311273 3.320004 4.665914 5.850577 7.182975

29 H 2.238240 3.320004 2.915244 4.316270 5.341298

30 H 4.335410 5.203347 2.899651 2.257663 1.080325

31 H 5.859268 6.187459 4.632868 3.319378 2.188607

32 Zn 3.113243 2.099779 3.474279 3.105789 4.342866

33 C 5.523903 5.170755 4.889353 3.579698 3.615273

34 C 6.787962 6.549467 5.982778 4.597564 4.210808

35 C 4.613926 3.728874 6.027365 6.792458 8.244455

36 C 7.910576 7.735881 7.014601 5.612333 5.001416

37 C 5.601637 4.852542 7.036270 7.897338 9.342306

38 C 7.840010 6.549467 8.372180 7.839071 8.794352

39 C 9.037721 7.735881 9.580287 9.029977 9.950346

40 C 2.428784 3.728874 1.424555 2.413304 2.891594

41 C 3.503590 4.852542 2.632836 3.510803 3.644647

42 H 4.511961 5.875240 3.699827 4.524524 4.473238

43 H 8.917586 8.786967 7.963052 6.559128 5.814428

44 H 10.096327 8.786967 10.647216 10.086291 10.982765

45 H 6.539899 5.875240 7.977576 8.898450 10.335541

21 22 23 24 25

21 C 0.000000

22 C 1.453642 0.000000

23 N 2.298016 1.371430 0.000000

24 H 9.648537 8.410561 7.362677 0.000000

25 H 9.458930 8.050857 7.362677 2.670188 0.000000

26 H 5.341298 4.316270 5.189101 9.164843 7.521565

27 H 7.182975 5.850577 6.179450 7.504387 5.375445

28 H 8.094949 7.549922 6.179450 5.375445 7.504387

29 H 6.516329 6.434458 5.189101 7.521565 9.164843

30 H 2.188607 3.319378 3.332541 10.293887 10.634567

31 H 1.080325 2.257663 3.332541 10.634567 10.293887

32 Zn 4.342866 3.105789 2.094025 5.317690 5.317690

33 C 2.536995 1.404256 2.473223 8.501425 7.695371

34 C 2.891594 2.413304 3.718770 9.861671 8.877675

35 C 8.794352 7.839071 6.551795 2.698538 5.071642

36 C 3.644647 3.510803 4.859425 11.022816 9.920500

37 C 9.950346 9.029977 7.728690 3.102076 5.719180

38 C 8.244455 6.792458 6.551795 5.071642 2.698538

39 C 9.342306 7.897338 7.728690 5.719180 3.102076

40 C 4.210808 4.597564 3.718770 8.877675 9.861671

41 C 5.001416 5.612333 4.859425 9.920500 11.022816

42 H 5.814428 6.559128 5.886836 10.873926 12.058039

43 H 4.473238 4.524524 5.886836 12.058039 10.873926

44 H 10.335541 8.898450 8.776695 6.420361 3.750599

45 H 10.982765 10.086291 8.776695 3.750599 6.420361

26 27 28 29 30

26 H 0.000000

27 H 2.688832 0.000000

28 H 10.615282 10.269100 0.000000

29 H 10.269100 10.615282 2.688832 0.000000

30 H 7.504387 9.164843 7.521565 5.375445 0.000000

31 H 5.375445 7.521565 9.164843 7.504387 2.670188

32 Zn 5.308300 5.308300 5.308300 5.308300 5.317690

33 C 2.915244 4.665914 8.484103 7.662108 4.632868

34 C 2.713957 5.103914 9.847081 8.847634 5.071642

35 C 9.847081 8.847634 2.713957 5.103914 8.877675

36 C 3.077481 5.715271 11.020428 9.912437 5.719180

37 C 11.020428 9.912437 3.077481 5.715271 9.920500

38 C 5.103914 2.713957 8.847634 9.847081 9.861671

39 C 5.715271 3.077481 9.912437 11.020428 11.022816

40 C 8.847634 9.847081 5.103914 2.713957 2.698538

41 C 9.912437 11.020428 5.715271 3.077481 3.102076

42 H 10.873751 12.060255 6.404669 3.715981 3.750599

43 H 3.715981 6.404669 12.060255 10.873751 6.420361

44 H 6.404669 3.715981 10.873751 12.060255 12.058039

45 H 12.060255 10.873751 3.715981 6.404669 10.873926

31 32 33 34 35

31 H 0.000000

32 Zn 5.317690 0.000000

33 C 2.899651 3.474279 0.000000

34 C 2.698538 4.898762 1.424555 0.000000

35 C 9.861671 4.898762 8.372180 9.796698 0.000000

36 C 3.102076 6.106893 2.632836 1.208382 11.004810

37 C 11.022816 6.106893 9.580287 11.004810 1.208382

38 C 8.877675 4.898762 6.027365 6.948881 6.905675

39 C 9.920500 6.106893 7.036270 7.835824 7.820863

40 C 5.071642 4.898762 5.982778 6.905675 6.948881

41 C 5.719180 6.106893 7.014601 7.820863 7.835824

42 H 6.420361 7.173835 7.963052 8.683511 8.689112

43 H 3.750599 7.173835 3.699827 2.275351 12.071736

44 H 10.873926 7.173835 7.977576 8.689112 8.683511

45 H 12.058039 7.173835 10.647216 12.071736 2.275351

36 37 38 39 40

36 C 0.000000

37 C 12.212967 0.000000

38 C 7.835824 7.820863 0.000000

39 C 8.625842 8.645890 1.208382 0.000000

40 C 7.820863 7.835824 9.796698 11.004810 0.000000

41 C 8.645890 8.625842 11.004810 12.212967 1.208382

42 H 9.437238 9.403879 12.071736 13.279907 2.275351

43 H 1.066991 13.279907 8.689112 9.403879 8.683511

44 H 9.403879 9.437238 2.275351 1.066991 12.071736

45 H 13.279907 1.066991 8.683511 9.437238 8.689112

41 42 43 44 45

41 C 0.000000

42 H 1.066991 0.000000

43 H 9.437238 10.169339 0.000000

44 H 13.279907 14.346850 10.120110 0.000000

45 H 9.403879 10.120110 14.346850 10.169339 0.000000

Stoichiometry C28H12N4Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C28H12)]

Deg. of freedom 34

Full point group C2V NOp 4

RotChk: IX=2 Diff= 3.77D-14

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.678398 4.289160 0.004905

2 6 0 1.108766 2.900715 -0.003904

3 7 0 0.000000 2.093630 -0.012392

4 6 0 -1.108766 2.900715 -0.003904

5 6 0 -0.678398 4.289160 0.004905

6 6 0 -2.444676 2.468007 0.002750

7 6 0 -2.909016 1.107324 0.008079

8 7 0 -2.099072 -0.000000 0.001392

9 6 0 -2.909016 -1.107324 0.008079

10 6 0 -4.274169 -0.690918 0.021675

11 6 0 -4.274169 0.690918 0.021675

12 6 0 2.444676 2.468007 0.002750

13 6 0 2.909016 1.107324 0.008079

14 6 0 4.274169 0.690918 0.021675

15 6 0 4.274169 -0.690918 0.021675

16 6 0 2.909016 -1.107324 0.008079

17 7 0 2.099072 0.000000 0.001392

18 6 0 2.444676 -2.468007 0.002750

19 6 0 1.108766 -2.900715 -0.003904

20 6 0 0.678398 -4.289160 0.004905

21 6 0 -0.678398 -4.289160 0.004905

22 6 0 -1.108766 -2.900715 -0.003904

23 7 0 0.000000 -2.093630 -0.012392

24 1 0 1.335094 5.146944 0.012648

25 1 0 -1.335094 5.146944 0.012648

26 1 0 -5.134550 -1.344416 0.030529

27 1 0 -5.134550 1.344416 0.030529

28 1 0 5.134550 1.344416 0.030529

29 1 0 5.134550 -1.344416 0.030529

30 1 0 1.335094 -5.146944 0.012648

31 1 0 -1.335094 -5.146944 0.012648

32 30 0 0.000000 0.000000 -0.053086

33 6 0 -2.444676 -2.468007 0.002750

34 6 0 -3.452837 -3.474441 0.010508

35 6 0 3.452837 3.474441 0.010508

36 6 0 -4.322945 -4.312921 0.017623

37 6 0 4.322945 4.312921 0.017623

38 6 0 -3.452837 3.474441 0.010508

39 6 0 -4.322945 4.312921 0.017623

40 6 0 3.452837 -3.474441 0.010508

41 6 0 4.322945 -4.312921 0.017623

42 1 0 5.084670 -5.060055 0.023646

43 1 0 -5.084670 -5.060055 0.023646

44 1 0 -5.084670 5.060055 0.023646

45 1 0 5.084670 5.060055 0.023646

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

Rotational constants (GHZ): 0.1459934 0.1454885 0.0728753

Leave Link 202 at Tue Jul 30 21:25:34 2019, MaxMem= 4294967296 cpu: 0.2

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

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

Pseudo-potential data read from rwf file.

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

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

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

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

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

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

111 alpha electrons 110 beta electrons

nuclear repulsion energy 3052.8562827810 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= 13 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= -0.1303553448 Hartrees.

Nuclear repulsion after empirical dispersion term = 3052.7259274362 Hartrees.

No density basis found on file 724.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

2nd derivatives : Analytical E(r).r(xy)/FMM algorithm (CHGder, D2EAlg=3).

Cavity 2nd derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3868

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.32D-05

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 74

GePol: Fraction of low-weight points (<1% of avg) = 1.91%

GePol: Cavity surface area = 416.402 Ang\*\*2

GePol: Cavity volume = 420.898 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0083720343 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3052.7342994705 Hartrees.

Leave Link 301 at Tue Jul 30 21:25:34 2019, MaxMem= 4294967296 cpu: 1.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16177 LenP2D= 44694.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.47D-05 NBF= 172 148 158 158

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

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Tue Jul 30 21:25:34 2019, MaxMem= 4294967296 cpu: 11.2

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Jul 30 21:25:34 2019, MaxMem= 4294967296 cpu: 1.3

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

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

B after Tr= 0.000000 -0.000000 0.000000

Rot= 1.000000 -0.000000 -0.000000 -0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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The electronic state of the initial guess is 2-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7630 S= 0.5065

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1359.67039963329

Leave Link 401 at Tue Jul 30 21:25:37 2019, MaxMem= 4294967296 cpu: 43.1

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1387497 IEndB= 1387497 NGot= 4294967296 MDV= 4294047352

LenX= 4294047352 LenY= 4293596440

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= 650000000 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= 44884272.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.00D-15 for 3865.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.13D-15 for 2182 1996.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.55D-15 for 3865.

Iteration 1 A^-1\*A deviation from orthogonality is 1.42D-14 for 3210 3156.

E= -1359.17554351861

DIIS: error= 3.86D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.17554351861 IErMin= 1 ErrMin= 3.86D-03

ErrMax= 3.86D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.97D-02 BMatP= 1.97D-02

IDIUse=3 WtCom= 9.61D-01 WtEn= 3.86D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.387 Goal= None Shift= 0.000

Gap= 0.438 Goal= None Shift= 0.000

GapD= 0.387 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

RMSDP=3.95D-04 MaxDP=2.00D-02 OVMax= 2.03D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.95D-04 CP: 9.98D-01

E= -1359.18232327502 Delta-E= -0.006779756410 Rises=F Damp=F

DIIS: error= 1.31D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.18232327502 IErMin= 2 ErrMin= 1.31D-03

ErrMax= 1.31D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.15D-04 BMatP= 1.97D-02

IDIUse=3 WtCom= 9.87D-01 WtEn= 1.31D-02

Coeff-Com: -0.154D-01 0.102D+01

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

Coeff: -0.152D-01 0.102D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=4.03D-05 MaxDP=9.30D-04 DE=-6.78D-03 OVMax= 2.53D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.73D-05 CP: 9.98D-01 1.04D+00

E= -1359.18239972745 Delta-E= -0.000076452428 Rises=F Damp=F

DIIS: error= 1.74D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.18239972745 IErMin= 2 ErrMin= 1.31D-03

ErrMax= 1.74D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.32D-04 BMatP= 4.15D-04

IDIUse=3 WtCom= 9.83D-01 WtEn= 1.74D-02

Coeff-Com: -0.235D-01 0.524D+00 0.499D+00

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

Coeff: -0.231D-01 0.515D+00 0.508D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.59D-05 MaxDP=5.95D-04 DE=-7.65D-05 OVMax= 1.18D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.12D-05 CP: 9.98D-01 1.04D+00 7.00D-01

E= -1359.18243907552 Delta-E= -0.000039348076 Rises=F Damp=F

DIIS: error= 2.77D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.18243907552 IErMin= 4 ErrMin= 2.77D-04

ErrMax= 2.77D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.60D-05 BMatP= 4.15D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.77D-03

Coeff-Com: -0.640D-02 0.983D-01 0.194D+00 0.715D+00

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

Coeff: -0.639D-02 0.980D-01 0.193D+00 0.715D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=4.57D-06 MaxDP=1.77D-04 DE=-3.93D-05 OVMax= 6.44D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.11D-06 CP: 9.98D-01 1.04D+00 7.01D-01 8.21D-01

E= -1359.18244082595 Delta-E= -0.000001750426 Rises=F Damp=F

DIIS: error= 4.97D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.18244082595 IErMin= 5 ErrMin= 4.97D-05

ErrMax= 4.97D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.18D-06 BMatP= 1.60D-05

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

Coeff-Com: -0.195D-02 0.168D-01 0.712D-01 0.395D+00 0.519D+00

Coeff: -0.195D-02 0.168D-01 0.712D-01 0.395D+00 0.519D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.63D-06 MaxDP=1.20D-04 DE=-1.75D-06 OVMax= 4.19D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.33D-06 CP: 9.98D-01 1.04D+00 7.04D-01 8.73D-01 8.25D-01

E= -1359.18244142716 Delta-E= -0.000000601209 Rises=F Damp=F

DIIS: error= 1.98D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.18244142716 IErMin= 6 ErrMin= 1.98D-05

ErrMax= 1.98D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.19D-07 BMatP= 3.18D-06

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

Coeff-Com: 0.380D-03-0.160D-01-0.435D-02 0.756D-01 0.331D+00 0.614D+00

Coeff: 0.380D-03-0.160D-01-0.435D-02 0.756D-01 0.331D+00 0.614D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=6.35D-07 MaxDP=3.82D-05 DE=-6.01D-07 OVMax= 1.18D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.85D-07 CP: 9.98D-01 1.04D+00 7.12D-01 8.84D-01 8.43D-01

CP: 6.52D-01

E= -1359.18244156040 Delta-E= -0.000000133239 Rises=F Damp=F

DIIS: error= 1.77D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.18244156040 IErMin= 7 ErrMin= 1.77D-06

ErrMax= 1.77D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.74D-09 BMatP= 6.19D-07

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

Coeff-Com: 0.182D-03-0.628D-02-0.277D-02 0.205D-01 0.111D+00 0.226D+00

Coeff-Com: 0.652D+00

Coeff: 0.182D-03-0.628D-02-0.277D-02 0.205D-01 0.111D+00 0.226D+00

Coeff: 0.652D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=9.12D-08 MaxDP=4.46D-06 DE=-1.33D-07 OVMax= 1.57D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.51D-08 CP: 9.98D-01 1.04D+00 7.12D-01 8.84D-01 8.46D-01

CP: 6.56D-01 9.47D-01

E= -1359.18244156142 Delta-E= -0.000000001023 Rises=F Damp=F

DIIS: error= 1.49D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.18244156142 IErMin= 8 ErrMin= 1.49D-06

ErrMax= 1.49D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.47D-09 BMatP= 6.74D-09

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

Coeff-Com: 0.409D-04-0.821D-03-0.773D-03-0.134D-02 0.537D-02 0.228D-01

Coeff-Com: 0.420D+00 0.555D+00

Coeff: 0.409D-04-0.821D-03-0.773D-03-0.134D-02 0.537D-02 0.228D-01

Coeff: 0.420D+00 0.555D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=4.39D-08 MaxDP=2.53D-06 DE=-1.02D-09 OVMax= 7.88D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.38D-08 CP: 9.98D-01 1.04D+00 7.13D-01 8.85D-01 8.46D-01

CP: 6.60D-01 9.88D-01 7.22D-01

E= -1359.18244156219 Delta-E= -0.000000000771 Rises=F Damp=F

DIIS: error= 4.05D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1359.18244156219 IErMin= 9 ErrMin= 4.05D-07

ErrMax= 4.05D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.70D-10 BMatP= 3.47D-09

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

Coeff-Com: -0.118D-04 0.705D-03 0.123D-03-0.413D-02-0.170D-01-0.295D-01

Coeff-Com: 0.861D-01 0.264D+00 0.700D+00

Coeff: -0.118D-04 0.705D-03 0.123D-03-0.413D-02-0.170D-01-0.295D-01

Coeff: 0.861D-01 0.264D+00 0.700D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.66D-08 MaxDP=5.64D-07 DE=-7.71D-10 OVMax= 3.02D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.43D-08 CP: 9.98D-01 1.04D+00 7.13D-01 8.85D-01 8.46D-01

CP: 6.60D-01 1.01D+00 7.72D-01 8.75D-01

E= -1359.18244156230 Delta-E= -0.000000000105 Rises=F Damp=F

DIIS: error= 2.22D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1359.18244156230 IErMin=10 ErrMin= 2.22D-07

ErrMax= 2.22D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.87D-11 BMatP= 2.70D-10

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

Coeff-Com: -0.115D-04 0.513D-03 0.156D-03-0.233D-02-0.108D-01-0.204D-01

Coeff-Com: 0.591D-02 0.973D-01 0.420D+00 0.510D+00

Coeff: -0.115D-04 0.513D-03 0.156D-03-0.233D-02-0.108D-01-0.204D-01

Coeff: 0.591D-02 0.973D-01 0.420D+00 0.510D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=6.09D-09 MaxDP=3.17D-07 DE=-1.05D-10 OVMax= 1.27D-06

Error on total polarization charges = 0.06717

SCF Done: E(UB3LYP) = -1359.18244156 A.U. after 10 cycles

NFock= 10 Conv=0.61D-08 -V/T= 1.9682

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7630 S= 0.5065

<L.S>= 0.000000000000E+00

KE= 1.403884039607D+03 PE=-9.375025072719D+03 EE= 3.559224292079D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.25

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7630, after 0.7501

Leave Link 502 at Tue Jul 30 21:26:37 2019, MaxMem= 4294967296 cpu: 928.5

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 636

NBasis= 636 NAE= 111 NBE= 110 NFC= 0 NFV= 0

NROrb= 636 NOA= 111 NOB= 110 NVA= 525 NVB= 526

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.13858970D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.38218185D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.14070572D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.88699701D-01

Leave Link 801 at Tue Jul 30 21:26:37 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 45.

Will process 46 centers per pass.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16177 LenP2D= 44694.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 11 by ecpmxn.

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

Leave Link 1101 at Tue Jul 30 21:26:41 2019, MaxMem= 4294967296 cpu: 45.2

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Tue Jul 30 21:26:41 2019, MaxMem= 4294967296 cpu: 1.1

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 45.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966832.

G2DrvN: will do 46 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

G2PCM: DoFxE=T DoFxN=T DoGrad=T DoDP/DQ/DG/TGxP=FFFF NFrqRd= 0 IEInf=0 SqF1=F DoCFld=F IF1Alg=4.

GePol: Maximum number of non-zero 1st derivatives = 256

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Tue Jul 30 21:28:38 2019, MaxMem= 4294967296 cpu: 1873.0

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=111111111111111111111111111111111111111111111

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Using symmetry in CPHF.

Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.

Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.

NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 4294965570 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 0.

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

IRaf= 650000000 NMat= 42 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

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

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

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

NMat0= 42 NMatS0= 42 NMatT0= 0 NMatD0= 42 NMtDS0= 0 NMtDT0= 0

Integrals replicated using symmetry in FoFCou.

There are 42 degrees of freedom in the 1st order CPHF. IDoFFX=4 NUNeed= 42.

42 vectors produced by pass 0 Test12= 2.77D-13 2.38D-09 XBig12= 8.03D+03 5.91D+01.

AX will form 42 AO Fock derivatives at one time.

42 vectors produced by pass 1 Test12= 2.77D-13 2.38D-09 XBig12= 1.07D+03 6.83D+00.

42 vectors produced by pass 2 Test12= 2.77D-13 2.38D-09 XBig12= 2.79D+02 5.64D+00.

42 vectors produced by pass 3 Test12= 2.77D-13 2.38D-09 XBig12= 7.54D+01 2.04D+00.

42 vectors produced by pass 4 Test12= 2.77D-13 2.38D-09 XBig12= 6.90D+00 4.66D-01.

42 vectors produced by pass 5 Test12= 2.77D-13 2.38D-09 XBig12= 2.49D-01 4.89D-02.

42 vectors produced by pass 6 Test12= 2.77D-13 2.38D-09 XBig12= 8.90D-03 7.88D-03.

42 vectors produced by pass 7 Test12= 2.77D-13 2.38D-09 XBig12= 2.00D-04 1.25D-03.

38 vectors produced by pass 8 Test12= 2.77D-13 2.38D-09 XBig12= 3.66D-06 1.36D-04.

23 vectors produced by pass 9 Test12= 2.77D-13 2.38D-09 XBig12= 4.75D-08 1.66D-05.

6 vectors produced by pass 10 Test12= 2.77D-13 2.38D-09 XBig12= 5.54D-10 1.50D-06.

2 vectors produced by pass 11 Test12= 2.77D-13 2.38D-09 XBig12= 6.71D-12 1.76D-07.

2 vectors produced by pass 12 Test12= 2.77D-13 2.38D-09 XBig12= 9.29D-14 2.72D-08.

InvSVY: IOpt=1 It= 1 EMax= 5.68D-14

Solved reduced A of dimension 407 with 42 vectors.

FullF1: Do perturbations 1 to 42.

Isotropic polarizability for W= 0.000000 1004.52 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Tue Jul 30 22:27:10 2019, MaxMem= 4294967296 cpu: 56205.2

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16177 LenP2D= 44694.

LDataN: DoStor=T MaxTD1= 7 Len= 274

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 256

Leave Link 701 at Tue Jul 30 22:27:45 2019, MaxMem= 4294967296 cpu: 549.2

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

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

Leave Link 702 at Tue Jul 30 22:27:45 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

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

wScrn= 0.000000 ICntrl= 100127 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Tue Jul 30 22:29:35 2019, MaxMem= 4294967296 cpu: 1763.1

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

Dipole =-5.48450174D-14-6.78734846D-13-1.03189888D-01

Polarizability= 1.65063649D+03-6.34000549D-06 1.17582098D+03

1.40455221D-05 9.72130296D-06 1.87108130D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000123221 0.001911189 -0.000017695

2 6 -0.000128443 0.000382306 -0.000068554

3 7 -0.000223276 0.000000000 -0.000581953

4 6 -0.000128443 -0.000382306 -0.000068554

5 6 -0.000123221 -0.001911189 -0.000017695

6 6 -0.000648999 -0.000360908 0.000109204

7 6 0.001346159 -0.000012960 -0.000053840

8 7 -0.000000000 -0.000298115 -0.001576685

9 6 -0.001346159 -0.000012960 -0.000053840

10 6 0.001671019 0.000015365 -0.000025304

11 6 -0.001671019 0.000015365 -0.000025304

12 6 -0.000648999 0.000360908 0.000109204

13 6 0.001346159 0.000012960 -0.000053840

14 6 -0.001671019 -0.000015365 -0.000025304

15 6 0.001671019 -0.000015365 -0.000025304

16 6 -0.001346159 0.000012960 -0.000053840

17 7 0.000000000 0.000298115 -0.001576685

18 6 0.000648999 0.000360908 0.000109204

19 6 0.000128443 0.000382306 -0.000068554

20 6 0.000123221 0.001911189 -0.000017695

21 6 0.000123221 -0.001911189 -0.000017695

22 6 0.000128443 -0.000382306 -0.000068554

23 7 0.000223276 0.000000000 -0.000581953

24 1 0.000044105 0.000083124 0.000005397

25 1 0.000044105 -0.000083124 0.000005397

26 1 0.000034588 0.000012225 0.000008727

27 1 -0.000034588 0.000012225 0.000008727

28 1 -0.000034588 -0.000012225 0.000008727

29 1 0.000034588 -0.000012225 0.000008727

30 1 -0.000044105 0.000083124 0.000005397

31 1 -0.000044105 -0.000083124 0.000005397

32 30 0.000000000 -0.000000000 0.004560319

33 6 0.000648999 -0.000360908 0.000109204

34 6 0.000093581 0.000242542 -0.000024103

35 6 -0.000093581 -0.000242542 -0.000024103

36 6 0.000213226 -0.000007398 -0.000002447

37 6 -0.000213226 0.000007398 -0.000002447

38 6 -0.000093581 0.000242542 -0.000024103

39 6 -0.000213226 -0.000007398 -0.000002447

40 6 0.000093581 -0.000242542 -0.000024103

41 6 0.000213226 0.000007398 -0.000002447

42 1 -0.000162541 -0.000030687 0.000007854

43 1 -0.000162541 0.000030687 0.000007854

44 1 0.000162541 0.000030687 0.000007854

45 1 0.000162541 -0.000030687 0.000007854

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

Cartesian Forces: Max 0.004560319 RMS 0.000685068

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

Leave Link 716 at Tue Jul 30 22:29:35 2019, MaxMem= 4294967296 cpu: 0.8

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.001898407 RMS 0.000319786

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 = .31979D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

ITU= 0 0

Eigenvalues --- 0.00159 0.00336 0.00423 0.00536 0.00666

Eigenvalues --- 0.00974 0.01116 0.01117 0.01121 0.01232

Eigenvalues --- 0.01246 0.01271 0.01282 0.01306 0.01308

Eigenvalues --- 0.01403 0.01505 0.01523 0.01764 0.01784

Eigenvalues --- 0.01892 0.01950 0.01963 0.01966 0.02008

Eigenvalues --- 0.02054 0.02100 0.02107 0.02129 0.02135

Eigenvalues --- 0.03000 0.03148 0.03192 0.03657 0.04006

Eigenvalues --- 0.04129 0.04137 0.04140 0.04152 0.04161

Eigenvalues --- 0.04357 0.04359 0.06078 0.06357 0.08292

Eigenvalues --- 0.08294 0.08311 0.08609 0.08912 0.08935

Eigenvalues --- 0.09000 0.09240 0.09313 0.09416 0.09625

Eigenvalues --- 0.09634 0.09665 0.09748 0.10421 0.10425

Eigenvalues --- 0.10451 0.10506 0.12201 0.13256 0.13363

Eigenvalues --- 0.13485 0.15778 0.16893 0.16958 0.19284

Eigenvalues --- 0.19874 0.20053 0.20141 0.20366 0.20610

Eigenvalues --- 0.20646 0.20849 0.21669 0.21885 0.21919

Eigenvalues --- 0.22029 0.26016 0.26194 0.27694 0.27952

Eigenvalues --- 0.28140 0.29508 0.30101 0.31812 0.32502

Eigenvalues --- 0.32766 0.32798 0.33625 0.35673 0.35719

Eigenvalues --- 0.35869 0.36112 0.36433 0.37021 0.37102

Eigenvalues --- 0.37155 0.37333 0.37416 0.37549 0.37878

Eigenvalues --- 0.38066 0.38400 0.38830 0.39203 0.40191

Eigenvalues --- 0.40193 0.40195 0.40198 0.41419 0.41539

Eigenvalues --- 0.42063 0.42628 0.45428 0.46114 0.46449

Eigenvalues --- 0.46729 0.50348 0.50373 0.53068 0.53466

Eigenvalues --- 1.03370 1.04131 1.04463 1.04696

En-DIIS/RFO-DIIS IScMMF= 0 using points: 2 1

RFO step: Lambda=-1.17436063D-04.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 5.02D-04 SmlDif= 1.00D-05

RMS Error= 0.1731963722D-02 NUsed= 2 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.07566 0.92434

Iteration 1 RMS(Cart)= 0.03187864 RMS(Int)= 0.00148247

Iteration 2 RMS(Cart)= 0.00297953 RMS(Int)= 0.00014433

Iteration 3 RMS(Cart)= 0.00000282 RMS(Int)= 0.00014432

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00014432

ITry= 1 IFail=0 DXMaxC= 4.05D-01 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 7.08D-04 for atom 37.

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

(Linear) (Quad) (Total)

R1 2.74699 0.00005 -0.00101 0.00001 -0.00096 2.74603

R2 2.56397 0.00190 0.00273 0.00044 0.00351 2.56748

R3 2.04152 0.00002 -0.00007 -0.00000 -0.00007 2.04145

R4 2.59163 0.00051 0.00229 0.00007 0.00232 2.59395

R5 2.65366 0.00001 -0.00132 0.00002 -0.00110 2.65256

R6 2.59163 0.00051 0.00229 0.00007 0.00232 2.59395

R7 3.95713 0.00060 -0.00340 0.00055 -0.00301 3.95413

R8 2.74699 0.00005 -0.00101 0.00001 -0.00096 2.74603

R9 2.65366 0.00001 -0.00132 0.00002 -0.00110 2.65256

R10 2.04152 0.00002 -0.00007 -0.00000 -0.00007 2.04145

R11 2.71694 0.00073 -0.00014 0.00032 0.00052 2.71746

R12 2.69202 -0.00009 -0.00056 -0.00004 -0.00064 2.69138

R13 2.59259 -0.00006 0.00050 -0.00006 0.00029 2.59288

R14 2.69723 -0.00015 -0.00164 0.00007 -0.00158 2.69565

R15 2.59259 -0.00006 0.00050 -0.00006 0.00029 2.59288

R16 3.96801 0.00041 -0.00217 0.00029 -0.00203 3.96598

R17 2.69723 -0.00015 -0.00164 0.00007 -0.00158 2.69565

R18 2.71694 0.00073 -0.00014 0.00032 0.00052 2.71746

R19 2.61129 0.00129 0.00281 0.00029 0.00344 2.61474

R20 2.04177 0.00001 -0.00007 -0.00000 -0.00007 2.04170

R21 2.04177 0.00001 -0.00007 -0.00000 -0.00007 2.04170

R22 2.71694 0.00073 -0.00014 0.00032 0.00052 2.71746

R23 2.69202 -0.00009 -0.00056 -0.00004 -0.00064 2.69138

R24 2.69723 -0.00015 -0.00164 0.00007 -0.00158 2.69565

R25 2.59259 -0.00006 0.00050 -0.00006 0.00029 2.59288

R26 2.61129 0.00128 0.00281 0.00030 0.00344 2.61474

R27 2.04177 0.00001 -0.00007 -0.00000 -0.00007 2.04170

R28 2.69723 -0.00015 -0.00164 0.00007 -0.00158 2.69565

R29 2.04177 0.00001 -0.00007 -0.00000 -0.00007 2.04170

R30 2.59259 -0.00006 0.00050 -0.00006 0.00029 2.59288

R31 2.71694 0.00073 -0.00014 0.00032 0.00052 2.71746

R32 3.96801 0.00041 -0.00217 0.00025 -0.00203 3.96598

R33 2.65366 0.00001 -0.00132 0.00002 -0.00110 2.65256

R34 2.69202 -0.00009 -0.00056 -0.00004 -0.00064 2.69138

R35 2.74699 0.00005 -0.00101 0.00001 -0.00096 2.74603

R36 2.59163 0.00051 0.00229 0.00007 0.00232 2.59395

R37 2.56397 0.00190 0.00273 0.00045 0.00351 2.56748

R38 2.04152 0.00002 -0.00007 -0.00000 -0.00007 2.04145

R39 2.74699 0.00005 -0.00101 0.00001 -0.00096 2.74603

R40 2.04152 0.00002 -0.00007 -0.00000 -0.00007 2.04145

R41 2.59163 0.00051 0.00229 0.00007 0.00232 2.59395

R42 2.65366 0.00001 -0.00132 0.00002 -0.00110 2.65256

R43 3.95713 0.00061 -0.00340 0.00051 -0.00301 3.95413

R44 2.69202 -0.00009 -0.00056 -0.00004 -0.00064 2.69138

R45 2.28351 0.00002 -0.00001 0.00001 -0.00000 2.28351

R46 2.28351 0.00002 -0.00001 0.00001 -0.00000 2.28351

R47 2.01632 -0.00014 -0.00031 -0.00003 -0.00037 2.01595

R48 2.01632 -0.00014 -0.00031 -0.00003 -0.00037 2.01595

R49 2.28351 0.00002 -0.00001 0.00001 -0.00000 2.28351

R50 2.01632 -0.00014 -0.00031 -0.00003 -0.00037 2.01595

R51 2.28351 0.00002 -0.00001 0.00001 -0.00000 2.28351

R52 2.01632 -0.00014 -0.00031 -0.00003 -0.00037 2.01595

A1 1.87136 -0.00015 -0.00068 -0.00003 -0.00068 1.87068

A2 2.18765 -0.00002 -0.00060 -0.00002 -0.00064 2.18701

A3 2.22417 0.00017 0.00127 0.00005 0.00131 2.22548

A4 1.89946 0.00005 0.00235 -0.00003 0.00212 1.90158

A5 2.18455 -0.00013 -0.00258 -0.00000 -0.00241 2.18214

A6 2.19915 0.00008 0.00022 0.00003 0.00030 2.19945

A7 1.88311 0.00020 -0.00335 0.00012 -0.00286 1.88025

A8 2.20001 -0.00010 0.00073 -0.00007 0.00060 2.20061

A9 2.20001 -0.00010 0.00073 -0.00005 0.00060 2.20061

A10 1.89946 0.00005 0.00235 -0.00003 0.00212 1.90158

A11 2.19915 0.00008 0.00022 0.00002 0.00030 2.19945

A12 2.18455 -0.00013 -0.00258 0.00000 -0.00241 2.18214

A13 1.87136 -0.00015 -0.00068 -0.00003 -0.00068 1.87068

A14 2.22417 0.00017 0.00127 0.00005 0.00131 2.22548

A15 2.18765 -0.00002 -0.00060 -0.00002 -0.00064 2.18701

A16 2.21291 -0.00008 -0.00359 0.00000 -0.00335 2.20956

A17 2.04383 -0.00031 0.00057 -0.00007 0.00030 2.04412

A18 2.02644 0.00040 0.00301 0.00007 0.00304 2.02948

A19 2.18118 0.00007 -0.00021 0.00005 -0.00014 2.18104

A20 2.19573 -0.00038 -0.00317 -0.00010 -0.00316 2.19256

A21 1.90628 0.00031 0.00334 0.00005 0.00328 1.90956

A22 1.87852 -0.00008 -0.00394 0.00004 -0.00361 1.87491

A23 2.20222 0.00004 0.00139 -0.00001 0.00133 2.20355

A24 2.20222 0.00004 0.00139 -0.00004 0.00133 2.20355

A25 1.90628 0.00031 0.00334 0.00005 0.00328 1.90956

A26 2.18118 0.00007 -0.00021 0.00006 -0.00014 2.18104

A27 2.19573 -0.00038 -0.00317 -0.00011 -0.00316 2.19256

A28 1.86684 -0.00027 -0.00137 -0.00007 -0.00147 1.86537

A29 2.19599 0.00010 0.00005 0.00001 0.00009 2.19608

A30 2.22035 0.00017 0.00132 0.00006 0.00137 2.22172

A31 1.86684 -0.00027 -0.00137 -0.00007 -0.00147 1.86537

A32 2.19599 0.00010 0.00005 0.00001 0.00009 2.19608

A33 2.22035 0.00017 0.00132 0.00006 0.00137 2.22172

A34 2.21291 -0.00008 -0.00359 0.00000 -0.00335 2.20956

A35 2.04383 -0.00031 0.00057 -0.00007 0.00030 2.04412

A36 2.02644 0.00040 0.00301 0.00006 0.00304 2.02948

A37 2.19573 -0.00038 -0.00317 -0.00009 -0.00316 2.19256

A38 2.18118 0.00007 -0.00021 0.00005 -0.00014 2.18104

A39 1.90628 0.00031 0.00334 0.00005 0.00328 1.90956

A40 1.86684 -0.00027 -0.00137 -0.00007 -0.00147 1.86537

A41 2.19599 0.00010 0.00005 0.00001 0.00009 2.19608

A42 2.22035 0.00017 0.00132 0.00006 0.00137 2.22172

A43 1.86684 -0.00027 -0.00137 -0.00007 -0.00147 1.86537

A44 2.22035 0.00017 0.00132 0.00006 0.00137 2.22172

A45 2.19599 0.00010 0.00005 0.00001 0.00009 2.19608

A46 1.90628 0.00031 0.00334 0.00004 0.00328 1.90956

A47 2.19573 -0.00038 -0.00317 -0.00010 -0.00316 2.19256

A48 2.18118 0.00007 -0.00021 0.00006 -0.00014 2.18104

A49 1.87852 -0.00008 -0.00394 0.00005 -0.00361 1.87491

A50 2.20222 0.00004 0.00139 -0.00001 0.00133 2.20355

A51 2.20222 0.00004 0.00139 -0.00004 0.00133 2.20355

A52 2.21291 -0.00009 -0.00359 0.00001 -0.00335 2.20956

A53 2.02644 0.00040 0.00301 0.00006 0.00304 2.02948

A54 2.04383 -0.00031 0.00057 -0.00007 0.00030 2.04412

A55 2.18455 -0.00013 -0.00258 0.00001 -0.00241 2.18214

A56 2.19915 0.00008 0.00022 0.00003 0.00030 2.19945

A57 1.89946 0.00005 0.00235 -0.00003 0.00212 1.90158

A58 1.87136 -0.00015 -0.00068 -0.00003 -0.00068 1.87068

A59 2.18765 -0.00002 -0.00060 -0.00002 -0.00064 2.18701

A60 2.22417 0.00017 0.00127 0.00005 0.00131 2.22548

A61 1.87136 -0.00015 -0.00068 -0.00003 -0.00068 1.87068

A62 2.22417 0.00017 0.00127 0.00005 0.00131 2.22548

A63 2.18765 -0.00002 -0.00060 -0.00002 -0.00064 2.18701

A64 1.89946 0.00005 0.00235 -0.00003 0.00212 1.90158

A65 2.18455 -0.00013 -0.00258 0.00001 -0.00241 2.18214

A66 2.19915 0.00008 0.00022 0.00002 0.00030 2.19945

A67 1.88311 0.00020 -0.00335 0.00012 -0.00286 1.88025

A68 2.20001 -0.00010 0.00073 -0.00008 0.00060 2.20061

A69 2.20001 -0.00010 0.00073 -0.00005 0.00060 2.20061

A70 1.57029 0.00003 -0.00369 -0.00003 -0.00310 1.56719

A71 1.57029 0.00002 -0.00369 -0.00001 -0.00310 1.56719

A72 1.57029 0.00002 -0.00369 -0.00001 -0.00310 1.56719

A73 1.57029 0.00002 -0.00369 0.00001 -0.00310 1.56719

A74 2.21291 -0.00008 -0.00359 0.00001 -0.00335 2.20956

A75 2.02644 0.00040 0.00301 0.00007 0.00304 2.02948

A76 2.04383 -0.00031 0.00057 -0.00007 0.00030 2.04412

A77 3.14058 0.00004 -0.00739 -0.00001 -0.00620 3.13439

A78 3.14058 0.00004 -0.00739 -0.00001 -0.00620 3.13439

A79 3.12394 -0.00007 0.00032 0.00010 0.00040 3.12434

A80 3.15924 0.00007 -0.00034 -0.00009 -0.00042 3.15883

A81 3.15043 -0.00019 -0.00310 -0.00022 -0.00356 3.14688

A82 3.15043 -0.00019 -0.00310 -0.00022 -0.00356 3.14688

A83 3.15924 0.00007 -0.00034 -0.00009 -0.00042 3.15883

A84 3.15043 -0.00019 -0.00310 -0.00022 -0.00356 3.14688

A85 3.12394 -0.00007 0.00032 0.00010 0.00040 3.12434

A86 3.15043 -0.00019 -0.00310 -0.00022 -0.00356 3.14688

A87 3.10274 0.00087 0.16194 -0.00081 0.16121 3.26394

A88 3.19348 -0.00118 -0.16964 0.00036 -0.16937 3.02410

A89 3.14189 0.00003 -0.00120 0.00015 -0.00106 3.14084

A90 3.14112 -0.00003 0.00173 -0.00015 0.00158 3.14270

A91 3.14140 0.00001 -0.00007 0.00003 -0.00003 3.14136

A92 3.14140 0.00001 -0.00007 0.00003 -0.00003 3.14136

A93 3.14206 0.00003 -0.00173 0.00015 -0.00158 3.14048

A94 3.14179 -0.00001 0.00007 -0.00003 0.00003 3.14182

A95 3.14129 -0.00003 0.00120 -0.00015 0.00106 3.14235

A96 3.14179 -0.00001 0.00007 -0.00003 0.00003 3.14182

D1 0.00259 -0.00015 -0.00265 -0.00006 -0.00271 -0.00011

D2 -3.13341 -0.00024 -0.01408 -0.00008 -0.01416 3.13562

D3 3.14158 -0.00002 0.00334 -0.00004 0.00330 -3.13831

D4 0.00558 -0.00012 -0.00809 -0.00006 -0.00816 -0.00259

D5 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D6 3.13891 0.00013 0.00616 0.00001 0.00617 -3.13810

D7 -3.13891 -0.00013 -0.00616 -0.00001 -0.00617 3.13810

D8 -0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D9 -0.00421 0.00024 0.00430 0.00009 0.00439 0.00018

D10 3.12635 0.00022 0.07602 -0.00042 0.07560 -3.08123

D11 3.13173 0.00034 0.01587 0.00011 0.01598 -3.13547

D12 -0.02089 0.00032 0.08758 -0.00040 0.08719 0.06630

D13 3.12976 0.00034 0.02522 0.00017 0.02540 -3.12803

D14 -0.00706 0.00006 0.01333 0.00021 0.01355 0.00649

D15 -0.00529 0.00023 0.01185 0.00015 0.01199 0.00670

D16 3.14108 -0.00005 -0.00004 0.00019 0.00015 3.14122

D17 0.00421 -0.00024 -0.00430 -0.00009 -0.00439 -0.00018

D18 -3.13173 -0.00034 -0.01587 -0.00011 -0.01598 3.13547

D19 -3.12635 -0.00022 -0.07602 0.00042 -0.07560 3.08123

D20 0.02089 -0.00032 -0.08758 0.00040 -0.08719 -0.06630

D21 3.12214 0.00060 0.04254 0.00012 0.04272 -3.11832

D22 0.03243 -0.00058 -0.12710 0.00048 -0.12665 -0.09422

D23 -0.03243 0.00058 0.12710 -0.00048 0.12665 0.09422

D24 -3.12214 -0.00060 -0.04254 -0.00012 -0.04272 3.11832

D25 -0.00259 0.00015 0.00265 0.00006 0.00271 0.00011

D26 -3.14158 0.00002 -0.00334 0.00004 -0.00330 3.13831

D27 3.13341 0.00024 0.01408 0.00008 0.01416 -3.13562

D28 -0.00558 0.00012 0.00809 0.00006 0.00816 0.00259

D29 0.00529 -0.00023 -0.01185 -0.00015 -0.01199 -0.00670

D30 -3.14108 0.00005 0.00004 -0.00019 -0.00015 -3.14122

D31 -3.12976 -0.00034 -0.02522 -0.00017 -0.02540 3.12803

D32 0.00706 -0.00006 -0.01333 -0.00021 -0.01355 -0.00649

D33 -0.00540 0.00025 0.01641 0.00019 0.01660 0.01121

D34 3.13567 0.00028 0.02610 -0.00005 0.02606 -3.12146

D35 3.14093 -0.00003 0.00462 0.00022 0.00485 -3.13740

D36 -0.00119 -0.00000 0.01431 -0.00001 0.01431 0.01312

D37 -3.14032 0.00007 0.00735 -0.00028 0.00708 -3.13325

D38 -0.02065 0.00028 0.07902 -0.00047 0.07856 0.05791

D39 0.00173 0.00005 -0.00100 -0.00008 -0.00107 0.00065

D40 3.12140 0.00026 0.07067 -0.00027 0.07041 -3.09138

D41 3.14099 -0.00005 -0.00780 0.00025 -0.00756 3.13343

D42 -0.00093 -0.00003 -0.00346 0.00017 -0.00329 -0.00422

D43 -0.00106 -0.00003 0.00062 0.00005 0.00066 -0.00040

D44 3.14020 -0.00001 0.00496 -0.00003 0.00493 -3.13805

D45 -0.00173 -0.00005 0.00100 0.00008 0.00107 -0.00065

D46 3.14032 -0.00007 -0.00735 0.00028 -0.00708 3.13325

D47 -3.12140 -0.00026 -0.07067 0.00026 -0.07041 3.09138

D48 0.02065 -0.00028 -0.07902 0.00047 -0.07856 -0.05791

D49 0.03237 -0.00056 -0.12336 0.00051 -0.12287 -0.09050

D50 3.13510 0.00031 0.03858 -0.00030 0.03834 -3.10974

D51 -3.13510 -0.00031 -0.03858 0.00030 -0.03834 3.10974

D52 -0.03237 0.00056 0.12336 -0.00051 0.12287 0.09050

D53 0.00106 0.00003 -0.00062 -0.00005 -0.00066 0.00040

D54 -3.14020 0.00001 -0.00496 0.00003 -0.00493 3.13805

D55 -3.14099 0.00005 0.00780 -0.00025 0.00756 -3.13343

D56 0.00093 0.00003 0.00346 -0.00017 0.00329 0.00422

D57 0.00540 -0.00025 -0.01641 -0.00018 -0.01660 -0.01121

D58 -3.14093 0.00003 -0.00462 -0.00022 -0.00485 3.13740

D59 -3.13567 -0.00028 -0.02610 0.00005 -0.02606 3.12146

D60 0.00119 0.00000 -0.01431 0.00001 -0.01431 -0.01312

D61 -0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D62 -3.14126 -0.00002 -0.00443 0.00009 -0.00435 3.13757

D63 3.14126 0.00002 0.00443 -0.00008 0.00435 -3.13757

D64 0.00000 -0.00000 0.00000 0.00000 -0.00000 0.00000

D65 -3.13567 -0.00028 -0.02610 0.00005 -0.02606 3.12146

D66 0.00540 -0.00025 -0.01641 -0.00019 -0.01660 -0.01121

D67 0.00119 0.00000 -0.01431 0.00001 -0.01431 -0.01312

D68 -3.14093 0.00003 -0.00462 -0.00022 -0.00485 3.13740

D69 -3.14099 0.00005 0.00780 -0.00025 0.00756 -3.13343

D70 0.00093 0.00003 0.00346 -0.00017 0.00329 0.00422

D71 0.00106 0.00003 -0.00062 -0.00005 -0.00066 0.00040

D72 -3.14020 0.00001 -0.00496 0.00003 -0.00493 3.13805

D73 3.14032 -0.00007 -0.00735 0.00028 -0.00708 3.13325

D74 0.02065 -0.00028 -0.07902 0.00047 -0.07856 -0.05791

D75 -0.00173 -0.00005 0.00100 0.00008 0.00107 -0.00065

D76 -3.12140 -0.00026 -0.07067 0.00027 -0.07041 3.09138

D77 -0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D78 -3.14126 -0.00002 -0.00443 0.00008 -0.00435 3.13757

D79 3.14126 0.00002 0.00443 -0.00009 0.00435 -3.13757

D80 0.00000 0.00000 0.00000 -0.00000 -0.00000 -0.00000

D81 -0.00106 -0.00003 0.00062 0.00005 0.00066 -0.00040

D82 3.14099 -0.00005 -0.00780 0.00025 -0.00756 3.13343

D83 3.14020 -0.00001 0.00496 -0.00003 0.00493 -3.13805

D84 -0.00093 -0.00003 -0.00346 0.00017 -0.00329 -0.00422

D85 0.00173 0.00005 -0.00100 -0.00008 -0.00107 0.00065

D86 3.12140 0.00026 0.07067 -0.00027 0.07041 -3.09138

D87 -3.14032 0.00007 0.00735 -0.00028 0.00708 -3.13325

D88 -0.02065 0.00028 0.07902 -0.00047 0.07856 0.05791

D89 3.13567 0.00028 0.02610 -0.00005 0.02606 -3.12146

D90 -0.00119 -0.00000 0.01431 -0.00001 0.01431 0.01312

D91 -0.00540 0.00025 0.01641 0.00018 0.01660 0.01121

D92 3.14093 -0.00003 0.00462 0.00022 0.00485 -3.13740

D93 -0.03237 0.00056 0.12336 -0.00052 0.12287 0.09050

D94 -3.13510 -0.00031 -0.03858 0.00030 -0.03834 3.10974

D95 3.13510 0.00031 0.03858 -0.00030 0.03834 -3.10974

D96 0.03237 -0.00056 -0.12336 0.00051 -0.12287 -0.09050

D97 -3.12976 -0.00034 -0.02522 -0.00017 -0.02540 3.12803

D98 0.00529 -0.00023 -0.01185 -0.00015 -0.01199 -0.00670

D99 0.00706 -0.00006 -0.01333 -0.00021 -0.01355 -0.00649

D100 -3.14108 0.00005 0.00004 -0.00018 -0.00015 -3.14122

D101 3.13341 0.00024 0.01408 0.00008 0.01416 -3.13562

D102 -0.00558 0.00012 0.00809 0.00006 0.00816 0.00259

D103 -0.00259 0.00015 0.00265 0.00006 0.00271 0.00011

D104 -3.14158 0.00002 -0.00334 0.00004 -0.00330 3.13831

D105 -3.13173 -0.00034 -0.01587 -0.00011 -0.01598 3.13547

D106 0.02089 -0.00032 -0.08758 0.00040 -0.08719 -0.06630

D107 0.00421 -0.00024 -0.00430 -0.00009 -0.00439 -0.00018

D108 -3.12635 -0.00022 -0.07602 0.00042 -0.07560 3.08123

D109 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D110 -3.13891 -0.00013 -0.00616 -0.00001 -0.00617 3.13810

D111 3.13891 0.00013 0.00616 0.00001 0.00617 -3.13810

D112 -0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D113 0.00259 -0.00015 -0.00265 -0.00006 -0.00271 -0.00011

D114 -3.13341 -0.00024 -0.01408 -0.00008 -0.01416 3.13562

D115 3.14158 -0.00002 0.00334 -0.00004 0.00330 -3.13831

D116 0.00558 -0.00012 -0.00809 -0.00006 -0.00816 -0.00259

D117 -0.00421 0.00024 0.00430 0.00009 0.00439 0.00018

D118 3.12635 0.00022 0.07602 -0.00042 0.07560 -3.08123

D119 3.13173 0.00034 0.01587 0.00011 0.01598 -3.13547

D120 -0.02089 0.00032 0.08758 -0.00040 0.08719 0.06630

D121 3.12976 0.00034 0.02522 0.00017 0.02540 -3.12803

D122 -0.00706 0.00006 0.01333 0.00021 0.01355 0.00649

D123 -0.00529 0.00023 0.01185 0.00015 0.01199 0.00670

D124 3.14108 -0.00005 -0.00004 0.00018 0.00015 3.14122

D125 -3.12214 -0.00060 -0.04254 -0.00012 -0.04272 3.11832

D126 -0.03243 0.00058 0.12710 -0.00048 0.12665 0.09422

D127 0.03243 -0.00058 -0.12710 0.00048 -0.12665 -0.09422

D128 3.12214 0.00060 0.04254 0.00012 0.04272 -3.11832

Item Value Threshold Converged?

Maximum Force 0.001898 0.000450 NO

RMS Force 0.000320 0.000300 NO

Maximum Displacement 0.404692 0.001800 NO

RMS Displacement 0.032118 0.001200 NO

Predicted change in Energy=-3.497823D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Jul 30 22:29:35 2019, MaxMem= 4294967296 cpu: 1.1

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -4.286056 0.679326 -0.028822

2 6 0 -2.897882 1.108602 -0.011499

3 7 0 -2.088507 0.000000 -0.001255

4 6 0 -2.897882 -1.108602 -0.011499

5 6 0 -4.286056 -0.679326 -0.028822

6 6 0 -2.467676 -2.444723 -0.013000

7 6 0 -1.105983 -2.906985 -0.011898

8 7 0 -0.000000 -2.095070 0.003444

9 6 0 1.105983 -2.906985 -0.011898

10 6 0 0.691829 -4.271788 -0.036808

11 6 0 -0.691829 -4.271788 -0.036808

12 6 0 -2.467676 2.444723 -0.013000

13 6 0 -1.105983 2.906985 -0.011898

14 6 0 -0.691829 4.271788 -0.036808

15 6 0 0.691829 4.271788 -0.036808

16 6 0 1.105983 2.906985 -0.011898

17 7 0 0.000000 2.095070 0.003444

18 6 0 2.467676 2.444723 -0.013000

19 6 0 2.897882 1.108602 -0.011499

20 6 0 4.286056 0.679326 -0.028822

21 6 0 4.286056 -0.679326 -0.028822

22 6 0 2.897882 -1.108602 -0.011499

23 7 0 2.088507 -0.000000 -0.001255

24 1 0 -5.142872 1.337127 -0.042503

25 1 0 -5.142872 -1.337127 -0.042503

26 1 0 1.346484 -5.131075 -0.055946

27 1 0 -1.346484 -5.131075 -0.055946

28 1 0 -1.346484 5.131075 -0.055946

29 1 0 1.346484 5.131075 -0.055946

30 1 0 5.142872 1.337127 -0.042503

31 1 0 5.142872 -1.337127 -0.042503

32 30 0 0.000000 0.000000 0.126891

33 6 0 2.467676 -2.444723 -0.013000

34 6 0 3.475284 -3.451193 -0.024873

35 6 0 -3.475284 3.451193 -0.024873

36 6 0 4.315334 -4.319739 -0.036115

37 6 0 -4.315334 4.319739 -0.036115

38 6 0 -3.475284 -3.451193 -0.024873

39 6 0 -4.315334 -4.319739 -0.036115

40 6 0 3.475284 3.451193 -0.024873

41 6 0 4.315334 4.319739 -0.036115

42 1 0 5.061000 5.082587 -0.046184

43 1 0 5.061000 -5.082587 -0.046184

44 1 0 -5.061000 -5.082587 -0.046184

45 1 0 -5.061000 5.082587 -0.046184

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.453136 0.000000

3 N 2.300318 1.372658 0.000000

4 C 2.263628 2.217204 1.372658 0.000000

5 C 1.358652 2.263628 2.300318 1.453136 0.000000

6 C 3.614753 3.579274 2.473980 1.403674 2.534440

7 C 4.793202 4.397254 3.068555 2.538718 3.882733

8 N 5.105741 4.319891 2.958244 3.061220 4.513939

9 C 6.475801 5.670615 4.319195 4.389205 5.834109

10 C 7.020892 6.468018 5.097029 4.784602 6.138826

11 C 6.118174 5.815144 4.494457 3.856560 5.081762

12 C 2.534440 1.403674 2.473980 3.579274 3.614753

13 C 3.882733 2.538718 3.068555 4.397254 4.793202

14 C 5.081762 3.856560 4.494457 5.815144 6.118174

15 C 6.138826 4.784602 5.097029 6.468018 7.020892

16 C 5.834109 4.389205 4.319195 5.670615 6.475801

17 N 4.513939 3.061220 2.958244 4.319891 5.105741

18 C 6.980671 5.529415 5.170649 6.435475 7.441292

19 C 7.196773 5.795765 5.108149 6.205391 7.403104

20 C 8.572112 7.196773 6.410718 7.403104 8.679115

21 C 8.679115 7.403104 6.410718 7.196773 8.572112

22 C 7.403104 6.205391 5.108149 5.795765 7.196773

23 N 6.410718 5.108149 4.177015 5.108149 6.410718

24 H 1.080289 2.256804 3.334480 3.320020 2.190982

25 H 2.190982 3.320020 3.334480 2.256804 1.080289

26 H 8.092404 7.546535 6.174956 5.847812 7.179436

27 H 6.511726 6.429804 5.184739 4.311508 5.334781

28 H 5.334781 4.311508 5.184739 6.429804 6.511726

29 H 7.179436 5.847812 6.174956 7.546535 8.092404

30 H 9.451856 8.044061 7.354078 8.404539 9.642145

31 H 9.642145 8.404539 7.354078 8.044061 9.451856

32 Zn 4.342350 3.105780 2.092435 3.105780 4.342350

33 C 7.441292 6.435475 5.170649 5.529415 6.980671

34 C 8.792018 7.836399 6.547294 6.790077 8.241459

35 C 2.888012 2.412737 3.719467 4.596226 4.209341

36 C 9.948599 9.027623 7.724671 7.895727 9.340052

37 C 3.640538 3.510153 4.860053 5.610406 4.999156

38 C 4.209341 4.596226 3.719467 2.412737 2.888012

39 C 4.999156 5.610406 4.860053 3.510153 3.640538

40 C 8.241459 6.790077 6.547294 7.836399 8.792018

41 C 9.340052 7.895727 7.724671 9.027623 9.948599

42 H 10.332302 8.895930 8.772124 10.083443 10.980319

43 H 10.980319 10.083443 8.772124 8.895930 10.332302

44 H 5.813818 6.558285 5.888159 4.524692 4.470967

45 H 4.470967 4.524692 5.888159 6.558285 5.813818

6 7 8 9 10

6 C 0.000000

7 C 1.438018 0.000000

8 N 2.492378 1.372093 0.000000

9 C 3.603432 2.211965 1.372093 0.000000

10 C 3.649822 2.257307 2.284370 1.426474 0.000000

11 C 2.548011 1.426474 2.284370 2.257307 1.383659

12 C 4.889447 5.522227 5.167148 6.435202 7.422571

13 C 5.522227 5.813971 5.122889 6.220534 7.400509

14 C 6.947353 7.190753 6.404462 7.400509 8.654894

15 C 7.422571 7.400509 6.404462 7.190753 8.543576

16 C 6.435202 6.220534 5.122889 5.813971 7.190753

17 N 5.167148 5.122889 4.190141 5.122889 6.404462

18 C 6.947257 6.435202 5.167148 5.522227 6.947353

19 C 6.435475 5.670615 4.319891 4.397254 5.815144

20 C 7.441292 6.475801 5.105741 4.793202 6.118174

21 C 6.980671 5.834109 4.513939 3.882733 5.081762

22 C 5.529415 4.389205 3.061220 2.538718 3.856560

23 N 5.170649 4.319195 2.958244 3.068555 4.494457

24 H 4.632487 5.857465 6.183140 7.553914 8.093435

25 H 2.895569 4.331497 5.198627 6.443103 6.531157

26 H 4.665420 3.311058 3.321727 2.237489 1.080423

27 H 2.911254 2.237489 3.321727 3.311058 2.212117

28 H 7.658436 8.041778 7.350763 8.403984 9.621274

29 H 8.481885 8.403984 7.350763 8.041778 9.425644

30 H 8.498453 7.553914 6.183140 5.857465 7.160429

31 H 7.690779 6.443103 5.198627 4.331497 5.331421

32 Zn 3.476444 3.113362 2.098704 3.113362 4.330542

33 C 4.935351 3.603432 2.492378 1.438018 2.548011

34 C 6.027594 4.613494 3.730612 2.431032 2.901919

35 C 5.981408 6.785292 6.545184 7.836746 8.775500

36 C 7.037431 5.602422 4.855185 3.506622 3.623822

37 C 7.012298 7.907343 7.731329 9.034202 9.944145

38 C 1.424217 2.431032 3.730612 4.613494 4.247158

39 C 2.632501 3.506622 4.855185 5.602422 5.007393

40 C 8.371423 7.836746 6.545184 6.785292 8.209274

41 C 9.579546 9.034202 7.731329 7.907343 9.324383

42 H 10.646241 10.092874 8.782650 8.914965 10.324440

43 H 7.977492 6.539579 5.877197 4.514043 4.443775

44 H 3.699291 4.514043 5.877197 6.539579 5.809693

45 H 7.961585 8.914965 8.782650 10.092874 10.981778

11 12 13 14 15

11 C 0.000000

12 C 6.947353 0.000000

13 C 7.190753 1.438018 0.000000

14 C 8.543576 2.548011 1.426474 0.000000

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17 N 6.404462 2.492378 1.372093 2.284370 2.284370

18 C 7.422571 4.935351 3.603432 3.649822 2.548011

19 C 6.468018 5.529415 4.389205 4.784602 3.856560

20 C 7.020892 6.980671 5.834109 6.138826 5.081762

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22 C 4.784602 6.435475 5.670615 6.468018 5.815144

23 N 5.097029 5.170649 4.319195 5.097029 4.494457

24 H 7.160429 2.895569 4.331497 5.331421 6.531157

25 H 5.331421 4.632487 5.857465 7.160429 8.093435

26 H 2.212117 8.481885 8.403984 9.621274 9.425644

27 H 1.080423 7.658436 8.041778 9.425644 9.621274

28 H 9.425644 2.911254 2.237489 1.080423 2.212117

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32 Zn 4.330542 3.476444 3.113362 4.330542 4.330542

33 C 3.649822 6.947257 6.435202 7.422571 6.947353

34 C 4.247158 8.371423 7.836746 8.775500 8.209274

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37 C 9.324383 2.632501 3.506622 3.623822 5.007393

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41 C 9.944145 7.037431 5.602422 5.007393 3.623822

42 H 10.981778 7.977492 6.539579 5.809693 4.443775

43 H 5.809693 10.646241 10.092874 10.981778 10.324440

44 H 4.443775 7.961585 8.914965 10.324440 10.981778

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16 17 18 19 20

16 C 0.000000

17 N 1.372093 0.000000

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22 C 4.397254 4.319891 3.579274 2.217204 2.263628

23 N 3.068555 2.958244 2.473980 1.372658 2.300318

24 H 6.443103 5.198627 7.690779 8.044061 9.451856

25 H 7.553914 6.183140 8.498453 8.404539 9.642145

26 H 8.041778 7.350763 7.658436 6.429804 6.511726

27 H 8.403984 7.350763 8.481885 7.546535 8.092404

28 H 3.311058 3.321727 4.665420 5.847812 7.179436

29 H 2.237489 3.321727 2.911254 4.311508 5.334781

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31 H 5.857465 6.183140 4.632487 3.320020 2.190982

32 Zn 3.113362 2.098704 3.476444 3.105780 4.342350

33 C 5.522227 5.167148 4.889447 3.579274 3.614753

34 C 6.785292 6.545184 5.981408 4.596226 4.209341

35 C 4.613494 3.730612 6.027594 6.790077 8.241459

36 C 7.907343 7.731329 7.012298 5.610406 4.999156

37 C 5.602422 4.855185 7.037431 7.895727 9.340052

38 C 7.836746 6.545184 8.371423 7.836399 8.792018

39 C 9.034202 7.731329 9.579546 9.027623 9.948599

40 C 2.431032 3.730612 1.424217 2.412737 2.888012

41 C 3.506622 4.855185 2.632501 3.510153 3.640538

42 H 4.514043 5.877197 3.699291 4.524692 4.470967

43 H 8.914965 8.782650 7.961585 6.558285 5.813818

44 H 10.092874 8.782650 10.646241 10.083443 10.980319

45 H 6.539579 5.877197 7.977492 8.895930 10.332302

21 22 23 24 25

21 C 0.000000

22 C 1.453136 0.000000

23 N 2.300318 1.372658 0.000000

24 H 9.642145 8.404539 7.354078 0.000000

25 H 9.451856 8.044061 7.354078 2.674253 0.000000

26 H 5.334781 4.311508 5.184739 9.162399 7.517045

27 H 7.179436 5.847812 6.174956 7.500025 5.367196

28 H 8.092404 7.546535 6.174956 5.367196 7.500025

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30 H 2.190982 3.320020 3.334480 10.285744 10.627708

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32 Zn 4.342350 3.105780 2.092435 5.316553 5.316553

33 C 2.534440 1.403674 2.473980 8.498453 7.690779

34 C 2.888012 2.412737 3.719467 9.859053 8.873680

35 C 8.792018 7.836399 6.547294 2.692664 5.070421

36 C 3.640538 3.510153 4.860053 11.020791 9.917343

37 C 9.948599 9.027623 7.724671 3.095292 5.717078

38 C 8.241459 6.790077 6.547294 5.070421 2.692664

39 C 9.340052 7.895727 7.724671 5.717078 3.095292

40 C 4.209341 4.596226 3.719467 8.873680 9.859053

41 C 4.999156 5.610406 4.860053 9.917343 11.020791

42 H 5.813818 6.558285 5.888159 10.869567 12.055362

43 H 4.470967 4.524692 5.888159 12.055362 10.869567

44 H 10.332302 8.895930 8.772124 6.420236 3.746356

45 H 10.980319 10.083443 8.772124 3.746356 6.420236

26 27 28 29 30

26 H 0.000000

27 H 2.692968 0.000000

28 H 10.609609 10.262150 0.000000

29 H 10.262150 10.609609 2.692968 0.000000

30 H 7.500025 9.162399 7.517045 5.367196 0.000000

31 H 5.367196 7.517045 9.162399 7.500025 2.674253

32 Zn 5.307954 5.307954 5.307954 5.307954 5.316553

33 C 2.911254 4.665420 8.481885 7.658436 4.632487

34 C 2.711966 5.106115 9.844070 8.842402 5.070421

35 C 9.844070 8.842402 2.711966 5.106115 8.873680

36 C 3.077781 5.719689 11.017008 9.906177 5.717078

37 C 11.017008 9.906177 3.077781 5.719689 9.917343

38 C 5.106115 2.711966 8.842402 9.844070 9.859053

39 C 5.719689 3.077781 9.906177 11.017008 11.020791

40 C 8.842402 9.844070 5.106115 2.711966 2.692664

41 C 9.906177 11.017008 5.719689 3.077781 3.095292

42 H 10.868147 12.057149 6.407675 3.714846 3.746356

43 H 3.714846 6.407675 12.057149 10.868147 6.420236

44 H 6.407675 3.714846 10.868147 12.057149 12.055362

45 H 12.057149 10.868147 3.714846 6.407675 10.869567

31 32 33 34 35

31 H 0.000000

32 Zn 5.316553 0.000000

33 C 2.895569 3.476444 0.000000

34 C 2.692664 4.900139 1.424217 0.000000

35 C 9.859053 4.900139 8.371423 9.795576 0.000000

36 C 3.095292 6.108095 2.632501 1.208381 11.003692

37 C 11.020791 6.108095 9.579546 11.003692 1.208381

38 C 8.873680 4.900139 6.027594 6.950567 6.902385

39 C 9.917343 6.108095 7.037431 7.838892 7.816213

40 C 5.070421 4.900139 5.981408 6.902385 6.950567

41 C 5.717078 6.108095 7.012298 7.816213 7.838892

42 H 6.420236 7.174703 7.961585 8.679881 8.690802

43 H 3.746356 7.174703 3.699291 2.275170 12.070376

44 H 10.869567 7.174703 7.977492 8.690802 8.679881

45 H 12.055362 7.174703 10.646241 12.070376 2.275170

36 37 38 39 40

36 C 0.000000

37 C 12.211839 0.000000

38 C 7.838892 7.816213 0.000000

39 C 8.630669 8.639477 1.208381 0.000000

40 C 7.816213 7.838892 9.795576 11.003692 0.000000

41 C 8.639477 8.630669 11.003692 12.211839 1.208381

42 H 9.431852 9.407321 12.070376 13.278534 2.275170

43 H 1.066797 13.278534 8.690802 9.407321 8.679881

44 H 9.407321 9.431852 2.275170 1.066797 12.070376

45 H 13.278534 1.066797 8.679881 9.431852 8.690802

41 42 43 44 45

41 C 0.000000

42 H 1.066797 0.000000

43 H 9.431852 10.165173 0.000000

44 H 13.278534 14.345231 10.122001 0.000000

45 H 9.407321 10.122001 14.345231 10.165173 0.000000

Stoichiometry C28H12N4Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C28H12)]

Deg. of freedom 34

Full point group C2V NOp 4

RotChk: IX=0 Diff= 1.31D-14

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.679326 4.286056 -0.026076

2 6 0 1.108602 2.897882 -0.008753

3 7 0 0.000000 2.088507 0.001491

4 6 0 -1.108602 2.897882 -0.008753

5 6 0 -0.679326 4.286056 -0.026076

6 6 0 -2.444723 2.467676 -0.010254

7 6 0 -2.906985 1.105983 -0.009152

8 7 0 -2.095070 0.000000 0.006189

9 6 0 -2.906985 -1.105983 -0.009152

10 6 0 -4.271788 -0.691829 -0.034062

11 6 0 -4.271788 0.691829 -0.034062

12 6 0 2.444723 2.467676 -0.010254

13 6 0 2.906985 1.105983 -0.009152

14 6 0 4.271788 0.691829 -0.034062

15 6 0 4.271788 -0.691829 -0.034062

16 6 0 2.906985 -1.105983 -0.009152

17 7 0 2.095070 -0.000000 0.006189

18 6 0 2.444723 -2.467676 -0.010254

19 6 0 1.108602 -2.897882 -0.008753

20 6 0 0.679326 -4.286056 -0.026076

21 6 0 -0.679326 -4.286056 -0.026076

22 6 0 -1.108602 -2.897882 -0.008753

23 7 0 -0.000000 -2.088507 0.001491

24 1 0 1.337127 5.142872 -0.039757

25 1 0 -1.337127 5.142872 -0.039757

26 1 0 -5.131075 -1.346484 -0.053200

27 1 0 -5.131075 1.346484 -0.053200

28 1 0 5.131075 1.346484 -0.053200

29 1 0 5.131075 -1.346484 -0.053200

30 1 0 1.337127 -5.142872 -0.039757

31 1 0 -1.337127 -5.142872 -0.039757

32 30 0 0.000000 0.000000 0.129637

33 6 0 -2.444723 -2.467676 -0.010254

34 6 0 -3.451193 -3.475284 -0.022127

35 6 0 3.451193 3.475284 -0.022127

36 6 0 -4.319739 -4.315334 -0.033370

37 6 0 4.319739 4.315334 -0.033370

38 6 0 -3.451193 3.475284 -0.022127

39 6 0 -4.319739 4.315334 -0.033370

40 6 0 3.451193 -3.475284 -0.022127

41 6 0 4.319739 -4.315334 -0.033370

42 1 0 5.082587 -5.061000 -0.043438

43 1 0 -5.082587 -5.061000 -0.043438

44 1 0 -5.082587 5.061000 -0.043438

45 1 0 5.082587 5.061000 -0.043438

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

Rotational constants (GHZ): 0.1461202 0.1455143 0.0729352

Leave Link 202 at Tue Jul 30 22:29:35 2019, MaxMem= 4294967296 cpu: 0.2

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

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

Pseudo-potential data read from rwf file.

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

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

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

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

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

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

111 alpha electrons 110 beta electrons

nuclear repulsion energy 3053.6697952690 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= 13 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= -0.1303953894 Hartrees.

Nuclear repulsion after empirical dispersion term = 3053.5393998795 Hartrees.

No density basis found on file 724.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

2nd derivatives : Analytical E(r).r(xy)/FMM algorithm (CHGder, D2EAlg=3).

Cavity 2nd derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3886

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.73D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 104

GePol: Fraction of low-weight points (<1% of avg) = 2.68%

GePol: Cavity surface area = 416.118 Ang\*\*2

GePol: Cavity volume = 420.680 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0083794312 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3053.5477793107 Hartrees.

Leave Link 301 at Tue Jul 30 22:29:35 2019, MaxMem= 4294967296 cpu: 1.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16185 LenP2D= 44720.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.45D-05 NBF= 172 148 158 158

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

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Tue Jul 30 22:29:36 2019, MaxMem= 4294967296 cpu: 11.0

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Jul 30 22:29:36 2019, MaxMem= 4294967296 cpu: 1.3

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

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

B after Tr= -0.000000 0.000000 -0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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Beta Orbitals:

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The electronic state of the initial guess is 2-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7630 S= 0.5065

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1359.66967768245

Leave Link 401 at Tue Jul 30 22:29:39 2019, MaxMem= 4294967296 cpu: 41.4

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1387497 IEndB= 1387497 NGot= 4294967296 MDV= 4294047352

LenX= 4294047352 LenY= 4293596440

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= 650000000 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= 45302988.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.77D-15 for 3865.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.71D-15 for 1081 852.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.55D-15 for 3865.

Iteration 1 A^-1\*A deviation from orthogonality is 1.72D-14 for 2278 2260.

E= -1359.17610625284

DIIS: error= 3.47D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.17610625284 IErMin= 1 ErrMin= 3.47D-03

ErrMax= 3.47D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.66D-02 BMatP= 1.66D-02

IDIUse=3 WtCom= 9.65D-01 WtEn= 3.47D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.387 Goal= None Shift= 0.000

Gap= 0.438 Goal= None Shift= 0.000

GapD= 0.387 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

RMSDP=3.65D-04 MaxDP=1.85D-02 OVMax= 1.88D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.65D-04 CP: 9.99D-01

E= -1359.18186544695 Delta-E= -0.005759194108 Rises=F Damp=F

DIIS: error= 6.10D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.18186544695 IErMin= 2 ErrMin= 6.10D-04

ErrMax= 6.10D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.23D-04 BMatP= 1.66D-02

IDIUse=3 WtCom= 9.94D-01 WtEn= 6.10D-03

Coeff-Com: -0.285D-01 0.103D+01

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

Coeff: -0.283D-01 0.103D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=3.32D-05 MaxDP=7.37D-04 DE=-5.76D-03 OVMax= 2.33D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.99D-05 CP: 9.99D-01 1.04D+00

E= -1359.18194008856 Delta-E= -0.000074641609 Rises=F Damp=F

DIIS: error= 7.69D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.18194008856 IErMin= 2 ErrMin= 6.10D-04

ErrMax= 7.69D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.16D-04 BMatP= 2.23D-04

IDIUse=3 WtCom= 9.92D-01 WtEn= 7.69D-03

Coeff-Com: -0.201D-01 0.430D+00 0.590D+00

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

Coeff: -0.199D-01 0.427D+00 0.593D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.06D-05 MaxDP=3.47D-04 DE=-7.46D-05 OVMax= 8.49D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 8.36D-06 CP: 9.99D-01 1.04D+00 7.87D-01

E= -1359.18195270163 Delta-E= -0.000012613075 Rises=F Damp=F

DIIS: error= 2.76D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.18195270163 IErMin= 4 ErrMin= 2.76D-04

ErrMax= 2.76D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.87D-05 BMatP= 1.16D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.76D-03

Coeff-Com: -0.637D-02 0.988D-01 0.305D+00 0.603D+00

Coeff-En: 0.000D+00 0.000D+00 0.800D-01 0.920D+00

Coeff: -0.635D-02 0.986D-01 0.304D+00 0.603D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=4.01D-06 MaxDP=2.05D-04 DE=-1.26D-05 OVMax= 5.19D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.59D-06 CP: 9.99D-01 1.04D+00 7.83D-01 7.92D-01

E= -1359.18195518167 Delta-E= -0.000002480035 Rises=F Damp=F

DIIS: error= 4.23D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.18195518167 IErMin= 5 ErrMin= 4.23D-05

ErrMax= 4.23D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.21D-06 BMatP= 1.87D-05

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

Coeff-Com: -0.158D-02 0.105D-01 0.106D+00 0.324D+00 0.561D+00

Coeff: -0.158D-02 0.105D-01 0.106D+00 0.324D+00 0.561D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.41D-06 MaxDP=9.67D-05 DE=-2.48D-06 OVMax= 3.00D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.08D-06 CP: 9.99D-01 1.04D+00 7.94D-01 8.51D-01 8.09D-01

E= -1359.18195561063 Delta-E= -0.000000428964 Rises=F Damp=F

DIIS: error= 2.86D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.18195561063 IErMin= 6 ErrMin= 2.86D-05

ErrMax= 2.86D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.90D-07 BMatP= 2.21D-06

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

Coeff-Com: 0.373D-03-0.160D-01 0.247D-02 0.814D-01 0.357D+00 0.575D+00

Coeff: 0.373D-03-0.160D-01 0.247D-02 0.814D-01 0.357D+00 0.575D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=5.59D-07 MaxDP=2.99D-05 DE=-4.29D-07 OVMax= 9.60D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.64D-07 CP: 9.99D-01 1.04D+00 8.02D-01 8.54D-01 8.32D-01

CP: 6.17D-01

E= -1359.18195570891 Delta-E= -0.000000098275 Rises=F Damp=F

DIIS: error= 1.70D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.18195570891 IErMin= 7 ErrMin= 1.70D-06

ErrMax= 1.70D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.77D-09 BMatP= 4.90D-07

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

Coeff-Com: 0.187D-03-0.648D-02-0.144D-02 0.239D-01 0.123D+00 0.225D+00

Coeff-Com: 0.637D+00

Coeff: 0.187D-03-0.648D-02-0.144D-02 0.239D-01 0.123D+00 0.225D+00

Coeff: 0.637D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=7.86D-08 MaxDP=3.71D-06 DE=-9.83D-08 OVMax= 1.11D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 7.21D-08 CP: 9.99D-01 1.04D+00 8.03D-01 8.55D-01 8.33D-01

CP: 6.32D-01 9.36D-01

E= -1359.18195571014 Delta-E= -0.000000001231 Rises=F Damp=F

DIIS: error= 1.31D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.18195571014 IErMin= 8 ErrMin= 1.31D-06

ErrMax= 1.31D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.62D-09 BMatP= 6.77D-09

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

Coeff-Com: 0.461D-04-0.104D-02-0.113D-02 0.184D-03 0.988D-02 0.326D-01

Coeff-Com: 0.388D+00 0.572D+00

Coeff: 0.461D-04-0.104D-02-0.113D-02 0.184D-03 0.988D-02 0.326D-01

Coeff: 0.388D+00 0.572D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=3.82D-08 MaxDP=2.13D-06 DE=-1.23D-09 OVMax= 6.01D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.33D-08 CP: 9.99D-01 1.04D+00 8.03D-01 8.55D-01 8.33D-01

CP: 6.34D-01 9.71D-01 8.02D-01

E= -1359.18195571069 Delta-E= -0.000000000553 Rises=F Damp=F

DIIS: error= 5.63D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1359.18195571069 IErMin= 9 ErrMin= 5.63D-07

ErrMax= 5.63D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.67D-10 BMatP= 2.62D-09

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

Coeff-Com: -0.107D-04 0.708D-03-0.311D-03-0.454D-02-0.191D-01-0.275D-01

Coeff-Com: 0.884D-01 0.321D+00 0.642D+00

Coeff: -0.107D-04 0.708D-03-0.311D-03-0.454D-02-0.191D-01-0.275D-01

Coeff: 0.884D-01 0.321D+00 0.642D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.82D-08 MaxDP=7.80D-07 DE=-5.53D-10 OVMax= 2.81D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.51D-08 CP: 9.99D-01 1.04D+00 8.03D-01 8.55D-01 8.33D-01

CP: 6.34D-01 9.94D-01 8.54D-01 7.96D-01

E= -1359.18195571078 Delta-E= -0.000000000094 Rises=F Damp=F

DIIS: error= 2.28D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1359.18195571078 IErMin=10 ErrMin= 2.28D-07

ErrMax= 2.28D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.89D-11 BMatP= 3.67D-10

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

Coeff-Com: -0.114D-04 0.503D-03-0.207D-04-0.241D-02-0.113D-01-0.187D-01

Coeff-Com: -0.887D-03 0.963D-01 0.334D+00 0.603D+00

Coeff: -0.114D-04 0.503D-03-0.207D-04-0.241D-02-0.113D-01-0.187D-01

Coeff: -0.887D-03 0.963D-01 0.334D+00 0.603D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=6.90D-09 MaxDP=3.23D-07 DE=-9.37D-11 OVMax= 1.13D-06

Error on total polarization charges = 0.06719

SCF Done: E(UB3LYP) = -1359.18195571 A.U. after 10 cycles

NFock= 10 Conv=0.69D-08 -V/T= 1.9682

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7630 S= 0.5065

<L.S>= 0.000000000000E+00

KE= 1.403876600940D+03 PE=-9.376706062394D+03 EE= 3.560099726432D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.26

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7630, after 0.7501

Leave Link 502 at Tue Jul 30 22:30:39 2019, MaxMem= 4294967296 cpu: 926.5

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 636

NBasis= 636 NAE= 111 NBE= 110 NFC= 0 NFV= 0

NROrb= 636 NOA= 111 NOB= 110 NVA= 525 NVB= 526

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.13706802D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.38384677D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.13693500D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.88571733D-01

Leave Link 801 at Tue Jul 30 22:30:39 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 45.

Will process 46 centers per pass.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16185 LenP2D= 44720.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 11 by ecpmxn.

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

Leave Link 1101 at Tue Jul 30 22:30:42 2019, MaxMem= 4294967296 cpu: 45.0

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Tue Jul 30 22:30:42 2019, MaxMem= 4294967296 cpu: 1.1

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 45.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966832.

G2DrvN: will do 46 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

G2PCM: DoFxE=T DoFxN=T DoGrad=T DoDP/DQ/DG/TGxP=FFFF NFrqRd= 0 IEInf=0 SqF1=F DoCFld=F IF1Alg=4.

GePol: Maximum number of non-zero 1st derivatives = 256

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Tue Jul 30 22:32:39 2019, MaxMem= 4294967296 cpu: 1871.3

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=111111111111111111111111111111111111111111111

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Using symmetry in CPHF.

Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.

Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.

NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 4294965570 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 0.

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

IRaf= 650000000 NMat= 42 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

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

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

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

NMat0= 42 NMatS0= 42 NMatT0= 0 NMatD0= 42 NMtDS0= 0 NMtDT0= 0

Integrals replicated using symmetry in FoFCou.

There are 42 degrees of freedom in the 1st order CPHF. IDoFFX=4 NUNeed= 42.

42 vectors produced by pass 0 Test12= 2.77D-13 2.38D-09 XBig12= 8.02D+03 5.90D+01.

AX will form 42 AO Fock derivatives at one time.

42 vectors produced by pass 1 Test12= 2.77D-13 2.38D-09 XBig12= 1.07D+03 6.83D+00.

42 vectors produced by pass 2 Test12= 2.77D-13 2.38D-09 XBig12= 2.79D+02 5.62D+00.

42 vectors produced by pass 3 Test12= 2.77D-13 2.38D-09 XBig12= 6.69D+01 1.73D+00.

42 vectors produced by pass 4 Test12= 2.77D-13 2.38D-09 XBig12= 5.16D+00 4.13D-01.

42 vectors produced by pass 5 Test12= 2.77D-13 2.38D-09 XBig12= 1.70D-01 3.95D-02.

42 vectors produced by pass 6 Test12= 2.77D-13 2.38D-09 XBig12= 5.69D-03 6.56D-03.

42 vectors produced by pass 7 Test12= 2.77D-13 2.38D-09 XBig12= 1.41D-04 1.06D-03.

38 vectors produced by pass 8 Test12= 2.77D-13 2.38D-09 XBig12= 2.46D-06 1.26D-04.

21 vectors produced by pass 9 Test12= 2.77D-13 2.38D-09 XBig12= 3.26D-08 1.63D-05.

5 vectors produced by pass 10 Test12= 2.77D-13 2.38D-09 XBig12= 4.09D-10 1.62D-06.

2 vectors produced by pass 11 Test12= 2.77D-13 2.38D-09 XBig12= 5.60D-12 1.79D-07.

2 vectors produced by pass 12 Test12= 2.77D-13 2.38D-09 XBig12= 7.29D-14 2.10D-08.

InvSVY: IOpt=1 It= 1 EMax= 5.68D-14

Solved reduced A of dimension 404 with 42 vectors.

FullF1: Do perturbations 1 to 42.

Isotropic polarizability for W= 0.000000 1004.26 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Tue Jul 30 23:31:45 2019, MaxMem= 4294967296 cpu: 56734.0

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16185 LenP2D= 44720.

LDataN: DoStor=T MaxTD1= 7 Len= 274

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 256

Leave Link 701 at Tue Jul 30 23:32:20 2019, MaxMem= 4294967296 cpu: 560.4

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

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

Leave Link 702 at Tue Jul 30 23:32:20 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

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

wScrn= 0.000000 ICntrl= 100127 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Tue Jul 30 23:34:10 2019, MaxMem= 4294967296 cpu: 1758.5

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

Dipole =-1.83367210D-13 6.90003610D-14 2.86127141D-01

Polarizability= 1.64901213D+03 1.71990208D-05 1.17647726D+03

-1.18790753D-05 3.18893196D-06 1.87280261D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000008243 -0.000134915 0.000000554

2 6 0.000010644 -0.000023131 -0.000002575

3 7 -0.000076077 0.000000000 0.000189395

4 6 0.000010644 0.000023131 -0.000002575

5 6 0.000008243 0.000134915 0.000000554

6 6 0.000045285 0.000030669 -0.000001063

7 6 -0.000097926 0.000007866 -0.000001508

8 7 -0.000000000 -0.000055859 0.000231476

9 6 0.000097926 0.000007866 -0.000001508

10 6 -0.000123016 -0.000006068 0.000000062

11 6 0.000123016 -0.000006068 0.000000062

12 6 0.000045285 -0.000030669 -0.000001063

13 6 -0.000097926 -0.000007866 -0.000001508

14 6 0.000123016 0.000006068 0.000000062

15 6 -0.000123016 0.000006068 0.000000062

16 6 0.000097926 -0.000007866 -0.000001508

17 7 0.000000000 0.000055859 0.000231476

18 6 -0.000045285 -0.000030669 -0.000001063

19 6 -0.000010644 -0.000023131 -0.000002575

20 6 -0.000008243 -0.000134915 0.000000554

21 6 -0.000008243 0.000134915 0.000000554

22 6 -0.000010644 0.000023131 -0.000002575

23 7 0.000076077 -0.000000000 0.000189395

24 1 -0.000003410 -0.000006170 -0.000000477

25 1 -0.000003410 0.000006170 -0.000000477

26 1 -0.000002736 -0.000001125 -0.000000402

27 1 0.000002736 -0.000001125 -0.000000402

28 1 0.000002736 0.000001125 -0.000000402

29 1 -0.000002736 0.000001125 -0.000000402

30 1 0.000003410 -0.000006170 -0.000000477

31 1 0.000003410 0.000006170 -0.000000477

32 30 -0.000000000 0.000000000 -0.000819668

33 6 -0.000045285 0.000030669 -0.000001063

34 6 -0.000006243 -0.000017853 0.000000112

35 6 0.000006243 0.000017853 0.000000112

36 6 -0.000016582 0.000001032 0.000000389

37 6 0.000016582 -0.000001032 0.000000389

38 6 0.000006243 -0.000017853 0.000000112

39 6 0.000016582 0.000001032 0.000000389

40 6 -0.000006243 0.000017853 0.000000112

41 6 -0.000016582 -0.000001032 0.000000389

42 1 0.000013228 0.000003516 -0.000000612

43 1 0.000013228 -0.000003516 -0.000000612

44 1 -0.000013228 -0.000003516 -0.000000612

45 1 -0.000013228 0.000003516 -0.000000612

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

Cartesian Forces: Max 0.000819668 RMS 0.000088571

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

Leave Link 716 at Tue Jul 30 23:34:10 2019, MaxMem= 4294967296 cpu: 0.8

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000182609 RMS 0.000036684

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 = .36684D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= 4.86D-04 DEPred=-3.50D-04 R=-1.39D+00

Trust test=-1.39D+00 RLast= 5.50D-01 DXMaxT set to 1.50D-01

ITU= -1 0 0

Eigenvalues --- -0.00918 0.00042 0.00120 0.00155 0.00311

Eigenvalues --- 0.00645 0.00758 0.00817 0.00837 0.01033

Eigenvalues --- 0.01119 0.01136 0.01230 0.01231 0.01264

Eigenvalues --- 0.01283 0.01476 0.01521 0.01522 0.01594

Eigenvalues --- 0.01616 0.01714 0.01943 0.01956 0.01975

Eigenvalues --- 0.02017 0.02108 0.02113 0.02127 0.02143

Eigenvalues --- 0.02825 0.02994 0.03190 0.03496 0.03992

Eigenvalues --- 0.04097 0.04139 0.04141 0.04153 0.04160

Eigenvalues --- 0.04300 0.04351 0.04933 0.05078 0.07587

Eigenvalues --- 0.08274 0.08303 0.08526 0.08527 0.09033

Eigenvalues --- 0.09047 0.09158 0.09167 0.09205 0.09611

Eigenvalues --- 0.09629 0.09640 0.09664 0.10406 0.10408

Eigenvalues --- 0.10442 0.10509 0.12437 0.12959 0.13042

Eigenvalues --- 0.13164 0.14880 0.16897 0.16929 0.19238

Eigenvalues --- 0.19849 0.20006 0.20100 0.20348 0.20637

Eigenvalues --- 0.20646 0.20806 0.21674 0.21881 0.21944

Eigenvalues --- 0.22020 0.25989 0.26257 0.27693 0.28015

Eigenvalues --- 0.28063 0.29415 0.30045 0.31747 0.32511

Eigenvalues --- 0.32740 0.32941 0.33570 0.35631 0.35688

Eigenvalues --- 0.35854 0.36103 0.36464 0.37030 0.37103

Eigenvalues --- 0.37163 0.37324 0.37398 0.37567 0.37780

Eigenvalues --- 0.38082 0.38311 0.38836 0.39197 0.40237

Eigenvalues --- 0.40240 0.40242 0.40243 0.41332 0.41469

Eigenvalues --- 0.42095 0.42606 0.45513 0.46272 0.46575

Eigenvalues --- 0.46834 0.50207 0.50222 0.52639 0.53057

Eigenvalues --- 1.03392 1.04135 1.04467 1.04699

Eigenvalue 1 is -9.18D-03 should be greater than 0.000000 Eigenvector:

A88 A87 D126 D127 D22

1 0.32296 -0.31642 -0.21479 0.21470 0.21459

D23 D96 D93 D52 D49

1 -0.21451 0.21133 -0.21124 -0.21114 0.21105

Use linear search instead of GDIIS.

Linear search step of 0.181 exceeds DXMaxT= 0.150 but not scaled.

RFO step: Lambda=-9.17964759D-03 EMin=-9.17850020D-03

I= 1 Eig= -9.18D-03 Dot1= -3.83D-05

I= 1 Stepn= -3.75D-01 RXN= 3.75D-01 EDone=F

Mixed 1 eigenvectors in step. Raw Step.Grad= 3.83D-05.

RFO eigenvector is Hessian eigenvector with negative curvature.

Taking step of 3.75D-01 in eigenvector direction(s). Step.Grad= 8.74D-06.

Quintic linear search produced a step of -0.75175.

Maximum step size ( 0.150) exceeded in Quadratic search.

-- Step size not scaled.

Iteration 1 RMS(Cart)= 0.01249189 RMS(Int)= 0.00120665

Iteration 2 RMS(Cart)= 0.00011569 RMS(Int)= 0.00120567

Iteration 3 RMS(Cart)= 0.00000004 RMS(Int)= 0.00120567

ITry= 1 IFail=0 DXMaxC= 6.12D-02 DCOld= 1.00D+10 DXMaxT= 1.50D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 5.97D-03 for atom 37.

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

(Linear) (Quad) (Total)

R1 2.74603 0.00000 0.00072 -0.00124 -0.00015 2.74588

R2 2.56748 -0.00013 -0.00264 -0.00110 -0.00100 2.56648

R3 2.04145 -0.00000 0.00005 -0.00006 -0.00001 2.04144

R4 2.59395 -0.00004 -0.00174 0.00214 0.00008 2.59403

R5 2.65256 0.00001 0.00083 -0.00295 -0.00048 2.65208

R6 2.59395 -0.00004 -0.00174 0.00211 0.00008 2.59403

R7 3.95413 0.00000 0.00226 -0.00399 -0.00298 3.95114

R8 2.74603 0.00000 0.00072 -0.00125 -0.00015 2.74588

R9 2.65256 0.00002 0.00083 -0.00298 -0.00048 2.65208

R10 2.04145 -0.00000 0.00005 -0.00006 -0.00001 2.04144

R11 2.71746 -0.00003 -0.00039 -0.00355 -0.00104 2.71642

R12 2.69138 0.00001 0.00048 -0.00009 0.00009 2.69147

R13 2.59288 0.00000 -0.00022 0.00188 0.00035 2.59323

R14 2.69565 0.00002 0.00119 -0.00115 -0.00009 2.69556

R15 2.59288 0.00000 -0.00022 0.00191 0.00035 2.59323

R16 3.96598 -0.00000 0.00153 -0.00225 -0.00211 3.96386

R17 2.69565 0.00002 0.00119 -0.00114 -0.00009 2.69556

R18 2.71746 -0.00003 -0.00039 -0.00352 -0.00104 2.71642

R19 2.61474 -0.00009 -0.00259 -0.00108 -0.00088 2.61386

R20 2.04170 -0.00000 0.00005 -0.00006 -0.00001 2.04170

R21 2.04170 -0.00000 0.00005 -0.00006 -0.00001 2.04170

R22 2.71746 -0.00003 -0.00039 -0.00353 -0.00104 2.71642

R23 2.69138 0.00001 0.00048 -0.00009 0.00009 2.69147

R24 2.69565 0.00002 0.00119 -0.00115 -0.00009 2.69556

R25 2.59288 0.00000 -0.00022 0.00186 0.00035 2.59323

R26 2.61474 -0.00009 -0.00259 -0.00105 -0.00088 2.61386

R27 2.04170 -0.00000 0.00005 -0.00006 -0.00001 2.04170

R28 2.69565 0.00002 0.00119 -0.00115 -0.00009 2.69556

R29 2.04170 -0.00000 0.00005 -0.00006 -0.00001 2.04170

R30 2.59288 0.00000 -0.00022 0.00189 0.00035 2.59323

R31 2.71746 -0.00003 -0.00039 -0.00350 -0.00104 2.71642

R32 3.96598 0.00000 0.00153 -0.00271 -0.00211 3.96386

R33 2.65256 0.00001 0.00083 -0.00295 -0.00048 2.65208

R34 2.69138 0.00001 0.00048 -0.00009 0.00009 2.69147

R35 2.74603 -0.00000 0.00072 -0.00124 -0.00015 2.74588

R36 2.59395 -0.00004 -0.00174 0.00213 0.00008 2.59403

R37 2.56748 -0.00013 -0.00264 -0.00108 -0.00100 2.56648

R38 2.04145 -0.00000 0.00005 -0.00006 -0.00001 2.04144

R39 2.74603 -0.00000 0.00072 -0.00125 -0.00015 2.74588

R40 2.04145 -0.00000 0.00005 -0.00006 -0.00001 2.04144

R41 2.59395 -0.00004 -0.00174 0.00210 0.00008 2.59403

R42 2.65256 0.00001 0.00083 -0.00297 -0.00048 2.65208

R43 3.95413 0.00001 0.00226 -0.00441 -0.00298 3.95114

R44 2.69138 0.00001 0.00048 -0.00009 0.00009 2.69147

R45 2.28351 -0.00000 0.00000 -0.00002 -0.00002 2.28349

R46 2.28351 -0.00000 0.00000 -0.00002 -0.00002 2.28349

R47 2.01595 0.00001 0.00028 -0.00001 0.00002 2.01598

R48 2.01595 0.00001 0.00028 -0.00001 0.00002 2.01598

R49 2.28351 -0.00000 0.00000 -0.00002 -0.00002 2.28349

R50 2.01595 0.00001 0.00028 -0.00001 0.00002 2.01598

R51 2.28351 -0.00000 0.00000 -0.00002 -0.00002 2.28349

R52 2.01595 0.00001 0.00028 -0.00001 0.00002 2.01598

A1 1.87068 0.00001 0.00051 -0.00073 -0.00000 1.87068

A2 2.18701 0.00000 0.00048 -0.00032 0.00004 2.18705

A3 2.22548 -0.00001 -0.00099 0.00103 -0.00004 2.22544

A4 1.90158 -0.00001 -0.00159 0.00370 0.00040 1.90198

A5 2.18214 0.00002 0.00181 -0.00366 -0.00049 2.18165

A6 2.19945 -0.00001 -0.00022 -0.00009 0.00009 2.19954

A7 1.88025 0.00000 0.00215 -0.00596 -0.00080 1.87945

A8 2.20061 -0.00000 -0.00045 0.00190 0.00088 2.20149

A9 2.20061 -0.00000 -0.00045 0.00213 0.00088 2.20149

A10 1.90158 -0.00001 -0.00159 0.00371 0.00040 1.90198

A11 2.19945 -0.00001 -0.00022 -0.00014 0.00009 2.19954

A12 2.18214 0.00002 0.00181 -0.00363 -0.00049 2.18165

A13 1.87068 0.00001 0.00051 -0.00073 -0.00000 1.87068

A14 2.22548 -0.00001 -0.00099 0.00103 -0.00004 2.22544

A15 2.18701 0.00000 0.00048 -0.00032 0.00004 2.18705

A16 2.20956 0.00002 0.00252 -0.00508 -0.00050 2.20907

A17 2.04412 0.00002 -0.00022 0.00234 0.00039 2.04451

A18 2.02948 -0.00004 -0.00229 0.00263 0.00001 2.02949

A19 2.18104 -0.00000 0.00011 -0.00031 -0.00008 2.18096

A20 2.19256 0.00004 0.00238 -0.00336 -0.00013 2.19243

A21 1.90956 -0.00003 -0.00246 0.00360 0.00017 1.90973

A22 1.87491 0.00002 0.00271 -0.00568 -0.00060 1.87432

A23 2.20355 -0.00001 -0.00100 0.00216 0.00068 2.20423

A24 2.20355 -0.00001 -0.00100 0.00194 0.00068 2.20423

A25 1.90956 -0.00003 -0.00246 0.00359 0.00017 1.90973

A26 2.18104 -0.00000 0.00011 -0.00027 -0.00008 2.18096

A27 2.19256 0.00004 0.00238 -0.00339 -0.00013 2.19243

A28 1.86537 0.00002 0.00111 -0.00076 0.00011 1.86548

A29 2.19608 -0.00001 -0.00007 -0.00032 -0.00007 2.19601

A30 2.22172 -0.00001 -0.00103 0.00106 -0.00005 2.22167

A31 1.86537 0.00002 0.00111 -0.00076 0.00011 1.86548

A32 2.19608 -0.00001 -0.00007 -0.00032 -0.00007 2.19601

A33 2.22172 -0.00001 -0.00103 0.00106 -0.00005 2.22167

A34 2.20956 0.00002 0.00252 -0.00504 -0.00050 2.20907

A35 2.04412 0.00002 -0.00022 0.00233 0.00039 2.04451

A36 2.02948 -0.00004 -0.00229 0.00260 0.00001 2.02949

A37 2.19256 0.00003 0.00238 -0.00330 -0.00013 2.19243

A38 2.18104 -0.00000 0.00011 -0.00034 -0.00008 2.18096

A39 1.90956 -0.00003 -0.00246 0.00357 0.00017 1.90973

A40 1.86537 0.00002 0.00111 -0.00076 0.00011 1.86548

A41 2.19608 -0.00001 -0.00007 -0.00031 -0.00007 2.19601

A42 2.22172 -0.00001 -0.00103 0.00105 -0.00005 2.22167

A43 1.86537 0.00002 0.00111 -0.00075 0.00011 1.86548

A44 2.22172 -0.00001 -0.00103 0.00105 -0.00005 2.22167

A45 2.19608 -0.00001 -0.00007 -0.00031 -0.00007 2.19601

A46 1.90956 -0.00003 -0.00246 0.00356 0.00017 1.90973

A47 2.19256 0.00003 0.00238 -0.00333 -0.00013 2.19243

A48 2.18104 -0.00000 0.00011 -0.00030 -0.00008 2.18096

A49 1.87491 0.00002 0.00271 -0.00563 -0.00060 1.87432

A50 2.20355 -0.00001 -0.00100 0.00213 0.00068 2.20423

A51 2.20355 -0.00001 -0.00100 0.00192 0.00068 2.20423

A52 2.20956 0.00002 0.00252 -0.00500 -0.00050 2.20907

A53 2.02948 -0.00004 -0.00229 0.00259 0.00001 2.02949

A54 2.04412 0.00002 -0.00022 0.00231 0.00039 2.04451

A55 2.18214 0.00002 0.00181 -0.00360 -0.00049 2.18165

A56 2.19945 -0.00001 -0.00022 -0.00012 0.00009 2.19954

A57 1.90158 -0.00001 -0.00159 0.00367 0.00040 1.90198

A58 1.87068 0.00001 0.00051 -0.00072 -0.00000 1.87068

A59 2.18701 0.00000 0.00048 -0.00032 0.00004 2.18705

A60 2.22548 -0.00001 -0.00099 0.00102 -0.00004 2.22544

A61 1.87068 0.00001 0.00051 -0.00073 -0.00000 1.87068

A62 2.22548 -0.00001 -0.00099 0.00103 -0.00004 2.22544

A63 2.18701 0.00000 0.00048 -0.00032 0.00004 2.18705

A64 1.90158 -0.00001 -0.00159 0.00368 0.00040 1.90198

A65 2.18214 0.00002 0.00181 -0.00357 -0.00049 2.18165

A66 2.19945 -0.00001 -0.00022 -0.00017 0.00009 2.19954

A67 1.88025 0.00000 0.00215 -0.00591 -0.00080 1.87945

A68 2.20061 0.00000 -0.00045 0.00187 0.00088 2.20149

A69 2.20061 -0.00000 -0.00045 0.00210 0.00088 2.20149

A70 1.56719 0.00001 0.00233 -0.00741 0.00023 1.56742

A71 1.56719 0.00001 0.00233 -0.00722 0.00023 1.56742

A72 1.56719 0.00001 0.00233 -0.00723 0.00023 1.56742

A73 1.56719 0.00001 0.00233 -0.00703 0.00023 1.56742

A74 2.20956 0.00002 0.00252 -0.00504 -0.00050 2.20907

A75 2.02948 -0.00004 -0.00229 0.00262 0.00001 2.02949

A76 2.04412 0.00002 -0.00022 0.00232 0.00039 2.04451

A77 3.13439 0.00002 0.00466 -0.01425 0.00045 3.13484

A78 3.13439 0.00002 0.00466 -0.01427 0.00045 3.13484

A79 3.12434 0.00000 -0.00030 0.00052 0.00011 3.12445

A80 3.15883 -0.00000 0.00031 -0.00056 -0.00015 3.15868

A81 3.14688 0.00001 0.00267 -0.00003 0.00063 3.14750

A82 3.14688 0.00001 0.00267 -0.00002 0.00063 3.14750

A83 3.15883 -0.00000 0.00031 -0.00058 -0.00015 3.15868

A84 3.14688 0.00001 0.00267 -0.00003 0.00063 3.14750

A85 3.12434 0.00000 -0.00030 0.00050 0.00011 3.12445

A86 3.14688 0.00001 0.00267 -0.00003 0.00063 3.14750

A87 3.26394 -0.00017 -0.12119 0.11866 -0.00194 3.26200

A88 3.02410 0.00018 0.12733 -0.12111 0.00556 3.02967

A89 3.14084 -0.00000 0.00080 -0.00217 -0.00134 3.13950

A90 3.14270 0.00000 -0.00119 0.00260 0.00145 3.14415

A91 3.14136 -0.00000 0.00002 -0.00029 -0.00008 3.14129

A92 3.14136 -0.00000 0.00002 -0.00032 -0.00008 3.14129

A93 3.14048 -0.00000 0.00119 -0.00263 -0.00145 3.13903

A94 3.14182 0.00000 -0.00002 0.00033 0.00008 3.14190

A95 3.14235 0.00000 -0.00080 0.00214 0.00134 3.14369

A96 3.14182 0.00000 -0.00002 0.00028 0.00008 3.14190

D1 -0.00011 0.00002 0.00203 -0.00473 -0.00272 -0.00283

D2 3.13562 0.00003 0.01065 -0.01398 -0.00333 3.13229

D3 -3.13831 0.00000 -0.00248 0.00110 -0.00137 -3.13968

D4 -0.00259 0.00001 0.00614 -0.00815 -0.00197 -0.00456

D5 0.00000 -0.00000 -0.00000 0.00000 -0.00000 0.00000

D6 -3.13810 -0.00002 -0.00464 0.00600 0.00139 -3.13671

D7 3.13810 0.00002 0.00464 -0.00600 -0.00139 3.13671

D8 -0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D9 0.00018 -0.00003 -0.00330 0.00765 0.00441 0.00459

D10 -3.08123 -0.00004 -0.05683 0.04121 -0.01561 -3.09684

D11 -3.13547 -0.00004 -0.01201 0.01704 0.00502 -3.13045

D12 0.06630 -0.00006 -0.06555 0.05059 -0.01499 0.05131

D13 -3.12803 -0.00005 -0.01909 0.02810 0.00905 -3.11899

D14 0.00649 -0.00001 -0.01018 0.00964 -0.00060 0.00589

D15 0.00670 -0.00004 -0.00902 0.01729 0.00834 0.01504

D16 3.14122 0.00001 -0.00011 -0.00117 -0.00131 3.13992

D17 -0.00018 0.00003 0.00330 -0.00765 -0.00441 -0.00459

D18 3.13547 0.00004 0.01201 -0.01704 -0.00502 3.13045

D19 3.08123 0.00004 0.05683 -0.04122 0.01561 3.09684

D20 -0.06630 0.00006 0.06555 -0.05060 0.01499 -0.05131

D21 -3.11832 -0.00008 -0.03212 0.04062 0.00900 -3.10932

D22 -0.09422 0.00010 0.09521 -0.08047 0.01456 -0.07966

D23 0.09422 -0.00010 -0.09521 0.08044 -0.01456 0.07966

D24 3.11832 0.00008 0.03212 -0.04065 -0.00900 3.10932

D25 0.00011 -0.00002 -0.00203 0.00472 0.00272 0.00283

D26 3.13831 -0.00000 0.00248 -0.00111 0.00137 3.13968

D27 -3.13562 -0.00003 -0.01065 0.01398 0.00333 -3.13229

D28 0.00259 -0.00001 -0.00614 0.00815 0.00197 0.00456

D29 -0.00670 0.00004 0.00902 -0.01726 -0.00834 -0.01504

D30 -3.14122 -0.00001 0.00011 0.00123 0.00131 -3.13992

D31 3.12803 0.00005 0.01909 -0.02808 -0.00905 3.11899

D32 -0.00649 0.00001 0.01018 -0.00959 0.00060 -0.00589

D33 0.01121 -0.00004 -0.01248 0.01880 0.00638 0.01759

D34 -3.12146 -0.00005 -0.01959 0.02971 0.01023 -3.11123

D35 -3.13740 0.00000 -0.00364 0.00044 -0.00319 -3.14059

D36 0.01312 -0.00000 -0.01075 0.01136 0.00066 0.01378

D37 -3.13325 -0.00003 -0.00532 0.01420 0.00889 -3.12436

D38 0.05791 -0.00005 -0.05906 0.04757 -0.01146 0.04645

D39 0.00065 -0.00002 0.00081 0.00476 0.00557 0.00623

D40 -3.09138 -0.00005 -0.05293 0.03813 -0.01478 -3.10615

D41 3.13343 0.00002 0.00568 -0.01244 -0.00679 3.12664

D42 -0.00422 0.00001 0.00247 -0.00730 -0.00484 -0.00906

D43 -0.00040 0.00001 -0.00050 -0.00294 -0.00345 -0.00385

D44 -3.13805 0.00000 -0.00371 0.00220 -0.00150 -3.13955

D45 -0.00065 0.00002 -0.00081 -0.00476 -0.00557 -0.00623

D46 3.13325 0.00003 0.00532 -0.01419 -0.00889 3.12436

D47 3.09138 0.00005 0.05293 -0.03812 0.01478 3.10615

D48 -0.05791 0.00005 0.05906 -0.04756 0.01146 -0.04645

D49 -0.09050 0.00010 0.09237 -0.07915 0.01300 -0.07750

D50 -3.10974 -0.00007 -0.02882 0.03949 0.01106 -3.09868

D51 3.10974 0.00007 0.02882 -0.03946 -0.01106 3.09868

D52 0.09050 -0.00010 -0.09237 0.07918 -0.01300 0.07750

D53 0.00040 -0.00001 0.00050 0.00295 0.00345 0.00385

D54 3.13805 -0.00000 0.00371 -0.00219 0.00150 3.13955

D55 -3.13343 -0.00002 -0.00568 0.01244 0.00679 -3.12664

D56 0.00422 -0.00001 -0.00247 0.00730 0.00484 0.00906

D57 -0.01121 0.00004 0.01248 -0.01883 -0.00638 -0.01759

D58 3.13740 -0.00000 0.00364 -0.00050 0.00319 3.14059

D59 3.12146 0.00005 0.01959 -0.02974 -0.01023 3.11123

D60 -0.01312 0.00000 0.01075 -0.01141 -0.00066 -0.01378

D61 -0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D62 3.13757 0.00001 0.00327 -0.00524 -0.00199 3.13559

D63 -3.13757 -0.00001 -0.00327 0.00524 0.00199 -3.13559

D64 0.00000 -0.00000 -0.00000 0.00000 -0.00000 0.00000

D65 3.12146 0.00005 0.01959 -0.02968 -0.01023 3.11123

D66 -0.01121 0.00004 0.01248 -0.01879 -0.00638 -0.01759

D67 -0.01312 0.00000 0.01075 -0.01136 -0.00066 -0.01378

D68 3.13740 -0.00000 0.00364 -0.00047 0.00319 3.14059

D69 -3.13343 -0.00002 -0.00568 0.01241 0.00679 -3.12664

D70 0.00422 -0.00001 -0.00247 0.00728 0.00484 0.00906

D71 0.00040 -0.00001 0.00050 0.00293 0.00345 0.00385

D72 3.13805 -0.00000 0.00371 -0.00219 0.00150 3.13955

D73 3.13325 0.00003 0.00532 -0.01415 -0.00889 3.12436

D74 -0.05791 0.00005 0.05906 -0.04763 0.01146 -0.04645

D75 -0.00065 0.00002 -0.00081 -0.00474 -0.00557 -0.00623

D76 3.09138 0.00005 0.05293 -0.03821 0.01478 3.10615

D77 -0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D78 3.13757 0.00001 0.00327 -0.00523 -0.00199 3.13559

D79 -3.13757 -0.00001 -0.00327 0.00523 0.00199 -3.13559

D80 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D81 -0.00040 0.00001 -0.00050 -0.00294 -0.00345 -0.00385

D82 3.13343 0.00002 0.00568 -0.01241 -0.00679 3.12664

D83 -3.13805 0.00000 -0.00371 0.00219 -0.00150 -3.13955

D84 -0.00422 0.00001 0.00247 -0.00728 -0.00484 -0.00906

D85 0.00065 -0.00002 0.00081 0.00474 0.00557 0.00623

D86 -3.09138 -0.00005 -0.05293 0.03821 -0.01478 -3.10615

D87 -3.13325 -0.00003 -0.00532 0.01415 0.00889 -3.12436

D88 0.05791 -0.00005 -0.05906 0.04762 -0.01146 0.04645

D89 -3.12146 -0.00005 -0.01959 0.02971 0.01023 -3.11123

D90 0.01312 -0.00000 -0.01075 0.01141 0.00066 0.01378

D91 0.01121 -0.00004 -0.01248 0.01882 0.00638 0.01759

D92 -3.13740 0.00000 -0.00364 0.00053 -0.00319 -3.14059

D93 0.09050 -0.00010 -0.09237 0.07922 -0.01300 0.07750

D94 3.10974 0.00007 0.02882 -0.03944 -0.01106 3.09868

D95 -3.10974 -0.00007 -0.02882 0.03941 0.01106 -3.09868

D96 -0.09050 0.00010 0.09237 -0.07925 0.01300 -0.07750

D97 3.12803 0.00005 0.01909 -0.02807 -0.00905 3.11899

D98 -0.00670 0.00004 0.00902 -0.01729 -0.00834 -0.01504

D99 -0.00649 0.00001 0.01018 -0.00964 0.00060 -0.00589

D100 -3.14122 -0.00001 0.00011 0.00114 0.00131 -3.13992

D101 -3.13562 -0.00003 -0.01065 0.01394 0.00333 -3.13229

D102 0.00259 -0.00001 -0.00614 0.00813 0.00197 0.00456

D103 0.00011 -0.00002 -0.00203 0.00471 0.00272 0.00283

D104 3.13831 -0.00000 0.00248 -0.00110 0.00137 3.13968

D105 3.13547 0.00004 0.01201 -0.01699 -0.00502 3.13045

D106 -0.06630 0.00006 0.06555 -0.05066 0.01499 -0.05131

D107 -0.00018 0.00003 0.00330 -0.00763 -0.00441 -0.00459

D108 3.08123 0.00004 0.05683 -0.04130 0.01561 3.09684

D109 0.00000 0.00000 -0.00000 -0.00000 -0.00000 0.00000

D110 3.13810 0.00002 0.00464 -0.00599 -0.00139 3.13671

D111 -3.13810 -0.00002 -0.00464 0.00599 0.00139 -3.13671

D112 -0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D113 -0.00011 0.00002 0.00203 -0.00471 -0.00272 -0.00283

D114 3.13562 0.00003 0.01065 -0.01394 -0.00333 3.13229

D115 -3.13831 0.00000 -0.00248 0.00111 -0.00137 -3.13968

D116 -0.00259 0.00001 0.00614 -0.00813 -0.00197 -0.00456

D117 0.00018 -0.00003 -0.00330 0.00763 0.00441 0.00459

D118 -3.08123 -0.00004 -0.05683 0.04130 -0.01561 -3.09684

D119 -3.13547 -0.00004 -0.01201 0.01699 0.00502 -3.13045

D120 0.06630 -0.00006 -0.06555 0.05067 -0.01499 0.05131

D121 -3.12803 -0.00005 -0.01909 0.02805 0.00905 -3.11899

D122 0.00649 -0.00001 -0.01018 0.00959 -0.00060 0.00589

D123 0.00670 -0.00004 -0.00902 0.01726 0.00834 0.01504

D124 3.14122 0.00001 -0.00011 -0.00120 -0.00131 3.13992

D125 3.11832 0.00008 0.03212 -0.04056 -0.00900 3.10932

D126 0.09422 -0.00010 -0.09521 0.08055 -0.01456 0.07966

D127 -0.09422 0.00010 0.09521 -0.08051 0.01456 -0.07966

D128 -3.11832 -0.00008 -0.03212 0.04060 0.00900 -3.10932

Item Value Threshold Converged?

Maximum Force 0.000183 0.000450 YES

RMS Force 0.000037 0.000300 YES

Maximum Displacement 0.060806 0.001800 NO

RMS Displacement 0.012444 0.001200 NO

Predicted change in Energy=-2.254677D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Jul 30 23:34:10 2019, MaxMem= 4294967296 cpu: 1.1

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -4.284483 0.679061 -0.032500

2 6 0 -2.896652 1.108312 -0.000123

3 7 0 -2.087056 0.000000 0.022442

4 6 0 -2.896652 -1.108312 -0.000123

5 6 0 -4.284483 -0.679061 -0.032500

6 6 0 -2.467086 -2.444374 -0.000801

7 6 0 -1.105891 -2.906361 0.004486

8 7 0 -0.000000 -2.094291 0.030904

9 6 0 1.105891 -2.906361 0.004486

10 6 0 0.691597 -4.270823 -0.031522

11 6 0 -0.691597 -4.270823 -0.031522

12 6 0 -2.467086 2.444374 -0.000801

13 6 0 -1.105891 2.906361 0.004486

14 6 0 -0.691597 4.270823 -0.031522

15 6 0 0.691597 4.270823 -0.031522

16 6 0 1.105891 2.906361 0.004486

17 7 0 0.000000 2.094291 0.030904

18 6 0 2.467086 2.444374 -0.000801

19 6 0 2.896652 1.108312 -0.000123

20 6 0 4.284483 0.679061 -0.032500

21 6 0 4.284483 -0.679061 -0.032500

22 6 0 2.896652 -1.108312 -0.000123

23 7 0 2.087056 -0.000000 0.022442

24 1 0 -5.141091 1.336822 -0.056667

25 1 0 -5.141091 -1.336822 -0.056667

26 1 0 1.346208 -5.129902 -0.059358

27 1 0 -1.346208 -5.129902 -0.059358

28 1 0 -1.346208 5.129902 -0.059358

29 1 0 1.346208 5.129902 -0.059358

30 1 0 5.141091 1.336822 -0.056667

31 1 0 5.141091 -1.336822 -0.056667

32 30 0 -0.000000 -0.000000 0.148444

33 6 0 2.467086 -2.444374 -0.000801

34 6 0 3.474521 -3.450769 -0.028555

35 6 0 -3.474521 3.450769 -0.028555

36 6 0 4.314467 -4.319078 -0.054901

37 6 0 -4.314467 4.319078 -0.054901

38 6 0 -3.474521 -3.450769 -0.028555

39 6 0 -4.314467 -4.319078 -0.054901

40 6 0 3.474521 3.450769 -0.028555

41 6 0 4.314467 4.319078 -0.054901

42 1 0 5.060529 5.081261 -0.078361

43 1 0 5.060529 -5.081261 -0.078361

44 1 0 -5.060529 -5.081261 -0.078361

45 1 0 -5.060529 5.081261 -0.078361

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.453058 0.000000

3 N 2.300614 1.372702 0.000000

4 C 2.263144 2.216623 1.372702 0.000000

5 C 1.358121 2.263144 2.300614 1.453058 0.000000

6 C 3.613831 3.578561 2.473849 1.403421 2.533824

7 C 4.791665 4.395957 3.067562 2.537681 3.881453

8 N 5.104144 4.318358 2.956675 3.060018 4.512614

9 C 6.474005 5.669036 4.317657 4.387864 5.832526

10 C 7.018740 6.466190 5.095464 4.783095 6.136948

11 C 6.116385 5.813634 4.493344 3.855480 5.080313

12 C 2.533824 1.403421 2.473849 3.578561 3.613831

13 C 3.881453 2.537681 3.067562 4.395957 4.791665

14 C 5.080313 3.855480 4.493344 5.813634 6.116385

15 C 6.136948 4.783095 5.095464 6.466190 7.018740

16 C 5.832526 4.387864 4.317657 5.669036 6.474005

17 N 4.512614 3.060018 2.956675 4.318358 5.104144

18 C 6.978611 5.527635 5.168724 6.433604 7.439121

19 C 7.194025 5.793304 5.105507 6.202885 7.400300

20 C 8.568965 7.194025 6.407858 7.400300 8.675924

21 C 8.675924 7.400300 6.407858 7.194025 8.568965

22 C 7.400300 6.202885 5.105507 5.793304 7.194025

23 N 6.407858 5.105507 4.174111 5.105507 6.407858

24 H 1.080283 2.256750 3.334738 3.319545 2.190466

25 H 2.190466 3.319545 3.334738 2.256750 1.080283

26 H 8.090083 7.544580 6.173321 5.846243 7.177422

27 H 6.509856 6.428273 5.183767 4.310519 5.333308

28 H 5.333308 4.310519 5.183767 6.428273 6.509856

29 H 7.177422 5.846243 6.173321 7.544580 8.090083

30 H 9.448527 8.041189 7.351153 8.401618 9.638765

31 H 9.638765 8.401618 7.351153 8.041189 9.448527

32 Zn 4.341734 3.104999 2.090856 3.104999 4.341734

33 C 7.439121 6.433604 5.168724 5.527635 6.978611

34 C 8.789633 7.834403 6.545345 6.788207 8.239206

35 C 2.887632 2.412850 3.719606 4.595645 4.208508

36 C 9.946045 9.025507 7.722687 7.893811 9.337674

37 C 3.640209 3.510301 4.860223 5.609791 4.998278

38 C 4.208508 4.595645 3.719606 2.412850 2.887632

39 C 4.998278 5.609791 4.860223 3.510301 3.640209

40 C 8.239206 6.788207 6.545345 7.834403 8.789633

41 C 9.337674 7.893811 7.722687 9.025507 9.946045

42 H 10.330088 8.894222 8.770254 10.081352 10.977826

43 H 10.977826 10.081352 8.770254 8.894222 10.330088

44 H 5.812543 6.557385 5.888202 4.524689 4.470316

45 H 4.470316 4.524689 5.888202 6.557385 5.812543

6 7 8 9 10

6 C 0.000000

7 C 1.437467 0.000000

8 N 2.492003 1.372279 0.000000

9 C 3.602725 2.211782 1.372279 0.000000

10 C 3.648855 2.256993 2.284622 1.426427 0.000000

11 C 2.547395 1.426427 2.284622 2.256993 1.383195

12 C 4.888748 5.521163 5.165946 6.434015 7.421057

13 C 5.521163 5.812721 5.121543 6.219301 7.398934

14 C 6.946018 7.189221 6.402880 7.398934 8.652915

15 C 7.421057 7.398934 6.402880 7.189221 8.541646

16 C 6.434015 6.219301 5.121543 5.812721 7.189221

17 N 5.165946 5.121543 4.188581 5.121543 6.402880

18 C 6.945928 6.434015 5.165946 5.521163 6.946018

19 C 6.433604 5.669036 4.318358 4.395957 5.813634

20 C 7.439121 6.474005 5.104144 4.791665 6.116385

21 C 6.978611 5.832526 4.512614 3.881453 5.080313

22 C 5.527635 4.387864 3.060018 2.537681 3.855480

23 N 5.168724 4.317657 2.956675 3.067562 4.493344

24 H 4.631507 5.855866 6.181506 7.552027 8.091141

25 H 2.894839 4.330130 5.197330 6.441426 6.529108

26 H 4.664408 3.310740 3.321951 2.237401 1.080420

27 H 2.910646 2.237401 3.321951 3.310740 2.211661

28 H 7.656987 8.040109 7.349108 8.402285 9.619099

29 H 8.480230 8.402285 7.349108 8.040109 9.423530

30 H 8.496171 7.552027 6.181506 5.855866 7.158512

31 H 7.688573 6.441426 5.197330 4.330130 5.329821

32 Zn 3.476169 3.112981 2.097586 3.112981 4.330199

33 C 4.934172 3.602725 2.492003 1.437467 2.547395

34 C 6.026300 4.612770 3.730397 2.430613 2.901234

35 C 5.980669 6.784143 6.543968 7.835455 8.773798

36 C 7.036114 5.601747 4.855065 3.506316 3.623266

37 C 7.011420 7.906038 7.730024 9.032760 9.942214

38 C 1.424263 2.430613 3.730397 4.612770 4.246062

39 C 2.632538 3.506316 4.855065 5.601747 5.006351

40 C 8.369956 7.835455 6.543968 6.784143 8.207780

41 C 9.577925 9.032760 7.730024 7.906038 9.322667

42 H 10.644538 10.091269 8.781198 8.913368 10.322366

43 H 7.976477 6.539250 5.877320 4.514002 4.443711

44 H 3.699343 4.514002 5.877320 6.539250 5.809128

45 H 7.960348 8.913368 8.781198 10.091269 10.979555

11 12 13 14 15

11 C 0.000000

12 C 6.946018 0.000000

13 C 7.189221 1.437467 0.000000

14 C 8.541646 2.547395 1.426427 0.000000

15 C 8.652915 3.648855 2.256993 1.383195 0.000000

16 C 7.398934 3.602725 2.211782 2.256993 1.426427

17 N 6.402880 2.492003 1.372279 2.284622 2.284622

18 C 7.421057 4.934172 3.602725 3.648855 2.547395

19 C 6.466190 5.527635 4.387864 4.783095 3.855480

20 C 7.018740 6.978611 5.832526 6.136948 5.080313

21 C 6.136948 7.439121 6.474005 7.018740 6.116385

22 C 4.783095 6.433604 5.669036 6.466190 5.813634

23 N 5.095464 5.168724 4.317657 5.095464 4.493344

24 H 7.158512 2.894839 4.330130 5.329821 6.529108

25 H 5.329821 4.631507 5.855866 7.158512 8.091141

26 H 2.211661 8.480230 8.402285 9.619099 9.423530

27 H 1.080420 7.656987 8.040109 9.423530 9.619099

28 H 9.423530 2.910646 2.237401 1.080420 2.211661

29 H 9.619099 4.664408 3.310740 2.211661 1.080420

30 H 8.091141 7.688573 6.441426 6.529108 5.329821

31 H 6.529108 8.496171 7.552027 8.091141 7.158512

32 Zn 4.330199 3.476169 3.112981 4.330199 4.330199

33 C 3.648855 6.945928 6.434015 7.421057 6.946018

34 C 4.246062 8.369956 7.835455 8.773798 8.207780

35 C 8.207780 1.424263 2.430613 2.901234 4.246062

36 C 5.006351 9.577925 9.032760 9.942214 9.322667

37 C 9.322667 2.632538 3.506316 3.623266 5.006351

38 C 2.901234 5.980669 6.784143 8.207780 8.773798

39 C 3.623266 7.011420 7.906038 9.322667 9.942214

40 C 8.773798 6.026300 4.612770 4.246062 2.901234

41 C 9.942214 7.036114 5.601747 5.006351 3.623266

42 H 10.979555 7.976477 6.539250 5.809128 4.443711

43 H 5.809128 10.644538 10.091269 10.979555 10.322366

44 H 4.443711 7.960348 8.913368 10.322366 10.979555

45 H 10.322366 3.699343 4.514002 4.443711 5.809128

16 17 18 19 20

16 C 0.000000

17 N 1.372279 0.000000

18 C 1.437467 2.492003 0.000000

19 C 2.537681 3.060018 1.403421 0.000000

20 C 3.881453 4.512614 2.533824 1.453058 0.000000

21 C 4.791665 5.104144 3.613831 2.263144 1.358121

22 C 4.395957 4.318358 3.578561 2.216623 2.263144

23 N 3.067562 2.956675 2.473849 1.372702 2.300614

24 H 6.441426 5.197330 7.688573 8.041189 9.448527

25 H 7.552027 6.181506 8.496171 8.401618 9.638765

26 H 8.040109 7.349108 7.656987 6.428273 6.509856

27 H 8.402285 7.349108 8.480230 7.544580 8.090083

28 H 3.310740 3.321951 4.664408 5.846243 7.177422

29 H 2.237401 3.321951 2.910646 4.310519 5.333308

30 H 4.330130 5.197330 2.894839 2.256750 1.080283

31 H 5.855866 6.181506 4.631507 3.319545 2.190466

32 Zn 3.112981 2.097586 3.476169 3.104999 4.341734

33 C 5.521163 5.165946 4.888748 3.578561 3.613831

34 C 6.784143 6.543968 5.980669 4.595645 4.208508

35 C 4.612770 3.730397 6.026300 6.788207 8.239206

36 C 7.906038 7.730024 7.011420 5.609791 4.998278

37 C 5.601747 4.855065 7.036114 7.893811 9.337674

38 C 7.835455 6.543968 8.369956 7.834403 8.789633

39 C 9.032760 7.730024 9.577925 9.025507 9.946045

40 C 2.430613 3.730397 1.424263 2.412850 2.887632

41 C 3.506316 4.855065 2.632538 3.510301 3.640209

42 H 4.514002 5.877320 3.699343 4.524689 4.470316

43 H 8.913368 8.781198 7.960348 6.557385 5.812543

44 H 10.091269 8.781198 10.644538 10.081352 10.977826

45 H 6.539250 5.877320 7.976477 8.894222 10.330088

21 22 23 24 25

21 C 0.000000

22 C 1.453058 0.000000

23 N 2.300614 1.372702 0.000000

24 H 9.638765 8.401618 7.351153 0.000000

25 H 9.448527 8.041189 7.351153 2.673643 0.000000

26 H 5.333308 4.310519 5.183767 9.159889 7.514819

27 H 7.177422 5.846243 6.173321 7.497977 5.365501

28 H 8.090083 7.544580 6.173321 5.365501 7.497977

29 H 6.509856 6.428273 5.183767 7.514819 9.159889

30 H 2.190466 3.319545 3.334738 10.282182 10.624106

31 H 1.080283 2.256750 3.334738 10.624106 10.282182

32 Zn 4.341734 3.104999 2.090856 5.316011 5.316011

33 C 2.533824 1.403421 2.473849 8.496171 7.688573

34 C 2.887632 2.412850 3.719606 9.856499 8.871208

35 C 8.789633 7.834403 6.545345 2.692029 5.069444

36 C 3.640209 3.510301 4.860223 11.018020 9.914707

37 C 9.946045 9.025507 7.722687 3.094699 5.715987

38 C 8.239206 6.788207 6.545345 5.069444 2.692029

39 C 9.337674 7.893811 7.722687 5.715987 3.094699

40 C 4.208508 4.595645 3.719606 8.871208 9.856499

41 C 4.998278 5.609791 4.860223 9.914707 11.018020

42 H 5.812543 6.557385 5.888202 10.867122 12.052606

43 H 4.470316 4.524689 5.888202 12.052606 10.867122

44 H 10.330088 8.894222 8.770254 6.418625 3.745369

45 H 10.977826 10.081352 8.770254 3.745369 6.418625

26 27 28 29 30

26 H 0.000000

27 H 2.692416 0.000000

28 H 10.607200 10.259804 0.000000

29 H 10.259804 10.607200 2.692416 0.000000

30 H 7.497977 9.159889 7.514819 5.365501 0.000000

31 H 5.365501 7.514819 9.159889 7.497977 2.673643

32 Zn 5.307669 5.307669 5.307669 5.307669 5.316011

33 C 2.910646 4.664408 8.480230 7.656987 4.631507

34 C 2.711117 5.104886 9.842169 8.840734 5.069444

35 C 9.842169 8.840734 2.711117 5.104886 8.871208

36 C 3.077014 5.718452 11.014830 9.904231 5.715987

37 C 11.014830 9.904231 3.077014 5.718452 9.914707

38 C 5.104886 2.711117 8.840734 9.842169 9.856499

39 C 5.718452 3.077014 9.904231 11.014830 11.018020

40 C 8.840734 9.842169 5.104886 2.711117 2.692029

41 C 9.904231 11.014830 5.718452 3.077014 3.094699

42 H 10.865745 12.054646 6.406950 3.714688 3.745369

43 H 3.714688 6.406950 12.054646 10.865745 6.418625

44 H 6.406950 3.714688 10.865745 12.054646 12.052606

45 H 12.054646 10.865745 3.714688 6.406950 10.867122

31 32 33 34 35

31 H 0.000000

32 Zn 5.316011 0.000000

33 C 2.894839 3.476169 0.000000

34 C 2.692029 4.900146 1.424263 0.000000

35 C 9.856499 4.900146 8.369956 9.793896 0.000000

36 C 3.094699 6.108224 2.632538 1.208372 11.001797

37 C 11.018020 6.108224 9.577925 11.001797 1.208372

38 C 8.871208 4.900146 6.026300 6.949042 6.901538

39 C 9.914707 6.108224 7.036114 7.837281 7.815159

40 C 5.069444 4.900146 5.980669 6.901538 6.949042

41 C 5.715987 6.108224 7.011420 7.815159 7.837281

42 H 6.418625 7.174929 7.960348 8.678332 8.689538

43 H 3.745369 7.174929 3.699343 2.275172 12.068351

44 H 10.867122 7.174929 7.976477 8.689538 8.678332

45 H 12.052606 7.174929 10.644538 12.068351 2.275172

36 37 38 39 40

36 C 0.000000

37 C 12.209677 0.000000

38 C 7.837281 7.815159 0.000000

39 C 8.628933 8.638155 1.208372 0.000000

40 C 7.815159 7.837281 9.793896 11.001797 0.000000

41 C 8.638155 8.628933 11.001797 12.209677 1.208372

42 H 9.429927 9.405957 12.068351 13.276199 2.275172

43 H 1.066810 13.276199 8.689538 9.405957 8.678332

44 H 9.405957 9.429927 2.275172 1.066810 12.068351

45 H 13.276199 1.066810 8.678332 9.429927 8.689538

41 42 43 44 45

41 C 0.000000

42 H 1.066810 0.000000

43 H 9.429927 10.162523 0.000000

44 H 13.276199 14.342688 10.121058 0.000000

45 H 9.405957 10.121058 14.342688 10.162523 0.000000

Stoichiometry C28H12N4Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C28H12)]

Deg. of freedom 34

Full point group C2V NOp 4

RotChk: IX=0 Diff= 1.53D-14

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.679061 4.284483 -0.036570

2 6 0 1.108312 2.896652 -0.004193

3 7 0 0.000000 2.087056 0.018372

4 6 0 -1.108312 2.896652 -0.004193

5 6 0 -0.679061 4.284483 -0.036570

6 6 0 -2.444374 2.467086 -0.004871

7 6 0 -2.906361 1.105891 0.000416

8 7 0 -2.094291 0.000000 0.026834

9 6 0 -2.906361 -1.105891 0.000416

10 6 0 -4.270823 -0.691597 -0.035592

11 6 0 -4.270823 0.691597 -0.035592

12 6 0 2.444374 2.467086 -0.004871

13 6 0 2.906361 1.105891 0.000416

14 6 0 4.270823 0.691597 -0.035592

15 6 0 4.270823 -0.691597 -0.035592

16 6 0 2.906361 -1.105891 0.000416

17 7 0 2.094291 -0.000000 0.026834

18 6 0 2.444374 -2.467086 -0.004871

19 6 0 1.108312 -2.896652 -0.004193

20 6 0 0.679061 -4.284483 -0.036570

21 6 0 -0.679061 -4.284483 -0.036570

22 6 0 -1.108312 -2.896652 -0.004193

23 7 0 -0.000000 -2.087056 0.018372

24 1 0 1.336822 5.141091 -0.060737

25 1 0 -1.336822 5.141091 -0.060737

26 1 0 -5.129902 -1.346208 -0.063427

27 1 0 -5.129902 1.346208 -0.063427

28 1 0 5.129902 1.346208 -0.063427

29 1 0 5.129902 -1.346208 -0.063427

30 1 0 1.336822 -5.141091 -0.060737

31 1 0 -1.336822 -5.141091 -0.060737

32 30 0 0.000000 0.000000 0.144374

33 6 0 -2.444374 -2.467086 -0.004871

34 6 0 -3.450769 -3.474521 -0.032625

35 6 0 3.450769 3.474521 -0.032625

36 6 0 -4.319078 -4.314467 -0.058971

37 6 0 4.319078 4.314467 -0.058971

38 6 0 -3.450769 3.474521 -0.032625

39 6 0 -4.319078 4.314467 -0.058971

40 6 0 3.450769 -3.474521 -0.032625

41 6 0 4.319078 -4.314467 -0.058971

42 1 0 5.081261 -5.060529 -0.082431

43 1 0 -5.081261 -5.060529 -0.082431

44 1 0 -5.081261 5.060529 -0.082431

45 1 0 5.081261 5.060529 -0.082431

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

Rotational constants (GHZ): 0.1461552 0.1455792 0.0729704

Leave Link 202 at Tue Jul 30 23:34:10 2019, MaxMem= 4294967296 cpu: 0.2

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

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

Pseudo-potential data read from rwf file.

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

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

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

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

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

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

111 alpha electrons 110 beta electrons

nuclear repulsion energy 3054.2361408698 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= 13 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= -0.1304119444 Hartrees.

Nuclear repulsion after empirical dispersion term = 3054.1057289254 Hartrees.

No density basis found on file 724.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

2nd derivatives : Analytical E(r).r(xy)/FMM algorithm (CHGder, D2EAlg=3).

Cavity 2nd derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3890

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.37D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 140

GePol: Fraction of low-weight points (<1% of avg) = 3.60%

GePol: Cavity surface area = 416.473 Ang\*\*2

GePol: Cavity volume = 420.786 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0083749908 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3054.1141039162 Hartrees.

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16185 LenP2D= 44720.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.45D-05 NBF= 172 148 158 158

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

Precomputing XC quadrature grid using

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

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

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

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Jul 30 23:34:11 2019, MaxMem= 4294967296 cpu: 1.3

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

Lowest energy guess from the checkpoint file: "ZnTSPsimanion.chk"

B after Tr= 0.000000 -0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 -0.000000 0.000000

Rot= 1.000000 -0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 2.48D-01

Max alpha theta= 1.307 degrees.

Max beta theta= 1.293 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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

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Beta Orbitals:

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

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

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

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The electronic state of the initial guess is 2-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7630 S= 0.5065

Leave Link 401 at Tue Jul 30 23:34:13 2019, MaxMem= 4294967296 cpu: 34.0

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1387497 IEndB= 1387497 NGot= 4294967296 MDV= 4294047352

LenX= 4294047352 LenY= 4293596440

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

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

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 650000000 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= 45396300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.77D-15 for 3887.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.69D-15 for 1823 1697.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.33D-15 for 3887.

Iteration 1 A^-1\*A deviation from orthogonality is 3.42D-14 for 2282 2264.

E= -1359.17444819070

DIIS: error= 2.86D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.17444819070 IErMin= 1 ErrMin= 2.86D-03

ErrMax= 2.86D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.93D-02 BMatP= 1.93D-02

IDIUse=3 WtCom= 9.71D-01 WtEn= 2.86D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 12.462 Goal= None Shift= 0.000

Gap= 12.341 Goal= None Shift= 0.000

GapD= 12.341 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=2.94D-04 MaxDP=1.31D-02 OVMax= 1.82D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.94D-04 CP: 1.00D+00

E= -1359.18182072892 Delta-E= -0.007372538223 Rises=F Damp=F

DIIS: error= 5.03D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.18182072892 IErMin= 2 ErrMin= 5.03D-04

ErrMax= 5.03D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.44D-04 BMatP= 1.93D-02

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.03D-03

Coeff-Com: -0.444D-01 0.104D+01

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

Coeff: -0.442D-01 0.104D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=3.18D-05 MaxDP=7.78D-04 DE=-7.37D-03 OVMax= 2.33D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.87D-05 CP: 1.00D+00 1.05D+00

E= -1359.18192085561 Delta-E= -0.000100126686 Rises=F Damp=F

DIIS: error= 6.63D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.18192085561 IErMin= 2 ErrMin= 5.03D-04

ErrMax= 6.63D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.49D-05 BMatP= 2.44D-04

IDIUse=3 WtCom= 9.93D-01 WtEn= 6.63D-03

Coeff-Com: -0.224D-01 0.386D+00 0.637D+00

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

Coeff: -0.222D-01 0.383D+00 0.639D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.01D-05 MaxDP=2.91D-04 DE=-1.00D-04 OVMax= 6.68D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 8.37D-06 CP: 1.00D+00 1.05D+00 8.05D-01

E= -1359.18192983972 Delta-E= -0.000008984113 Rises=F Damp=F

DIIS: error= 3.12D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.18192983972 IErMin= 4 ErrMin= 3.12D-04

ErrMax= 3.12D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.92D-05 BMatP= 8.49D-05

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.12D-03

Coeff-Com: -0.617D-02 0.811D-01 0.334D+00 0.591D+00

Coeff-En: 0.000D+00 0.000D+00 0.945D-01 0.905D+00

Coeff: -0.615D-02 0.808D-01 0.334D+00 0.592D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=3.76D-06 MaxDP=1.55D-04 DE=-8.98D-06 OVMax= 4.04D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.46D-06 CP: 1.00D+00 1.05D+00 8.15D-01 8.34D-01

E= -1359.18193213857 Delta-E= -0.000002298844 Rises=F Damp=F

DIIS: error= 3.41D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.18193213857 IErMin= 5 ErrMin= 3.41D-05

ErrMax= 3.41D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.55D-06 BMatP= 1.92D-05

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

Coeff-Com: -0.102D-02 0.132D-02 0.101D+00 0.284D+00 0.616D+00

Coeff: -0.102D-02 0.132D-02 0.101D+00 0.284D+00 0.616D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.34D-06 MaxDP=8.25D-05 DE=-2.30D-06 OVMax= 2.53D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.44D-07 CP: 1.00D+00 1.05D+00 8.30D-01 8.82D-01 7.92D-01

E= -1359.18193238839 Delta-E= -0.000000249822 Rises=F Damp=F

DIIS: error= 2.71D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.18193238839 IErMin= 6 ErrMin= 2.71D-05

ErrMax= 2.71D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.88D-07 BMatP= 1.55D-06

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

Coeff-Com: 0.503D-03-0.157D-01 0.501D-02 0.839D-01 0.420D+00 0.506D+00

Coeff: 0.503D-03-0.157D-01 0.501D-02 0.839D-01 0.420D+00 0.506D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=5.43D-07 MaxDP=3.15D-05 DE=-2.50D-07 OVMax= 1.02D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.35D-07 CP: 1.00D+00 1.05D+00 8.37D-01 8.80D-01 8.16D-01

CP: 5.36D-01

E= -1359.18193250937 Delta-E= -0.000000120978 Rises=F Damp=F

DIIS: error= 2.21D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.18193250937 IErMin= 7 ErrMin= 2.21D-06

ErrMax= 2.21D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.21D-09 BMatP= 5.88D-07

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

Coeff-Com: 0.217D-03-0.591D-02-0.385D-03 0.246D-01 0.142D+00 0.195D+00

Coeff-Com: 0.644D+00

Coeff: 0.217D-03-0.591D-02-0.385D-03 0.246D-01 0.142D+00 0.195D+00

Coeff: 0.644D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=7.00D-08 MaxDP=4.29D-06 DE=-1.21D-07 OVMax= 1.16D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.67D-08 CP: 1.00D+00 1.05D+00 8.38D-01 8.81D-01 8.18D-01

CP: 5.47D-01 9.65D-01

E= -1359.18193251025 Delta-E= -0.000000000888 Rises=F Damp=F

DIIS: error= 1.71D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.18193251025 IErMin= 8 ErrMin= 1.71D-06

ErrMax= 1.71D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.31D-09 BMatP= 6.21D-09

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

Coeff-Com: 0.307D-04-0.362D-03-0.124D-02-0.239D-02-0.322D-03 0.167D-01

Coeff-Com: 0.431D+00 0.556D+00

Coeff: 0.307D-04-0.362D-03-0.124D-02-0.239D-02-0.322D-03 0.167D-01

Coeff: 0.431D+00 0.556D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=3.86D-08 MaxDP=1.96D-06 DE=-8.88D-10 OVMax= 6.44D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.06D-08 CP: 1.00D+00 1.05D+00 8.38D-01 8.81D-01 8.18D-01

CP: 5.55D-01 1.01D+00 7.23D-01

E= -1359.18193251104 Delta-E= -0.000000000790 Rises=F Damp=F

DIIS: error= 4.64D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1359.18193251104 IErMin= 9 ErrMin= 4.64D-07

ErrMax= 4.64D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.83D-10 BMatP= 3.31D-09

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

Coeff-Com: -0.171D-04 0.723D-03-0.586D-03-0.504D-02-0.226D-01-0.224D-01

Coeff-Com: 0.121D+00 0.289D+00 0.640D+00

Coeff: -0.171D-04 0.723D-03-0.586D-03-0.504D-02-0.226D-01-0.224D-01

Coeff: 0.121D+00 0.289D+00 0.640D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.68D-08 MaxDP=7.10D-07 DE=-7.90D-10 OVMax= 2.43D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.33D-08 CP: 1.00D+00 1.05D+00 8.38D-01 8.81D-01 8.18D-01

CP: 5.55D-01 1.04D+00 7.85D-01 8.02D-01

E= -1359.18193251115 Delta-E= -0.000000000101 Rises=F Damp=F

DIIS: error= 1.61D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1359.18193251115 IErMin=10 ErrMin= 1.61D-07

ErrMax= 1.61D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.74D-11 BMatP= 2.83D-10

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

Coeff-Com: -0.124D-04 0.403D-03-0.132D-03-0.218D-02-0.112D-01-0.135D-01

Coeff-Com: 0.415D-02 0.697D-01 0.315D+00 0.638D+00

Coeff: -0.124D-04 0.403D-03-0.132D-03-0.218D-02-0.112D-01-0.135D-01

Coeff: 0.415D-02 0.697D-01 0.315D+00 0.638D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=6.26D-09 MaxDP=2.63D-07 DE=-1.01D-10 OVMax= 8.98D-07

Error on total polarization charges = 0.06716

SCF Done: E(UB3LYP) = -1359.18193251 A.U. after 10 cycles

NFock= 10 Conv=0.63D-08 -V/T= 1.9682

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7630 S= 0.5065

<L.S>= 0.000000000000E+00

KE= 1.403890364666D+03 PE=-9.377861211997D+03 EE= 3.560674810904D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.26

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7630, after 0.7501

Leave Link 502 at Tue Jul 30 23:35:15 2019, MaxMem= 4294967296 cpu: 959.2

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 636

NBasis= 636 NAE= 111 NBE= 110 NFC= 0 NFV= 0

NROrb= 636 NOA= 111 NOB= 110 NVA= 525 NVB= 526

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.13680966D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.38363027D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.13667421D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.88705781D-01

Leave Link 801 at Tue Jul 30 23:35:16 2019, MaxMem= 4294967296 cpu: 0.7

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 45.

Will process 46 centers per pass.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16185 LenP2D= 44720.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 11 by ecpmxn.

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

Leave Link 1101 at Tue Jul 30 23:35:19 2019, MaxMem= 4294967296 cpu: 44.8

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Tue Jul 30 23:35:19 2019, MaxMem= 4294967296 cpu: 1.1

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 45.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966832.

G2DrvN: will do 46 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

G2PCM: DoFxE=T DoFxN=T DoGrad=T DoDP/DQ/DG/TGxP=FFFF NFrqRd= 0 IEInf=0 SqF1=F DoCFld=F IF1Alg=4.

GePol: Maximum number of non-zero 1st derivatives = 257

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Tue Jul 30 23:37:16 2019, MaxMem= 4294967296 cpu: 1880.6

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=111111111111111111111111111111111111111111111

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Using symmetry in CPHF.

Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.

Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.

NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 4294965570 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 0.

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

IRaf= 650000000 NMat= 42 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

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

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

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

NMat0= 42 NMatS0= 42 NMatT0= 0 NMatD0= 42 NMtDS0= 0 NMtDT0= 0

Integrals replicated using symmetry in FoFCou.

There are 42 degrees of freedom in the 1st order CPHF. IDoFFX=4 NUNeed= 42.

42 vectors produced by pass 0 Test12= 2.77D-13 2.38D-09 XBig12= 8.01D+03 5.90D+01.

AX will form 42 AO Fock derivatives at one time.

42 vectors produced by pass 1 Test12= 2.77D-13 2.38D-09 XBig12= 1.07D+03 6.81D+00.

42 vectors produced by pass 2 Test12= 2.77D-13 2.38D-09 XBig12= 2.78D+02 5.62D+00.

42 vectors produced by pass 3 Test12= 2.77D-13 2.38D-09 XBig12= 6.50D+01 1.71D+00.

42 vectors produced by pass 4 Test12= 2.77D-13 2.38D-09 XBig12= 4.49D+00 4.30D-01.

42 vectors produced by pass 5 Test12= 2.77D-13 2.38D-09 XBig12= 1.44D-01 4.14D-02.

42 vectors produced by pass 6 Test12= 2.77D-13 2.38D-09 XBig12= 4.88D-03 6.22D-03.

42 vectors produced by pass 7 Test12= 2.77D-13 2.38D-09 XBig12= 1.23D-04 1.00D-03.

38 vectors produced by pass 8 Test12= 2.77D-13 2.38D-09 XBig12= 2.15D-06 1.21D-04.

21 vectors produced by pass 9 Test12= 2.77D-13 2.38D-09 XBig12= 3.03D-08 1.55D-05.

4 vectors produced by pass 10 Test12= 2.77D-13 2.38D-09 XBig12= 3.64D-10 1.50D-06.

2 vectors produced by pass 11 Test12= 2.77D-13 2.38D-09 XBig12= 4.82D-12 1.65D-07.

2 vectors produced by pass 12 Test12= 2.77D-13 2.38D-09 XBig12= 6.88D-14 2.18D-08.

InvSVY: IOpt=1 It= 1 EMax= 1.14D-13

Solved reduced A of dimension 403 with 42 vectors.

FullF1: Do perturbations 1 to 42.

Isotropic polarizability for W= 0.000000 1003.31 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Wed Jul 31 00:10:45 2019, MaxMem= 4294967296 cpu: 32145.3

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16185 LenP2D= 44720.

LDataN: DoStor=T MaxTD1= 7 Len= 274

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 257

Leave Link 701 at Wed Jul 31 00:11:20 2019, MaxMem= 4294967296 cpu: 561.3

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

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

Leave Link 702 at Wed Jul 31 00:11:20 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

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

wScrn= 0.000000 ICntrl= 100127 IOpCl= 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 Wed Jul 31 00:13:11 2019, MaxMem= 4294967296 cpu: 1764.0

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

Dipole = 5.78148640D-13 3.01189629D-13 2.26870479D-01

Polarizability= 1.64746082D+03 2.05980942D-05 1.17507727D+03

-9.28085889D-06 3.45679015D-06 1.87395073D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000019976 0.000283225 -0.000024734

2 6 -0.000042669 0.000061413 0.000384354

3 7 -0.000659949 0.000000000 -0.000346950

4 6 -0.000042669 -0.000061413 0.000384354

5 6 -0.000019976 -0.000283225 -0.000024734

6 6 -0.000112283 -0.000023677 -0.000251556

7 6 0.000187537 0.000005821 0.000400369

8 7 0.000000000 -0.000681786 -0.000424457

9 6 -0.000187537 0.000005821 0.000400369

10 6 0.000202464 -0.000038246 -0.000054832

11 6 -0.000202464 -0.000038246 -0.000054832

12 6 -0.000112283 0.000023677 -0.000251556

13 6 0.000187537 -0.000005821 0.000400369

14 6 -0.000202464 0.000038246 -0.000054832

15 6 0.000202464 0.000038246 -0.000054832

16 6 -0.000187537 -0.000005821 0.000400369

17 7 -0.000000000 0.000681786 -0.000424457

18 6 0.000112283 0.000023677 -0.000251556

19 6 0.000042669 0.000061413 0.000384354

20 6 0.000019976 0.000283225 -0.000024734

21 6 0.000019976 -0.000283225 -0.000024734

22 6 0.000042669 -0.000061413 0.000384354

23 7 0.000659949 0.000000000 -0.000346950

24 1 0.000009450 0.000014151 0.000006886

25 1 0.000009450 -0.000014151 0.000006886

26 1 0.000007072 0.000004660 0.000002397

27 1 -0.000007072 0.000004660 0.000002397

28 1 -0.000007072 -0.000004660 0.000002397

29 1 0.000007072 -0.000004660 0.000002397

30 1 -0.000009450 0.000014151 0.000006886

31 1 -0.000009450 -0.000014151 0.000006886

32 30 -0.000000000 0.000000000 -0.000626501

33 6 0.000112283 -0.000023677 -0.000251556

34 6 0.000007291 0.000022456 0.000072281

35 6 -0.000007291 -0.000022456 0.000072281

36 6 0.000028487 0.000003676 0.000006541

37 6 -0.000028487 -0.000003676 0.000006541

38 6 -0.000007291 0.000022456 0.000072281

39 6 -0.000028487 0.000003676 0.000006541

40 6 0.000007291 -0.000022456 0.000072281

41 6 0.000028487 -0.000003676 0.000006541

42 1 -0.000008457 0.000005020 0.000000623

43 1 -0.000008457 -0.000005020 0.000000623

44 1 0.000008457 -0.000005020 0.000000623

45 1 0.000008457 0.000005020 0.000000623

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

Cartesian Forces: Max 0.000681786 RMS 0.000193042

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

Leave Link 716 at Wed Jul 31 00:13:11 2019, MaxMem= 4294967296 cpu: 0.8

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000539224 RMS 0.000112623

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 = .11262D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Second derivative matrix not updated -- analytic derivatives used.

ITU= 0 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quintic linear search produced a step of -0.75032.

Iteration 1 RMS(Cart)= 0.03103858 RMS(Int)= 0.00084926

Iteration 2 RMS(Cart)= 0.00179326 RMS(Int)= 0.00029507

Iteration 3 RMS(Cart)= 0.00000087 RMS(Int)= 0.00029507

ITry= 1 IFail=0 DXMaxC= 3.34D-01 DCOld= 1.00D+10 DXMaxT= 1.50D-01 DXLimC= 3.00D+00 Rises=T

ClnCor: largest displacement from symmetrization is 1.46D-03 for atom 37.

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

(Linear) (Quad) (Total)

R1 2.74588 0.00003 0.00083 0.00000 0.00092 2.74681

R2 2.56648 0.00035 -0.00188 0.00000 -0.00120 2.56528

R3 2.04144 0.00000 0.00006 0.00000 0.00006 2.04150

R4 2.59403 0.00006 -0.00180 0.00000 -0.00188 2.59215

R5 2.65208 0.00014 0.00119 0.00000 0.00161 2.65369

R6 2.59403 0.00006 -0.00180 0.00000 -0.00188 2.59215

R7 3.95114 0.00054 0.00449 0.00000 0.00419 3.95533

R8 2.74588 0.00003 0.00083 0.00000 0.00092 2.74681

R9 2.65208 0.00014 0.00119 0.00000 0.00161 2.65369

R10 2.04144 0.00000 0.00006 0.00000 0.00006 2.04150

R11 2.71642 0.00027 0.00039 0.00000 0.00113 2.71755

R12 2.69147 0.00000 0.00041 0.00000 0.00035 2.69182

R13 2.59323 -0.00002 -0.00048 0.00000 -0.00081 2.59242

R14 2.69556 0.00004 0.00126 0.00000 0.00123 2.69679

R15 2.59323 -0.00002 -0.00048 0.00000 -0.00081 2.59242

R16 3.96386 0.00052 0.00311 0.00000 0.00279 3.96665

R17 2.69556 0.00004 0.00126 0.00000 0.00123 2.69679

R18 2.71642 0.00027 0.00039 0.00000 0.00113 2.71755

R19 2.61386 0.00023 -0.00193 0.00000 -0.00123 2.61263

R20 2.04170 0.00000 0.00006 0.00000 0.00006 2.04175

R21 2.04170 0.00000 0.00006 0.00000 0.00006 2.04175

R22 2.71642 0.00027 0.00039 0.00000 0.00113 2.71755

R23 2.69147 0.00000 0.00041 0.00000 0.00035 2.69182

R24 2.69556 0.00004 0.00126 0.00000 0.00123 2.69679

R25 2.59323 -0.00002 -0.00048 0.00000 -0.00081 2.59242

R26 2.61386 0.00023 -0.00193 0.00000 -0.00123 2.61263

R27 2.04170 0.00000 0.00006 0.00000 0.00006 2.04175

R28 2.69556 0.00004 0.00126 0.00000 0.00123 2.69679

R29 2.04170 0.00000 0.00006 0.00000 0.00006 2.04175

R30 2.59323 -0.00002 -0.00048 0.00000 -0.00081 2.59242

R31 2.71642 0.00027 0.00039 0.00000 0.00113 2.71755

R32 3.96386 0.00052 0.00311 0.00000 0.00279 3.96665

R33 2.65208 0.00013 0.00119 0.00000 0.00161 2.65369

R34 2.69147 0.00000 0.00041 0.00000 0.00035 2.69182

R35 2.74588 0.00002 0.00083 0.00000 0.00092 2.74681

R36 2.59403 0.00006 -0.00180 0.00000 -0.00188 2.59215

R37 2.56648 0.00035 -0.00188 0.00000 -0.00120 2.56528

R38 2.04144 0.00000 0.00006 0.00000 0.00006 2.04150

R39 2.74588 0.00002 0.00083 0.00000 0.00092 2.74681

R40 2.04144 0.00000 0.00006 0.00000 0.00006 2.04150

R41 2.59403 0.00006 -0.00180 0.00000 -0.00188 2.59215

R42 2.65208 0.00014 0.00119 0.00000 0.00161 2.65369

R43 3.95114 0.00054 0.00449 0.00000 0.00419 3.95533

R44 2.69147 0.00000 0.00041 0.00000 0.00035 2.69182

R45 2.28349 0.00001 0.00001 0.00000 0.00001 2.28351

R46 2.28349 0.00001 0.00001 0.00000 0.00001 2.28351

R47 2.01598 -0.00000 0.00026 0.00000 0.00021 2.01619

R48 2.01598 -0.00000 0.00026 0.00000 0.00021 2.01619

R49 2.28349 0.00001 0.00001 0.00000 0.00001 2.28351

R50 2.01598 -0.00000 0.00026 0.00000 0.00021 2.01619

R51 2.28349 0.00001 0.00001 0.00000 0.00001 2.28351

R52 2.01598 -0.00000 0.00026 0.00000 0.00021 2.01619

A1 1.87068 -0.00001 0.00051 0.00000 0.00056 1.87125

A2 2.18705 -0.00001 0.00045 0.00000 0.00042 2.18747

A3 2.22544 0.00002 -0.00095 0.00000 -0.00098 2.22447

A4 1.90198 -0.00007 -0.00189 0.00000 -0.00231 1.89967

A5 2.18165 0.00004 0.00218 0.00000 0.00255 2.18420

A6 2.19954 0.00002 -0.00029 0.00000 -0.00022 2.19931

A7 1.87945 0.00015 0.00275 0.00000 0.00350 1.88294

A8 2.20149 -0.00008 -0.00111 0.00000 -0.00137 2.20012

A9 2.20149 -0.00008 -0.00111 0.00000 -0.00137 2.20012

A10 1.90198 -0.00007 -0.00189 0.00000 -0.00231 1.89967

A11 2.19954 0.00003 -0.00029 0.00000 -0.00022 2.19931

A12 2.18165 0.00004 0.00218 0.00000 0.00255 2.18420

A13 1.87068 -0.00001 0.00051 0.00000 0.00056 1.87125

A14 2.22544 0.00002 -0.00095 0.00000 -0.00098 2.22447

A15 2.18705 -0.00001 0.00045 0.00000 0.00042 2.18747

A16 2.20907 0.00008 0.00288 0.00000 0.00339 2.21245

A17 2.04451 -0.00009 -0.00052 0.00000 -0.00093 2.04358

A18 2.02949 0.00001 -0.00229 0.00000 -0.00235 2.02715

A19 2.18096 0.00002 0.00016 0.00000 0.00017 2.18113

A20 2.19243 0.00002 0.00247 0.00000 0.00271 2.19514

A21 1.90973 -0.00004 -0.00259 0.00000 -0.00282 1.90691

A22 1.87432 0.00012 0.00316 0.00000 0.00374 1.87806

A23 2.20423 -0.00006 -0.00151 0.00000 -0.00169 2.20254

A24 2.20423 -0.00006 -0.00151 0.00000 -0.00169 2.20254

A25 1.90973 -0.00004 -0.00259 0.00000 -0.00282 1.90691

A26 2.18096 0.00002 0.00016 0.00000 0.00017 2.18113

A27 2.19243 0.00002 0.00247 0.00000 0.00271 2.19514

A28 1.86548 -0.00002 0.00102 0.00000 0.00096 1.86644

A29 2.19601 0.00000 -0.00001 0.00000 0.00007 2.19608

A30 2.22167 0.00002 -0.00099 0.00000 -0.00101 2.22066

A31 1.86548 -0.00002 0.00102 0.00000 0.00096 1.86644

A32 2.19601 0.00000 -0.00001 0.00000 0.00007 2.19608

A33 2.22167 0.00002 -0.00099 0.00000 -0.00101 2.22066

A34 2.20907 0.00008 0.00288 0.00000 0.00339 2.21245

A35 2.04451 -0.00009 -0.00052 0.00000 -0.00093 2.04358

A36 2.02949 0.00001 -0.00229 0.00000 -0.00235 2.02715

A37 2.19243 0.00001 0.00247 0.00000 0.00271 2.19514

A38 2.18096 0.00002 0.00016 0.00000 0.00017 2.18113

A39 1.90973 -0.00004 -0.00259 0.00000 -0.00282 1.90691

A40 1.86548 -0.00002 0.00102 0.00000 0.00096 1.86644

A41 2.19601 0.00000 -0.00001 0.00000 0.00007 2.19608

A42 2.22167 0.00002 -0.00099 0.00000 -0.00101 2.22066

A43 1.86548 -0.00002 0.00102 0.00000 0.00096 1.86644

A44 2.22167 0.00002 -0.00099 0.00000 -0.00101 2.22066

A45 2.19601 0.00000 -0.00001 0.00000 0.00007 2.19608

A46 1.90973 -0.00004 -0.00259 0.00000 -0.00282 1.90691

A47 2.19243 0.00002 0.00247 0.00000 0.00271 2.19514

A48 2.18096 0.00002 0.00016 0.00000 0.00017 2.18113

A49 1.87432 0.00012 0.00316 0.00000 0.00374 1.87806

A50 2.20423 -0.00006 -0.00151 0.00000 -0.00169 2.20254

A51 2.20423 -0.00006 -0.00151 0.00000 -0.00169 2.20254

A52 2.20907 0.00008 0.00288 0.00000 0.00339 2.21245

A53 2.02949 0.00001 -0.00229 0.00000 -0.00235 2.02715

A54 2.04451 -0.00009 -0.00052 0.00000 -0.00093 2.04358

A55 2.18165 0.00004 0.00218 0.00000 0.00255 2.18420

A56 2.19954 0.00003 -0.00029 0.00000 -0.00022 2.19931

A57 1.90198 -0.00007 -0.00189 0.00000 -0.00231 1.89967

A58 1.87068 -0.00001 0.00051 0.00000 0.00056 1.87125

A59 2.18705 -0.00001 0.00045 0.00000 0.00042 2.18747

A60 2.22544 0.00002 -0.00095 0.00000 -0.00098 2.22447

A61 1.87068 -0.00001 0.00051 0.00000 0.00056 1.87125

A62 2.22544 0.00002 -0.00095 0.00000 -0.00098 2.22447

A63 2.18705 -0.00001 0.00045 0.00000 0.00042 2.18747

A64 1.90198 -0.00007 -0.00189 0.00000 -0.00231 1.89967

A65 2.18165 0.00004 0.00218 0.00000 0.00255 2.18420

A66 2.19954 0.00003 -0.00029 0.00000 -0.00022 2.19931

A67 1.87945 0.00015 0.00275 0.00000 0.00350 1.88294

A68 2.20149 -0.00008 -0.00111 0.00000 -0.00137 2.20012

A69 2.20149 -0.00008 -0.00111 0.00000 -0.00137 2.20012

A70 1.56742 0.00002 0.00216 0.00000 0.00338 1.57080

A71 1.56742 0.00002 0.00216 0.00000 0.00338 1.57080

A72 1.56742 0.00002 0.00216 0.00000 0.00338 1.57080

A73 1.56742 0.00001 0.00216 0.00000 0.00338 1.57080

A74 2.20907 0.00008 0.00288 0.00000 0.00339 2.21245

A75 2.02949 0.00001 -0.00229 0.00000 -0.00235 2.02715

A76 2.04451 -0.00009 -0.00052 0.00000 -0.00093 2.04358

A77 3.13484 0.00003 0.00431 0.00000 0.00676 3.14160

A78 3.13484 0.00003 0.00431 0.00000 0.00676 3.14160

A79 3.12445 0.00001 -0.00038 0.00000 -0.00041 3.12404

A80 3.15868 -0.00001 0.00043 0.00000 0.00047 3.15915

A81 3.14750 -0.00002 0.00220 0.00000 0.00170 3.14920

A82 3.14750 -0.00002 0.00220 0.00000 0.00170 3.14920

A83 3.15868 -0.00001 0.00043 0.00000 0.00047 3.15915

A84 3.14750 -0.00002 0.00220 0.00000 0.00170 3.14920

A85 3.12445 0.00001 -0.00038 0.00000 -0.00041 3.12404

A86 3.14750 -0.00002 0.00220 0.00000 0.00170 3.14920

A87 3.26200 -0.00034 -0.11950 0.00000 -0.11951 3.14250

A88 3.02967 0.00029 0.12291 0.00000 0.12290 3.15256

A89 3.13950 0.00002 0.00180 0.00000 0.00180 3.14130

A90 3.14415 -0.00002 -0.00228 0.00000 -0.00228 3.14188

A91 3.14129 0.00000 0.00008 0.00000 0.00007 3.14136

A92 3.14129 0.00000 0.00008 0.00000 0.00007 3.14136

A93 3.13903 0.00002 0.00228 0.00000 0.00228 3.14131

A94 3.14190 -0.00000 -0.00008 0.00000 -0.00007 3.14183

A95 3.14369 -0.00002 -0.00180 0.00000 -0.00180 3.14189

A96 3.14190 -0.00000 -0.00008 0.00000 -0.00007 3.14183

D1 -0.00283 0.00007 0.00407 0.00000 0.00408 0.00124

D2 3.13229 0.00007 0.01312 0.00000 0.01313 -3.13776

D3 -3.13968 0.00002 -0.00145 0.00000 -0.00144 -3.14113

D4 -0.00456 0.00002 0.00761 0.00000 0.00761 0.00305

D5 -0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13671 -0.00005 -0.00567 0.00000 -0.00568 3.14079

D7 3.13671 0.00005 0.00567 0.00000 0.00568 -3.14079

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00459 -0.00011 -0.00660 0.00000 -0.00660 -0.00202

D10 -3.09684 0.00001 -0.04501 0.00000 -0.04501 3.14133

D11 -3.13045 -0.00011 -0.01576 0.00000 -0.01577 3.13696

D12 0.05131 0.00001 -0.05417 0.00000 -0.05418 -0.00288

D13 -3.11899 -0.00013 -0.02584 0.00000 -0.02585 3.13835

D14 0.00589 0.00005 -0.00972 0.00000 -0.00973 -0.00384

D15 0.01504 -0.00013 -0.01525 0.00000 -0.01526 -0.00022

D16 3.13992 0.00004 0.00087 0.00000 0.00087 3.14078

D17 -0.00459 0.00011 0.00660 0.00000 0.00660 0.00202

D18 3.13045 0.00011 0.01576 0.00000 0.01577 -3.13696

D19 3.09684 -0.00001 0.04501 0.00000 0.04501 -3.14133

D20 -0.05131 -0.00001 0.05417 0.00000 0.05418 0.00288

D21 -3.10932 -0.00021 -0.03881 0.00000 -0.03879 3.13508

D22 -0.07966 0.00008 0.08410 0.00000 0.08411 0.00445

D23 0.07966 -0.00008 -0.08410 0.00000 -0.08411 -0.00445

D24 3.10932 0.00021 0.03881 0.00000 0.03879 -3.13508

D25 0.00283 -0.00007 -0.00407 0.00000 -0.00408 -0.00124

D26 3.13968 -0.00002 0.00145 0.00000 0.00144 3.14113

D27 -3.13229 -0.00007 -0.01312 0.00000 -0.01313 3.13776

D28 0.00456 -0.00002 -0.00761 0.00000 -0.00761 -0.00305

D29 -0.01504 0.00013 0.01525 0.00000 0.01526 0.00022

D30 -3.13992 -0.00004 -0.00087 0.00000 -0.00087 -3.14078

D31 3.11899 0.00013 0.02584 0.00000 0.02585 -3.13835

D32 -0.00589 -0.00005 0.00972 0.00000 0.00973 0.00384

D33 0.01759 -0.00011 -0.01725 0.00000 -0.01725 0.00034

D34 -3.11123 -0.00012 -0.02723 0.00000 -0.02723 -3.13846

D35 -3.14059 0.00006 -0.00125 0.00000 -0.00125 3.14135

D36 0.01378 0.00006 -0.01123 0.00000 -0.01123 0.00255

D37 -3.12436 -0.00016 -0.01198 0.00000 -0.01199 -3.13635

D38 0.04645 -0.00002 -0.05035 0.00000 -0.05035 -0.00390

D39 0.00623 -0.00015 -0.00338 0.00000 -0.00338 0.00284

D40 -3.10615 -0.00002 -0.04174 0.00000 -0.04174 3.13529

D41 3.12664 0.00010 0.01077 0.00000 0.01077 3.13741

D42 -0.00906 0.00003 0.00610 0.00000 0.00610 -0.00296

D43 -0.00385 0.00010 0.00209 0.00000 0.00210 -0.00176

D44 -3.13955 0.00003 -0.00257 0.00000 -0.00257 3.14106

D45 -0.00623 0.00015 0.00338 0.00000 0.00338 -0.00284

D46 3.12436 0.00016 0.01198 0.00000 0.01199 3.13635

D47 3.10615 0.00002 0.04174 0.00000 0.04174 -3.13529

D48 -0.04645 0.00002 0.05035 0.00000 0.05035 0.00390

D49 -0.07750 0.00009 0.08244 0.00000 0.08245 0.00495

D50 -3.09868 -0.00025 -0.03707 0.00000 -0.03706 -3.13574

D51 3.09868 0.00025 0.03707 0.00000 0.03706 3.13574

D52 0.07750 -0.00009 -0.08244 0.00000 -0.08245 -0.00495

D53 0.00385 -0.00010 -0.00209 0.00000 -0.00210 0.00176

D54 3.13955 -0.00003 0.00257 0.00000 0.00257 -3.14106

D55 -3.12664 -0.00010 -0.01077 0.00000 -0.01077 -3.13741

D56 0.00906 -0.00003 -0.00610 0.00000 -0.00610 0.00296

D57 -0.01759 0.00011 0.01725 0.00000 0.01725 -0.00034

D58 3.14059 -0.00006 0.00125 0.00000 0.00125 -3.14135

D59 3.11123 0.00012 0.02723 0.00000 0.02723 3.13846

D60 -0.01378 -0.00006 0.01123 0.00000 0.01123 -0.00255

D61 -0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D62 3.13559 0.00007 0.00476 0.00000 0.00476 3.14035

D63 -3.13559 -0.00007 -0.00476 0.00000 -0.00476 -3.14035

D64 0.00000 -0.00000 -0.00000 0.00000 -0.00000 0.00000

D65 3.11123 0.00012 0.02723 0.00000 0.02723 3.13846

D66 -0.01759 0.00011 0.01725 0.00000 0.01725 -0.00034

D67 -0.01378 -0.00006 0.01123 0.00000 0.01123 -0.00255

D68 3.14059 -0.00006 0.00125 0.00000 0.00125 -3.14135

D69 -3.12664 -0.00010 -0.01077 0.00000 -0.01077 -3.13741

D70 0.00906 -0.00003 -0.00610 0.00000 -0.00610 0.00296

D71 0.00385 -0.00010 -0.00209 0.00000 -0.00210 0.00176

D72 3.13955 -0.00003 0.00257 0.00000 0.00257 -3.14106

D73 3.12436 0.00016 0.01198 0.00000 0.01199 3.13635

D74 -0.04645 0.00002 0.05035 0.00000 0.05035 0.00390

D75 -0.00623 0.00015 0.00338 0.00000 0.00338 -0.00284

D76 3.10615 0.00002 0.04174 0.00000 0.04174 -3.13529

D77 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D78 3.13559 0.00007 0.00476 0.00000 0.00476 3.14035

D79 -3.13559 -0.00007 -0.00476 0.00000 -0.00476 -3.14035

D80 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D81 -0.00385 0.00010 0.00209 0.00000 0.00210 -0.00176

D82 3.12664 0.00010 0.01077 0.00000 0.01077 3.13741

D83 -3.13955 0.00003 -0.00257 0.00000 -0.00257 3.14106

D84 -0.00906 0.00003 0.00610 0.00000 0.00610 -0.00296

D85 0.00623 -0.00015 -0.00338 0.00000 -0.00338 0.00284

D86 -3.10615 -0.00002 -0.04174 0.00000 -0.04174 3.13529

D87 -3.12436 -0.00016 -0.01198 0.00000 -0.01199 -3.13635

D88 0.04645 -0.00002 -0.05035 0.00000 -0.05035 -0.00390

D89 -3.11123 -0.00012 -0.02723 0.00000 -0.02723 -3.13846

D90 0.01378 0.00006 -0.01123 0.00000 -0.01123 0.00255

D91 0.01759 -0.00011 -0.01725 0.00000 -0.01725 0.00034

D92 -3.14059 0.00006 -0.00125 0.00000 -0.00125 3.14135

D93 0.07750 -0.00009 -0.08244 0.00000 -0.08245 -0.00495

D94 3.09868 0.00025 0.03707 0.00000 0.03706 3.13574

D95 -3.09868 -0.00025 -0.03707 0.00000 -0.03706 -3.13574

D96 -0.07750 0.00009 0.08244 0.00000 0.08245 0.00495

D97 3.11899 0.00013 0.02584 0.00000 0.02585 -3.13835

D98 -0.01504 0.00013 0.01525 0.00000 0.01526 0.00022

D99 -0.00589 -0.00005 0.00972 0.00000 0.00973 0.00384

D100 -3.13992 -0.00004 -0.00087 0.00000 -0.00087 -3.14078

D101 -3.13229 -0.00007 -0.01312 0.00000 -0.01313 3.13776

D102 0.00456 -0.00002 -0.00761 0.00000 -0.00761 -0.00305

D103 0.00283 -0.00007 -0.00407 0.00000 -0.00408 -0.00124

D104 3.13968 -0.00002 0.00145 0.00000 0.00144 3.14113

D105 3.13045 0.00011 0.01576 0.00000 0.01577 -3.13696

D106 -0.05131 -0.00001 0.05417 0.00000 0.05418 0.00288

D107 -0.00459 0.00011 0.00660 0.00000 0.00660 0.00202

D108 3.09684 -0.00001 0.04501 0.00000 0.04501 -3.14133

D109 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D110 3.13671 0.00005 0.00567 0.00000 0.00568 -3.14079

D111 -3.13671 -0.00005 -0.00567 0.00000 -0.00568 3.14079

D112 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D113 -0.00283 0.00007 0.00407 0.00000 0.00408 0.00124

D114 3.13229 0.00007 0.01312 0.00000 0.01313 -3.13776

D115 -3.13968 0.00002 -0.00145 0.00000 -0.00144 -3.14113

D116 -0.00456 0.00002 0.00761 0.00000 0.00761 0.00305

D117 0.00459 -0.00011 -0.00660 0.00000 -0.00660 -0.00202

D118 -3.09684 0.00001 -0.04501 0.00000 -0.04501 3.14133

D119 -3.13045 -0.00011 -0.01576 0.00000 -0.01577 3.13696

D120 0.05131 0.00001 -0.05417 0.00000 -0.05418 -0.00288

D121 -3.11899 -0.00013 -0.02584 0.00000 -0.02585 3.13835

D122 0.00589 0.00005 -0.00972 0.00000 -0.00973 -0.00384

D123 0.01504 -0.00013 -0.01525 0.00000 -0.01526 -0.00022

D124 3.13992 0.00004 0.00087 0.00000 0.00087 3.14078

D125 3.10932 0.00021 0.03881 0.00000 0.03879 -3.13508

D126 0.07966 -0.00008 -0.08410 0.00000 -0.08411 -0.00445

D127 -0.07966 0.00008 0.08410 0.00000 0.08411 0.00445

D128 -3.10932 -0.00021 -0.03881 0.00000 -0.03879 3.13508

Item Value Threshold Converged?

Maximum Force 0.000539 0.000450 NO

RMS Force 0.000113 0.000300 YES

Maximum Displacement 0.334287 0.001800 NO

RMS Displacement 0.030897 0.001200 NO

Predicted change in Energy=-5.480583D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Wed Jul 31 00:13:11 2019, MaxMem= 4294967296 cpu: 0.9

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -4.288889 0.678744 -0.030053

2 6 0 -2.900457 1.108924 -0.028619

3 7 0 -2.093071 0.000000 -0.029399

4 6 0 -2.900457 -1.108924 -0.028619

5 6 0 -4.288889 -0.678744 -0.030053

6 6 0 -2.468128 -2.444984 -0.023776

7 6 0 -1.107063 -2.909204 -0.018476

8 7 0 -0.000000 -2.099031 -0.016941

9 6 0 1.107063 -2.909204 -0.018476

10 6 0 0.691273 -4.274367 -0.017231

11 6 0 -0.691273 -4.274367 -0.017231

12 6 0 -2.468128 2.444984 -0.023776

13 6 0 -1.107063 2.909204 -0.018476

14 6 0 -0.691273 4.274367 -0.017231

15 6 0 0.691273 4.274367 -0.017231

16 6 0 1.107063 2.909204 -0.018476

17 7 0 0.000000 2.099031 -0.016941

18 6 0 2.468128 2.444984 -0.023776

19 6 0 2.900457 1.108924 -0.028619

20 6 0 4.288889 0.678744 -0.030053

21 6 0 4.288889 -0.678744 -0.030053

22 6 0 2.900457 -1.108924 -0.028619

23 7 0 2.093071 -0.000000 -0.029399

24 1 0 -5.146504 1.335688 -0.030254

25 1 0 -5.146504 -1.335688 -0.030254

26 1 0 1.345031 -5.134582 -0.017519

27 1 0 -1.345031 -5.134582 -0.017519

28 1 0 -1.345031 5.134582 -0.017519

29 1 0 1.345031 5.134582 -0.017519

30 1 0 5.146504 1.335688 -0.030254

31 1 0 5.146504 -1.335688 -0.030254

32 30 0 0.000000 0.000000 -0.028453

33 6 0 2.468128 -2.444984 -0.023776

34 6 0 3.475017 -3.452571 -0.024854

35 6 0 -3.475017 3.452571 -0.024854

36 6 0 4.314036 -4.322184 -0.026066

37 6 0 -4.314036 4.322184 -0.026066

38 6 0 -3.475017 -3.452571 -0.024854

39 6 0 -4.314036 -4.322184 -0.026066

40 6 0 3.475017 3.452571 -0.024854

41 6 0 4.314036 4.322184 -0.026066

42 1 0 5.060654 5.084337 -0.027376

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45 1 0 -5.060654 5.084337 -0.027376

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.453547 0.000000

3 N 2.298328 1.371709 0.000000

4 C 2.263515 2.217848 1.371709 0.000000

5 C 1.357488 2.263515 2.298328 1.453547 0.000000

6 C 3.615644 3.580111 2.473589 1.404275 2.536693

7 C 4.795574 4.400196 3.071775 2.541137 3.885756

8 N 5.109870 4.324785 2.964293 3.064816 4.517959

9 C 6.479954 5.675004 4.324864 4.393327 5.838782

10 C 7.023922 6.471512 5.101267 4.787555 6.142530

11 C 6.121790 5.818973 4.498377 3.860136 5.086404

12 C 2.536693 1.404275 2.473589 3.580111 3.615644

13 C 3.885756 2.541137 3.071775 4.400196 4.795574

14 C 5.086404 3.860136 4.498377 5.818973 6.121790

15 C 6.142530 4.787555 5.101267 6.471512 7.023922

16 C 5.838782 4.393327 4.324864 5.675004 6.479954

17 N 4.517959 3.064816 2.964293 4.324785 5.109870

18 C 6.984047 5.532340 5.175182 6.438322 7.444124

19 C 7.202204 5.800914 5.115177 6.210431 7.408269

20 C 8.577777 7.202204 6.417951 7.408269 8.684529

21 C 8.684529 7.408269 6.417951 7.202204 8.577777

22 C 7.408269 6.210431 5.115177 5.800914 7.202204

23 N 6.417951 5.115177 4.186142 5.115177 6.417951

24 H 1.080314 2.257466 3.332794 3.319768 2.189393

25 H 2.189393 3.319768 3.332794 2.257466 1.080314

26 H 8.095429 7.550210 6.179371 5.850660 7.183015

27 H 6.516227 6.434349 5.188799 4.315715 5.340500

28 H 5.340500 4.315715 5.188799 6.434349 6.516227

29 H 7.183015 5.850660 6.179371 7.550210 8.095429

30 H 9.458235 8.050156 7.361760 8.410096 9.648035

31 H 9.648035 8.410096 7.361760 8.050156 9.458235

32 Zn 4.342265 3.105215 2.093071 3.105215 4.342265

33 C 7.444124 6.438322 5.175182 5.532340 6.984047

34 C 8.794659 7.839255 6.551631 6.792596 8.244536

35 C 2.890767 2.413051 3.718877 4.597540 4.210722

36 C 9.950860 9.030274 7.728668 7.897718 9.342643

37 C 3.643529 3.510449 4.859421 5.612054 5.000993

38 C 4.210722 4.597540 3.718877 2.413051 2.890767

39 C 5.000993 5.612054 4.859421 3.510449 3.643529

40 C 8.244536 6.792596 6.551631 7.839255 8.794659

41 C 9.342643 7.897718 7.728668 9.030274 9.950860

42 H 10.335531 8.898495 8.776461 10.086416 10.983035

43 H 10.983035 10.086416 8.776461 8.898495 10.335531

44 H 5.814528 6.559187 5.887023 4.524419 4.472682

45 H 4.472682 4.524419 5.887023 6.559187 5.814528

6 7 8 9 10

6 C 0.000000

7 C 1.438064 0.000000

8 N 2.492265 1.371850 0.000000

9 C 3.605207 2.214125 1.371850 0.000000

10 C 3.650822 2.257804 2.282530 1.427078 0.000000

11 C 2.550275 1.427078 2.282530 2.257804 1.382545

12 C 4.889967 5.524478 5.171051 6.438117 7.425061

13 C 5.524478 5.818409 5.129134 6.225450 7.405249

14 C 6.950319 7.195594 6.410777 7.405249 8.659808

15 C 7.425061 7.405249 6.410777 7.195594 8.548734

16 C 6.438117 6.225450 5.129134 5.818409 7.195594

17 N 5.171051 5.129134 4.198062 5.129134 6.410777

18 C 6.948266 6.438117 5.171051 5.524478 6.950319

19 C 6.438322 5.675004 4.324785 4.400196 5.818973

20 C 7.444124 6.479954 5.109870 4.795574 6.121790

21 C 6.984047 5.838782 4.517959 3.885756 5.086404

22 C 5.532340 4.393327 3.064816 2.541137 3.860136

23 N 5.175182 4.324864 2.964293 3.071775 4.498377

24 H 4.633273 5.859722 6.187405 7.558197 8.096451

25 H 2.899013 4.335110 5.202824 6.448503 6.535721

26 H 4.666280 3.311355 3.320193 2.238065 1.080450

27 H 2.914674 2.238065 3.320193 3.311355 2.210544

28 H 7.662324 8.047306 7.357599 8.409237 9.626778

29 H 8.484695 8.409237 7.357599 8.047306 9.431634

30 H 8.501538 7.558197 6.187405 5.859722 7.163935

31 H 7.695012 6.448503 5.202824 4.335110 5.337143

32 Zn 3.474136 3.112741 2.099062 3.112741 4.329919

33 C 4.936256 3.605207 2.492265 1.438064 2.550275

34 C 6.027952 4.614189 3.729326 2.429505 2.902522

35 C 5.982891 6.788184 6.549511 7.840133 8.778587

36 C 7.037161 5.602221 4.853184 3.504461 3.623090

37 C 7.014409 7.910608 7.735825 9.037773 9.947556

38 C 1.424450 2.429505 3.729326 4.614189 4.246572

39 C 2.632729 3.504461 4.853184 5.602221 5.005545

40 C 8.372701 7.840133 6.549511 6.788184 8.213091

41 C 9.580830 9.037773 7.735825 7.910608 9.328729

42 H 10.647688 10.096411 8.786985 8.917829 10.328453

43 H 7.978018 6.540032 5.875575 4.512446 4.443833

44 H 3.699648 4.512446 5.875575 6.540032 5.808685

45 H 7.963158 8.917829 8.786985 10.096411 10.984995

11 12 13 14 15

11 C 0.000000

12 C 6.950319 0.000000

13 C 7.195594 1.438064 0.000000

14 C 8.548734 2.550275 1.427078 0.000000

15 C 8.659808 3.650822 2.257804 1.382545 0.000000

16 C 7.405249 3.605207 2.214125 2.257804 1.427078

17 N 6.410777 2.492265 1.371850 2.282530 2.282530

18 C 7.425061 4.936256 3.605207 3.650822 2.550275

19 C 6.471512 5.532340 4.393327 4.787555 3.860136

20 C 7.023922 6.984047 5.838782 6.142530 5.086404

21 C 6.142530 7.444124 6.479954 7.023922 6.121790

22 C 4.787555 6.438322 5.675004 6.471512 5.818973

23 N 5.101267 5.175182 4.324864 5.101267 4.498377

24 H 7.163935 2.899013 4.335110 5.337143 6.535721

25 H 5.337143 4.633273 5.859722 7.163935 8.096451

26 H 2.210544 8.484695 8.409237 9.626778 9.431634

27 H 1.080450 7.662324 8.047306 9.431634 9.626778

28 H 9.431634 2.914674 2.238065 1.080450 2.210544

29 H 9.626778 4.666280 3.311355 2.210544 1.080450

30 H 8.096451 7.695012 6.448503 6.535721 5.337143

31 H 6.535721 8.501538 7.558197 8.096451 7.163935

32 Zn 4.329919 3.474136 3.112741 4.329919 4.329919

33 C 3.650822 6.948266 6.438117 7.425061 6.950319

34 C 4.246572 8.372701 7.840133 8.778587 8.213091

35 C 8.213091 1.424450 2.429505 2.902522 4.246572

36 C 5.005545 9.580830 9.037773 9.947556 9.328729

37 C 9.328729 2.632729 3.504461 3.623090 5.005545

38 C 2.902522 5.982891 6.788184 8.213091 8.778587

39 C 3.623090 7.014409 7.910608 9.328729 9.947556

40 C 8.778587 6.027952 4.614189 4.246572 2.902522

41 C 9.947556 7.037161 5.602221 5.005545 3.623090

42 H 10.984995 7.978018 6.540032 5.808685 4.443833

43 H 5.808685 10.647688 10.096411 10.984995 10.328453

44 H 4.443833 7.963158 8.917829 10.328453 10.984995

45 H 10.328453 3.699648 4.512446 4.443833 5.808685

16 17 18 19 20

16 C 0.000000

17 N 1.371850 0.000000

18 C 1.438064 2.492265 0.000000

19 C 2.541137 3.064816 1.404275 0.000000

20 C 3.885756 4.517959 2.536693 1.453547 0.000000

21 C 4.795574 5.109870 3.615644 2.263515 1.357488

22 C 4.400196 4.324785 3.580111 2.217848 2.263515

23 N 3.071775 2.964293 2.473589 1.371709 2.298328

24 H 6.448503 5.202824 7.695012 8.050156 9.458235

25 H 7.558197 6.187405 8.501538 8.410096 9.648035

26 H 8.047306 7.357599 7.662324 6.434349 6.516227

27 H 8.409237 7.357599 8.484695 7.550210 8.095429

28 H 3.311355 3.320193 4.666280 5.850660 7.183015

29 H 2.238065 3.320193 2.914674 4.315715 5.340500

30 H 4.335110 5.202824 2.899013 2.257466 1.080314

31 H 5.859722 6.187405 4.633273 3.319768 2.189393

32 Zn 3.112741 2.099062 3.474136 3.105215 4.342265

33 C 5.524478 5.171051 4.889967 3.580111 3.615644

34 C 6.788184 6.549511 5.982891 4.597540 4.210722

35 C 4.614189 3.729326 6.027952 6.792596 8.244536

36 C 7.910608 7.735825 7.014409 5.612054 5.000993

37 C 5.602221 4.853184 7.037161 7.897718 9.342643

38 C 7.840133 6.549511 8.372701 7.839255 8.794659

39 C 9.037773 7.735825 9.580830 9.030274 9.950860

40 C 2.429505 3.729326 1.424450 2.413051 2.890767

41 C 3.504461 4.853184 2.632729 3.510449 3.643529

42 H 4.512446 5.875575 3.699648 4.524419 4.472682

43 H 8.917829 8.786985 7.963158 6.559187 5.814528

44 H 10.096411 8.786985 10.647688 10.086416 10.983035

45 H 6.540032 5.875575 7.978018 8.898495 10.335531

21 22 23 24 25

21 C 0.000000

22 C 1.453547 0.000000

23 N 2.298328 1.371709 0.000000

24 H 9.648035 8.410096 7.361760 0.000000

25 H 9.458235 8.050156 7.361760 2.671375 0.000000

26 H 5.340500 4.315715 5.188799 9.165402 7.521423

27 H 7.183015 5.850660 6.179371 7.504382 5.374287

28 H 8.095429 7.550210 6.179371 5.374287 7.504382

29 H 6.516227 6.434349 5.188799 7.521423 9.165402

30 H 2.189393 3.319768 3.332794 10.293009 10.634015

31 H 1.080314 2.257466 3.332794 10.634015 10.293009

32 Zn 4.342265 3.105215 2.093071 5.317008 5.317008

33 C 2.536693 1.404275 2.473589 8.501538 7.695012

34 C 2.890767 2.413051 3.718877 9.861951 8.877604

35 C 8.794659 7.839255 6.551631 2.697239 5.071619

36 C 3.643529 3.510449 4.859421 11.023309 9.920736

37 C 9.950860 9.030274 7.728668 3.100352 5.718788

38 C 8.244536 6.792596 6.551631 5.071619 2.697239

39 C 9.342643 7.897718 7.728668 5.718788 3.100352

40 C 4.210722 4.597540 3.718877 8.877604 9.861951

41 C 5.000993 5.612054 4.859421 9.920736 11.023309

42 H 5.814528 6.559187 5.887023 10.873751 12.058309

43 H 4.472682 4.524419 5.887023 12.058309 10.873751

44 H 10.335531 8.898495 8.776461 6.420600 3.749634

45 H 10.983035 10.086416 8.776461 3.749634 6.420600

26 27 28 29 30

26 H 0.000000

27 H 2.690063 0.000000

28 H 10.615657 10.269164 0.000000

29 H 10.269164 10.615657 2.690063 0.000000

30 H 7.504382 9.165402 7.521423 5.374287 0.000000

31 H 5.374287 7.521423 9.165402 7.504382 2.671375

32 Zn 5.307840 5.307840 5.307840 5.307840 5.317008

33 C 2.914674 4.666280 8.484695 7.662324 4.633273

34 C 2.714047 5.105103 9.847442 8.847378 5.071619

35 C 9.847442 8.847378 2.714047 5.105103 8.877604

36 C 3.078157 5.717089 11.020687 9.911886 5.718788

37 C 11.020687 9.911886 3.078157 5.717089 9.920736

38 C 5.105103 2.714047 8.847378 9.847442 9.861951

39 C 5.717089 3.078157 9.911886 11.020687 11.023309

40 C 8.847378 9.847442 5.105103 2.714047 2.697239

41 C 9.911886 11.020687 5.717089 3.078157 3.100352

42 H 10.873466 12.060648 6.405890 3.715976 3.749634

43 H 3.715976 6.405890 12.060648 10.873466 6.420600

44 H 6.405890 3.715976 10.873466 12.060648 12.058309

45 H 12.060648 10.873466 3.715976 6.405890 10.873751

31 32 33 34 35

31 H 0.000000

32 Zn 5.317008 0.000000

33 C 2.899013 3.474136 0.000000

34 C 2.697239 4.898571 1.424450 0.000000

35 C 9.861951 4.898571 8.372701 9.797140 0.000000

36 C 3.100352 6.106733 2.632729 1.208380 11.005279

37 C 11.023309 6.106733 9.580830 11.005279 1.208380

38 C 8.877604 4.898571 6.027952 6.950033 6.905143

39 C 9.920736 6.106733 7.037161 7.837446 7.819896

40 C 5.071619 4.898571 5.982891 6.905143 6.950033

41 C 5.718788 6.106733 7.014409 7.819896 7.837446

42 H 6.420600 7.173612 7.963158 8.682918 8.690244

43 H 3.749634 7.173612 3.699648 2.275283 12.072137

44 H 10.873751 7.173612 7.978018 8.690244 8.682918

45 H 12.058309 7.173612 10.647688 12.072137 2.275283

36 37 38 39 40

36 C 0.000000

37 C 12.213465 0.000000

38 C 7.837446 7.819896 0.000000

39 C 8.628072 8.644368 1.208380 0.000000

40 C 7.819896 7.837446 9.797140 11.005279 0.000000

41 C 8.644368 8.628072 11.005279 12.213465 1.208380

42 H 9.436105 9.405620 12.072137 13.280341 2.275283

43 H 1.066920 13.280341 8.690244 9.405620 8.682918

44 H 9.405620 9.436105 2.275283 1.066920 12.072137

45 H 13.280341 1.066920 8.682918 9.436105 8.690244

41 42 43 44 45

41 C 0.000000

42 H 1.066920 0.000000

43 H 9.436105 10.168675 0.000000

44 H 13.280341 14.347224 10.121309 0.000000

45 H 9.405620 10.121309 14.347224 10.168675 0.000000

Stoichiometry C28H12N4Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C28H12)]

Deg. of freedom 34

Full point group C2V NOp 4

RotChk: IX=2 Diff= 4.99D-14

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.678744 4.288889 -0.005428

2 6 0 1.108924 2.900457 -0.003994

3 7 0 0.000000 2.093071 -0.004774

4 6 0 -1.108924 2.900457 -0.003994

5 6 0 -0.678744 4.288889 -0.005428

6 6 0 -2.444984 2.468128 0.000849

7 6 0 -2.909204 1.107063 0.006149

8 7 0 -2.099031 -0.000000 0.007684

9 6 0 -2.909204 -1.107063 0.006149

10 6 0 -4.274367 -0.691273 0.007394

11 6 0 -4.274367 0.691273 0.007394

12 6 0 2.444984 2.468128 0.000849

13 6 0 2.909204 1.107063 0.006149

14 6 0 4.274367 0.691273 0.007394

15 6 0 4.274367 -0.691273 0.007394

16 6 0 2.909204 -1.107063 0.006149

17 7 0 2.099031 0.000000 0.007684

18 6 0 2.444984 -2.468128 0.000849

19 6 0 1.108924 -2.900457 -0.003994

20 6 0 0.678744 -4.288889 -0.005428

21 6 0 -0.678744 -4.288889 -0.005428

22 6 0 -1.108924 -2.900457 -0.003994

23 7 0 0.000000 -2.093071 -0.004774

24 1 0 1.335688 5.146504 -0.005629

25 1 0 -1.335688 5.146504 -0.005629

26 1 0 -5.134582 -1.345031 0.007106

27 1 0 -5.134582 1.345031 0.007106

28 1 0 5.134582 1.345031 0.007106

29 1 0 5.134582 -1.345031 0.007106

30 1 0 1.335688 -5.146504 -0.005629

31 1 0 -1.335688 -5.146504 -0.005629

32 30 0 0.000000 0.000000 -0.003828

33 6 0 -2.444984 -2.468128 0.000849

34 6 0 -3.452571 -3.475017 -0.000229

35 6 0 3.452571 3.475017 -0.000229

36 6 0 -4.322184 -4.314036 -0.001441

37 6 0 4.322184 4.314036 -0.001441

38 6 0 -3.452571 3.475017 -0.000229

39 6 0 -4.322184 4.314036 -0.001441

40 6 0 3.452571 -3.475017 -0.000229

41 6 0 4.322184 -4.314036 -0.001441

42 1 0 5.084337 -5.060654 -0.002751

43 1 0 -5.084337 -5.060654 -0.002751

44 1 0 -5.084337 5.060654 -0.002751

45 1 0 5.084337 5.060654 -0.002751

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

Rotational constants (GHZ): 0.1460102 0.1454795 0.0728724

Leave Link 202 at Wed Jul 31 00:13:11 2019, MaxMem= 4294967296 cpu: 0.2

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

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

Pseudo-potential data read from rwf file.

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

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

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

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

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

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

111 alpha electrons 110 beta electrons

nuclear repulsion energy 3052.8595405349 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= 13 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= -0.1303625490 Hartrees.

Nuclear repulsion after empirical dispersion term = 3052.7291779859 Hartrees.

No density basis found on file 724.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

2nd derivatives : Analytical E(r).r(xy)/FMM algorithm (CHGder, D2EAlg=3).

Cavity 2nd derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3878

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.69D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 84

GePol: Fraction of low-weight points (<1% of avg) = 2.17%

GePol: Cavity surface area = 416.364 Ang\*\*2

GePol: Cavity volume = 420.929 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0083754010 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3052.7375533869 Hartrees.

Leave Link 301 at Wed Jul 31 00:13:11 2019, MaxMem= 4294967296 cpu: 1.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16177 LenP2D= 44694.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.47D-05 NBF= 172 148 158 158

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

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Wed Jul 31 00:13:12 2019, MaxMem= 4294967296 cpu: 10.8

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

DipDrv: MaxL=1.

Leave Link 303 at Wed Jul 31 00:13:12 2019, MaxMem= 4294967296 cpu: 1.3

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

Lowest energy guess from the checkpoint file: "ZnTSPsimanion.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= -0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 -0.000000 -0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 2.50D-01

Max alpha theta= 1.636 degrees.

Max beta theta= 1.622 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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

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Beta Orbitals:

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The electronic state of the initial guess is 2-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7630 S= 0.5065

Leave Link 401 at Wed Jul 31 00:13:14 2019, MaxMem= 4294967296 cpu: 34.3

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1387497 IEndB= 1387497 NGot= 4294967296 MDV= 4294047352

LenX= 4294047352 LenY= 4293596440

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

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

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 650000000 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= 45116652.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.00D-15 for 3852.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.46D-15 for 2186 2000.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.11D-15 for 3852.

Iteration 1 A^-1\*A deviation from orthogonality is 1.33D-14 for 3834 3688.

E= -1359.18266030725

DIIS: error= 1.94D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.18266030725 IErMin= 1 ErrMin= 1.94D-04

ErrMax= 1.94D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.19D-05 BMatP= 1.19D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.94D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 12.252 Goal= None Shift= 0.000

Gap= 12.349 Goal= None Shift= 0.000

RMSDP=1.04D-05 MaxDP=2.91D-04 OVMax= 6.46D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.04D-05 CP: 1.00D+00

E= -1359.18266278723 Delta-E= -0.000002479980 Rises=F Damp=F

DIIS: error= 2.93D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.18266278723 IErMin= 1 ErrMin= 1.94D-04

ErrMax= 2.93D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.12D-05 BMatP= 1.19D-05

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.93D-03

Coeff-Com: 0.490D+00 0.510D+00

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

Coeff: 0.489D+00 0.511D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=3.11D-06 MaxDP=1.21D-04 DE=-2.48D-06 OVMax= 1.80D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.99D-06 CP: 1.00D+00 9.19D-01

E= -1359.18266382224 Delta-E= -0.000001035018 Rises=F Damp=F

DIIS: error= 6.31D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.18266382224 IErMin= 3 ErrMin= 6.31D-05

ErrMax= 6.31D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.08D-07 BMatP= 1.12D-05

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

Coeff-Com: 0.491D-02 0.183D+00 0.812D+00

Coeff: 0.491D-02 0.183D+00 0.812D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=4.73D-07 MaxDP=2.65D-05 DE=-1.04D-06 OVMax= 1.02D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.33D-07 CP: 1.00D+00 9.36D-01 1.01D+00

E= -1359.18266386800 Delta-E= -0.000000045757 Rises=F Damp=F

DIIS: error= 9.22D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.18266386800 IErMin= 4 ErrMin= 9.22D-06

ErrMax= 9.22D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.44D-08 BMatP= 6.08D-07

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

Coeff-Com: -0.458D-02 0.101D+00 0.436D+00 0.468D+00

Coeff: -0.458D-02 0.101D+00 0.436D+00 0.468D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=2.04D-07 MaxDP=1.61D-05 DE=-4.58D-08 OVMax= 4.56D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.86D-07 CP: 1.00D+00 9.37D-01 1.01D+00 8.11D-01

E= -1359.18266388071 Delta-E= -0.000000012706 Rises=F Damp=F

DIIS: error= 3.28D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.18266388071 IErMin= 5 ErrMin= 3.28D-06

ErrMax= 3.28D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.92D-09 BMatP= 7.44D-08

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

Coeff-Com: -0.297D-02 0.251D-01 0.714D-01 0.263D+00 0.643D+00

Coeff: -0.297D-02 0.251D-01 0.714D-01 0.263D+00 0.643D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.17D-07 MaxDP=4.65D-06 DE=-1.27D-08 OVMax= 1.83D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 5.86D-08 CP: 1.00D+00 9.40D-01 9.88D-01 8.26D-01 6.28D-01

E= -1359.18266388297 Delta-E= -0.000000002266 Rises=F Damp=F

DIIS: error= 6.19D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.18266388297 IErMin= 6 ErrMin= 6.19D-07

ErrMax= 6.19D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.83D-10 BMatP= 9.92D-09

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

Coeff-Com: -0.867D-03 0.553D-02 0.566D-02 0.779D-01 0.277D+00 0.635D+00

Coeff: -0.867D-03 0.553D-02 0.566D-02 0.779D-01 0.277D+00 0.635D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.98D-08 MaxDP=7.80D-07 DE=-2.27D-09 OVMax= 5.10D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.74D-08 CP: 1.00D+00 9.40D-01 9.87D-01 8.28D-01 6.64D-01

CP: 8.94D-01

E= -1359.18266388308 Delta-E= -0.000000000103 Rises=F Damp=F

DIIS: error= 3.49D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.18266388308 IErMin= 7 ErrMin= 3.49D-07

ErrMax= 3.49D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-10 BMatP= 3.83D-10

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

Coeff-Com: -0.360D-05-0.136D-02-0.920D-02-0.244D-02 0.549D-01 0.373D+00

Coeff-Com: 0.585D+00

Coeff: -0.360D-05-0.136D-02-0.920D-02-0.244D-02 0.549D-01 0.373D+00

Coeff: 0.585D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=1.11D-08 MaxDP=5.20D-07 DE=-1.03D-10 OVMax= 2.00D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 9.25D-09 CP: 1.00D+00 9.40D-01 9.89D-01 8.35D-01 6.84D-01

CP: 8.95D-01 9.30D-01

E= -1359.18266388314 Delta-E= -0.000000000061 Rises=F Damp=F

DIIS: error= 1.88D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.18266388314 IErMin= 8 ErrMin= 1.88D-07

ErrMax= 1.88D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.21D-11 BMatP= 1.10D-10

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

Coeff-Com: 0.180D-03-0.202D-02-0.568D-02-0.179D-01-0.280D-01 0.598D-01

Coeff-Com: 0.306D+00 0.688D+00

Coeff: 0.180D-03-0.202D-02-0.568D-02-0.179D-01-0.280D-01 0.598D-01

Coeff: 0.306D+00 0.688D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.089 Goal= None Shift= 0.000

RMSDP=6.13D-09 MaxDP=3.35D-07 DE=-6.09D-11 OVMax= 1.69D-06

Error on total polarization charges = 0.06716

SCF Done: E(UB3LYP) = -1359.18266388 A.U. after 8 cycles

NFock= 8 Conv=0.61D-08 -V/T= 1.9682

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7630 S= 0.5065

<L.S>= 0.000000000000E+00

KE= 1.403878170588D+03 PE=-9.375015489576D+03 EE= 3.559217101718D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.26

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7630, after 0.7501

Leave Link 502 at Wed Jul 31 00:14:06 2019, MaxMem= 4294967296 cpu: 791.3

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 636

NBasis= 636 NAE= 111 NBE= 110 NFC= 0 NFV= 0

NROrb= 636 NOA= 111 NOB= 110 NVA= 525 NVB= 526

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.15161228D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.38268662D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.15136971D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.88604697D-01

Leave Link 801 at Wed Jul 31 00:14:06 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 45.

Will process 46 centers per pass.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16177 LenP2D= 44694.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 11 by ecpmxn.

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

Leave Link 1101 at Wed Jul 31 00:14:09 2019, MaxMem= 4294967296 cpu: 44.7

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Wed Jul 31 00:14:09 2019, MaxMem= 4294967296 cpu: 1.1

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 45.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966832.

G2DrvN: will do 46 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

G2PCM: DoFxE=T DoFxN=T DoGrad=T DoDP/DQ/DG/TGxP=FFFF NFrqRd= 0 IEInf=0 SqF1=F DoCFld=F IF1Alg=4.

GePol: Maximum number of non-zero 1st derivatives = 256

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Wed Jul 31 00:16:06 2019, MaxMem= 4294967296 cpu: 1879.2

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=111111111111111111111111111111111111111111111

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Using symmetry in CPHF.

Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.

Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.

NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 4294965570 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 0.

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

IRaf= 650000000 NMat= 42 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

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

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

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

NMat0= 42 NMatS0= 42 NMatT0= 0 NMatD0= 42 NMtDS0= 0 NMtDT0= 0

Integrals replicated using symmetry in FoFCou.

There are 42 degrees of freedom in the 1st order CPHF. IDoFFX=4 NUNeed= 42.

42 vectors produced by pass 0 Test12= 2.77D-13 2.38D-09 XBig12= 8.04D+03 5.91D+01.

AX will form 42 AO Fock derivatives at one time.

42 vectors produced by pass 1 Test12= 2.77D-13 2.38D-09 XBig12= 1.07D+03 6.84D+00.

42 vectors produced by pass 2 Test12= 2.77D-13 2.38D-09 XBig12= 2.80D+02 5.65D+00.

42 vectors produced by pass 3 Test12= 2.77D-13 2.38D-09 XBig12= 8.13D+01 2.08D+00.

42 vectors produced by pass 4 Test12= 2.77D-13 2.38D-09 XBig12= 8.70D+00 4.89D-01.

42 vectors produced by pass 5 Test12= 2.77D-13 2.38D-09 XBig12= 3.06D-01 6.01D-02.

42 vectors produced by pass 6 Test12= 2.77D-13 2.38D-09 XBig12= 1.23D-02 9.15D-03.

42 vectors produced by pass 7 Test12= 2.77D-13 2.38D-09 XBig12= 2.61D-04 1.43D-03.

37 vectors produced by pass 8 Test12= 2.77D-13 2.38D-09 XBig12= 4.82D-06 1.63D-04.

23 vectors produced by pass 9 Test12= 2.77D-13 2.38D-09 XBig12= 6.69D-08 2.10D-05.

7 vectors produced by pass 10 Test12= 2.77D-13 2.38D-09 XBig12= 9.02D-10 2.17D-06.

2 vectors produced by pass 11 Test12= 2.77D-13 2.38D-09 XBig12= 9.77D-12 1.94D-07.

2 vectors produced by pass 12 Test12= 2.77D-13 2.38D-09 XBig12= 1.31D-13 3.41D-08.

1 vectors produced by pass 13 Test12= 2.77D-13 2.38D-09 XBig12= 3.39D-15 2.70D-09.

InvSVY: IOpt=1 It= 1 EMax= 8.53D-14

Solved reduced A of dimension 408 with 42 vectors.

FullF1: Do perturbations 1 to 42.

Isotropic polarizability for W= 0.000000 1005.00 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Wed Jul 31 00:47:20 2019, MaxMem= 4294967296 cpu: 29980.8

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16177 LenP2D= 44694.

LDataN: DoStor=T MaxTD1= 7 Len= 274

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 256

Leave Link 701 at Wed Jul 31 00:47:55 2019, MaxMem= 4294967296 cpu: 554.0

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

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

Leave Link 702 at Wed Jul 31 00:47:55 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

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

wScrn= 0.000000 ICntrl= 100127 IOpCl= 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 Wed Jul 31 00:49:45 2019, MaxMem= 4294967296 cpu: 1766.4

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

Dipole =-3.61030650D-13-1.84435800D-13-2.05150195D-02

Polarizability= 1.65129133D+03 2.55415542D-06 1.17661803D+03

1.26297420D-05 4.02036671D-06 1.87088917D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000101523 0.001224129 -0.000020954

2 6 -0.000055634 0.000195867 0.000039864

3 7 -0.001224618 -0.000000000 0.000192135

4 6 -0.000055634 -0.000195867 0.000039864

5 6 -0.000101523 -0.001224129 -0.000020954

6 6 -0.000424526 -0.000224927 0.000013695

7 6 0.000893935 0.000031286 0.000054852

8 7 -0.000000000 -0.001113711 -0.000618476

9 6 -0.000893935 0.000031286 0.000054852

10 6 0.001042855 -0.000034588 -0.000032637

11 6 -0.001042855 -0.000034588 -0.000032637

12 6 -0.000424526 0.000224927 0.000013695

13 6 0.000893935 -0.000031286 0.000054852

14 6 -0.001042855 0.000034588 -0.000032637

15 6 0.001042855 0.000034588 -0.000032637

16 6 -0.000893935 -0.000031286 0.000054852

17 7 0.000000000 0.001113711 -0.000618476

18 6 0.000424526 0.000224927 0.000013695

19 6 0.000055634 0.000195867 0.000039864

20 6 0.000101523 0.001224129 -0.000020954

21 6 0.000101523 -0.001224129 -0.000020954

22 6 0.000055634 -0.000195867 0.000039864

23 7 0.001224618 0.000000000 0.000192135

24 1 0.000023084 0.000053057 0.000005896

25 1 0.000023084 -0.000053057 0.000005896

26 1 0.000022702 0.000002549 0.000007085

27 1 -0.000022702 0.000002549 0.000007085

28 1 -0.000022702 -0.000002549 0.000007085

29 1 0.000022702 -0.000002549 0.000007085

30 1 -0.000023084 0.000053057 0.000005896

31 1 -0.000023084 -0.000053057 0.000005896

32 30 -0.000000000 0.000000000 0.000553554

33 6 0.000424526 -0.000224927 0.000013695

34 6 0.000045976 0.000166722 0.000005623

35 6 -0.000045976 -0.000166722 0.000005623

36 6 0.000143603 -0.000016895 -0.000003623

37 6 -0.000143603 0.000016895 -0.000003623

38 6 -0.000045976 0.000166722 0.000005623

39 6 -0.000143603 -0.000016895 -0.000003623

40 6 0.000045976 -0.000166722 0.000005623

41 6 0.000143603 0.000016895 -0.000003623

42 1 -0.000099898 -0.000017252 0.000004980

43 1 -0.000099898 0.000017252 0.000004980

44 1 0.000099898 0.000017252 0.000004980

45 1 0.000099898 -0.000017252 0.000004980

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

Cartesian Forces: Max 0.001224618 RMS 0.000399913

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

Leave Link 716 at Wed Jul 31 00:49:45 2019, MaxMem= 4294967296 cpu: 0.8

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.001297632 RMS 0.000220626

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 = .22063D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

ITU= 0 0 -1 0 0

Eigenvalues --- 0.00143 0.00338 0.00452 0.00556 0.00648

Eigenvalues --- 0.00959 0.01111 0.01121 0.01158 0.01222

Eigenvalues --- 0.01231 0.01278 0.01283 0.01341 0.01367

Eigenvalues --- 0.01506 0.01522 0.01543 0.01829 0.01918

Eigenvalues --- 0.01939 0.01940 0.01964 0.01994 0.02004

Eigenvalues --- 0.02090 0.02099 0.02113 0.02125 0.02403

Eigenvalues --- 0.03000 0.03136 0.03193 0.03620 0.04004

Eigenvalues --- 0.04124 0.04126 0.04136 0.04140 0.04149

Eigenvalues --- 0.04353 0.04359 0.06226 0.06295 0.08273

Eigenvalues --- 0.08284 0.08298 0.08562 0.08838 0.08872

Eigenvalues --- 0.08931 0.09192 0.09260 0.09575 0.09619

Eigenvalues --- 0.09634 0.09663 0.09986 0.10417 0.10420

Eigenvalues --- 0.10450 0.10503 0.12248 0.13224 0.13555

Eigenvalues --- 0.13577 0.15993 0.16909 0.16972 0.19304

Eigenvalues --- 0.19864 0.20044 0.20137 0.20375 0.20618

Eigenvalues --- 0.20652 0.20841 0.21650 0.21863 0.21909

Eigenvalues --- 0.21997 0.26015 0.26201 0.27699 0.27968

Eigenvalues --- 0.28127 0.29502 0.30068 0.31776 0.32506

Eigenvalues --- 0.32772 0.32819 0.33617 0.35654 0.35715

Eigenvalues --- 0.35860 0.36108 0.36439 0.37024 0.37102

Eigenvalues --- 0.37158 0.37333 0.37410 0.37554 0.37837

Eigenvalues --- 0.38069 0.38373 0.38833 0.39205 0.40205

Eigenvalues --- 0.40208 0.40210 0.40212 0.41355 0.41473

Eigenvalues --- 0.42028 0.42573 0.45438 0.46132 0.46450

Eigenvalues --- 0.46726 0.50295 0.50316 0.52914 0.53317

Eigenvalues --- 1.03374 1.04129 1.04462 1.04694

En-DIIS/RFO-DIIS IScMMF= 0 using points: 5 4

RFO step: Lambda=-2.78871698D-05.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 7.31D-04 SmlDif= 1.00D-05

RMS Error= 0.5192642450D-03 NUsed= 2 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.54414 0.45586

Iteration 1 RMS(Cart)= 0.00947810 RMS(Int)= 0.00028865

Iteration 2 RMS(Cart)= 0.00031309 RMS(Int)= 0.00023852

Iteration 3 RMS(Cart)= 0.00000007 RMS(Int)= 0.00023852

ITry= 1 IFail=0 DXMaxC= 1.20D-01 DCOld= 1.00D+10 DXMaxT= 1.50D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.08D-03 for atom 37.

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

(Linear) (Quad) (Total)

R1 2.74681 0.00008 -0.00042 0.00031 -0.00003 2.74678

R2 2.56528 0.00130 0.00055 0.00180 0.00289 2.56817

R3 2.04150 0.00001 -0.00003 0.00001 -0.00002 2.04148

R4 2.59215 0.00025 0.00086 -0.00019 0.00057 2.59273

R5 2.65369 0.00020 -0.00074 0.00080 0.00043 2.65413

R6 2.59215 0.00025 0.00086 -0.00020 0.00057 2.59273

R7 3.95533 0.00116 -0.00191 0.00510 0.00284 3.95817

R8 2.74681 0.00008 -0.00042 0.00031 -0.00003 2.74678

R9 2.65369 0.00020 -0.00074 0.00080 0.00043 2.65413

R10 2.04150 0.00001 -0.00003 0.00001 -0.00002 2.04148

R11 2.71755 0.00068 -0.00051 0.00173 0.00184 2.71939

R12 2.69182 -0.00005 -0.00016 -0.00018 -0.00039 2.69143

R13 2.59242 -0.00008 0.00037 -0.00070 -0.00056 2.59186

R14 2.69679 -0.00002 -0.00056 0.00007 -0.00051 2.69627

R15 2.59242 -0.00008 0.00037 -0.00069 -0.00056 2.59186

R16 3.96665 0.00091 -0.00127 0.00344 0.00185 3.96850

R17 2.69679 -0.00002 -0.00056 0.00007 -0.00051 2.69627

R18 2.71755 0.00068 -0.00051 0.00174 0.00184 2.71939

R19 2.61263 0.00089 0.00056 0.00165 0.00276 2.61539

R20 2.04175 0.00001 -0.00003 0.00001 -0.00002 2.04173

R21 2.04175 0.00001 -0.00003 0.00001 -0.00002 2.04173

R22 2.71755 0.00068 -0.00051 0.00174 0.00184 2.71939

R23 2.69182 -0.00005 -0.00016 -0.00018 -0.00039 2.69143

R24 2.69679 -0.00002 -0.00056 0.00007 -0.00051 2.69627

R25 2.59242 -0.00008 0.00037 -0.00070 -0.00056 2.59186

R26 2.61263 0.00089 0.00056 0.00165 0.00276 2.61539

R27 2.04175 0.00001 -0.00003 0.00001 -0.00002 2.04173

R28 2.69679 -0.00002 -0.00056 0.00007 -0.00051 2.69627

R29 2.04175 0.00001 -0.00003 0.00001 -0.00002 2.04173

R30 2.59242 -0.00008 0.00037 -0.00070 -0.00056 2.59186

R31 2.71755 0.00068 -0.00051 0.00174 0.00184 2.71939

R32 3.96665 0.00091 -0.00127 0.00339 0.00185 3.96850

R33 2.65369 0.00020 -0.00074 0.00080 0.00043 2.65413

R34 2.69182 -0.00005 -0.00016 -0.00018 -0.00039 2.69143

R35 2.74681 0.00008 -0.00042 0.00031 -0.00003 2.74678

R36 2.59215 0.00025 0.00086 -0.00019 0.00057 2.59273

R37 2.56528 0.00130 0.00055 0.00180 0.00289 2.56817

R38 2.04150 0.00001 -0.00003 0.00001 -0.00002 2.04148

R39 2.74681 0.00008 -0.00042 0.00031 -0.00003 2.74678

R40 2.04150 0.00001 -0.00003 0.00001 -0.00002 2.04148

R41 2.59215 0.00025 0.00086 -0.00020 0.00057 2.59273

R42 2.65369 0.00020 -0.00074 0.00080 0.00043 2.65413

R43 3.95533 0.00116 -0.00191 0.00506 0.00284 3.95817

R44 2.69182 -0.00005 -0.00016 -0.00018 -0.00039 2.69143

R45 2.28351 0.00003 -0.00001 0.00005 0.00004 2.28355

R46 2.28351 0.00003 -0.00001 0.00005 0.00004 2.28355

R47 2.01619 -0.00008 -0.00009 -0.00011 -0.00025 2.01593

R48 2.01619 -0.00008 -0.00009 -0.00011 -0.00025 2.01593

R49 2.28351 0.00003 -0.00001 0.00005 0.00004 2.28355

R50 2.01619 -0.00008 -0.00009 -0.00011 -0.00025 2.01593

R51 2.28351 0.00003 -0.00001 0.00005 0.00004 2.28355

R52 2.01619 -0.00008 -0.00009 -0.00011 -0.00025 2.01593

A1 1.87125 -0.00009 -0.00026 -0.00004 -0.00026 1.87098

A2 2.18747 -0.00001 -0.00019 -0.00003 -0.00024 2.18723

A3 2.22447 0.00010 0.00044 0.00007 0.00050 2.22497

A4 1.89967 -0.00006 0.00105 -0.00064 0.00008 1.89975

A5 2.18420 0.00001 -0.00116 0.00058 -0.00025 2.18395

A6 2.19931 0.00006 0.00010 0.00006 0.00017 2.19948

A7 1.88294 0.00031 -0.00159 0.00135 0.00037 1.88331

A8 2.20012 -0.00015 0.00062 -0.00070 -0.00035 2.19977

A9 2.20012 -0.00015 0.00062 -0.00067 -0.00035 2.19977

A10 1.89967 -0.00006 0.00105 -0.00063 0.00008 1.89975

A11 2.19931 0.00006 0.00010 0.00005 0.00017 2.19948

A12 2.18420 0.00001 -0.00116 0.00058 -0.00025 2.18395

A13 1.87125 -0.00009 -0.00026 -0.00004 -0.00026 1.87098

A14 2.22447 0.00010 0.00044 0.00007 0.00050 2.22497

A15 2.18747 -0.00001 -0.00019 -0.00003 -0.00024 2.18723

A16 2.21245 0.00008 -0.00154 0.00080 -0.00035 2.21211

A17 2.04358 -0.00026 0.00042 -0.00090 -0.00078 2.04280

A18 2.02715 0.00018 0.00107 0.00010 0.00113 2.02828

A19 2.18113 0.00007 -0.00008 0.00025 0.00018 2.18130

A20 2.19514 -0.00017 -0.00123 -0.00009 -0.00114 2.19400

A21 1.90691 0.00010 0.00129 -0.00015 0.00096 1.90787

A22 1.87806 0.00012 -0.00171 0.00089 -0.00038 1.87768

A23 2.20254 -0.00006 0.00077 -0.00038 0.00011 2.20266

A24 2.20254 -0.00006 0.00077 -0.00040 0.00011 2.20266

A25 1.90691 0.00010 0.00129 -0.00015 0.00096 1.90787

A26 2.18113 0.00007 -0.00008 0.00026 0.00018 2.18130

A27 2.19514 -0.00017 -0.00123 -0.00010 -0.00114 2.19400

A28 1.86644 -0.00016 -0.00044 -0.00028 -0.00077 1.86568

A29 2.19608 0.00006 -0.00003 0.00019 0.00023 2.19631

A30 2.22066 0.00010 0.00046 0.00009 0.00054 2.22120

A31 1.86644 -0.00016 -0.00044 -0.00028 -0.00077 1.86568

A32 2.19608 0.00006 -0.00003 0.00019 0.00023 2.19631

A33 2.22066 0.00010 0.00046 0.00009 0.00054 2.22120

A34 2.21245 0.00008 -0.00154 0.00081 -0.00035 2.21211

A35 2.04358 -0.00026 0.00042 -0.00090 -0.00078 2.04280

A36 2.02715 0.00018 0.00107 0.00009 0.00113 2.02828

A37 2.19514 -0.00017 -0.00123 -0.00009 -0.00114 2.19400

A38 2.18113 0.00007 -0.00008 0.00025 0.00018 2.18130

A39 1.90691 0.00010 0.00129 -0.00016 0.00096 1.90787

A40 1.86644 -0.00016 -0.00044 -0.00028 -0.00077 1.86568

A41 2.19608 0.00006 -0.00003 0.00019 0.00023 2.19631

A42 2.22066 0.00010 0.00046 0.00009 0.00054 2.22120

A43 1.86644 -0.00016 -0.00044 -0.00028 -0.00077 1.86568

A44 2.22066 0.00010 0.00046 0.00009 0.00054 2.22120

A45 2.19608 0.00006 -0.00003 0.00019 0.00023 2.19631

A46 1.90691 0.00010 0.00129 -0.00016 0.00096 1.90787

A47 2.19514 -0.00017 -0.00123 -0.00009 -0.00114 2.19400

A48 2.18113 0.00007 -0.00008 0.00026 0.00018 2.18130

A49 1.87806 0.00012 -0.00171 0.00089 -0.00038 1.87768

A50 2.20254 -0.00006 0.00077 -0.00038 0.00011 2.20266

A51 2.20254 -0.00006 0.00077 -0.00041 0.00011 2.20266

A52 2.21245 0.00008 -0.00154 0.00081 -0.00035 2.21211

A53 2.02715 0.00018 0.00107 0.00009 0.00113 2.02828

A54 2.04358 -0.00026 0.00042 -0.00090 -0.00078 2.04280

A55 2.18420 0.00001 -0.00116 0.00059 -0.00025 2.18395

A56 2.19931 0.00006 0.00010 0.00005 0.00017 2.19948

A57 1.89967 -0.00006 0.00105 -0.00064 0.00008 1.89975

A58 1.87125 -0.00009 -0.00026 -0.00004 -0.00026 1.87098

A59 2.18747 -0.00001 -0.00019 -0.00003 -0.00024 2.18723

A60 2.22447 0.00010 0.00044 0.00007 0.00050 2.22497

A61 1.87125 -0.00009 -0.00026 -0.00004 -0.00026 1.87098

A62 2.22447 0.00010 0.00044 0.00007 0.00050 2.22497

A63 2.18747 -0.00001 -0.00019 -0.00003 -0.00024 2.18723

A64 1.89967 -0.00006 0.00105 -0.00064 0.00008 1.89975

A65 2.18420 0.00001 -0.00116 0.00059 -0.00025 2.18395

A66 2.19931 0.00006 0.00010 0.00005 0.00017 2.19948

A67 1.88294 0.00031 -0.00159 0.00136 0.00037 1.88331

A68 2.20012 -0.00015 0.00062 -0.00070 -0.00035 2.19977

A69 2.20012 -0.00015 0.00062 -0.00067 -0.00035 2.19977

A70 1.57080 -0.00000 -0.00154 -0.00004 -0.00060 1.57020

A71 1.57080 -0.00000 -0.00154 -0.00001 -0.00060 1.57020

A72 1.57080 -0.00000 -0.00154 -0.00002 -0.00060 1.57020

A73 1.57080 -0.00000 -0.00154 0.00001 -0.00060 1.57020

A74 2.21245 0.00008 -0.00154 0.00081 -0.00035 2.21211

A75 2.02715 0.00018 0.00107 0.00010 0.00113 2.02828

A76 2.04358 -0.00026 0.00042 -0.00090 -0.00078 2.04280

A77 3.14160 -0.00000 -0.00308 -0.00001 -0.00119 3.14040

A78 3.14160 -0.00000 -0.00308 -0.00001 -0.00119 3.14040

A79 3.12404 -0.00005 0.00019 0.00021 0.00038 3.12441

A80 3.15915 0.00005 -0.00022 -0.00021 -0.00038 3.15877

A81 3.14920 -0.00012 -0.00077 -0.00132 -0.00247 3.14673

A82 3.14920 -0.00012 -0.00077 -0.00131 -0.00247 3.14673

A83 3.15915 0.00005 -0.00022 -0.00021 -0.00038 3.15877

A84 3.14920 -0.00012 -0.00077 -0.00131 -0.00247 3.14673

A85 3.12404 -0.00005 0.00019 0.00021 0.00038 3.12441

A86 3.14920 -0.00012 -0.00077 -0.00132 -0.00247 3.14673

A87 3.14250 -0.00002 0.05448 -0.00506 0.04947 3.19196

A88 3.15256 -0.00024 -0.05602 -0.00210 -0.05820 3.09436

A89 3.14130 0.00001 -0.00082 0.00139 0.00057 3.14187

A90 3.14188 -0.00001 0.00104 -0.00146 -0.00042 3.14146

A91 3.14136 0.00001 -0.00003 0.00009 0.00005 3.14141

A92 3.14136 0.00001 -0.00003 0.00008 0.00005 3.14141

A93 3.14131 0.00001 -0.00104 0.00146 0.00042 3.14172

A94 3.14183 -0.00001 0.00003 -0.00008 -0.00005 3.14177

A95 3.14189 -0.00001 0.00082 -0.00139 -0.00057 3.14132

A96 3.14183 -0.00001 0.00003 -0.00009 -0.00005 3.14177

D1 0.00124 -0.00005 -0.00186 0.00086 -0.00099 0.00025

D2 -3.13776 -0.00009 -0.00599 0.00056 -0.00542 3.14000

D3 -3.14113 -0.00001 0.00066 0.00038 0.00104 -3.14009

D4 0.00305 -0.00005 -0.00347 0.00008 -0.00339 -0.00034

D5 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D6 3.14079 0.00004 0.00259 -0.00050 0.00209 -3.14031

D7 -3.14079 -0.00004 -0.00259 0.00050 -0.00209 3.14031

D8 -0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D9 -0.00202 0.00008 0.00301 -0.00140 0.00161 -0.00041

D10 3.14133 0.00002 0.02052 0.00547 0.02599 -3.11587

D11 3.13696 0.00012 0.00719 -0.00110 0.00609 -3.14014

D12 -0.00288 0.00006 0.02470 0.00577 0.03047 0.02759

D13 3.13835 0.00006 0.01178 -0.00372 0.00806 -3.13678

D14 -0.00384 0.00004 0.00443 0.00202 0.00645 0.00262

D15 -0.00022 0.00002 0.00696 -0.00407 0.00287 0.00265

D16 3.14078 -0.00001 -0.00039 0.00167 0.00127 -3.14114

D17 0.00202 -0.00008 -0.00301 0.00140 -0.00161 0.00041

D18 -3.13696 -0.00012 -0.00719 0.00110 -0.00609 3.14014

D19 -3.14133 -0.00002 -0.02052 -0.00547 -0.02599 3.11587

D20 0.00288 -0.00006 -0.02470 -0.00577 -0.03047 -0.02759

D21 3.13508 0.00015 0.01768 -0.00299 0.01475 -3.13336

D22 0.00445 -0.00008 -0.03834 -0.00509 -0.04345 -0.03900

D23 -0.00445 0.00008 0.03834 0.00509 0.04345 0.03900

D24 -3.13508 -0.00015 -0.01768 0.00299 -0.01475 3.13336

D25 -0.00124 0.00005 0.00186 -0.00086 0.00099 -0.00025

D26 3.14113 0.00001 -0.00066 -0.00038 -0.00104 3.14009

D27 3.13776 0.00009 0.00599 -0.00056 0.00542 -3.14000

D28 -0.00305 0.00005 0.00347 -0.00008 0.00339 0.00034

D29 0.00022 -0.00002 -0.00696 0.00407 -0.00287 -0.00265

D30 -3.14078 0.00001 0.00039 -0.00167 -0.00127 3.14114

D31 -3.13835 -0.00006 -0.01178 0.00372 -0.00806 3.13678

D32 0.00384 -0.00004 -0.00443 -0.00202 -0.00645 -0.00262

D33 0.00034 0.00004 0.00786 -0.00337 0.00450 0.00484

D34 -3.13846 0.00002 0.01241 -0.00726 0.00516 -3.13330

D35 3.14135 0.00001 0.00057 0.00233 0.00291 -3.13893

D36 0.00255 -0.00001 0.00512 -0.00156 0.00357 0.00612

D37 -3.13635 -0.00011 0.00547 -0.00746 -0.00200 -3.13835

D38 -0.00390 0.00002 0.02295 0.00449 0.02745 0.02355

D39 0.00284 -0.00009 0.00154 -0.00412 -0.00257 0.00027

D40 3.13529 0.00004 0.01903 0.00784 0.02688 -3.12102

D41 3.13741 0.00008 -0.00491 0.00592 0.00101 3.13842

D42 -0.00296 0.00003 -0.00278 0.00421 0.00143 -0.00153

D43 -0.00176 0.00005 -0.00096 0.00255 0.00159 -0.00017

D44 3.14106 0.00001 0.00117 0.00083 0.00201 -3.14012

D45 -0.00284 0.00009 -0.00154 0.00412 0.00257 -0.00027

D46 3.13635 0.00011 -0.00547 0.00746 0.00200 3.13835

D47 -3.13529 -0.00004 -0.01903 -0.00784 -0.02688 3.12102

D48 0.00390 -0.00002 -0.02295 -0.00449 -0.02745 -0.02355

D49 0.00495 -0.00006 -0.03758 -0.00453 -0.04213 -0.03718

D50 -3.13574 -0.00009 0.01689 -0.00960 0.00734 -3.12840

D51 3.13574 0.00009 -0.01689 0.00960 -0.00734 3.12840

D52 -0.00495 0.00006 0.03758 0.00453 0.04213 0.03718

D53 0.00176 -0.00005 0.00096 -0.00255 -0.00159 0.00017

D54 -3.14106 -0.00001 -0.00117 -0.00083 -0.00201 3.14012

D55 -3.13741 -0.00008 0.00491 -0.00592 -0.00101 -3.13842

D56 0.00296 -0.00003 0.00278 -0.00421 -0.00143 0.00153

D57 -0.00034 -0.00004 -0.00786 0.00337 -0.00450 -0.00484

D58 -3.14135 -0.00001 -0.00057 -0.00233 -0.00291 3.13893

D59 3.13846 -0.00002 -0.01241 0.00726 -0.00516 3.13330

D60 -0.00255 0.00001 -0.00512 0.00156 -0.00357 -0.00612

D61 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D62 3.14035 0.00005 -0.00217 0.00174 -0.00043 3.13992

D63 -3.14035 -0.00005 0.00217 -0.00174 0.00043 -3.13992

D64 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D65 3.13846 -0.00002 -0.01241 0.00726 -0.00516 3.13330

D66 -0.00034 -0.00004 -0.00786 0.00337 -0.00450 -0.00484

D67 -0.00255 0.00001 -0.00512 0.00156 -0.00357 -0.00612

D68 -3.14135 -0.00001 -0.00057 -0.00233 -0.00291 3.13893

D69 -3.13741 -0.00008 0.00491 -0.00592 -0.00101 -3.13842

D70 0.00296 -0.00003 0.00278 -0.00421 -0.00143 0.00153

D71 0.00176 -0.00005 0.00096 -0.00255 -0.00159 0.00017

D72 -3.14106 -0.00001 -0.00117 -0.00083 -0.00201 3.14012

D73 3.13635 0.00011 -0.00547 0.00746 0.00200 3.13835

D74 0.00390 -0.00002 -0.02295 -0.00449 -0.02745 -0.02355

D75 -0.00284 0.00009 -0.00154 0.00412 0.00257 -0.00027

D76 -3.13529 -0.00004 -0.01903 -0.00784 -0.02688 3.12102

D77 0.00000 0.00000 -0.00000 0.00000 -0.00000 0.00000

D78 3.14035 0.00005 -0.00217 0.00174 -0.00043 3.13992

D79 -3.14035 -0.00005 0.00217 -0.00174 0.00043 -3.13992

D80 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D81 -0.00176 0.00005 -0.00096 0.00255 0.00159 -0.00017

D82 3.13741 0.00008 -0.00491 0.00592 0.00101 3.13842

D83 3.14106 0.00001 0.00117 0.00083 0.00201 -3.14012

D84 -0.00296 0.00003 -0.00278 0.00421 0.00143 -0.00153

D85 0.00284 -0.00009 0.00154 -0.00412 -0.00257 0.00027

D86 3.13529 0.00004 0.01903 0.00784 0.02688 -3.12102

D87 -3.13635 -0.00011 0.00547 -0.00746 -0.00200 -3.13835

D88 -0.00390 0.00002 0.02295 0.00449 0.02745 0.02355

D89 -3.13846 0.00002 0.01241 -0.00726 0.00516 -3.13330

D90 0.00255 -0.00001 0.00512 -0.00156 0.00357 0.00612

D91 0.00034 0.00004 0.00786 -0.00337 0.00450 0.00484

D92 3.14135 0.00001 0.00057 0.00233 0.00291 -3.13893

D93 -0.00495 0.00006 0.03758 0.00453 0.04213 0.03718

D94 3.13574 0.00009 -0.01689 0.00959 -0.00734 3.12840

D95 -3.13574 -0.00009 0.01689 -0.00960 0.00734 -3.12840

D96 0.00495 -0.00006 -0.03758 -0.00453 -0.04213 -0.03718

D97 -3.13835 -0.00006 -0.01178 0.00373 -0.00806 3.13678

D98 0.00022 -0.00002 -0.00696 0.00407 -0.00287 -0.00265

D99 0.00384 -0.00004 -0.00443 -0.00202 -0.00645 -0.00262

D100 -3.14078 0.00001 0.00039 -0.00167 -0.00127 3.14114

D101 3.13776 0.00009 0.00599 -0.00056 0.00542 -3.14000

D102 -0.00305 0.00005 0.00347 -0.00008 0.00339 0.00034

D103 -0.00124 0.00005 0.00186 -0.00086 0.00099 -0.00025

D104 3.14113 0.00001 -0.00066 -0.00038 -0.00104 3.14009

D105 -3.13696 -0.00012 -0.00719 0.00110 -0.00609 3.14014

D106 0.00288 -0.00006 -0.02470 -0.00578 -0.03047 -0.02759

D107 0.00202 -0.00008 -0.00301 0.00140 -0.00161 0.00041

D108 -3.14133 -0.00002 -0.02052 -0.00547 -0.02599 3.11587

D109 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D110 -3.14079 -0.00004 -0.00259 0.00050 -0.00209 3.14031

D111 3.14079 0.00004 0.00259 -0.00050 0.00209 -3.14031

D112 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D113 0.00124 -0.00005 -0.00186 0.00086 -0.00099 0.00025

D114 -3.13776 -0.00009 -0.00599 0.00056 -0.00542 3.14000

D115 -3.14113 -0.00001 0.00066 0.00038 0.00104 -3.14009

D116 0.00305 -0.00005 -0.00347 0.00008 -0.00339 -0.00034

D117 -0.00202 0.00008 0.00301 -0.00140 0.00161 -0.00041

D118 3.14133 0.00002 0.02052 0.00547 0.02599 -3.11587

D119 3.13696 0.00012 0.00719 -0.00110 0.00609 -3.14014

D120 -0.00288 0.00006 0.02470 0.00578 0.03047 0.02759

D121 3.13835 0.00006 0.01178 -0.00373 0.00806 -3.13678

D122 -0.00384 0.00004 0.00443 0.00202 0.00645 0.00262

D123 -0.00022 0.00002 0.00696 -0.00407 0.00287 0.00265

D124 3.14078 -0.00001 -0.00039 0.00167 0.00127 -3.14114

D125 -3.13508 -0.00015 -0.01768 0.00299 -0.01475 3.13336

D126 -0.00445 0.00008 0.03834 0.00509 0.04345 0.03900

D127 0.00445 -0.00008 -0.03834 -0.00509 -0.04345 -0.03900

D128 3.13508 0.00015 0.01768 -0.00299 0.01475 -3.13336

Item Value Threshold Converged?

Maximum Force 0.001298 0.000450 NO

RMS Force 0.000221 0.000300 YES

Maximum Displacement 0.120210 0.001800 NO

RMS Displacement 0.009484 0.001200 NO

Predicted change in Energy=-2.051809D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Wed Jul 31 00:49:45 2019, MaxMem= 4294967296 cpu: 1.1

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -4.289779 0.679509 -0.027076

2 6 0 -2.901261 1.109319 -0.020877

3 7 0 -2.093909 0.000000 -0.017603

4 6 0 -2.901261 -1.109319 -0.020877

5 6 0 -4.289779 -0.679509 -0.027076

6 6 0 -2.468833 -2.445597 -0.020775

7 6 0 -1.106669 -2.909645 -0.020307

8 7 0 -0.000000 -2.099455 -0.014444

9 6 0 1.106669 -2.909645 -0.020307

10 6 0 0.692003 -4.274832 -0.029825

11 6 0 -0.692003 -4.274832 -0.029825

12 6 0 -2.468833 2.445597 -0.020775

13 6 0 -1.106669 2.909645 -0.020307

14 6 0 -0.692003 4.274832 -0.029825

15 6 0 0.692003 4.274832 -0.029825

16 6 0 1.106669 2.909645 -0.020307

17 7 0 0.000000 2.099455 -0.014444

18 6 0 2.468833 2.445597 -0.020775

19 6 0 2.901261 1.109319 -0.020877

20 6 0 4.289779 0.679509 -0.027076

21 6 0 4.289779 -0.679509 -0.027076

22 6 0 2.901261 -1.109319 -0.020877

23 7 0 2.093909 -0.000000 -0.017603

24 1 0 -5.147043 1.336876 -0.032007

25 1 0 -5.147043 -1.336876 -0.032007

26 1 0 1.346218 -5.134656 -0.037256

27 1 0 -1.346218 -5.134656 -0.037256

28 1 0 -1.346218 5.134656 -0.037256

29 1 0 1.346218 5.134656 -0.037256

30 1 0 5.147043 1.336876 -0.032007

31 1 0 5.147043 -1.336876 -0.032007

32 30 0 0.000000 -0.000000 0.035159

33 6 0 2.468833 -2.445597 -0.020775

34 6 0 3.476349 -3.452260 -0.023958

35 6 0 -3.476349 3.452260 -0.023958

36 6 0 4.316379 -4.320923 -0.026436

37 6 0 -4.316379 4.320923 -0.026436

38 6 0 -3.476349 -3.452260 -0.023958

39 6 0 -4.316379 -4.320923 -0.026436

40 6 0 3.476349 3.452260 -0.023958

41 6 0 4.316379 4.320923 -0.026436

42 1 0 5.061893 5.083968 -0.028764

43 1 0 5.061893 -5.083968 -0.028764

44 1 0 -5.061893 -5.083968 -0.028764

45 1 0 -5.061893 5.083968 -0.028764

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.453532 0.000000

3 N 2.298623 1.372012 0.000000

4 C 2.264492 2.218637 1.372012 0.000000

5 C 1.359018 2.264492 2.298623 1.453532 0.000000

6 C 3.616928 3.581120 2.474171 1.404505 2.536720

7 C 4.797318 4.401435 3.072569 2.541995 3.886610

8 N 5.111263 4.325921 2.965161 3.065572 4.518696

9 C 6.481028 5.675877 4.325476 4.393709 5.839110

10 C 7.025927 6.473076 5.102514 4.788748 6.143656

11 C 6.122866 5.819792 4.498853 3.860230 5.086290

12 C 2.536720 1.404505 2.474171 3.581120 3.616928

13 C 3.886610 2.541995 3.072569 4.401435 4.797318

14 C 5.086290 3.860230 4.498853 5.819792 6.122866

15 C 6.143656 4.788748 5.102514 6.473076 7.025927

16 C 5.839110 4.393709 4.325476 5.675877 6.481028

17 N 4.518696 3.065572 2.965161 4.325921 5.111263

18 C 6.985552 5.533855 5.176830 6.440135 7.446151

19 C 7.203876 5.802523 5.116867 6.212216 7.410196

20 C 8.579558 7.203876 6.419758 7.410196 8.686526

21 C 8.686526 7.410196 6.419758 7.203876 8.579558

22 C 7.410196 6.212216 5.116867 5.802523 7.203876

23 N 6.419758 5.116867 4.187818 5.116867 6.419758

24 H 1.080305 2.257308 3.333028 3.320772 2.191058

25 H 2.191058 3.320772 3.333028 2.257308 1.080305

26 H 8.097474 7.551726 6.180579 5.851896 7.184212

27 H 6.516837 6.434722 5.188845 4.315294 5.339755

28 H 5.339755 4.315294 5.188845 6.434722 6.516837

29 H 7.184212 5.851896 6.180579 7.551726 8.097474

30 H 9.459692 8.051529 7.363344 8.411849 9.649842

31 H 9.649842 8.411849 7.363344 8.051529 9.459692

32 Zn 4.343709 3.106613 2.094574 3.106613 4.343709

33 C 7.446151 6.440135 5.176830 5.533855 6.985552

34 C 8.796833 7.841041 6.553314 6.794358 8.246266

35 C 2.889607 2.412491 3.718774 4.597688 4.211080

36 C 9.953405 9.032269 7.730605 7.899922 9.344830

37 C 3.641512 3.509557 4.858995 5.611605 5.000503

38 C 4.211080 4.597688 3.718774 2.412491 2.889607

39 C 5.000503 5.611605 4.858995 3.509557 3.641512

40 C 8.246266 6.794358 6.553314 7.841041 8.796833

41 C 9.344830 7.899922 7.730605 9.032269 9.953405

42 H 10.336974 8.899985 8.777947 10.088047 10.985055

43 H 10.985055 10.088047 8.777947 8.899985 10.336974

44 H 5.814966 6.559359 5.886916 4.523962 4.471624

45 H 4.471624 4.523962 5.886916 6.559359 5.814966

6 7 8 9 10

6 C 0.000000

7 C 1.439038 0.000000

8 N 2.492988 1.371553 0.000000

9 C 3.605490 2.213338 1.371553 0.000000

10 C 3.651995 2.258107 2.282842 1.426806 0.000000

11 C 2.550159 1.426806 2.282842 2.258107 1.384006

12 C 4.891194 5.525767 5.172299 6.439164 7.426650

13 C 5.525767 5.819290 5.129896 6.225994 7.406215

14 C 6.951358 7.196440 6.411758 7.406215 8.660960

15 C 7.426650 7.406215 6.411758 7.196440 8.549664

16 C 6.439164 6.225994 5.129896 5.819290 7.196440

17 N 5.172299 5.129896 4.198911 5.129896 6.411758

18 C 6.950131 6.439164 5.172299 5.525767 6.951358

19 C 6.440135 5.675877 4.325921 4.401435 5.819792

20 C 7.446151 6.481028 5.111263 4.797318 6.122866

21 C 6.985552 5.839110 4.518696 3.886610 5.086290

22 C 5.533855 4.393709 3.065572 2.541995 3.860230

23 N 5.176830 4.325476 2.965161 3.072569 4.498853

24 H 4.634656 5.861544 6.188759 7.559232 8.098502

25 H 2.898654 4.335707 5.203257 6.448461 6.536516

26 H 4.667540 3.311739 3.320431 2.237933 1.080440

27 H 2.914030 2.237933 3.320431 3.311739 2.212170

28 H 7.662947 8.047884 7.358341 8.409977 9.627713

29 H 8.486172 8.409977 7.358341 8.047884 9.432206

30 H 8.503458 7.559232 6.188759 5.861544 7.165100

31 H 7.696165 6.448461 5.203257 4.335707 5.336569

32 Zn 3.475516 3.113491 2.100041 3.113491 4.330968

33 C 4.937666 3.605490 2.492988 1.439038 2.550159

34 C 6.029807 4.615030 3.730305 2.431014 2.903316

35 C 5.983295 6.788905 6.550316 7.840785 8.779701

36 C 7.039601 5.603677 4.854502 3.506277 3.624670

37 C 7.014218 7.910966 7.736442 9.038285 9.948412

38 C 1.424244 2.431014 3.730305 4.615030 4.248743

39 C 2.632548 3.506277 4.854502 5.603677 5.008595

40 C 8.374361 7.840785 6.550316 6.788905 8.213439

41 C 9.582532 9.038285 7.736442 7.910966 9.328619

42 H 10.649237 10.096984 8.787749 8.918616 10.328750

43 H 7.979530 6.540559 5.876247 4.513485 4.444170

44 H 3.699328 4.513485 5.876247 6.540559 5.810510

45 H 7.963565 8.918616 8.787749 10.096984 10.986103

11 12 13 14 15

11 C 0.000000

12 C 6.951358 0.000000

13 C 7.196440 1.439038 0.000000

14 C 8.549664 2.550159 1.426806 0.000000

15 C 8.660960 3.651995 2.258107 1.384006 0.000000

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17 N 6.411758 2.492988 1.371553 2.282842 2.282842

18 C 7.426650 4.937666 3.605490 3.651995 2.550159

19 C 6.473076 5.533855 4.393709 4.788748 3.860230

20 C 7.025927 6.985552 5.839110 6.143656 5.086290

21 C 6.143656 7.446151 6.481028 7.025927 6.122866

22 C 4.788748 6.440135 5.675877 6.473076 5.819792

23 N 5.102514 5.176830 4.325476 5.102514 4.498853

24 H 7.165100 2.898654 4.335707 5.336569 6.536516

25 H 5.336569 4.634656 5.861544 7.165100 8.098502

26 H 2.212170 8.486172 8.409977 9.627713 9.432206

27 H 1.080440 7.662947 8.047884 9.432206 9.627713

28 H 9.432206 2.914030 2.237933 1.080440 2.212170

29 H 9.627713 4.667540 3.311739 2.212170 1.080440

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32 Zn 4.330968 3.475516 3.113491 4.330968 4.330968

33 C 3.651995 6.950131 6.439164 7.426650 6.951358

34 C 4.248743 8.374361 7.840785 8.779701 8.213439

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36 C 5.008595 9.582532 9.038285 9.948412 9.328619

37 C 9.328619 2.632548 3.506277 3.624670 5.008595

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39 C 3.624670 7.014218 7.910966 9.328619 9.948412

40 C 8.779701 6.029807 4.615030 4.248743 2.903316

41 C 9.948412 7.039601 5.603677 5.008595 3.624670

42 H 10.986103 7.979530 6.540559 5.810510 4.444170

43 H 5.810510 10.649237 10.096984 10.986103 10.328750

44 H 4.444170 7.963565 8.918616 10.328750 10.986103

45 H 10.328750 3.699328 4.513485 4.444170 5.810510

16 17 18 19 20

16 C 0.000000

17 N 1.371553 0.000000

18 C 1.439038 2.492988 0.000000

19 C 2.541995 3.065572 1.404505 0.000000

20 C 3.886610 4.518696 2.536720 1.453532 0.000000

21 C 4.797318 5.111263 3.616928 2.264492 1.359018

22 C 4.401435 4.325921 3.581120 2.218637 2.264492

23 N 3.072569 2.965161 2.474171 1.372012 2.298623

24 H 6.448461 5.203257 7.696165 8.051529 9.459692

25 H 7.559232 6.188759 8.503458 8.411849 9.649842

26 H 8.047884 7.358341 7.662947 6.434722 6.516837

27 H 8.409977 7.358341 8.486172 7.551726 8.097474

28 H 3.311739 3.320431 4.667540 5.851896 7.184212

29 H 2.237933 3.320431 2.914030 4.315294 5.339755

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31 H 5.861544 6.188759 4.634656 3.320772 2.191058

32 Zn 3.113491 2.100041 3.475516 3.106613 4.343709

33 C 5.525767 5.172299 4.891194 3.581120 3.616928

34 C 6.788905 6.550316 5.983295 4.597688 4.211080

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37 C 5.603677 4.854502 7.039601 7.899922 9.344830

38 C 7.840785 6.550316 8.374361 7.841041 8.796833

39 C 9.038285 7.736442 9.582532 9.032269 9.953405

40 C 2.431014 3.730305 1.424244 2.412491 2.889607

41 C 3.506277 4.854502 2.632548 3.509557 3.641512

42 H 4.513485 5.876247 3.699328 4.523962 4.471624

43 H 8.918616 8.787749 7.963565 6.559359 5.814966

44 H 10.096984 8.787749 10.649237 10.088047 10.985055

45 H 6.540559 5.876247 7.979530 8.899985 10.336974

21 22 23 24 25

21 C 0.000000

22 C 1.453532 0.000000

23 N 2.298623 1.372012 0.000000

24 H 9.649842 8.411849 7.363344 0.000000

25 H 9.459692 8.051529 7.363344 2.673753 0.000000

26 H 5.339755 4.315294 5.188845 9.167508 7.522340

27 H 7.184212 5.851896 6.180579 7.505133 5.373027

28 H 8.097474 7.551726 6.180579 5.373027 7.505133

29 H 6.516837 6.434722 5.188845 7.522340 9.167508

30 H 2.191058 3.320772 3.333028 10.294086 10.635655

31 H 1.080305 2.257308 3.333028 10.635655 10.294086

32 Zn 4.343709 3.106613 2.094574 5.318252 5.318252

33 C 2.536720 1.404505 2.474171 8.503458 7.696165

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35 C 8.796833 7.841041 6.553314 2.695576 5.072190

36 C 3.641512 3.509557 4.858995 11.025746 9.922748

37 C 9.953405 9.032269 7.730605 3.097510 5.718455

38 C 8.246266 6.794358 6.553314 5.072190 2.695576

39 C 9.344830 7.899922 7.730605 5.718455 3.097510

40 C 4.211080 4.597688 3.718774 8.879066 9.864015

41 C 5.000503 5.611605 4.858995 9.922748 11.025746

42 H 5.814966 6.559359 5.886916 10.874883 12.060250

43 H 4.471624 4.523962 5.886916 12.060250 10.874883

44 H 10.336974 8.899985 8.777947 6.421410 3.748060

45 H 10.985055 10.088047 8.777947 3.748060 6.421410

26 27 28 29 30

26 H 0.000000

27 H 2.692437 0.000000

28 H 10.616401 10.269311 0.000000

29 H 10.269311 10.616401 2.692437 0.000000

30 H 7.505133 9.167508 7.522340 5.373027 0.000000

31 H 5.373027 7.522340 9.167508 7.505133 2.673753

32 Zn 5.308694 5.308694 5.308694 5.308694 5.318252

33 C 2.914030 4.667540 8.486172 7.662947 4.634656

34 C 2.714422 5.107621 9.848475 8.847190 5.072190

35 C 9.848475 8.847190 2.714422 5.107621 8.879066

36 C 3.079631 5.720777 11.021484 9.911102 5.718455

37 C 11.021484 9.911102 3.079631 5.720777 9.922748

38 C 5.107621 2.714422 8.847190 9.848475 9.864015

39 C 5.720777 3.079631 9.911102 11.021484 11.025746

40 C 8.847190 9.848475 5.107621 2.714422 2.695576

41 C 9.911102 11.021484 5.720777 3.079631 3.097510

42 H 10.873205 12.061684 6.408318 3.716030 3.748060

43 H 3.716030 6.408318 12.061684 10.873205 6.421410

44 H 6.408318 3.716030 10.873205 12.061684 12.060250

45 H 12.061684 10.873205 3.716030 6.408318 10.874883

31 32 33 34 35

31 H 0.000000

32 Zn 5.318252 0.000000

33 C 2.898654 3.475516 0.000000

34 C 2.695576 4.899653 1.424244 0.000000

35 C 9.864015 4.899653 8.374361 9.798593 0.000000

36 C 3.097510 6.107806 2.632548 1.208400 11.006771

37 C 11.025746 6.107806 9.582532 11.006771 1.208400

38 C 8.879066 4.899653 6.029807 6.952698 6.904521

39 C 9.922748 6.107806 7.039601 7.840994 7.818442

40 C 5.072190 4.899653 5.983295 6.904521 6.952698

41 C 5.718455 6.107806 7.014218 7.818442 7.840994

42 H 6.421410 7.174509 7.963565 8.682233 8.692760

43 H 3.748060 7.174509 3.699328 2.275180 12.073475

44 H 10.874883 7.174509 7.979530 8.692760 8.682233

45 H 12.060250 7.174509 10.649237 12.073475 2.275180

36 37 38 39 40

36 C 0.000000

37 C 12.214991 0.000000

38 C 7.840994 7.818442 0.000000

39 C 8.632757 8.641847 1.208400 0.000000

40 C 7.818442 7.840994 9.798593 11.006771 0.000000

41 C 8.641847 8.632757 11.006771 12.214991 1.208400

42 H 9.434393 9.409263 12.073475 13.281716 2.275180

43 H 1.066787 13.281716 8.692760 9.409263 8.682233

44 H 9.409263 9.434393 2.275180 1.066787 12.073475

45 H 13.281716 1.066787 8.682233 9.434393 8.692760

41 42 43 44 45

41 C 0.000000

42 H 1.066787 0.000000

43 H 9.434393 10.167935 0.000000

44 H 13.281716 14.348448 10.123787 0.000000

45 H 9.409263 10.123787 14.348448 10.167935 0.000000

Stoichiometry C28H12N4Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C28H12)]

Deg. of freedom 34

Full point group C2V NOp 4

RotChk: IX=0 Diff= 1.67D-13

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.679509 4.289779 -0.010907

2 6 0 1.109319 2.901261 -0.004709

3 7 0 0.000000 2.093909 -0.001434

4 6 0 -1.109319 2.901261 -0.004709

5 6 0 -0.679509 4.289779 -0.010907

6 6 0 -2.445597 2.468833 -0.004607

7 6 0 -2.909645 1.106669 -0.004139

8 7 0 -2.099455 0.000000 0.001725

9 6 0 -2.909645 -1.106669 -0.004139

10 6 0 -4.274832 -0.692003 -0.013656

11 6 0 -4.274832 0.692003 -0.013656

12 6 0 2.445597 2.468833 -0.004607

13 6 0 2.909645 1.106669 -0.004139

14 6 0 4.274832 0.692003 -0.013656

15 6 0 4.274832 -0.692003 -0.013656

16 6 0 2.909645 -1.106669 -0.004139

17 7 0 2.099455 -0.000000 0.001725

18 6 0 2.445597 -2.468833 -0.004607

19 6 0 1.109319 -2.901261 -0.004709

20 6 0 0.679509 -4.289779 -0.010907

21 6 0 -0.679509 -4.289779 -0.010907

22 6 0 -1.109319 -2.901261 -0.004709

23 7 0 -0.000000 -2.093909 -0.001434

24 1 0 1.336876 5.147043 -0.015838

25 1 0 -1.336876 5.147043 -0.015838

26 1 0 -5.134656 -1.346218 -0.021088

27 1 0 -5.134656 1.346218 -0.021088

28 1 0 5.134656 1.346218 -0.021088

29 1 0 5.134656 -1.346218 -0.021088

30 1 0 1.336876 -5.147043 -0.015838

31 1 0 -1.336876 -5.147043 -0.015838

32 30 0 0.000000 0.000000 0.051327

33 6 0 -2.445597 -2.468833 -0.004607

34 6 0 -3.452260 -3.476349 -0.007790

35 6 0 3.452260 3.476349 -0.007790

36 6 0 -4.320923 -4.316379 -0.010268

37 6 0 4.320923 4.316379 -0.010268

38 6 0 -3.452260 3.476349 -0.007790

39 6 0 -4.320923 4.316379 -0.010268

40 6 0 3.452260 -3.476349 -0.007790

41 6 0 4.320923 -4.316379 -0.010268

42 1 0 5.083968 -5.061893 -0.012596

43 1 0 -5.083968 -5.061893 -0.012596

44 1 0 -5.083968 5.061893 -0.012596

45 1 0 5.083968 5.061893 -0.012596

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

Rotational constants (GHZ): 0.1460034 0.1453728 0.0728478

Leave Link 202 at Wed Jul 31 00:49:46 2019, MaxMem= 4294967296 cpu: 0.2

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

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

Pseudo-potential data read from rwf file.

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

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

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

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

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

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

111 alpha electrons 110 beta electrons

nuclear repulsion energy 3052.2875112999 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= 13 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= -0.1303499983 Hartrees.

Nuclear repulsion after empirical dispersion term = 3052.1571613015 Hartrees.

No density basis found on file 724.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

2nd derivatives : Analytical E(r).r(xy)/FMM algorithm (CHGder, D2EAlg=3).

Cavity 2nd derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3874

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.12D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 84

GePol: Fraction of low-weight points (<1% of avg) = 2.17%

GePol: Cavity surface area = 416.395 Ang\*\*2

GePol: Cavity volume = 420.969 Ang\*\*3

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

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

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PCM non-electrostatic energy = 0.0083847238 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3052.1655460254 Hartrees.

Leave Link 301 at Wed Jul 31 00:49:46 2019, MaxMem= 4294967296 cpu: 1.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16173 LenP2D= 44686.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.47D-05 NBF= 172 148 158 158

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

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Wed Jul 31 00:49:46 2019, MaxMem= 4294967296 cpu: 10.8

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

DipDrv: MaxL=1.

Leave Link 303 at Wed Jul 31 00:49:46 2019, MaxMem= 4294967296 cpu: 1.3

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

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

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 1.000000 0.000000 -0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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The electronic state of the initial guess is 2-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7630 S= 0.5065

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1359.66926568194

Leave Link 401 at Wed Jul 31 00:49:49 2019, MaxMem= 4294967296 cpu: 41.2

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1387497 IEndB= 1387497 NGot= 4294967296 MDV= 4294047352

LenX= 4294047352 LenY= 4293596440

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= 650000000 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= 45023628.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.11D-15 for 3871.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.81D-15 for 999 855.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.33D-15 for 3871.

Iteration 1 A^-1\*A deviation from orthogonality is 4.97D-15 for 3178 3160.

E= -1359.18202070211

DIIS: error= 1.18D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.18202070211 IErMin= 1 ErrMin= 1.18D-03

ErrMax= 1.18D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.32D-03 BMatP= 1.32D-03

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

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.388 Goal= None Shift= 0.000

Gap= 0.438 Goal= None Shift= 0.000

GapD= 0.388 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

RMSDP=1.20D-04 MaxDP=6.33D-03 OVMax= 5.45D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.20D-04 CP: 1.00D+00

E= -1359.18244030979 Delta-E= -0.000419607680 Rises=F Damp=F

DIIS: error= 8.82D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.18244030979 IErMin= 2 ErrMin= 8.82D-05

ErrMax= 8.82D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.52D-05 BMatP= 1.32D-03

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

Coeff-Com: -0.203D-01 0.102D+01

Coeff: -0.203D-01 0.102D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=9.89D-06 MaxDP=2.41D-04 DE=-4.20D-04 OVMax= 7.33D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 8.67D-06 CP: 1.00D+00 1.04D+00

E= -1359.18244477438 Delta-E= -0.000004464590 Rises=F Damp=F

DIIS: error= 8.20D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.18244477438 IErMin= 3 ErrMin= 8.20D-05

ErrMax= 8.20D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.34D-06 BMatP= 1.52D-05

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

Coeff-Com: -0.165D-01 0.445D+00 0.572D+00

Coeff: -0.165D-01 0.445D+00 0.572D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=3.40D-06 MaxDP=1.81D-04 DE=-4.46D-06 OVMax= 7.02D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.71D-06 CP: 1.00D+00 1.04D+00 7.63D-01

E= -1359.18244621712 Delta-E= -0.000001442735 Rises=F Damp=F

DIIS: error= 6.15D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.18244621712 IErMin= 4 ErrMin= 6.15D-05

ErrMax= 6.15D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.35D-06 BMatP= 9.34D-06

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

Coeff-Com: -0.746D-02 0.142D+00 0.377D+00 0.488D+00

Coeff: -0.746D-02 0.142D+00 0.377D+00 0.488D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=1.42D-06 MaxDP=9.49D-05 DE=-1.44D-06 OVMax= 3.14D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.10D-06 CP: 1.00D+00 1.04D+00 7.70D-01 6.68D-01

E= -1359.18244696843 Delta-E= -0.000000751310 Rises=F Damp=F

DIIS: error= 8.84D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.18244696843 IErMin= 5 ErrMin= 8.84D-06

ErrMax= 8.84D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.23D-07 BMatP= 3.35D-06

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

Coeff-Com: -0.109D-02 0.263D-02 0.909D-01 0.207D+00 0.700D+00

Coeff: -0.109D-02 0.263D-02 0.909D-01 0.207D+00 0.700D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=3.23D-07 MaxDP=1.52D-05 DE=-7.51D-07 OVMax= 4.56D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.66D-07 CP: 1.00D+00 1.04D+00 7.82D-01 7.12D-01 9.15D-01

E= -1359.18244699530 Delta-E= -0.000000026869 Rises=F Damp=F

DIIS: error= 3.18D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.18244699530 IErMin= 6 ErrMin= 3.18D-06

ErrMax= 3.18D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.81D-08 BMatP= 1.23D-07

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

Coeff-Com: 0.285D-03-0.156D-01 0.387D-02 0.501D-01 0.349D+00 0.613D+00

Coeff: 0.285D-03-0.156D-01 0.387D-02 0.501D-01 0.349D+00 0.613D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=1.22D-07 MaxDP=5.56D-06 DE=-2.69D-08 OVMax= 1.42D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 8.05D-08 CP: 1.00D+00 1.04D+00 7.88D-01 7.20D-01 9.19D-01

CP: 7.34D-01

E= -1359.18244699957 Delta-E= -0.000000004268 Rises=F Damp=F

DIIS: error= 9.07D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.18244699957 IErMin= 7 ErrMin= 9.07D-07

ErrMax= 9.07D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.84D-10 BMatP= 1.81D-08

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

Coeff-Com: 0.166D-03-0.696D-02-0.125D-02 0.146D-01 0.126D+00 0.268D+00

Coeff-Com: 0.600D+00

Coeff: 0.166D-03-0.696D-02-0.125D-02 0.146D-01 0.126D+00 0.268D+00

Coeff: 0.600D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=3.11D-08 MaxDP=1.26D-06 DE=-4.27D-09 OVMax= 4.61D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.87D-08 CP: 1.00D+00 1.04D+00 7.88D-01 7.21D-01 9.22D-01

CP: 7.38D-01 8.98D-01

E= -1359.18244699968 Delta-E= -0.000000000116 Rises=F Damp=F

DIIS: error= 6.71D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.18244699968 IErMin= 8 ErrMin= 6.71D-07

ErrMax= 6.71D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.98D-10 BMatP= 7.84D-10

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

Coeff-Com: 0.451D-04-0.107D-02-0.140D-02-0.127D-02 0.517D-02 0.356D-01

Coeff-Com: 0.376D+00 0.587D+00

Coeff: 0.451D-04-0.107D-02-0.140D-02-0.127D-02 0.517D-02 0.356D-01

Coeff: 0.376D+00 0.587D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=1.49D-08 MaxDP=8.63D-07 DE=-1.16D-10 OVMax= 3.48D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.29D-08 CP: 1.00D+00 1.04D+00 7.89D-01 7.21D-01 9.22D-01

CP: 7.48D-01 9.65D-01 8.80D-01

E= -1359.18244699984 Delta-E= -0.000000000161 Rises=F Damp=F

DIIS: error= 2.48D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1359.18244699984 IErMin= 9 ErrMin= 2.48D-07

ErrMax= 2.48D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.42D-11 BMatP= 2.98D-10

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

Coeff-Com: -0.190D-04 0.129D-02-0.347D-03-0.465D-02-0.316D-01-0.537D-01

Coeff-Com: 0.561D-01 0.319D+00 0.714D+00

Coeff: -0.190D-04 0.129D-02-0.347D-03-0.465D-02-0.316D-01-0.537D-01

Coeff: 0.561D-01 0.319D+00 0.714D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=8.50D-09 MaxDP=4.90D-07 DE=-1.61D-10 OVMax= 2.23D-06

Error on total polarization charges = 0.06718

SCF Done: E(UB3LYP) = -1359.18244700 A.U. after 9 cycles

NFock= 9 Conv=0.85D-08 -V/T= 1.9682

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7631 S= 0.5065

<L.S>= 0.000000000000E+00

KE= 1.403854552527D+03 PE=-9.373860468409D+03 EE= 3.558657922857D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.26

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7631, after 0.7501

Leave Link 502 at Wed Jul 31 00:50:44 2019, MaxMem= 4294967296 cpu: 841.8

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 636

NBasis= 636 NAE= 111 NBE= 110 NFC= 0 NFV= 0

NROrb= 636 NOA= 111 NOB= 110 NVA= 525 NVB= 526

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.13767955D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.38365040D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.13995891D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.88362612D-01

Leave Link 801 at Wed Jul 31 00:50:44 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 45.

Will process 46 centers per pass.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16173 LenP2D= 44686.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 11 by ecpmxn.

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

Leave Link 1101 at Wed Jul 31 00:50:47 2019, MaxMem= 4294967296 cpu: 45.0

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Wed Jul 31 00:50:47 2019, MaxMem= 4294967296 cpu: 1.1

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 45.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966832.

G2DrvN: will do 46 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

G2PCM: DoFxE=T DoFxN=T DoGrad=T DoDP/DQ/DG/TGxP=FFFF NFrqRd= 0 IEInf=0 SqF1=F DoCFld=F IF1Alg=4.

GePol: Maximum number of non-zero 1st derivatives = 255

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Wed Jul 31 00:52:44 2019, MaxMem= 4294967296 cpu: 1877.0

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=111111111111111111111111111111111111111111111

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Using symmetry in CPHF.

Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.

Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.

NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 4294965570 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 0.

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

IRaf= 650000000 NMat= 42 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

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

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

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

NMat0= 42 NMatS0= 42 NMatT0= 0 NMatD0= 42 NMtDS0= 0 NMtDT0= 0

Integrals replicated using symmetry in FoFCou.

There are 42 degrees of freedom in the 1st order CPHF. IDoFFX=4 NUNeed= 42.

42 vectors produced by pass 0 Test12= 2.77D-13 2.38D-09 XBig12= 8.06D+03 5.92D+01.

AX will form 42 AO Fock derivatives at one time.

42 vectors produced by pass 1 Test12= 2.77D-13 2.38D-09 XBig12= 1.08D+03 6.86D+00.

42 vectors produced by pass 2 Test12= 2.77D-13 2.38D-09 XBig12= 2.82D+02 5.66D+00.

42 vectors produced by pass 3 Test12= 2.77D-13 2.38D-09 XBig12= 7.68D+01 2.04D+00.

42 vectors produced by pass 4 Test12= 2.77D-13 2.38D-09 XBig12= 7.10D+00 4.61D-01.

42 vectors produced by pass 5 Test12= 2.77D-13 2.38D-09 XBig12= 2.51D-01 5.05D-02.

42 vectors produced by pass 6 Test12= 2.77D-13 2.38D-09 XBig12= 8.71D-03 7.32D-03.

42 vectors produced by pass 7 Test12= 2.77D-13 2.38D-09 XBig12= 1.92D-04 1.18D-03.

38 vectors produced by pass 8 Test12= 2.77D-13 2.38D-09 XBig12= 3.43D-06 1.33D-04.

23 vectors produced by pass 9 Test12= 2.77D-13 2.38D-09 XBig12= 4.45D-08 1.74D-05.

5 vectors produced by pass 10 Test12= 2.77D-13 2.38D-09 XBig12= 5.08D-10 1.54D-06.

2 vectors produced by pass 11 Test12= 2.77D-13 2.38D-09 XBig12= 5.99D-12 1.58D-07.

2 vectors produced by pass 12 Test12= 2.77D-13 2.38D-09 XBig12= 8.22D-14 1.93D-08.

InvSVY: IOpt=1 It= 1 EMax= 2.84D-14

Solved reduced A of dimension 406 with 42 vectors.

FullF1: Do perturbations 1 to 42.

Isotropic polarizability for W= 0.000000 1006.32 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Wed Jul 31 01:49:54 2019, MaxMem= 4294967296 cpu: 54876.7

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16173 LenP2D= 44686.

LDataN: DoStor=T MaxTD1= 7 Len= 274

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 255

Leave Link 701 at Wed Jul 31 01:50:29 2019, MaxMem= 4294967296 cpu: 552.8

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

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

Leave Link 702 at Wed Jul 31 01:50:29 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

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

wScrn= 0.000000 ICntrl= 100127 IOpCl= 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 Wed Jul 31 01:52:19 2019, MaxMem= 4294967296 cpu: 1768.7

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

Dipole = 2.23196461D-13 4.68097783D-14 1.19723985D-01

Polarizability= 1.65285348D+03 1.15335693D-05 1.17897021D+03

-1.35064373D-05-5.23966165D-06 1.87125315D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000011684 -0.000214517 -0.000001175

2 6 0.000023202 -0.000031235 -0.000007684

3 7 -0.000346472 0.000000000 0.001316370

4 6 0.000023202 0.000031235 -0.000007684

5 6 0.000011684 0.000214517 -0.000001175

6 6 0.000073852 0.000052908 -0.000004040

7 6 -0.000160854 0.000022565 -0.000007916

8 7 -0.000000000 -0.000226094 0.001200912

9 6 0.000160854 0.000022565 -0.000007916

10 6 -0.000196340 -0.000011234 -0.000000653

11 6 0.000196340 -0.000011234 -0.000000653

12 6 0.000073852 -0.000052908 -0.000004040

13 6 -0.000160854 -0.000022565 -0.000007916

14 6 0.000196340 0.000011234 -0.000000653

15 6 -0.000196340 0.000011234 -0.000000653

16 6 0.000160854 -0.000022565 -0.000007916

17 7 -0.000000000 0.000226094 0.001200912

18 6 -0.000073852 -0.000052908 -0.000004040

19 6 -0.000023202 -0.000031235 -0.000007684

20 6 -0.000011684 -0.000214517 -0.000001175

21 6 -0.000011684 0.000214517 -0.000001175

22 6 -0.000023202 0.000031235 -0.000007684

23 7 0.000346472 -0.000000000 0.001316370

24 1 -0.000007995 -0.000009504 -0.000000411

25 1 -0.000007995 0.000009504 -0.000000411

26 1 -0.000003686 -0.000003808 -0.000000360

27 1 0.000003686 -0.000003808 -0.000000360

28 1 0.000003686 0.000003808 -0.000000360

29 1 -0.000003686 0.000003808 -0.000000360

30 1 0.000007995 -0.000009504 -0.000000411

31 1 0.000007995 0.000009504 -0.000000411

32 30 0.000000000 -0.000000000 -0.004947941

33 6 -0.000073852 0.000052908 -0.000004040

34 6 -0.000013488 -0.000019350 0.000009875

35 6 0.000013488 0.000019350 0.000009875

36 6 -0.000028683 -0.000000326 -0.000006356

37 6 0.000028683 0.000000326 -0.000006356

38 6 0.000013488 -0.000019350 0.000009875

39 6 0.000028683 -0.000000326 -0.000006356

40 6 -0.000013488 0.000019350 0.000009875

41 6 -0.000028683 0.000000326 -0.000006356

42 1 0.000020586 0.000006607 -0.000002936

43 1 0.000020586 -0.000006607 -0.000002936

44 1 -0.000020586 -0.000006607 -0.000002936

45 1 -0.000020586 0.000006607 -0.000002936

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

Cartesian Forces: Max 0.004947941 RMS 0.000484330

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

Leave Link 716 at Wed Jul 31 01:52:19 2019, MaxMem= 4294967296 cpu: 0.8

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.001085513 RMS 0.000197286

Search for a local minimum.

Step number 6 out of a maximum of 270

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

RMS Force = .19729D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= 2.17D-04 DEPred=-2.05D-04 R=-1.06D+00

Trust test=-1.06D+00 RLast= 1.88D-01 DXMaxT set to 7.50D-02

ITU= -1 0 0 -1 0 0

Eigenvalues --- 0.00140 0.00336 0.00433 0.00482 0.00605

Eigenvalues --- 0.00935 0.01075 0.01120 0.01137 0.01156

Eigenvalues --- 0.01165 0.01230 0.01271 0.01276 0.01319

Eigenvalues --- 0.01398 0.01504 0.01520 0.01677 0.01744

Eigenvalues --- 0.01834 0.01925 0.01937 0.01966 0.01985

Eigenvalues --- 0.02005 0.02088 0.02099 0.02119 0.02122

Eigenvalues --- 0.02998 0.03115 0.03193 0.03569 0.03999

Eigenvalues --- 0.04120 0.04121 0.04125 0.04135 0.04147

Eigenvalues --- 0.04341 0.04356 0.06112 0.06202 0.08247

Eigenvalues --- 0.08251 0.08261 0.08598 0.08838 0.08874

Eigenvalues --- 0.09045 0.09152 0.09207 0.09327 0.09609

Eigenvalues --- 0.09628 0.09652 0.09718 0.10408 0.10408

Eigenvalues --- 0.10442 0.10500 0.12366 0.13246 0.13360

Eigenvalues --- 0.13407 0.15720 0.16905 0.16957 0.19276

Eigenvalues --- 0.19818 0.20051 0.20094 0.20350 0.20631

Eigenvalues --- 0.20660 0.20823 0.21622 0.21826 0.21896

Eigenvalues --- 0.21977 0.25998 0.26211 0.27691 0.27986

Eigenvalues --- 0.28013 0.29411 0.30003 0.31700 0.32499

Eigenvalues --- 0.32761 0.32846 0.33590 0.35684 0.35695

Eigenvalues --- 0.35845 0.36108 0.36446 0.37028 0.37101

Eigenvalues --- 0.37160 0.37327 0.37391 0.37567 0.37855

Eigenvalues --- 0.38051 0.38323 0.38809 0.39208 0.40235

Eigenvalues --- 0.40238 0.40241 0.40241 0.41201 0.41320

Eigenvalues --- 0.41936 0.42485 0.45407 0.46133 0.46474

Eigenvalues --- 0.46684 0.50187 0.50193 0.52584 0.53003

Eigenvalues --- 1.03372 1.04117 1.04449 1.04682

En-DIIS/RFO-DIIS IScMMF= 0 using points: 6 5 4

RFO step: Lambda=-1.02939164D-04.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=T DC= 7.31D-04 SmlDif= 1.00D-05

RMS Error= 0.1953554865D-02 NUsed= 3 EDIIS=F

DidBck=T Rises=T RFO-DIIS coefs: 0.01145 0.64543 0.34313

Iteration 1 RMS(Cart)= 0.00285669 RMS(Int)= 0.00019071

Iteration 2 RMS(Cart)= 0.00002924 RMS(Int)= 0.00019009

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00019009

ITry= 1 IFail=0 DXMaxC= 3.86D-02 DCOld= 1.00D+10 DXMaxT= 7.50D-02 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 9.28D-04 for atom 37.

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

(Linear) (Quad) (Total)

R1 2.74678 0.00001 -0.00029 0.00041 0.00018 2.74696

R2 2.56817 -0.00018 -0.00245 0.00206 0.00005 2.56822

R3 2.04148 0.00000 -0.00000 0.00002 0.00001 2.04149

R4 2.59273 -0.00008 0.00008 -0.00036 -0.00032 2.59241

R5 2.65413 0.00005 -0.00098 0.00095 0.00025 2.65438

R6 2.59273 -0.00008 0.00008 -0.00036 -0.00032 2.59241

R7 3.95817 0.00015 -0.00424 0.00616 0.00172 3.95989

R8 2.74678 0.00001 -0.00029 0.00041 0.00018 2.74696

R9 2.65413 0.00005 -0.00098 0.00095 0.00025 2.65438

R10 2.04148 0.00000 -0.00000 0.00002 0.00001 2.04149

R11 2.71939 -0.00002 -0.00221 0.00205 0.00031 2.71970

R12 2.69143 0.00000 0.00026 -0.00021 0.00001 2.69144

R13 2.59186 -0.00001 0.00083 -0.00074 -0.00014 2.59172

R14 2.69627 0.00004 0.00009 0.00007 0.00014 2.69641

R15 2.59186 -0.00001 0.00083 -0.00074 -0.00014 2.59172

R16 3.96850 0.00006 -0.00279 0.00345 0.00043 3.96894

R17 2.69627 0.00004 0.00009 0.00007 0.00014 2.69641

R18 2.71939 -0.00002 -0.00221 0.00205 0.00031 2.71970

R19 2.61539 -0.00012 -0.00231 0.00187 0.00003 2.61542

R20 2.04173 0.00000 -0.00000 0.00001 0.00001 2.04174

R21 2.04173 0.00000 -0.00000 0.00001 0.00001 2.04174

R22 2.71939 -0.00002 -0.00221 0.00205 0.00031 2.71970

R23 2.69143 0.00000 0.00026 -0.00021 0.00001 2.69144

R24 2.69627 0.00004 0.00009 0.00007 0.00014 2.69641

R25 2.59186 -0.00000 0.00083 -0.00074 -0.00014 2.59172

R26 2.61539 -0.00012 -0.00231 0.00188 0.00003 2.61542

R27 2.04173 0.00000 -0.00000 0.00001 0.00001 2.04174

R28 2.69627 0.00004 0.00009 0.00007 0.00014 2.69641

R29 2.04173 0.00000 -0.00000 0.00001 0.00001 2.04174

R30 2.59186 -0.00001 0.00083 -0.00074 -0.00014 2.59172

R31 2.71939 -0.00002 -0.00221 0.00205 0.00031 2.71970

R32 3.96850 0.00007 -0.00279 0.00343 0.00043 3.96894

R33 2.65413 0.00004 -0.00098 0.00095 0.00025 2.65438

R34 2.69143 0.00000 0.00026 -0.00021 0.00001 2.69144

R35 2.74678 0.00001 -0.00029 0.00041 0.00018 2.74696

R36 2.59273 -0.00008 0.00008 -0.00036 -0.00032 2.59241

R37 2.56817 -0.00018 -0.00245 0.00206 0.00005 2.56822

R38 2.04148 0.00000 -0.00000 0.00002 0.00001 2.04149

R39 2.74678 0.00001 -0.00029 0.00041 0.00018 2.74696

R40 2.04148 0.00000 -0.00000 0.00002 0.00001 2.04149

R41 2.59273 -0.00008 0.00008 -0.00036 -0.00032 2.59241

R42 2.65413 0.00005 -0.00098 0.00095 0.00025 2.65438

R43 3.95817 0.00015 -0.00424 0.00615 0.00172 3.95989

R44 2.69143 0.00000 0.00026 -0.00021 0.00001 2.69144

R45 2.28355 -0.00000 -0.00004 0.00005 0.00001 2.28356

R46 2.28355 -0.00000 -0.00004 0.00005 0.00001 2.28356

R47 2.01593 0.00002 0.00018 -0.00013 0.00001 2.01595

R48 2.01593 0.00002 0.00018 -0.00013 0.00001 2.01595

R49 2.28355 -0.00000 -0.00004 0.00005 0.00001 2.28356

R50 2.01593 0.00002 0.00018 -0.00013 0.00001 2.01595

R51 2.28355 -0.00000 -0.00004 0.00005 0.00001 2.28356

R52 2.01593 0.00002 0.00018 -0.00013 0.00001 2.01595

A1 1.87098 0.00002 0.00007 -0.00005 0.00005 1.87103

A2 2.18723 0.00000 0.00009 0.00001 0.00008 2.18731

A3 2.22497 -0.00002 -0.00016 0.00005 -0.00013 2.22484

A4 1.89975 -0.00004 0.00071 -0.00079 -0.00035 1.89939

A5 2.18395 0.00006 -0.00063 0.00086 0.00046 2.18441

A6 2.19948 -0.00002 -0.00009 -0.00006 -0.00010 2.19938

A7 1.88331 0.00004 -0.00157 0.00170 0.00061 1.88392

A8 2.19977 -0.00002 0.00081 -0.00088 -0.00021 2.19956

A9 2.19977 -0.00002 0.00081 -0.00087 -0.00021 2.19956

A10 1.89975 -0.00004 0.00071 -0.00079 -0.00035 1.89939

A11 2.19948 -0.00001 -0.00009 -0.00007 -0.00010 2.19938

A12 2.18395 0.00006 -0.00063 0.00086 0.00046 2.18441

A13 1.87098 0.00002 0.00007 -0.00005 0.00005 1.87103

A14 2.22497 -0.00002 -0.00016 0.00005 -0.00013 2.22484

A15 2.18723 0.00000 0.00009 0.00001 0.00008 2.18731

A16 2.21211 0.00006 -0.00082 0.00100 0.00050 2.21260

A17 2.04280 0.00002 0.00109 -0.00106 -0.00023 2.04257

A18 2.02828 -0.00008 -0.00031 0.00007 -0.00027 2.02801

A19 2.18130 0.00001 -0.00023 0.00040 0.00017 2.18147

A20 2.19400 0.00007 0.00019 -0.00017 0.00019 2.19420

A21 1.90787 -0.00008 0.00002 -0.00022 -0.00036 1.90751

A22 1.87768 0.00007 -0.00091 0.00104 0.00053 1.87821

A23 2.20266 -0.00004 0.00047 -0.00060 -0.00021 2.20244

A24 2.20266 -0.00003 0.00047 -0.00061 -0.00021 2.20244

A25 1.90787 -0.00008 0.00002 -0.00022 -0.00036 1.90751

A26 2.18130 0.00001 -0.00023 0.00040 0.00017 2.18147

A27 2.19400 0.00007 0.00019 -0.00017 0.00019 2.19420

A28 1.86568 0.00004 0.00043 -0.00030 0.00009 1.86577

A29 2.19631 -0.00001 -0.00025 0.00023 0.00003 2.19634

A30 2.22120 -0.00002 -0.00018 0.00007 -0.00013 2.22107

A31 1.86568 0.00004 0.00043 -0.00030 0.00009 1.86577

A32 2.19631 -0.00001 -0.00025 0.00023 0.00003 2.19634

A33 2.22120 -0.00002 -0.00018 0.00007 -0.00013 2.22107

A34 2.21211 0.00006 -0.00082 0.00100 0.00050 2.21260

A35 2.04280 0.00002 0.00109 -0.00106 -0.00023 2.04257

A36 2.02828 -0.00008 -0.00031 0.00007 -0.00027 2.02801

A37 2.19400 0.00006 0.00019 -0.00017 0.00019 2.19420

A38 2.18130 0.00001 -0.00023 0.00040 0.00017 2.18147

A39 1.90787 -0.00007 0.00002 -0.00022 -0.00036 1.90751

A40 1.86568 0.00004 0.00043 -0.00030 0.00009 1.86577

A41 2.19631 -0.00001 -0.00025 0.00023 0.00003 2.19634

A42 2.22120 -0.00002 -0.00018 0.00007 -0.00013 2.22107

A43 1.86568 0.00004 0.00043 -0.00030 0.00009 1.86577

A44 2.22120 -0.00002 -0.00018 0.00007 -0.00013 2.22107

A45 2.19631 -0.00001 -0.00025 0.00023 0.00003 2.19634

A46 1.90787 -0.00007 0.00002 -0.00022 -0.00036 1.90751

A47 2.19400 0.00006 0.00019 -0.00017 0.00019 2.19420

A48 2.18130 0.00001 -0.00023 0.00040 0.00017 2.18147

A49 1.87768 0.00007 -0.00091 0.00104 0.00053 1.87821

A50 2.20266 -0.00004 0.00047 -0.00060 -0.00021 2.20244

A51 2.20266 -0.00003 0.00047 -0.00061 -0.00021 2.20244

A52 2.21211 0.00006 -0.00082 0.00100 0.00050 2.21260

A53 2.02828 -0.00008 -0.00031 0.00007 -0.00027 2.02801

A54 2.04280 0.00002 0.00109 -0.00106 -0.00023 2.04257

A55 2.18395 0.00006 -0.00063 0.00086 0.00046 2.18441

A56 2.19948 -0.00001 -0.00009 -0.00006 -0.00010 2.19938

A57 1.89975 -0.00004 0.00071 -0.00080 -0.00035 1.89939

A58 1.87098 0.00002 0.00007 -0.00005 0.00005 1.87103

A59 2.18723 0.00000 0.00009 0.00001 0.00008 2.18731

A60 2.22497 -0.00002 -0.00016 0.00005 -0.00013 2.22484

A61 1.87098 0.00002 0.00007 -0.00005 0.00005 1.87103

A62 2.22497 -0.00002 -0.00016 0.00005 -0.00013 2.22484

A63 2.18723 0.00000 0.00009 0.00001 0.00008 2.18731

A64 1.89975 -0.00004 0.00071 -0.00080 -0.00035 1.89939

A65 2.18395 0.00006 -0.00063 0.00086 0.00046 2.18441

A66 2.19948 -0.00001 -0.00009 -0.00007 -0.00010 2.19938

A67 1.88331 0.00004 -0.00157 0.00170 0.00061 1.88392

A68 2.19977 -0.00002 0.00081 -0.00088 -0.00021 2.19956

A69 2.19977 -0.00002 0.00081 -0.00087 -0.00021 2.19956

A70 1.57020 0.00003 -0.00057 0.00011 0.00034 1.57054

A71 1.57020 0.00003 -0.00057 0.00012 0.00034 1.57054

A72 1.57020 0.00003 -0.00057 0.00012 0.00034 1.57054

A73 1.57020 0.00002 -0.00057 0.00013 0.00034 1.57054

A74 2.21211 0.00006 -0.00082 0.00100 0.00050 2.21260

A75 2.02828 -0.00008 -0.00031 0.00007 -0.00027 2.02801

A76 2.04280 0.00002 0.00109 -0.00106 -0.00023 2.04257

A77 3.14040 0.00005 -0.00114 0.00025 0.00067 3.14108

A78 3.14040 0.00005 -0.00114 0.00024 0.00067 3.14108

A79 3.12441 -0.00000 -0.00023 0.00021 -0.00004 3.12437

A80 3.15877 0.00000 0.00021 -0.00020 0.00004 3.15881

A81 3.14673 0.00002 0.00186 -0.00148 0.00006 3.14679

A82 3.14673 0.00002 0.00186 -0.00148 0.00006 3.14679

A83 3.15877 0.00000 0.00021 -0.00020 0.00004 3.15881

A84 3.14673 0.00002 0.00186 -0.00148 0.00006 3.14679

A85 3.12441 -0.00000 -0.00023 0.00021 -0.00004 3.12437

A86 3.14673 0.00002 0.00186 -0.00148 0.00006 3.14679

A87 3.19196 -0.00109 -0.00789 -0.00935 -0.01721 3.17476

A88 3.09436 0.00105 0.01536 0.00069 0.01602 3.11038

A89 3.14187 -0.00003 -0.00118 0.00115 -0.00003 3.14184

A90 3.14146 0.00003 0.00119 -0.00122 -0.00002 3.14144

A91 3.14141 -0.00001 -0.00008 0.00012 0.00004 3.14146

A92 3.14141 -0.00001 -0.00008 0.00012 0.00004 3.14146

A93 3.14172 -0.00003 -0.00119 0.00122 0.00002 3.14174

A94 3.14177 0.00001 0.00008 -0.00012 -0.00004 3.14173

A95 3.14132 0.00003 0.00118 -0.00115 0.00003 3.14135

A96 3.14177 0.00001 0.00008 -0.00012 -0.00004 3.14173

D1 0.00025 0.00008 -0.00042 0.00033 -0.00008 0.00017

D2 3.14000 0.00014 0.00085 -0.00030 0.00055 3.14055

D3 -3.14009 0.00001 -0.00053 0.00003 -0.00050 -3.14059

D4 -0.00034 0.00007 0.00074 -0.00061 0.00014 -0.00020

D5 -0.00000 -0.00000 0.00000 0.00000 -0.00000 -0.00000

D6 -3.14031 -0.00007 -0.00011 -0.00031 -0.00043 -3.14073

D7 3.14031 0.00007 0.00011 0.00031 0.00043 3.14073

D8 0.00000 0.00000 -0.00000 -0.00000 0.00000 0.00000

D9 -0.00041 -0.00013 0.00068 -0.00054 0.00014 -0.00028

D10 -3.11587 -0.00027 -0.01025 0.00143 -0.00881 -3.12468

D11 -3.14014 -0.00019 -0.00060 0.00010 -0.00051 -3.14065

D12 0.02759 -0.00033 -0.01153 0.00208 -0.00946 0.01814

D13 -3.13678 -0.00029 0.00090 -0.00249 -0.00159 -3.13837

D14 0.00262 -0.00004 -0.00304 0.00225 -0.00078 0.00183

D15 0.00265 -0.00023 0.00240 -0.00324 -0.00085 0.00181

D16 -3.14114 0.00003 -0.00155 0.00151 -0.00004 -3.14118

D17 0.00041 0.00013 -0.00068 0.00054 -0.00014 0.00028

D18 3.14014 0.00019 0.00060 -0.00010 0.00051 3.14065

D19 3.11587 0.00027 0.01025 -0.00143 0.00881 3.12468

D20 -0.02759 0.00033 0.01153 -0.00208 0.00946 -0.01814

D21 -3.13336 -0.00044 -0.00127 -0.00149 -0.00274 -3.13610

D22 -0.03900 0.00061 0.01409 -0.00080 0.01328 -0.02572

D23 0.03900 -0.00061 -0.01409 0.00080 -0.01328 0.02572

D24 3.13336 0.00044 0.00127 0.00149 0.00274 3.13610

D25 -0.00025 -0.00008 0.00042 -0.00033 0.00008 -0.00017

D26 3.14009 -0.00001 0.00053 -0.00003 0.00050 3.14059

D27 -3.14000 -0.00014 -0.00085 0.00030 -0.00055 -3.14055

D28 0.00034 -0.00007 -0.00074 0.00061 -0.00014 0.00020

D29 -0.00265 0.00023 -0.00240 0.00324 0.00085 -0.00181

D30 3.14114 -0.00003 0.00155 -0.00151 0.00004 3.14118

D31 3.13678 0.00029 -0.00090 0.00249 0.00159 3.13837

D32 -0.00262 0.00004 0.00304 -0.00225 0.00078 -0.00183

D33 0.00484 -0.00022 0.00147 -0.00313 -0.00166 0.00317

D34 -3.13330 -0.00030 0.00424 -0.00713 -0.00289 -3.13618

D35 -3.13893 0.00003 -0.00244 0.00158 -0.00086 -3.13980

D36 0.00612 -0.00004 0.00032 -0.00242 -0.00209 0.00403

D37 -3.13835 -0.00022 0.00609 -0.00727 -0.00118 -3.13953

D38 0.02355 -0.00034 -0.00986 0.00193 -0.00794 0.01561

D39 0.00027 -0.00016 0.00371 -0.00383 -0.00012 0.00014

D40 -3.12102 -0.00027 -0.01225 0.00536 -0.00688 -3.12790

D41 3.13842 0.00016 -0.00470 0.00584 0.00114 3.13956

D42 -0.00153 0.00008 -0.00351 0.00408 0.00057 -0.00095

D43 -0.00017 0.00010 -0.00229 0.00237 0.00008 -0.00009

D44 -3.14012 0.00001 -0.00110 0.00061 -0.00049 -3.14061

D45 -0.00027 0.00016 -0.00371 0.00383 0.00012 -0.00014

D46 3.13835 0.00022 -0.00609 0.00727 0.00118 3.13953

D47 3.12102 0.00027 0.01225 -0.00536 0.00688 3.12790

D48 -0.02355 0.00034 0.00986 -0.00193 0.00794 -0.01561

D49 -0.03718 0.00061 0.01336 -0.00075 0.01260 -0.02458

D50 -3.12840 -0.00048 0.00546 -0.01010 -0.00461 -3.13301

D51 3.12840 0.00048 -0.00546 0.01010 0.00461 3.13301

D52 0.03718 -0.00061 -0.01336 0.00075 -0.01260 0.02458

D53 0.00017 -0.00010 0.00229 -0.00237 -0.00008 0.00009

D54 3.14012 -0.00001 0.00110 -0.00061 0.00049 3.14061

D55 -3.13842 -0.00016 0.00470 -0.00583 -0.00114 -3.13956

D56 0.00153 -0.00008 0.00351 -0.00408 -0.00057 0.00095

D57 -0.00484 0.00022 -0.00147 0.00313 0.00166 -0.00317

D58 3.13893 -0.00003 0.00244 -0.00158 0.00086 3.13980

D59 3.13330 0.00030 -0.00424 0.00713 0.00289 3.13618

D60 -0.00612 0.00004 -0.00032 0.00242 0.00209 -0.00403

D61 -0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D62 3.13992 0.00009 -0.00121 0.00179 0.00058 3.14050

D63 -3.13992 -0.00009 0.00121 -0.00179 -0.00058 -3.14050

D64 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D65 3.13330 0.00030 -0.00424 0.00713 0.00289 3.13618

D66 -0.00484 0.00022 -0.00147 0.00313 0.00166 -0.00317

D67 -0.00612 0.00004 -0.00032 0.00241 0.00209 -0.00403

D68 3.13893 -0.00003 0.00244 -0.00158 0.00086 3.13980

D69 -3.13842 -0.00016 0.00470 -0.00584 -0.00114 -3.13956

D70 0.00153 -0.00008 0.00351 -0.00408 -0.00057 0.00095

D71 0.00017 -0.00010 0.00229 -0.00237 -0.00008 0.00009

D72 3.14012 -0.00001 0.00110 -0.00061 0.00049 3.14061

D73 3.13835 0.00022 -0.00609 0.00727 0.00118 3.13953

D74 -0.02355 0.00034 0.00986 -0.00193 0.00794 -0.01561

D75 -0.00027 0.00016 -0.00371 0.00383 0.00012 -0.00014

D76 3.12102 0.00027 0.01225 -0.00536 0.00688 3.12790

D77 -0.00000 -0.00000 -0.00000 0.00000 0.00000 0.00000

D78 3.13992 0.00009 -0.00121 0.00179 0.00058 3.14050

D79 -3.13992 -0.00009 0.00121 -0.00179 -0.00058 -3.14050

D80 0.00000 -0.00000 -0.00000 -0.00000 -0.00000 0.00000

D81 -0.00017 0.00010 -0.00229 0.00237 0.00008 -0.00009

D82 3.13842 0.00016 -0.00470 0.00584 0.00114 3.13956

D83 -3.14012 0.00001 -0.00110 0.00061 -0.00049 -3.14061

D84 -0.00153 0.00008 -0.00351 0.00408 0.00057 -0.00095

D85 0.00027 -0.00016 0.00371 -0.00383 -0.00012 0.00014

D86 -3.12102 -0.00027 -0.01225 0.00536 -0.00688 -3.12790

D87 -3.13835 -0.00022 0.00609 -0.00727 -0.00118 -3.13953

D88 0.02355 -0.00034 -0.00986 0.00193 -0.00794 0.01561

D89 -3.13330 -0.00030 0.00424 -0.00713 -0.00289 -3.13618

D90 0.00612 -0.00004 0.00032 -0.00241 -0.00209 0.00403

D91 0.00484 -0.00022 0.00147 -0.00313 -0.00166 0.00317

D92 -3.13893 0.00003 -0.00244 0.00158 -0.00086 -3.13980

D93 0.03718 -0.00061 -0.01336 0.00075 -0.01260 0.02458

D94 3.12840 0.00048 -0.00546 0.01010 0.00461 3.13301

D95 -3.12840 -0.00048 0.00546 -0.01010 -0.00461 -3.13301

D96 -0.03718 0.00061 0.01336 -0.00075 0.01260 -0.02458

D97 3.13678 0.00029 -0.00090 0.00250 0.00159 3.13837

D98 -0.00265 0.00023 -0.00240 0.00324 0.00085 -0.00181

D99 -0.00262 0.00004 0.00304 -0.00225 0.00078 -0.00183

D100 3.14114 -0.00003 0.00155 -0.00151 0.00004 3.14118

D101 -3.14000 -0.00014 -0.00085 0.00030 -0.00055 -3.14055

D102 0.00034 -0.00007 -0.00074 0.00061 -0.00014 0.00020

D103 -0.00025 -0.00008 0.00042 -0.00033 0.00008 -0.00017

D104 3.14009 -0.00001 0.00053 -0.00003 0.00050 3.14059

D105 3.14014 0.00019 0.00060 -0.00010 0.00051 3.14065

D106 -0.02759 0.00033 0.01153 -0.00208 0.00946 -0.01814

D107 0.00041 0.00014 -0.00068 0.00054 -0.00014 0.00028

D108 3.11587 0.00027 0.01025 -0.00144 0.00881 3.12468

D109 -0.00000 0.00000 0.00000 -0.00000 -0.00000 -0.00000

D110 3.14031 0.00007 0.00011 0.00031 0.00043 3.14073

D111 -3.14031 -0.00007 -0.00011 -0.00031 -0.00043 -3.14073

D112 0.00000 -0.00000 -0.00000 0.00000 0.00000 0.00000

D113 0.00025 0.00008 -0.00042 0.00034 -0.00008 0.00017

D114 3.14000 0.00014 0.00085 -0.00030 0.00055 3.14055

D115 -3.14009 0.00001 -0.00053 0.00003 -0.00050 -3.14059

D116 -0.00034 0.00007 0.00074 -0.00061 0.00014 -0.00020

D117 -0.00041 -0.00014 0.00068 -0.00054 0.00014 -0.00028

D118 -3.11587 -0.00027 -0.01025 0.00144 -0.00881 -3.12468

D119 -3.14014 -0.00019 -0.00060 0.00010 -0.00051 -3.14065

D120 0.02759 -0.00033 -0.01153 0.00208 -0.00946 0.01814

D121 -3.13678 -0.00029 0.00090 -0.00250 -0.00159 -3.13837

D122 0.00262 -0.00004 -0.00304 0.00225 -0.00078 0.00183

D123 0.00265 -0.00023 0.00240 -0.00324 -0.00085 0.00181

D124 -3.14114 0.00003 -0.00155 0.00151 -0.00004 -3.14118

D125 3.13336 0.00044 0.00127 0.00149 0.00274 3.13610

D126 0.03900 -0.00061 -0.01409 0.00080 -0.01328 0.02572

D127 -0.03900 0.00061 0.01409 -0.00080 0.01328 -0.02572

D128 -3.13336 -0.00044 -0.00127 -0.00149 -0.00274 -3.13610

Item Value Threshold Converged?

Maximum Force 0.001086 0.000450 NO

RMS Force 0.000197 0.000300 YES

Maximum Displacement 0.038590 0.001800 NO

RMS Displacement 0.002859 0.001200 NO

Predicted change in Energy=-1.518533D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Wed Jul 31 01:52:20 2019, MaxMem= 4294967296 cpu: 1.0

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -4.290711 0.679521 -0.026277

2 6 0 -2.902116 1.109428 -0.022175

3 7 0 -2.095197 0.000000 -0.020011

4 6 0 -2.902116 -1.109428 -0.022175

5 6 0 -4.290711 -0.679521 -0.026277

6 6 0 -2.469104 -2.445654 -0.022090

7 6 0 -1.106825 -2.909881 -0.021824

8 7 0 -0.000000 -2.100016 -0.018040

9 6 0 1.106825 -2.909881 -0.021824

10 6 0 0.692010 -4.275121 -0.028008

11 6 0 -0.692010 -4.275121 -0.028008

12 6 0 -2.469104 2.445654 -0.022090

13 6 0 -1.106825 2.909881 -0.021824

14 6 0 -0.692010 4.275121 -0.028008

15 6 0 0.692010 4.275121 -0.028008

16 6 0 1.106825 2.909881 -0.021824

17 7 0 0.000000 2.100016 -0.018040

18 6 0 2.469104 2.445654 -0.022090

19 6 0 2.902116 1.109428 -0.022175

20 6 0 4.290711 0.679521 -0.026277

21 6 0 4.290711 -0.679521 -0.026277

22 6 0 2.902116 -1.109428 -0.022175

23 7 0 2.095197 -0.000000 -0.020011

24 1 0 -5.148075 1.336782 -0.029549

25 1 0 -5.148075 -1.336782 -0.029549

26 1 0 1.346118 -5.135049 -0.032844

27 1 0 -1.346118 -5.135049 -0.032844

28 1 0 -1.346118 5.135049 -0.032844

29 1 0 1.346118 5.135049 -0.032844

30 1 0 5.148075 1.336782 -0.029549

31 1 0 5.148075 -1.336782 -0.029549

32 30 0 -0.000000 0.000000 0.014738

33 6 0 2.469104 -2.445654 -0.022090

34 6 0 3.476446 -3.452505 -0.024052

35 6 0 -3.476446 3.452505 -0.024052

36 6 0 4.316288 -4.321359 -0.025493

37 6 0 -4.316288 4.321359 -0.025493

38 6 0 -3.476446 -3.452505 -0.024052

39 6 0 -4.316288 -4.321359 -0.025493

40 6 0 3.476446 3.452505 -0.024052

41 6 0 4.316288 4.321359 -0.025493

42 1 0 5.061687 5.084527 -0.026874

43 1 0 5.061687 -5.084527 -0.026874

44 1 0 -5.061687 -5.084527 -0.026874

45 1 0 -5.061687 5.084527 -0.026874

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.453628 0.000000

3 N 2.298275 1.371842 0.000000

4 C 2.264631 2.218855 1.371842 0.000000

5 C 1.359043 2.264631 2.298275 1.453628 0.000000

6 C 3.617318 3.581355 2.474072 1.404635 2.537222

7 C 4.798016 4.402035 3.073157 2.542577 3.887371

8 N 5.112347 4.326987 2.966466 3.066522 4.519743

9 C 6.482070 5.676835 4.326703 4.394683 5.840199

10 C 7.026805 6.473881 5.103454 4.789507 6.144578

11 C 6.123653 5.820478 4.499517 3.860857 5.087140

12 C 2.537222 1.404635 2.474072 3.581355 3.617318

13 C 3.887371 2.542577 3.073157 4.402035 4.798016

14 C 5.087140 3.860857 4.499517 5.820478 6.123653

15 C 6.144578 4.789507 5.103454 6.473881 7.026805

16 C 5.840199 4.394683 4.326703 5.676835 6.482070

17 N 4.519743 3.066522 2.966466 4.326987 5.112347

18 C 6.986726 5.534935 5.178231 6.441165 7.447271

19 C 7.205664 5.804231 5.118982 6.213889 7.411957

20 C 8.581422 7.205664 6.421964 7.411957 8.688372

21 C 8.688372 7.411957 6.421964 7.205664 8.581422

22 C 7.411957 6.213889 5.118982 5.804231 7.205664

23 N 6.421964 5.118982 4.190395 5.118982 6.421964

24 H 1.080312 2.257449 3.332737 3.320893 2.191018

25 H 2.191018 3.320893 3.332737 2.257449 1.080312

26 H 8.098340 7.552555 6.181549 5.852626 7.185097

27 H 6.517661 6.435428 5.189414 4.315886 5.340637

28 H 5.340637 4.315886 5.189414 6.435428 6.517661

29 H 7.185097 5.852626 6.181549 7.552555 8.098340

30 H 9.461642 8.053403 7.365600 8.413653 9.651744

31 H 9.651744 8.413653 7.365600 8.053403 9.461642

32 Zn 4.344380 3.107164 2.095486 3.107164 4.344380

33 C 7.447271 6.441165 5.178231 5.534935 6.986726

34 C 8.797862 7.842020 6.554618 6.795297 8.247313

35 C 2.890064 2.412441 3.718556 4.597944 4.211493

36 C 9.954358 9.033206 7.731838 7.900751 9.345770

37 C 3.641927 3.509472 4.858746 5.611893 5.000946

38 C 4.211493 4.597944 3.718556 2.412441 2.890064

39 C 5.000946 5.611893 4.858746 3.509472 3.641927

40 C 8.247313 6.795297 6.554618 7.842020 8.797862

41 C 9.345770 7.900751 7.731838 9.033206 9.954358

42 H 10.337863 8.900763 8.779149 10.088967 10.985973

43 H 10.985973 10.088967 8.779149 8.900763 10.337863

44 H 5.815381 6.559638 5.886639 4.523846 4.471966

45 H 4.471966 4.523846 5.886639 6.559638 5.815381

6 7 8 9 10

6 C 0.000000

7 C 1.439205 0.000000

8 N 2.493182 1.371481 0.000000

9 C 3.605937 2.213651 1.371481 0.000000

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12 C 4.891308 5.526080 5.172969 6.439645 7.427078

13 C 5.526080 5.819762 5.130706 6.226547 7.406760

14 C 6.951756 7.196969 6.412592 7.406760 8.661532

15 C 7.427078 7.406760 6.412592 7.196969 8.550241

16 C 6.439645 6.226547 5.130706 5.819762 7.196969

17 N 5.172969 5.130706 4.200031 5.130706 6.412592

18 C 6.950597 6.439645 5.172969 5.526080 6.951756

19 C 6.441165 5.676835 4.326987 4.402035 5.820478

20 C 7.447271 6.482070 5.112347 4.798016 6.123653

21 C 6.986726 5.840199 4.519743 3.887371 5.087140

22 C 5.534935 4.394683 3.066522 2.542577 3.860857

23 N 5.178231 4.326703 2.966466 3.073157 4.499517

24 H 4.635058 5.862244 6.189861 7.560290 8.099385

25 H 2.899403 4.336634 5.204357 6.449688 6.537616

26 H 4.667856 3.311861 3.320193 2.238025 1.080444

27 H 2.914457 2.238025 3.320193 3.311861 2.212118

28 H 7.663438 8.048496 7.359240 8.410586 9.628358

29 H 8.486642 8.410586 7.359240 8.048496 9.432877

30 H 8.504604 7.560290 6.189861 5.862244 7.165889

31 H 7.697471 6.449688 5.204357 4.336634 5.337635

32 Zn 3.475494 3.113488 2.100272 3.113488 4.330977

33 C 4.938209 3.605937 2.493182 1.439205 2.550499

34 C 6.030201 4.615281 3.730273 2.430956 2.903411

35 C 5.983563 6.789335 6.551046 7.841323 8.780219

36 C 7.039874 5.603788 4.854355 3.506128 3.624574

37 C 7.014597 7.911479 7.737212 9.038861 9.948996

38 C 1.424251 2.430956 3.730273 4.615281 4.248851

39 C 2.632559 3.506128 4.854355 5.603788 5.008512

40 C 8.374835 7.841323 6.551046 6.789335 8.213970

41 C 9.583007 9.038861 7.737212 7.911479 9.329248

42 H 10.649717 10.097581 8.788538 8.919166 10.329428

43 H 7.979755 6.540615 5.876058 4.513318 4.444009

44 H 3.699346 4.513318 5.876058 6.540615 5.810349

45 H 7.963990 8.919166 8.788538 10.097581 10.986721

11 12 13 14 15

11 C 0.000000

12 C 6.951756 0.000000

13 C 7.196969 1.439205 0.000000

14 C 8.550241 2.550499 1.426881 0.000000

15 C 8.661532 3.652345 2.258257 1.384019 0.000000

16 C 7.406760 3.605937 2.213651 2.258257 1.426881

17 N 6.412592 2.493182 1.371481 2.282555 2.282555

18 C 7.427078 4.938209 3.605937 3.652345 2.550499

19 C 6.473881 5.534935 4.394683 4.789507 3.860857

20 C 7.026805 6.986726 5.840199 6.144578 5.087140

21 C 6.144578 7.447271 6.482070 7.026805 6.123653

22 C 4.789507 6.441165 5.676835 6.473881 5.820478

23 N 5.103454 5.178231 4.326703 5.103454 4.499517

24 H 7.165889 2.899403 4.336634 5.337635 6.537616

25 H 5.337635 4.635058 5.862244 7.165889 8.099385

26 H 2.212118 8.486642 8.410586 9.628358 9.432877

27 H 1.080444 7.663438 8.048496 9.432877 9.628358

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30 H 8.099385 7.697471 6.449688 6.537616 5.337635

31 H 6.537616 8.504604 7.560290 8.099385 7.165889

32 Zn 4.330977 3.475494 3.113488 4.330977 4.330977

33 C 3.652345 6.950597 6.439645 7.427078 6.951756

34 C 4.248851 8.374835 7.841323 8.780219 8.213970

35 C 8.213970 1.424251 2.430956 2.903411 4.248851

36 C 5.008512 9.583007 9.038861 9.948996 9.329248

37 C 9.329248 2.632559 3.506128 3.624574 5.008512

38 C 2.903411 5.983563 6.789335 8.213970 8.780219

39 C 3.624574 7.014597 7.911479 9.329248 9.948996

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42 H 10.986721 7.979755 6.540615 5.810349 4.444009

43 H 5.810349 10.649717 10.097581 10.986721 10.329428

44 H 4.444009 7.963990 8.919166 10.329428 10.986721

45 H 10.329428 3.699346 4.513318 4.444009 5.810349

16 17 18 19 20

16 C 0.000000

17 N 1.371481 0.000000

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19 C 2.542577 3.066522 1.404635 0.000000

20 C 3.887371 4.519743 2.537222 1.453628 0.000000

21 C 4.798016 5.112347 3.617318 2.264631 1.359043

22 C 4.402035 4.326987 3.581355 2.218855 2.264631

23 N 3.073157 2.966466 2.474072 1.371842 2.298275

24 H 6.449688 5.204357 7.697471 8.053403 9.461642

25 H 7.560290 6.189861 8.504604 8.413653 9.651744

26 H 8.048496 7.359240 7.663438 6.435428 6.517661

27 H 8.410586 7.359240 8.486642 7.552555 8.098340

28 H 3.311861 3.320193 4.667856 5.852626 7.185097

29 H 2.238025 3.320193 2.914457 4.315886 5.340637

30 H 4.336634 5.204357 2.899403 2.257449 1.080312

31 H 5.862244 6.189861 4.635058 3.320893 2.191018

32 Zn 3.113488 2.100272 3.475494 3.107164 4.344380

33 C 5.526080 5.172969 4.891308 3.581355 3.617318

34 C 6.789335 6.551046 5.983563 4.597944 4.211493

35 C 4.615281 3.730273 6.030201 6.795297 8.247313

36 C 7.911479 7.737212 7.014597 5.611893 5.000946

37 C 5.603788 4.854355 7.039874 7.900751 9.345770

38 C 7.841323 6.551046 8.374835 7.842020 8.797862

39 C 9.038861 7.737212 9.583007 9.033206 9.954358

40 C 2.430956 3.730273 1.424251 2.412441 2.890064

41 C 3.506128 4.854355 2.632559 3.509472 3.641927

42 H 4.513318 5.876058 3.699346 4.523846 4.471966

43 H 8.919166 8.788538 7.963990 6.559638 5.815381

44 H 10.097581 8.788538 10.649717 10.088967 10.985973

45 H 6.540615 5.876058 7.979755 8.900763 10.337863

21 22 23 24 25

21 C 0.000000

22 C 1.453628 0.000000

23 N 2.298275 1.371842 0.000000

24 H 9.651744 8.413653 7.365600 0.000000

25 H 9.461642 8.053403 7.365600 2.673564 0.000000

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27 H 7.185097 5.852626 6.181549 7.505963 5.374172

28 H 8.098340 7.552555 6.181549 5.374172 7.505963

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31 H 1.080312 2.257449 3.332737 10.637605 10.296149

32 Zn 4.344380 3.107164 2.095486 5.318987 5.318987

33 C 2.537222 1.404635 2.474072 8.504604 7.697471

34 C 2.890064 2.412441 3.718556 9.865072 8.880240

35 C 8.797862 7.842020 6.554618 2.696416 5.072637

36 C 3.641927 3.509472 4.858746 11.026728 9.923804

37 C 9.954358 9.033206 7.731838 3.098320 5.718955

38 C 8.247313 6.795297 6.554618 5.072637 2.696416

39 C 9.345770 7.900751 7.731838 5.718955 3.098320

40 C 4.211493 4.597944 3.718556 8.880240 9.865072

41 C 5.000946 5.611893 4.858746 9.923804 11.026728

42 H 5.815381 6.559638 5.886639 10.875883 12.061196

43 H 4.471966 4.523846 5.886639 12.061196 10.875883

44 H 10.337863 8.900763 8.779149 6.421891 3.748742

45 H 10.985973 10.088967 8.779149 3.748742 6.421891

26 27 28 29 30

26 H 0.000000

27 H 2.692236 0.000000

28 H 10.617112 10.270099 0.000000

29 H 10.270099 10.617112 2.692236 0.000000

30 H 7.505963 9.168377 7.523389 5.374172 0.000000

31 H 5.374172 7.523389 9.168377 7.505963 2.673564

32 Zn 5.308769 5.308769 5.308769 5.308769 5.318987

33 C 2.914457 4.667856 8.486642 7.663438 4.635058

34 C 2.714651 5.107656 9.849025 8.847851 5.072637

35 C 9.849025 8.847851 2.714651 5.107656 8.880240

36 C 3.079620 5.720576 11.022094 9.911893 5.718955

37 C 11.022094 9.911893 3.079620 5.720576 9.923804

38 C 5.107656 2.714651 8.847851 9.849025 9.865072

39 C 5.720576 3.079620 9.911893 11.022094 11.026728

40 C 8.847851 9.849025 5.107656 2.714651 2.696416

41 C 9.911893 11.022094 5.720576 3.079620 3.098320

42 H 10.874062 12.062327 6.408006 3.715917 3.748742

43 H 3.715917 6.408006 12.062327 10.874062 6.421891

44 H 6.408006 3.715917 10.874062 12.062327 12.061196

45 H 12.062327 10.874062 3.715917 6.408006 10.875883

31 32 33 34 35

31 H 0.000000

32 Zn 5.318987 0.000000

33 C 2.899403 3.475494 0.000000

34 C 2.696416 4.899691 1.424251 0.000000

35 C 9.865072 4.899691 8.374835 9.799075 0.000000

36 C 3.098320 6.107872 2.632559 1.208405 11.007255

37 C 11.026728 6.107872 9.583007 11.007255 1.208405

38 C 8.880240 4.899691 6.030201 6.952892 6.905011

39 C 9.923804 6.107872 7.039874 7.841021 7.819098

40 C 5.072637 4.899691 5.983563 6.905011 6.952892

41 C 5.718955 6.107872 7.014597 7.819098 7.841021

42 H 6.421891 7.174595 7.963990 8.682967 8.692710

43 H 3.748742 7.174595 3.699346 2.275191 12.073965

44 H 10.875883 7.174595 7.979755 8.692710 8.682967

45 H 12.061196 7.174595 10.649717 12.073965 2.275191

36 37 38 39 40

36 C 0.000000

37 C 12.215480 0.000000

38 C 7.841021 7.819098 0.000000

39 C 8.632576 8.642718 1.208405 0.000000

40 C 7.819098 7.841021 9.799075 11.007255 0.000000

41 C 8.642718 8.632576 11.007255 12.215480 1.208405

42 H 9.435376 9.408976 12.073965 13.282210 2.275191

43 H 1.066793 13.282210 8.692710 9.408976 8.682967

44 H 9.408976 9.435376 2.275191 1.066793 12.073965

45 H 13.282210 1.066793 8.682967 9.435376 8.692710

41 42 43 44 45

41 C 0.000000

42 H 1.066793 0.000000

43 H 9.435376 10.169055 0.000000

44 H 13.282210 14.348950 10.123373 0.000000

45 H 9.408976 10.123373 14.348950 10.169055 0.000000

Stoichiometry C28H12N4Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C28H12)]

Deg. of freedom 34

Full point group C2V NOp 4

RotChk: IX=0 Diff= 1.31D-14

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.679521 4.290711 -0.007262

2 6 0 1.109428 2.902116 -0.003159

3 7 0 0.000000 2.095197 -0.000996

4 6 0 -1.109428 2.902116 -0.003159

5 6 0 -0.679521 4.290711 -0.007262

6 6 0 -2.445654 2.469104 -0.003075

7 6 0 -2.909881 1.106825 -0.002808

8 7 0 -2.100016 0.000000 0.000976

9 6 0 -2.909881 -1.106825 -0.002808

10 6 0 -4.275121 -0.692010 -0.008993

11 6 0 -4.275121 0.692010 -0.008993

12 6 0 2.445654 2.469104 -0.003075

13 6 0 2.909881 1.106825 -0.002808

14 6 0 4.275121 0.692010 -0.008993

15 6 0 4.275121 -0.692010 -0.008993

16 6 0 2.909881 -1.106825 -0.002808

17 7 0 2.100016 -0.000000 0.000976

18 6 0 2.445654 -2.469104 -0.003075

19 6 0 1.109428 -2.902116 -0.003159

20 6 0 0.679521 -4.290711 -0.007262

21 6 0 -0.679521 -4.290711 -0.007262

22 6 0 -1.109428 -2.902116 -0.003159

23 7 0 -0.000000 -2.095197 -0.000996

24 1 0 1.336782 5.148075 -0.010533

25 1 0 -1.336782 5.148075 -0.010533

26 1 0 -5.135049 -1.346118 -0.013829

27 1 0 -5.135049 1.346118 -0.013829

28 1 0 5.135049 1.346118 -0.013829

29 1 0 5.135049 -1.346118 -0.013829

30 1 0 1.336782 -5.148075 -0.010533

31 1 0 -1.336782 -5.148075 -0.010533

32 30 0 0.000000 0.000000 0.033753

33 6 0 -2.445654 -2.469104 -0.003075

34 6 0 -3.452505 -3.476446 -0.005037

35 6 0 3.452505 3.476446 -0.005037

36 6 0 -4.321359 -4.316288 -0.006477

37 6 0 4.321359 4.316288 -0.006477

38 6 0 -3.452505 3.476446 -0.005037

39 6 0 -4.321359 4.316288 -0.006477

40 6 0 3.452505 -3.476446 -0.005037

41 6 0 4.321359 -4.316288 -0.006477

42 1 0 5.084527 -5.061687 -0.007858

43 1 0 -5.084527 -5.061687 -0.007858

44 1 0 -5.084527 5.061687 -0.007858

45 1 0 5.084527 5.061687 -0.007858

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

Rotational constants (GHZ): 0.1459838 0.1453406 0.0728325

Leave Link 202 at Wed Jul 31 01:52:20 2019, MaxMem= 4294967296 cpu: 0.2

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

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

Pseudo-potential data read from rwf file.

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

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

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

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

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

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

111 alpha electrons 110 beta electrons

nuclear repulsion energy 3052.0217856572 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= 13 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= -0.1303404405 Hartrees.

Nuclear repulsion after empirical dispersion term = 3051.8914452168 Hartrees.

No density basis found on file 724.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

2nd derivatives : Analytical E(r).r(xy)/FMM algorithm (CHGder, D2EAlg=3).

Cavity 2nd derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3874

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.77D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 76

GePol: Fraction of low-weight points (<1% of avg) = 1.96%

GePol: Cavity surface area = 416.454 Ang\*\*2

GePol: Cavity volume = 421.024 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0083853783 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3051.8998305951 Hartrees.

Leave Link 301 at Wed Jul 31 01:52:20 2019, MaxMem= 4294967296 cpu: 1.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16173 LenP2D= 44686.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.47D-05 NBF= 172 148 158 158

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

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Wed Jul 31 01:52:20 2019, MaxMem= 4294967296 cpu: 10.9

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

DipDrv: MaxL=1.

Leave Link 303 at Wed Jul 31 01:52:21 2019, MaxMem= 4294967296 cpu: 1.3

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

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

B after Tr= 0.000000 0.000000 -0.000000

Rot= 1.000000 -0.000000 -0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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The electronic state of the initial guess is 2-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7631 S= 0.5065

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1359.66919700971

Leave Link 401 at Wed Jul 31 01:52:23 2019, MaxMem= 4294967296 cpu: 41.8

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1387497 IEndB= 1387497 NGot= 4294967296 MDV= 4294047352

LenX= 4294047352 LenY= 4293596440

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= 650000000 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= 45023628.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.22D-15 for 3871.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.70D-15 for 2186 2000.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.77D-15 for 3871.

Iteration 1 A^-1\*A deviation from orthogonality is 1.02D-11 for 3865 3855.

E= -1359.18254632322

DIIS: error= 3.58D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.18254632322 IErMin= 1 ErrMin= 3.58D-04

ErrMax= 3.58D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.34D-04 BMatP= 1.34D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.58D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.388 Goal= None Shift= 0.000

Gap= 0.438 Goal= None Shift= 0.000

RMSDP=3.66D-05 MaxDP=1.93D-03 OVMax= 1.72D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.66D-05 CP: 1.00D+00

E= -1359.18258963416 Delta-E= -0.000043310934 Rises=F Damp=F

DIIS: error= 3.55D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.18258963416 IErMin= 2 ErrMin= 3.55D-05

ErrMax= 3.55D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.62D-06 BMatP= 1.34D-04

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

Coeff-Com: -0.233D-01 0.102D+01

Coeff: -0.233D-01 0.102D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=3.45D-06 MaxDP=7.46D-05 DE=-4.33D-05 OVMax= 2.34D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.15D-06 CP: 1.00D+00 1.04D+00

E= -1359.18259012334 Delta-E= -0.000000489180 Rises=F Damp=F

DIIS: error= 4.73D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.18259012334 IErMin= 2 ErrMin= 3.55D-05

ErrMax= 4.73D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.06D-06 BMatP= 1.62D-06

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

Coeff-Com: -0.175D-01 0.456D+00 0.561D+00

Coeff: -0.175D-01 0.456D+00 0.561D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=1.25D-06 MaxDP=6.24D-05 DE=-4.89D-07 OVMax= 2.06D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 8.54D-07 CP: 1.00D+00 1.04D+00 7.13D-01

E= -1359.18259026950 Delta-E= -0.000000146165 Rises=F Damp=F

DIIS: error= 1.66D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.18259026950 IErMin= 4 ErrMin= 1.66D-05

ErrMax= 1.66D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.80D-07 BMatP= 1.06D-06

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

Coeff-Com: -0.720D-02 0.129D+00 0.344D+00 0.534D+00

Coeff: -0.720D-02 0.129D+00 0.344D+00 0.534D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=4.14D-07 MaxDP=3.09D-05 DE=-1.46D-07 OVMax= 8.57D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.37D-07 CP: 1.00D+00 1.04D+00 7.32D-01 7.28D-01

E= -1359.18259032501 Delta-E= -0.000000055507 Rises=F Damp=F

DIIS: error= 5.93D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.18259032501 IErMin= 5 ErrMin= 5.93D-06

ErrMax= 5.93D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.64D-08 BMatP= 2.80D-07

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

Coeff-Com: -0.166D-02 0.140D-01 0.110D+00 0.255D+00 0.622D+00

Coeff: -0.166D-02 0.140D-01 0.110D+00 0.255D+00 0.622D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=1.14D-07 MaxDP=6.75D-06 DE=-5.55D-08 OVMax= 1.85D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.25D-08 CP: 1.00D+00 1.04D+00 7.38D-01 7.81D-01 8.73D-01

E= -1359.18259032780 Delta-E= -0.000000002793 Rises=F Damp=F

DIIS: error= 3.51D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.18259032780 IErMin= 6 ErrMin= 3.51D-06

ErrMax= 3.51D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.39D-09 BMatP= 1.64D-08

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

Coeff-Com: 0.312D-03-0.163D-01 0.355D-02 0.525D-01 0.358D+00 0.602D+00

Coeff: 0.312D-03-0.163D-01 0.355D-02 0.525D-01 0.358D+00 0.602D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=4.76D-08 MaxDP=1.60D-06 DE=-2.79D-09 OVMax= 6.78D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.74D-08 CP: 1.00D+00 1.04D+00 7.45D-01 7.87D-01 8.96D-01

CP: 6.64D-01

E= -1359.18259032834 Delta-E= -0.000000000539 Rises=F Damp=F

DIIS: error= 2.65D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.18259032834 IErMin= 7 ErrMin= 2.65D-07

ErrMax= 2.65D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.15D-10 BMatP= 3.39D-09

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

Coeff-Com: 0.202D-03-0.830D-02-0.110D-02 0.173D-01 0.153D+00 0.288D+00

Coeff-Com: 0.550D+00

Coeff: 0.202D-03-0.830D-02-0.110D-02 0.173D-01 0.153D+00 0.288D+00

Coeff: 0.550D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=1.11D-08 MaxDP=3.82D-07 DE=-5.39D-10 OVMax= 2.43D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 9.62D-09 CP: 1.00D+00 1.04D+00 7.46D-01 7.87D-01 8.95D-01

CP: 6.94D-01 8.71D-01

E= -1359.18259032837 Delta-E= -0.000000000034 Rises=F Damp=F

DIIS: error= 1.60D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.18259032837 IErMin= 8 ErrMin= 1.60D-07

ErrMax= 1.60D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.11D-11 BMatP= 1.15D-10

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

Coeff-Com: 0.434D-04-0.905D-03-0.112D-02-0.257D-02 0.348D-02 0.219D-01

Coeff-Com: 0.336D+00 0.643D+00

Coeff: 0.434D-04-0.905D-03-0.112D-02-0.257D-02 0.348D-02 0.219D-01

Coeff: 0.336D+00 0.643D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=5.02D-09 MaxDP=2.04D-07 DE=-3.37D-11 OVMax= 1.13D-06

Error on total polarization charges = 0.06718

SCF Done: E(UB3LYP) = -1359.18259033 A.U. after 8 cycles

NFock= 8 Conv=0.50D-08 -V/T= 1.9682

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7631 S= 0.5065

<L.S>= 0.000000000000E+00

KE= 1.403851233297D+03 PE=-9.373310995148D+03 EE= 3.558377340927D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.26

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7631, after 0.7501

Leave Link 502 at Wed Jul 31 01:53:12 2019, MaxMem= 4294967296 cpu: 753.0

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 636

NBasis= 636 NAE= 111 NBE= 110 NFC= 0 NFV= 0

NROrb= 636 NOA= 111 NOB= 110 NVA= 525 NVB= 526

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.14196301D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.38356337D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.14358740D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.88325654D-01

Leave Link 801 at Wed Jul 31 01:53:12 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 45.

Will process 46 centers per pass.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16173 LenP2D= 44686.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 11 by ecpmxn.

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

Leave Link 1101 at Wed Jul 31 01:53:15 2019, MaxMem= 4294967296 cpu: 44.3

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Wed Jul 31 01:53:16 2019, MaxMem= 4294967296 cpu: 1.1

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 45.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966832.

G2DrvN: will do 46 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

G2PCM: DoFxE=T DoFxN=T DoGrad=T DoDP/DQ/DG/TGxP=FFFF NFrqRd= 0 IEInf=0 SqF1=F DoCFld=F IF1Alg=4.

GePol: Maximum number of non-zero 1st derivatives = 255

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Wed Jul 31 01:55:13 2019, MaxMem= 4294967296 cpu: 1871.3

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=111111111111111111111111111111111111111111111

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Using symmetry in CPHF.

Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.

Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.

NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 4294965570 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 0.

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

IRaf= 650000000 NMat= 42 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

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

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

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

NMat0= 42 NMatS0= 42 NMatT0= 0 NMatD0= 42 NMtDS0= 0 NMtDT0= 0

Integrals replicated using symmetry in FoFCou.

There are 42 degrees of freedom in the 1st order CPHF. IDoFFX=4 NUNeed= 42.

42 vectors produced by pass 0 Test12= 2.77D-13 2.38D-09 XBig12= 8.06D+03 5.92D+01.

AX will form 42 AO Fock derivatives at one time.

42 vectors produced by pass 1 Test12= 2.77D-13 2.38D-09 XBig12= 1.08D+03 6.87D+00.

42 vectors produced by pass 2 Test12= 2.77D-13 2.38D-09 XBig12= 2.82D+02 5.66D+00.

42 vectors produced by pass 3 Test12= 2.77D-13 2.38D-09 XBig12= 7.90D+01 2.09D+00.

42 vectors produced by pass 4 Test12= 2.77D-13 2.38D-09 XBig12= 7.96D+00 4.81D-01.

42 vectors produced by pass 5 Test12= 2.77D-13 2.38D-09 XBig12= 2.79D-01 5.52D-02.

42 vectors produced by pass 6 Test12= 2.77D-13 2.38D-09 XBig12= 1.02D-02 7.62D-03.

42 vectors produced by pass 7 Test12= 2.77D-13 2.38D-09 XBig12= 2.19D-04 1.24D-03.

38 vectors produced by pass 8 Test12= 2.77D-13 2.38D-09 XBig12= 4.00D-06 1.45D-04.

23 vectors produced by pass 9 Test12= 2.77D-13 2.38D-09 XBig12= 5.16D-08 1.89D-05.

6 vectors produced by pass 10 Test12= 2.77D-13 2.38D-09 XBig12= 6.03D-10 1.83D-06.

2 vectors produced by pass 11 Test12= 2.77D-13 2.38D-09 XBig12= 7.02D-12 1.60D-07.

2 vectors produced by pass 12 Test12= 2.77D-13 2.38D-09 XBig12= 1.01D-13 2.42D-08.

InvSVY: IOpt=1 It= 1 EMax= 1.56D-13

Solved reduced A of dimension 407 with 42 vectors.

FullF1: Do perturbations 1 to 42.

Isotropic polarizability for W= 0.000000 1006.71 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Wed Jul 31 02:51:10 2019, MaxMem= 4294967296 cpu: 53722.8

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16173 LenP2D= 44686.

LDataN: DoStor=T MaxTD1= 7 Len= 274

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 255

Leave Link 701 at Wed Jul 31 02:51:45 2019, MaxMem= 4294967296 cpu: 551.8

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

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

Leave Link 702 at Wed Jul 31 02:51:45 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

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

wScrn= 0.000000 ICntrl= 100127 IOpCl= 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 Wed Jul 31 02:53:35 2019, MaxMem= 4294967296 cpu: 1766.9

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

Dipole = 9.34946565D-14 2.25278129D-13 7.92314215D-02

Polarizability= 1.65355102D+03 3.32801471D-06 1.17944191D+03

-1.76340713D-05-5.54915523D-06 1.87123929D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000006045 -0.000181650 -0.000000361

2 6 0.000022704 -0.000046213 -0.000005771

3 7 -0.000263227 0.000000000 0.000919630

4 6 0.000022704 0.000046213 -0.000005771

5 6 0.000006045 0.000181650 -0.000000361

6 6 0.000060254 0.000041220 -0.000003675

7 6 -0.000123898 0.000013935 -0.000005834

8 7 0.000000000 -0.000219174 0.000836980

9 6 0.000123898 0.000013935 -0.000005834

10 6 -0.000172121 -0.000014128 -0.000000576

11 6 0.000172121 -0.000014128 -0.000000576

12 6 0.000060254 -0.000041220 -0.000003675

13 6 -0.000123898 -0.000013935 -0.000005834

14 6 0.000172121 0.000014128 -0.000000576

15 6 -0.000172121 0.000014128 -0.000000576

16 6 0.000123898 -0.000013935 -0.000005834

17 7 0.000000000 0.000219174 0.000836980

18 6 -0.000060254 -0.000041220 -0.000003675

19 6 -0.000022704 -0.000046213 -0.000005771

20 6 -0.000006045 -0.000181650 -0.000000361

21 6 -0.000006045 0.000181650 -0.000000361

22 6 -0.000022704 0.000046213 -0.000005771

23 7 0.000263227 0.000000000 0.000919630

24 1 -0.000006317 -0.000008049 -0.000000103

25 1 -0.000006317 0.000008049 -0.000000103

26 1 -0.000003271 -0.000003516 -0.000000250

27 1 0.000003271 -0.000003516 -0.000000250

28 1 0.000003271 0.000003516 -0.000000250

29 1 -0.000003271 0.000003516 -0.000000250

30 1 0.000006317 -0.000008049 -0.000000103

31 1 0.000006317 0.000008049 -0.000000103

32 30 -0.000000000 0.000000000 -0.003448169

33 6 -0.000060254 0.000041220 -0.000003675

34 6 -0.000011235 -0.000017579 0.000007535

35 6 0.000011235 0.000017579 0.000007535

36 6 -0.000021429 -0.000002228 -0.000005126

37 6 0.000021429 0.000002228 -0.000005126

38 6 0.000011235 -0.000017579 0.000007535

39 6 0.000021429 -0.000002228 -0.000005126

40 6 -0.000011235 0.000017579 0.000007535

41 6 -0.000021429 0.000002228 -0.000005126

42 1 0.000016014 0.000004058 -0.000002102

43 1 0.000016014 -0.000004058 -0.000002102

44 1 -0.000016014 -0.000004058 -0.000002102

45 1 -0.000016014 0.000004058 -0.000002102

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

Cartesian Forces: Max 0.003448169 RMS 0.000339591

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

Leave Link 716 at Wed Jul 31 02:53:35 2019, MaxMem= 4294967296 cpu: 0.8

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000756514 RMS 0.000138533

Search for a local minimum.

Step number 7 out of a maximum of 270

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

RMS Force = .13853D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -1.43D-04 DEPred=-1.52D-04 R= 9.44D-01

TightC=F SS= 1.41D+00 RLast= 5.68D-02 DXNew= 1.2613D-01 1.7053D-01

Trust test= 9.44D-01 RLast= 5.68D-02 DXMaxT set to 1.26D-01

ITU= 1 -1 0 0 -1 0 0

Eigenvalues --- 0.00144 0.00339 0.00458 0.00559 0.00674

Eigenvalues --- 0.00957 0.01120 0.01121 0.01166 0.01230

Eigenvalues --- 0.01255 0.01277 0.01335 0.01351 0.01415

Eigenvalues --- 0.01506 0.01520 0.01559 0.01920 0.01925

Eigenvalues --- 0.01966 0.01986 0.02005 0.02056 0.02061

Eigenvalues --- 0.02094 0.02106 0.02122 0.02155 0.02636

Eigenvalues --- 0.03000 0.03194 0.03251 0.03724 0.04000

Eigenvalues --- 0.04120 0.04122 0.04135 0.04135 0.04147

Eigenvalues --- 0.04357 0.04364 0.06362 0.06411 0.08260

Eigenvalues --- 0.08271 0.08283 0.08597 0.08841 0.08874

Eigenvalues --- 0.09065 0.09267 0.09293 0.09546 0.09610

Eigenvalues --- 0.09628 0.09656 0.09900 0.10407 0.10410

Eigenvalues --- 0.10442 0.10500 0.12358 0.13246 0.13517

Eigenvalues --- 0.13559 0.15983 0.16909 0.16968 0.19292

Eigenvalues --- 0.19818 0.20056 0.20102 0.20353 0.20630

Eigenvalues --- 0.20661 0.20827 0.21618 0.21820 0.21890

Eigenvalues --- 0.21968 0.26001 0.26203 0.27692 0.27972

Eigenvalues --- 0.28025 0.29426 0.30006 0.31698 0.32498

Eigenvalues --- 0.32766 0.32824 0.33595 0.35684 0.35692

Eigenvalues --- 0.35844 0.36111 0.36442 0.37027 0.37100

Eigenvalues --- 0.37159 0.37328 0.37391 0.37564 0.37857

Eigenvalues --- 0.38045 0.38329 0.38805 0.39209 0.40233

Eigenvalues --- 0.40237 0.40240 0.40240 0.41186 0.41301

Eigenvalues --- 0.41916 0.42463 0.45392 0.46111 0.46454

Eigenvalues --- 0.46658 0.50185 0.50191 0.52586 0.53003

Eigenvalues --- 1.03367 1.04113 1.04445 1.04678

En-DIIS/RFO-DIIS IScMMF= 0 using points: 7 6 5 4

RFO step: Lambda=-3.23683643D-05.

NNeg= 0 NP= 4 Switch= 2.50D-03 Rises=F DC= 7.31D-04 SmlDif= 1.00D-05

RMS Error= 0.8680189756D-03 NUsed= 4 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 3.31641 -2.31493 -0.00369 0.00221

Iteration 1 RMS(Cart)= 0.00642385 RMS(Int)= 0.00014624

Iteration 2 RMS(Cart)= 0.00015296 RMS(Int)= 0.00012240

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00012240

ITry= 1 IFail=0 DXMaxC= 8.77D-02 DCOld= 1.00D+10 DXMaxT= 1.26D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 5.61D-04 for atom 37.

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

(Linear) (Quad) (Total)

R1 2.74696 0.00001 0.00042 0.00007 0.00044 2.74740

R2 2.56822 -0.00016 0.00012 -0.00020 -0.00037 2.56785

R3 2.04149 0.00000 0.00003 -0.00000 0.00003 2.04153

R4 2.59241 -0.00007 -0.00074 -0.00011 -0.00079 2.59161

R5 2.65438 0.00005 0.00057 0.00017 0.00057 2.65494

R6 2.59241 -0.00007 -0.00074 -0.00010 -0.00079 2.59161

R7 3.95989 0.00011 0.00399 -0.00026 0.00390 3.96380

R8 2.74696 0.00001 0.00042 0.00007 0.00044 2.74740

R9 2.65438 0.00005 0.00057 0.00017 0.00057 2.65494

R10 2.04149 0.00000 0.00003 -0.00000 0.00003 2.04153

R11 2.71970 -0.00001 0.00073 0.00002 0.00045 2.72016

R12 2.69144 0.00001 0.00003 0.00004 0.00011 2.69155

R13 2.59172 -0.00001 -0.00032 -0.00015 -0.00036 2.59136

R14 2.69641 0.00004 0.00032 0.00018 0.00052 2.69694

R15 2.59172 -0.00001 -0.00032 -0.00016 -0.00036 2.59136

R16 3.96894 0.00010 0.00100 0.00140 0.00257 3.97151

R17 2.69641 0.00004 0.00032 0.00018 0.00052 2.69694

R18 2.71970 -0.00001 0.00073 0.00001 0.00045 2.72016

R19 2.61542 -0.00011 0.00007 -0.00021 -0.00041 2.61500

R20 2.04174 0.00000 0.00002 0.00001 0.00003 2.04177

R21 2.04174 0.00000 0.00002 0.00001 0.00003 2.04177

R22 2.71970 -0.00001 0.00073 0.00002 0.00045 2.72016

R23 2.69144 0.00001 0.00003 0.00004 0.00011 2.69155

R24 2.69641 0.00004 0.00032 0.00018 0.00052 2.69694

R25 2.59172 -0.00001 -0.00032 -0.00015 -0.00036 2.59136

R26 2.61542 -0.00011 0.00007 -0.00021 -0.00041 2.61500

R27 2.04174 0.00000 0.00002 0.00001 0.00003 2.04177

R28 2.69641 0.00004 0.00032 0.00018 0.00052 2.69694

R29 2.04174 0.00000 0.00002 0.00001 0.00003 2.04177

R30 2.59172 -0.00001 -0.00032 -0.00015 -0.00036 2.59136

R31 2.71970 -0.00001 0.00073 0.00001 0.00045 2.72016

R32 3.96894 0.00010 0.00100 0.00150 0.00257 3.97151

R33 2.65438 0.00005 0.00057 0.00016 0.00057 2.65494

R34 2.69144 0.00001 0.00003 0.00004 0.00011 2.69155

R35 2.74696 0.00001 0.00042 0.00007 0.00044 2.74740

R36 2.59241 -0.00007 -0.00074 -0.00011 -0.00079 2.59161

R37 2.56822 -0.00016 0.00012 -0.00021 -0.00037 2.56785

R38 2.04149 0.00000 0.00003 -0.00000 0.00003 2.04153

R39 2.74696 0.00001 0.00042 0.00007 0.00044 2.74740

R40 2.04149 0.00000 0.00003 -0.00000 0.00003 2.04153

R41 2.59241 -0.00007 -0.00074 -0.00010 -0.00079 2.59161

R42 2.65438 0.00005 0.00057 0.00017 0.00057 2.65494

R43 3.95989 0.00012 0.00399 -0.00016 0.00390 3.96380

R44 2.69144 0.00001 0.00003 0.00004 0.00011 2.69155

R45 2.28356 0.00000 0.00002 0.00001 0.00003 2.28358

R46 2.28356 0.00000 0.00002 0.00001 0.00003 2.28358

R47 2.01595 0.00001 0.00002 0.00001 0.00006 2.01601

R48 2.01595 0.00001 0.00002 0.00001 0.00006 2.01601

R49 2.28356 0.00000 0.00002 0.00001 0.00003 2.28358

R50 2.01595 0.00001 0.00002 0.00001 0.00006 2.01601

R51 2.28356 0.00000 0.00002 0.00001 0.00003 2.28358

R52 2.01595 0.00001 0.00002 0.00001 0.00006 2.01601

A1 1.87103 0.00002 0.00011 0.00004 0.00013 1.87116

A2 2.18731 0.00000 0.00019 0.00002 0.00022 2.18753

A3 2.22484 -0.00002 -0.00030 -0.00006 -0.00035 2.22449

A4 1.89939 -0.00003 -0.00081 -0.00010 -0.00074 1.89866

A5 2.18441 0.00004 0.00105 -0.00005 0.00085 2.18526

A6 2.19938 -0.00001 -0.00024 0.00016 -0.00012 2.19926

A7 1.88392 0.00003 0.00141 0.00014 0.00121 1.88514

A8 2.19956 -0.00001 -0.00049 -0.00004 -0.00054 2.19902

A9 2.19956 -0.00002 -0.00049 -0.00010 -0.00054 2.19902

A10 1.89939 -0.00003 -0.00081 -0.00011 -0.00074 1.89866

A11 2.19938 -0.00001 -0.00024 0.00017 -0.00012 2.19926

A12 2.18441 0.00004 0.00105 -0.00006 0.00085 2.18526

A13 1.87103 0.00002 0.00011 0.00004 0.00013 1.87116

A14 2.22484 -0.00002 -0.00030 -0.00006 -0.00035 2.22449

A15 2.18731 0.00000 0.00019 0.00002 0.00022 2.18753

A16 2.21260 0.00005 0.00115 0.00024 0.00118 2.21378

A17 2.04257 0.00001 -0.00052 -0.00002 -0.00038 2.04219

A18 2.02801 -0.00006 -0.00062 -0.00022 -0.00080 2.02721

A19 2.18147 -0.00000 0.00039 -0.00020 0.00016 2.18164

A20 2.19420 0.00006 0.00044 0.00038 0.00074 2.19493

A21 1.90751 -0.00006 -0.00082 -0.00018 -0.00090 1.90662

A22 1.87821 0.00006 0.00122 0.00026 0.00124 1.87945

A23 2.20244 -0.00003 -0.00048 -0.00015 -0.00058 2.20187

A24 2.20244 -0.00003 -0.00048 -0.00010 -0.00058 2.20187

A25 1.90751 -0.00006 -0.00082 -0.00017 -0.00090 1.90662

A26 2.18147 -0.00000 0.00039 -0.00021 0.00016 2.18164

A27 2.19420 0.00006 0.00044 0.00039 0.00074 2.19493

A28 1.86577 0.00003 0.00021 0.00005 0.00028 1.86605

A29 2.19634 -0.00001 0.00008 0.00003 0.00008 2.19643

A30 2.22107 -0.00002 -0.00029 -0.00007 -0.00036 2.22071

A31 1.86577 0.00003 0.00021 0.00005 0.00028 1.86605

A32 2.19634 -0.00001 0.00008 0.00003 0.00008 2.19643

A33 2.22107 -0.00002 -0.00029 -0.00008 -0.00036 2.22071

A34 2.21260 0.00005 0.00115 0.00022 0.00118 2.21378

A35 2.04257 0.00001 -0.00052 -0.00002 -0.00038 2.04219

A36 2.02801 -0.00006 -0.00062 -0.00021 -0.00080 2.02721

A37 2.19420 0.00006 0.00044 0.00036 0.00074 2.19493

A38 2.18147 -0.00000 0.00039 -0.00019 0.00016 2.18164

A39 1.90751 -0.00006 -0.00082 -0.00017 -0.00090 1.90662

A40 1.86577 0.00003 0.00021 0.00005 0.00028 1.86605

A41 2.19634 -0.00001 0.00008 0.00003 0.00008 2.19643

A42 2.22107 -0.00002 -0.00029 -0.00007 -0.00036 2.22071

A43 1.86577 0.00003 0.00021 0.00005 0.00028 1.86605

A44 2.22107 -0.00002 -0.00029 -0.00007 -0.00036 2.22071

A45 2.19634 -0.00001 0.00008 0.00003 0.00008 2.19643

A46 1.90751 -0.00006 -0.00082 -0.00016 -0.00090 1.90662

A47 2.19420 0.00006 0.00044 0.00037 0.00074 2.19493

A48 2.18147 -0.00000 0.00039 -0.00020 0.00016 2.18164

A49 1.87821 0.00005 0.00122 0.00024 0.00124 1.87945

A50 2.20244 -0.00003 -0.00048 -0.00015 -0.00058 2.20187

A51 2.20244 -0.00003 -0.00048 -0.00009 -0.00058 2.20187

A52 2.21260 0.00005 0.00115 0.00021 0.00118 2.21378

A53 2.02801 -0.00006 -0.00062 -0.00020 -0.00080 2.02721

A54 2.04257 0.00001 -0.00052 -0.00001 -0.00038 2.04219

A55 2.18441 0.00004 0.00105 -0.00007 0.00085 2.18526

A56 2.19938 -0.00001 -0.00024 0.00016 -0.00012 2.19926

A57 1.89939 -0.00003 -0.00081 -0.00009 -0.00074 1.89866

A58 1.87103 0.00002 0.00011 0.00003 0.00013 1.87116

A59 2.18731 0.00000 0.00019 0.00002 0.00022 2.18753

A60 2.22484 -0.00002 -0.00030 -0.00005 -0.00035 2.22449

A61 1.87103 0.00002 0.00011 0.00004 0.00013 1.87116

A62 2.22484 -0.00002 -0.00030 -0.00006 -0.00035 2.22449

A63 2.18731 0.00000 0.00019 0.00002 0.00022 2.18753

A64 1.89939 -0.00003 -0.00081 -0.00010 -0.00074 1.89866

A65 2.18441 0.00004 0.00105 -0.00008 0.00085 2.18526

A66 2.19938 -0.00001 -0.00024 0.00018 -0.00012 2.19926

A67 1.88392 0.00003 0.00141 0.00012 0.00121 1.88514

A68 2.19956 -0.00001 -0.00049 -0.00003 -0.00054 2.19902

A69 2.19956 -0.00002 -0.00049 -0.00009 -0.00054 2.19902

A70 1.57054 0.00001 0.00077 0.00005 0.00025 1.57079

A71 1.57054 0.00001 0.00077 0.00000 0.00025 1.57079

A72 1.57054 0.00001 0.00077 -0.00000 0.00025 1.57079

A73 1.57054 0.00001 0.00077 -0.00005 0.00025 1.57079

A74 2.21260 0.00005 0.00115 0.00022 0.00118 2.21378

A75 2.02801 -0.00006 -0.00062 -0.00021 -0.00080 2.02721

A76 2.04257 0.00001 -0.00052 -0.00001 -0.00038 2.04219

A77 3.14108 0.00002 0.00154 -0.00005 0.00050 3.14157

A78 3.14108 0.00002 0.00154 -0.00005 0.00050 3.14157

A79 3.12437 -0.00000 -0.00010 -0.00007 -0.00015 3.12422

A80 3.15881 0.00000 0.00009 0.00006 0.00015 3.15897

A81 3.14679 0.00002 0.00014 0.00020 0.00053 3.14732

A82 3.14679 0.00002 0.00014 0.00020 0.00053 3.14732

A83 3.15881 0.00000 0.00009 0.00007 0.00015 3.15897

A84 3.14679 0.00002 0.00014 0.00020 0.00053 3.14732

A85 3.12437 -0.00000 -0.00010 -0.00006 -0.00015 3.12422

A86 3.14679 0.00002 0.00014 0.00020 0.00053 3.14732

A87 3.17476 -0.00076 -0.03952 -0.00001 -0.03953 3.13523

A88 3.11038 0.00073 0.03675 0.00002 0.03679 3.14717

A89 3.14184 -0.00002 -0.00007 -0.00015 -0.00022 3.14162

A90 3.14144 0.00002 -0.00004 0.00014 0.00011 3.14155

A91 3.14146 -0.00000 0.00010 0.00005 0.00015 3.14160

A92 3.14146 -0.00000 0.00010 0.00005 0.00015 3.14160

A93 3.14174 -0.00002 0.00004 -0.00014 -0.00011 3.14164

A94 3.14173 0.00000 -0.00010 -0.00005 -0.00015 3.14158

A95 3.14135 0.00002 0.00007 0.00015 0.00022 3.14157

A96 3.14173 0.00000 -0.00010 -0.00005 -0.00015 3.14158

D1 0.00017 0.00006 -0.00020 -0.00005 -0.00026 -0.00009

D2 3.14055 0.00010 0.00124 -0.00014 0.00109 -3.14154

D3 -3.14059 0.00001 -0.00115 -0.00005 -0.00121 3.14139

D4 -0.00020 0.00005 0.00029 -0.00015 0.00014 -0.00006

D5 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D6 -3.14073 -0.00005 -0.00097 -0.00000 -0.00097 3.14148

D7 3.14073 0.00005 0.00097 0.00000 0.00097 -3.14148

D8 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 -0.00028 -0.00009 0.00033 0.00008 0.00043 0.00015

D10 -3.12468 -0.00019 -0.02028 0.00008 -0.02019 3.13831

D11 -3.14065 -0.00013 -0.00113 0.00018 -0.00094 -3.14159

D12 0.01814 -0.00023 -0.02174 0.00017 -0.02156 -0.00342

D13 -3.13837 -0.00021 -0.00361 -0.00006 -0.00366 3.14116

D14 0.00183 -0.00003 -0.00178 -0.00019 -0.00197 -0.00013

D15 0.00181 -0.00016 -0.00192 -0.00016 -0.00207 -0.00027

D16 -3.14118 0.00002 -0.00010 -0.00029 -0.00038 -3.14156

D17 0.00028 0.00009 -0.00033 -0.00008 -0.00043 -0.00015

D18 3.14065 0.00013 0.00113 -0.00018 0.00094 3.14159

D19 3.12468 0.00019 0.02028 -0.00008 0.02019 -3.13831

D20 -0.01814 0.00023 0.02174 -0.00017 0.02156 0.00342

D21 -3.13610 -0.00031 -0.00624 -0.00001 -0.00627 3.14082

D22 -0.02572 0.00042 0.03051 0.00001 0.03052 0.00480

D23 0.02572 -0.00042 -0.03051 -0.00001 -0.03052 -0.00480

D24 3.13610 0.00031 0.00624 0.00001 0.00627 -3.14082

D25 -0.00017 -0.00006 0.00020 0.00005 0.00026 0.00009

D26 3.14059 -0.00001 0.00115 0.00005 0.00121 -3.14139

D27 -3.14055 -0.00010 -0.00124 0.00014 -0.00109 3.14154

D28 0.00020 -0.00005 -0.00029 0.00015 -0.00014 0.00006

D29 -0.00181 0.00016 0.00192 0.00016 0.00207 0.00027

D30 3.14118 -0.00002 0.00010 0.00029 0.00038 3.14156

D31 3.13837 0.00021 0.00361 0.00006 0.00366 -3.14116

D32 -0.00183 0.00003 0.00178 0.00019 0.00197 0.00013

D33 0.00317 -0.00016 -0.00381 0.00010 -0.00370 -0.00053

D34 -3.13618 -0.00021 -0.00662 0.00015 -0.00647 3.14053

D35 -3.13980 0.00002 -0.00200 -0.00002 -0.00203 3.14136

D36 0.00403 -0.00003 -0.00481 0.00002 -0.00479 -0.00077

D37 -3.13953 -0.00016 -0.00271 0.00008 -0.00262 3.14103

D38 0.01561 -0.00023 -0.01823 -0.00033 -0.01856 -0.00294

D39 0.00014 -0.00011 -0.00029 0.00004 -0.00025 -0.00010

D40 -3.12790 -0.00019 -0.01581 -0.00037 -0.01618 3.13911

D41 3.13956 0.00011 0.00262 -0.00006 0.00255 -3.14107

D42 -0.00095 0.00005 0.00132 -0.00006 0.00126 0.00030

D43 -0.00009 0.00007 0.00018 -0.00002 0.00015 0.00006

D44 -3.14061 0.00001 -0.00113 -0.00002 -0.00115 3.14143

D45 -0.00014 0.00011 0.00029 -0.00004 0.00025 0.00010

D46 3.13953 0.00016 0.00271 -0.00008 0.00262 -3.14103

D47 3.12790 0.00019 0.01581 0.00036 0.01618 -3.13911

D48 -0.01561 0.00023 0.01823 0.00032 0.01856 0.00294

D49 -0.02458 0.00043 0.02894 0.00024 0.02917 0.00459

D50 -3.13301 -0.00033 -0.01059 0.00023 -0.01036 3.13982

D51 3.13301 0.00033 0.01059 -0.00023 0.01036 -3.13982

D52 0.02458 -0.00043 -0.02894 -0.00024 -0.02917 -0.00459

D53 0.00009 -0.00007 -0.00018 0.00002 -0.00015 -0.00006

D54 3.14061 -0.00001 0.00113 0.00002 0.00115 -3.14143

D55 -3.13956 -0.00011 -0.00262 0.00006 -0.00255 3.14107

D56 0.00095 -0.00005 -0.00132 0.00006 -0.00126 -0.00030

D57 -0.00317 0.00016 0.00381 -0.00010 0.00370 0.00053

D58 3.13980 -0.00002 0.00200 0.00003 0.00203 -3.14136

D59 3.13618 0.00021 0.00662 -0.00015 0.00647 -3.14053

D60 -0.00403 0.00003 0.00481 -0.00002 0.00479 0.00077

D61 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D62 3.14050 0.00006 0.00133 -0.00000 0.00132 -3.14136

D63 -3.14050 -0.00006 -0.00133 0.00000 -0.00132 3.14136

D64 0.00000 0.00000 0.00000 0.00000 -0.00000 -0.00000

D65 3.13618 0.00021 0.00662 -0.00015 0.00647 -3.14053

D66 -0.00317 0.00016 0.00381 -0.00011 0.00370 0.00053

D67 -0.00403 0.00003 0.00481 -0.00002 0.00479 0.00077

D68 3.13980 -0.00002 0.00200 0.00002 0.00203 -3.14136

D69 -3.13956 -0.00011 -0.00262 0.00007 -0.00255 3.14107

D70 0.00095 -0.00005 -0.00132 0.00006 -0.00126 -0.00030

D71 0.00009 -0.00007 -0.00018 0.00002 -0.00015 -0.00006

D72 3.14061 -0.00001 0.00113 0.00002 0.00115 -3.14143

D73 3.13953 0.00016 0.00271 -0.00008 0.00262 -3.14103

D74 -0.01561 0.00023 0.01823 0.00033 0.01856 0.00294

D75 -0.00014 0.00011 0.00029 -0.00004 0.00025 0.00010

D76 3.12790 0.00019 0.01581 0.00037 0.01618 -3.13911

D77 -0.00000 -0.00000 -0.00000 -0.00000 0.00000 0.00000

D78 3.14050 0.00006 0.00133 -0.00000 0.00132 -3.14136

D79 -3.14050 -0.00006 -0.00133 0.00000 -0.00132 3.14136

D80 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D81 -0.00009 0.00007 0.00018 -0.00002 0.00015 0.00006

D82 3.13956 0.00011 0.00262 -0.00007 0.00255 -3.14107

D83 -3.14061 0.00001 -0.00113 -0.00002 -0.00115 3.14143

D84 -0.00095 0.00005 0.00132 -0.00006 0.00126 0.00030

D85 0.00014 -0.00011 -0.00029 0.00004 -0.00025 -0.00010

D86 -3.12790 -0.00019 -0.01581 -0.00037 -0.01618 3.13911

D87 -3.13953 -0.00016 -0.00271 0.00008 -0.00262 3.14103

D88 0.01561 -0.00023 -0.01823 -0.00033 -0.01856 -0.00294

D89 -3.13618 -0.00021 -0.00662 0.00015 -0.00647 3.14053

D90 0.00403 -0.00003 -0.00481 0.00002 -0.00479 -0.00077

D91 0.00317 -0.00016 -0.00381 0.00010 -0.00370 -0.00053

D92 -3.13980 0.00002 -0.00200 -0.00003 -0.00203 3.14136

D93 0.02458 -0.00043 -0.02894 -0.00025 -0.02917 -0.00459

D94 3.13301 0.00033 0.01059 -0.00024 0.01036 -3.13982

D95 -3.13301 -0.00033 -0.01059 0.00024 -0.01036 3.13982

D96 -0.02458 0.00043 0.02894 0.00025 0.02917 0.00459

D97 3.13837 0.00021 0.00361 0.00005 0.00366 -3.14116

D98 -0.00181 0.00016 0.00192 0.00016 0.00207 0.00027

D99 -0.00183 0.00003 0.00178 0.00019 0.00197 0.00013

D100 3.14118 -0.00002 0.00010 0.00030 0.00038 3.14156

D101 -3.14055 -0.00010 -0.00124 0.00014 -0.00109 3.14154

D102 0.00020 -0.00005 -0.00029 0.00015 -0.00014 0.00006

D103 -0.00017 -0.00006 0.00020 0.00005 0.00026 0.00009

D104 3.14059 -0.00001 0.00115 0.00006 0.00121 -3.14139

D105 3.14065 0.00013 0.00113 -0.00018 0.00094 3.14159

D106 -0.01814 0.00023 0.02174 -0.00017 0.02156 0.00342

D107 0.00028 0.00009 -0.00033 -0.00008 -0.00043 -0.00015

D108 3.12468 0.00019 0.02028 -0.00007 0.02019 -3.13831

D109 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D110 3.14073 0.00005 0.00097 0.00000 0.00097 -3.14148

D111 -3.14073 -0.00005 -0.00097 -0.00000 -0.00097 3.14148

D112 -0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D113 0.00017 0.00006 -0.00020 -0.00005 -0.00026 -0.00009

D114 3.14055 0.00010 0.00124 -0.00015 0.00109 -3.14154

D115 -3.14059 0.00001 -0.00115 -0.00006 -0.00121 3.14139

D116 -0.00020 0.00005 0.00029 -0.00015 0.00014 -0.00006

D117 -0.00028 -0.00009 0.00033 0.00008 0.00043 0.00015

D118 -3.12468 -0.00019 -0.02028 0.00007 -0.02019 3.13831

D119 -3.14065 -0.00013 -0.00113 0.00018 -0.00094 -3.14159

D120 0.01814 -0.00023 -0.02174 0.00017 -0.02156 -0.00342

D121 -3.13837 -0.00021 -0.00361 -0.00005 -0.00366 3.14116

D122 0.00183 -0.00003 -0.00178 -0.00018 -0.00197 -0.00013

D123 0.00181 -0.00016 -0.00192 -0.00016 -0.00207 -0.00027

D124 -3.14118 0.00002 -0.00010 -0.00029 -0.00038 -3.14156

D125 3.13610 0.00031 0.00624 0.00000 0.00627 -3.14082

D126 0.02572 -0.00042 -0.03051 -0.00002 -0.03052 -0.00480

D127 -0.02572 0.00042 0.03051 0.00002 0.03052 0.00480

D128 -3.13610 -0.00031 -0.00624 -0.00000 -0.00627 3.14082

Item Value Threshold Converged?

Maximum Force 0.000757 0.000450 NO

RMS Force 0.000139 0.000300 YES

Maximum Displacement 0.087722 0.001800 NO

RMS Displacement 0.006393 0.001200 NO

Predicted change in Energy=-9.603132D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Wed Jul 31 02:53:35 2019, MaxMem= 4294967296 cpu: 1.0

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -4.292311 0.679424 -0.023908

2 6 0 -2.903541 1.109578 -0.024679

3 7 0 -2.097540 0.000000 -0.025008

4 6 0 -2.903541 -1.109578 -0.024679

5 6 0 -4.292311 -0.679424 -0.023908

6 6 0 -2.469470 -2.445776 -0.024865

7 6 0 -1.107175 -2.910700 -0.025122

8 7 0 -0.000000 -2.101625 -0.025822

9 6 0 1.107175 -2.910700 -0.025122

10 6 0 0.691900 -4.276102 -0.024076

11 6 0 -0.691900 -4.276102 -0.024076

12 6 0 -2.469470 2.445776 -0.024865

13 6 0 -1.107175 2.910700 -0.025122

14 6 0 -0.691900 4.276102 -0.024076

15 6 0 0.691900 4.276102 -0.024076

16 6 0 1.107175 2.910700 -0.025122

17 7 0 0.000000 2.101625 -0.025822

18 6 0 2.469470 2.445776 -0.024865

19 6 0 2.903541 1.109578 -0.024679

20 6 0 4.292311 0.679424 -0.023908

21 6 0 4.292311 -0.679424 -0.023908

22 6 0 2.903541 -1.109578 -0.024679

23 7 0 2.097540 -0.000000 -0.025008

24 1 0 -5.149923 1.336395 -0.023335

25 1 0 -5.149923 -1.336395 -0.023335

26 1 0 1.345707 -5.136293 -0.023222

27 1 0 -1.345707 -5.136293 -0.023222

28 1 0 -1.345707 5.136293 -0.023222

29 1 0 1.345707 5.136293 -0.023222

30 1 0 5.149923 1.336395 -0.023335

31 1 0 5.149923 -1.336395 -0.023335

32 30 0 0.000000 0.000000 -0.031683

33 6 0 2.469470 -2.445776 -0.024865

34 6 0 3.476508 -3.453015 -0.024413

35 6 0 -3.476508 3.453015 -0.024413

36 6 0 4.315930 -4.322298 -0.023987

37 6 0 -4.315930 4.322298 -0.023987

38 6 0 -3.476508 -3.453015 -0.024413

39 6 0 -4.315930 -4.322298 -0.023987

40 6 0 3.476508 3.453015 -0.024413

41 6 0 4.315930 4.322298 -0.023987

42 1 0 5.061378 5.085464 -0.023605

43 1 0 5.061378 -5.085464 -0.023605

44 1 0 -5.061378 -5.085464 -0.023605

45 1 0 -5.061378 5.085464 -0.023605

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.453862 0.000000

3 N 2.297529 1.371423 0.000000

4 C 2.264776 2.219156 1.371423 0.000000

5 C 1.358847 2.264776 2.297529 1.453862 0.000000

6 C 3.617958 3.581754 2.473894 1.404935 2.538257

7 C 4.799383 4.403359 3.074573 2.543811 3.888918

8 N 5.114506 4.329247 2.969259 3.068340 4.521791

9 C 6.484091 5.678775 4.329246 4.396577 5.842349

10 C 7.028485 6.475550 5.105490 4.791041 6.146418

11 C 6.125373 5.822105 4.501208 3.862413 5.089111

12 C 2.538257 1.404935 2.473894 3.581754 3.617958

13 C 3.888918 2.543811 3.074573 4.403359 4.799383

14 C 5.089111 3.862413 4.501208 5.822105 6.125373

15 C 6.146418 4.791041 5.105490 6.475550 7.028485

16 C 5.842349 4.396577 4.329246 5.678775 6.484091

17 N 4.521791 3.068340 2.969259 4.329247 5.114506

18 C 6.988683 5.536667 5.180676 6.442810 7.449064

19 C 7.208698 5.807083 5.122692 6.216660 7.414905

20 C 8.584622 7.208698 6.425870 7.414905 8.691501

21 C 8.691501 7.414905 6.425870 7.208698 8.584622

22 C 7.414905 6.216660 5.122692 5.807083 7.208698

23 N 6.425870 5.122692 4.195079 5.122692 6.425870

24 H 1.080329 2.257804 3.332116 3.320996 2.190668

25 H 2.190668 3.320996 3.332116 2.257804 1.080329

26 H 8.099988 7.554271 6.183644 5.854105 7.186858

27 H 6.519589 6.437216 5.191027 4.317555 5.342861

28 H 5.342861 4.317555 5.191027 6.437216 6.519589

29 H 7.186858 5.854105 6.183644 7.554271 8.099988

30 H 9.465061 8.056658 7.369645 8.416714 9.655014

31 H 9.655014 8.416714 7.369645 8.056658 9.465061

32 Zn 4.345758 3.108338 2.097550 3.108338 4.345758

33 C 7.449064 6.442810 5.180676 5.536667 6.988683

34 C 8.799523 7.843614 6.556929 6.796817 8.249082

35 C 2.891080 2.412465 3.718181 4.598429 4.212195

36 C 9.955854 9.034713 7.734006 7.902046 9.347317

37 C 3.642950 3.509474 4.858345 5.612496 5.001777

38 C 4.212195 4.598429 3.718181 2.412465 2.891080

39 C 5.001777 5.612496 4.858345 3.509474 3.642950

40 C 8.249082 6.796817 6.556929 7.843614 8.799523

41 C 9.347317 7.902046 7.734006 9.034713 9.955854

42 H 10.339473 8.902113 8.781347 10.090515 10.987513

43 H 10.987513 10.090515 8.781347 8.902113 10.339473

44 H 5.815961 6.560092 5.886110 4.523708 4.472657

45 H 4.472657 4.523708 5.886110 6.560092 5.815961

6 7 8 9 10

6 C 0.000000

7 C 1.439445 0.000000

8 N 2.493336 1.371291 0.000000

9 C 3.606736 2.214350 1.371291 0.000000

10 C 3.652993 2.258539 2.281903 1.427157 0.000000

11 C 2.551441 1.427157 2.281903 2.258539 1.383800

12 C 4.891552 5.526996 5.174664 6.440825 7.428184

13 C 5.526996 5.821400 5.133151 6.228326 7.408563

14 C 6.952942 7.198790 6.415149 7.408563 8.663435

15 C 7.428184 7.408563 6.415149 7.198790 8.552205

16 C 6.440825 6.228326 5.133151 5.821400 7.198790

17 N 5.174664 5.133151 4.203250 5.133151 6.415149

18 C 6.951289 6.440825 5.174664 5.526996 6.952942

19 C 6.442810 5.678775 4.329247 4.403359 5.822105

20 C 7.449064 6.484091 5.114506 4.799383 6.125373

21 C 6.988683 5.842349 4.521791 3.888918 5.089111

22 C 5.536667 4.396577 3.068340 2.543811 3.862413

23 N 5.180676 4.329246 2.969259 3.074573 4.501208

24 H 4.635693 5.863585 6.192067 7.562347 8.101051

25 H 2.900957 4.338461 5.206466 6.452109 6.539784

26 H 4.668453 3.312083 3.319660 2.238339 1.080459

27 H 2.915772 2.238339 3.319660 3.312083 2.211734

28 H 7.664895 8.050528 7.361955 8.412534 9.630422

29 H 8.487835 8.412534 7.361955 8.050528 9.435075

30 H 8.506467 7.562347 6.192067 5.863585 7.167572

31 H 7.699732 6.452109 5.206466 4.338461 5.340023

32 Zn 3.475651 3.114170 2.101633 3.114170 4.331724

33 C 4.938941 3.606736 2.493336 1.439445 2.551441

34 C 6.030687 4.615653 3.729928 2.430606 2.903707

35 C 5.984134 6.790479 6.552873 7.842641 8.781508

36 C 7.040098 5.603809 4.853724 3.505526 3.624324

37 C 7.015428 7.912797 7.739124 9.040261 9.950419

38 C 1.424309 2.430606 3.729928 4.615653 4.248894

39 C 2.632631 3.505526 4.853724 5.603809 5.008043

40 C 8.375583 7.842641 6.552873 6.790479 8.215430

41 C 9.583761 9.040261 7.739124 7.912797 9.330920

42 H 10.650505 10.098995 8.790439 8.920447 10.331083

43 H 7.980077 6.540692 5.875445 4.512795 4.443805

44 H 3.699451 4.512795 5.875445 6.540692 5.809929

45 H 7.964771 8.920447 8.790439 10.098995 10.988136

11 12 13 14 15

11 C 0.000000

12 C 6.952942 0.000000

13 C 7.198790 1.439445 0.000000

14 C 8.552205 2.551441 1.427157 0.000000

15 C 8.663435 3.652993 2.258539 1.383800 0.000000

16 C 7.408563 3.606736 2.214350 2.258539 1.427157

17 N 6.415149 2.493336 1.371291 2.281903 2.281903

18 C 7.428184 4.938941 3.606736 3.652993 2.551441

19 C 6.475550 5.536667 4.396577 4.791041 3.862413

20 C 7.028485 6.988683 5.842349 6.146418 5.089111

21 C 6.146418 7.449064 6.484091 7.028485 6.125373

22 C 4.791041 6.442810 5.678775 6.475550 5.822105

23 N 5.105490 5.180676 4.329246 5.105490 4.501208

24 H 7.167572 2.900957 4.338461 5.340023 6.539784

25 H 5.340023 4.635693 5.863585 7.167572 8.101051

26 H 2.211734 8.487835 8.412534 9.630422 9.435075

27 H 1.080459 7.664895 8.050528 9.435075 9.630422

28 H 9.435075 2.915772 2.238339 1.080459 2.211734

29 H 9.630422 4.668453 3.312083 2.211734 1.080459

30 H 8.101051 7.699732 6.452109 6.539784 5.340023

31 H 6.539784 8.506467 7.562347 8.101051 7.167572

32 Zn 4.331724 3.475651 3.114170 4.331724 4.331724

33 C 3.652993 6.951289 6.440825 7.428184 6.952942

34 C 4.248894 8.375583 7.842641 8.781508 8.215430

35 C 8.215430 1.424309 2.430606 2.903707 4.248894

36 C 5.008043 9.583761 9.040261 9.950419 9.330920

37 C 9.330920 2.632631 3.505526 3.624324 5.008043

38 C 2.903707 5.984134 6.790479 8.215430 8.781508

39 C 3.624324 7.015428 7.912797 9.330920 9.950419

40 C 8.781508 6.030687 4.615653 4.248894 2.903707

41 C 9.950419 7.040098 5.603809 5.008043 3.624324

42 H 10.988136 7.980077 6.540692 5.809929 4.443805

43 H 5.809929 10.650505 10.098995 10.988136 10.331083

44 H 4.443805 7.964771 8.920447 10.331083 10.988136

45 H 10.331083 3.699451 4.512795 4.443805 5.809929

16 17 18 19 20

16 C 0.000000

17 N 1.371291 0.000000

18 C 1.439445 2.493336 0.000000

19 C 2.543811 3.068340 1.404935 0.000000

20 C 3.888918 4.521791 2.538257 1.453862 0.000000

21 C 4.799383 5.114506 3.617958 2.264776 1.358847

22 C 4.403359 4.329247 3.581754 2.219156 2.264776

23 N 3.074573 2.969259 2.473894 1.371423 2.297529

24 H 6.452109 5.206466 7.699732 8.056658 9.465061

25 H 7.562347 6.192067 8.506467 8.416714 9.655014

26 H 8.050528 7.361955 7.664895 6.437216 6.519589

27 H 8.412534 7.361955 8.487835 7.554271 8.099988

28 H 3.312083 3.319660 4.668453 5.854105 7.186858

29 H 2.238339 3.319660 2.915772 4.317555 5.342861

30 H 4.338461 5.206466 2.900957 2.257804 1.080329

31 H 5.863585 6.192067 4.635693 3.320996 2.190668

32 Zn 3.114170 2.101633 3.475651 3.108338 4.345758

33 C 5.526996 5.174664 4.891552 3.581754 3.617958

34 C 6.790479 6.552873 5.984134 4.598429 4.212195

35 C 4.615653 3.729928 6.030687 6.796817 8.249082

36 C 7.912797 7.739124 7.015428 5.612496 5.001777

37 C 5.603809 4.853724 7.040098 7.902046 9.347317

38 C 7.842641 6.552873 8.375583 7.843614 8.799523

39 C 9.040261 7.739124 9.583761 9.034713 9.955854

40 C 2.430606 3.729928 1.424309 2.412465 2.891080

41 C 3.505526 4.853724 2.632631 3.509474 3.642950

42 H 4.512795 5.875445 3.699451 4.523708 4.472657

43 H 8.920447 8.790439 7.964771 6.560092 5.815961

44 H 10.098995 8.790439 10.650505 10.090515 10.987513

45 H 6.540692 5.875445 7.980077 8.902113 10.339473

21 22 23 24 25

21 C 0.000000

22 C 1.453862 0.000000

23 N 2.297529 1.371423 0.000000

24 H 9.655014 8.416714 7.369645 0.000000

25 H 9.465061 8.056658 7.369645 2.672790 0.000000

26 H 5.342861 4.317555 5.191027 9.169999 7.525452

27 H 7.186858 5.854105 6.183644 7.507846 5.376921

28 H 8.099988 7.554271 6.183644 5.376921 7.507846

29 H 6.519589 6.437216 5.191027 7.525452 9.169999

30 H 2.190668 3.320996 3.332116 10.299846 10.640988

31 H 1.080329 2.257804 3.332116 10.640988 10.299846

32 Zn 4.345758 3.108338 2.097550 5.320501 5.320501

33 C 2.538257 1.404935 2.473894 8.506467 7.699732

34 C 2.891080 2.412465 3.718181 9.866801 8.882308

35 C 8.799523 7.843614 6.556929 2.698221 5.073339

36 C 3.642950 3.509474 4.858345 11.028289 9.925622

37 C 9.955854 9.034713 7.734006 3.100187 5.719821

38 C 8.249082 6.796817 6.556929 5.073339 2.698221

39 C 9.347317 7.902046 7.734006 5.719821 3.100187

40 C 4.212195 4.598429 3.718181 8.882308 9.866801

41 C 5.001777 5.612496 4.858345 9.925622 11.028289

42 H 5.815961 6.560092 5.886110 10.877784 12.062792

43 H 4.472657 4.523708 5.886110 12.062792 10.877784

44 H 10.339473 8.902113 8.781347 6.422470 3.750115

45 H 10.987513 10.090515 8.781347 3.750115 6.422470

26 27 28 29 30

26 H 0.000000

27 H 2.691413 0.000000

28 H 10.619309 10.272585 0.000000

29 H 10.272585 10.619309 2.691413 0.000000

30 H 7.507846 9.169999 7.525452 5.376921 0.000000

31 H 5.376921 7.525452 9.169999 7.507846 2.672790

32 Zn 5.309661 5.309661 5.309661 5.309661 5.320501

33 C 2.915772 4.668453 8.487835 7.664895 4.635693

34 C 2.715463 5.107561 9.850379 8.849662 5.073339

35 C 9.850379 8.849662 2.715463 5.107561 8.882308

36 C 3.079742 5.719853 11.023568 9.913988 5.719821

37 C 11.023568 9.913988 3.079742 5.719853 9.925622

38 C 5.107561 2.715463 8.849662 9.850379 9.866801

39 C 5.719853 3.079742 9.913988 11.023568 11.028289

40 C 8.849662 9.850379 5.107561 2.715463 2.698221

41 C 9.913988 11.023568 5.719853 3.079742 3.100187

42 H 10.876145 12.063791 6.407286 3.716019 3.750115

43 H 3.716019 6.407286 12.063791 10.876145 6.422470

44 H 6.407286 3.716019 10.876145 12.063791 12.062792

45 H 12.063791 10.876145 3.716019 6.407286 10.877784

31 32 33 34 35

31 H 0.000000

32 Zn 5.320501 0.000000

33 C 2.900957 3.475651 0.000000

34 C 2.698221 4.899946 1.424309 0.000000

35 C 9.866801 4.899946 8.375583 9.799882 0.000000

36 C 3.100187 6.108156 2.632631 1.208421 11.008068

37 C 11.028289 6.108156 9.583761 11.008068 1.208421

38 C 8.882308 4.899946 6.030687 6.953016 6.906030

39 C 9.925622 6.108156 7.040098 7.840774 7.820493

40 C 5.073339 4.899946 5.984134 6.906030 6.953016

41 C 5.719821 6.108156 7.015428 7.820493 7.840774

42 H 6.422470 7.174926 7.964771 8.684322 8.692548

43 H 3.750115 7.174926 3.699451 2.275237 12.074814

44 H 10.877784 7.174926 7.980077 8.692548 8.684322

45 H 12.062792 7.174926 10.650505 12.074814 2.275237

36 37 38 39 40

36 C 0.000000

37 C 12.216301 0.000000

38 C 7.840774 7.820493 0.000000

39 C 8.631859 8.644595 1.208421 0.000000

40 C 7.820493 7.840774 9.799882 11.008068 0.000000

41 C 8.644595 8.631859 11.008068 12.216301 1.208421

42 H 9.437250 9.408311 12.074814 13.283068 2.275237

43 H 1.066826 13.283068 8.692548 9.408311 8.684322

44 H 9.408311 9.437250 2.275237 1.066826 12.074814

45 H 13.283068 1.066826 8.684322 9.437250 8.692548

41 42 43 44 45

41 C 0.000000

42 H 1.066826 0.000000

43 H 9.437250 10.170929 0.000000

44 H 13.283068 14.349843 10.122756 0.000000

45 H 9.408311 10.122756 14.349843 10.170929 0.000000

Stoichiometry C28H12N4Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C28H12)]

Deg. of freedom 34

Full point group C2V NOp 4

RotChk: IX=2 Diff= 1.76D-14

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.679424 4.292311 0.001504

2 6 0 1.109578 2.903541 0.000733

3 7 0 0.000000 2.097540 0.000404

4 6 0 -1.109578 2.903541 0.000733

5 6 0 -0.679424 4.292311 0.001504

6 6 0 -2.445776 2.469470 0.000547

7 6 0 -2.910700 1.107175 0.000290

8 7 0 -2.101625 -0.000000 -0.000410

9 6 0 -2.910700 -1.107175 0.000290

10 6 0 -4.276102 -0.691900 0.001335

11 6 0 -4.276102 0.691900 0.001335

12 6 0 2.445776 2.469470 0.000547

13 6 0 2.910700 1.107175 0.000290

14 6 0 4.276102 0.691900 0.001335

15 6 0 4.276102 -0.691900 0.001335

16 6 0 2.910700 -1.107175 0.000290

17 7 0 2.101625 0.000000 -0.000410

18 6 0 2.445776 -2.469470 0.000547

19 6 0 1.109578 -2.903541 0.000733

20 6 0 0.679424 -4.292311 0.001504

21 6 0 -0.679424 -4.292311 0.001504

22 6 0 -1.109578 -2.903541 0.000733

23 7 0 0.000000 -2.097540 0.000404

24 1 0 1.336395 5.149923 0.002076

25 1 0 -1.336395 5.149923 0.002076

26 1 0 -5.136293 -1.345707 0.002190

27 1 0 -5.136293 1.345707 0.002190

28 1 0 5.136293 1.345707 0.002190

29 1 0 5.136293 -1.345707 0.002190

30 1 0 1.336395 -5.149923 0.002076

31 1 0 -1.336395 -5.149923 0.002076

32 30 0 0.000000 0.000000 -0.006271

33 6 0 -2.445776 -2.469470 0.000547

34 6 0 -3.453015 -3.476508 0.000999

35 6 0 3.453015 3.476508 0.000999

36 6 0 -4.322298 -4.315930 0.001424

37 6 0 4.322298 4.315930 0.001424

38 6 0 -3.453015 3.476508 0.000999

39 6 0 -4.322298 4.315930 0.001424

40 6 0 3.453015 -3.476508 0.000999

41 6 0 4.322298 -4.315930 0.001424

42 1 0 5.085464 -5.061378 0.001807

43 1 0 -5.085464 -5.061378 0.001807

44 1 0 -5.085464 5.061378 0.001807

45 1 0 5.085464 5.061378 0.001807

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

Rotational constants (GHZ): 0.1459239 0.1452863 0.0728023

Leave Link 202 at Wed Jul 31 02:53:35 2019, MaxMem= 4294967296 cpu: 0.2

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

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

Pseudo-potential data read from rwf file.

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

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

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

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

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

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

111 alpha electrons 110 beta electrons

nuclear repulsion energy 3051.4531422961 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= 13 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= -0.1303156416 Hartrees.

Nuclear repulsion after empirical dispersion term = 3051.3228266546 Hartrees.

No density basis found on file 724.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

2nd derivatives : Analytical E(r).r(xy)/FMM algorithm (CHGder, D2EAlg=3).

Cavity 2nd derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3878

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.56D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 84

GePol: Fraction of low-weight points (<1% of avg) = 2.17%

GePol: Cavity surface area = 416.559 Ang\*\*2

GePol: Cavity volume = 421.105 Ang\*\*3

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

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

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PCM non-electrostatic energy = 0.0083857235 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3051.3312123781 Hartrees.

Leave Link 301 at Wed Jul 31 02:53:36 2019, MaxMem= 4294967296 cpu: 1.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16169 LenP2D= 44682.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.48D-05 NBF= 172 148 158 158

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

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Wed Jul 31 02:53:36 2019, MaxMem= 4294967296 cpu: 10.9

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

DipDrv: MaxL=1.

Leave Link 303 at Wed Jul 31 02:53:36 2019, MaxMem= 4294967296 cpu: 1.3

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

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

B after Tr= 0.000000 -0.000000 0.000000

Rot= 1.000000 0.000000 -0.000000 -0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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The electronic state of the initial guess is 2-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7631 S= 0.5065

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1359.66911876527

Leave Link 401 at Wed Jul 31 02:53:39 2019, MaxMem= 4294967296 cpu: 41.8

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1387497 IEndB= 1387497 NGot= 4294967296 MDV= 4294047352

LenX= 4294047352 LenY= 4293596440

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= 650000000 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= 45116652.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.33D-15 for 3866.

Iteration 1 A\*A^-1 deviation from orthogonality is 7.77D-15 for 3860 540.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.66D-15 for 3866.

Iteration 1 A^-1\*A deviation from orthogonality is 1.66D-14 for 3746 3604.

E= -1359.18247818723

DIIS: error= 8.24D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.18247818723 IErMin= 1 ErrMin= 8.24D-04

ErrMax= 8.24D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.69D-04 BMatP= 6.69D-04

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.24D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.387 Goal= None Shift= 0.000

Gap= 0.438 Goal= None Shift= 0.000

RMSDP=8.40D-05 MaxDP=4.43D-03 OVMax= 3.83D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 8.40D-05 CP: 1.00D+00

E= -1359.18269248721 Delta-E= -0.000214299979 Rises=F Damp=F

DIIS: error= 6.56D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.18269248721 IErMin= 2 ErrMin= 6.56D-05

ErrMax= 6.56D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.37D-06 BMatP= 6.69D-04

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

Coeff-Com: -0.235D-01 0.102D+01

Coeff: -0.235D-01 0.102D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=7.21D-06 MaxDP=1.73D-04 DE=-2.14D-04 OVMax= 5.30D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 6.45D-06 CP: 1.00D+00 1.04D+00

E= -1359.18269508502 Delta-E= -0.000002597808 Rises=F Damp=F

DIIS: error= 5.09D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.18269508502 IErMin= 3 ErrMin= 5.09D-05

ErrMax= 5.09D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.28D-06 BMatP= 7.37D-06

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

Coeff-Com: -0.154D-01 0.396D+00 0.619D+00

Coeff: -0.154D-01 0.396D+00 0.619D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=2.58D-06 MaxDP=9.18D-05 DE=-2.60D-06 OVMax= 3.30D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.90D-06 CP: 1.00D+00 1.04D+00 7.30D-01

E= -1359.18269549954 Delta-E= -0.000000414522 Rises=F Damp=F

DIIS: error= 3.50D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.18269549954 IErMin= 4 ErrMin= 3.50D-05

ErrMax= 3.50D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.44D-06 BMatP= 3.28D-06

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

Coeff-Com: -0.688D-02 0.124D+00 0.400D+00 0.483D+00

Coeff: -0.688D-02 0.124D+00 0.400D+00 0.483D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=9.28D-07 MaxDP=4.71D-05 DE=-4.15D-07 OVMax= 1.54D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 7.15D-07 CP: 1.00D+00 1.04D+00 7.56D-01 7.01D-01

E= -1359.18269580602 Delta-E= -0.000000306479 Rises=F Damp=F

DIIS: error= 7.43D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.18269580602 IErMin= 5 ErrMin= 7.43D-06

ErrMax= 7.43D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.16D-08 BMatP= 1.44D-06

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

Coeff-Com: -0.661D-03-0.513D-02 0.779D-01 0.180D+00 0.748D+00

Coeff: -0.661D-03-0.513D-02 0.779D-01 0.180D+00 0.748D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=2.10D-07 MaxDP=9.07D-06 DE=-3.06D-07 OVMax= 2.51D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.63D-07 CP: 1.00D+00 1.04D+00 7.68D-01 7.42D-01 9.08D-01

E= -1359.18269581312 Delta-E= -0.000000007103 Rises=F Damp=F

DIIS: error= 7.12D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.18269581312 IErMin= 6 ErrMin= 7.12D-06

ErrMax= 7.12D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.39D-08 BMatP= 4.16D-08

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

Coeff-Com: 0.315D-03-0.166D-01 0.536D-02 0.573D-01 0.448D+00 0.505D+00

Coeff: 0.315D-03-0.166D-01 0.536D-02 0.573D-01 0.448D+00 0.505D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=8.08D-08 MaxDP=3.31D-06 DE=-7.10D-09 OVMax= 1.11D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.20D-08 CP: 1.00D+00 1.04D+00 7.73D-01 7.49D-01 9.17D-01

CP: 6.78D-01

E= -1359.18269581536 Delta-E= -0.000000002238 Rises=F Damp=F

DIIS: error= 4.41D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.18269581536 IErMin= 7 ErrMin= 4.41D-07

ErrMax= 4.41D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.30D-10 BMatP= 1.39D-08

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

Coeff-Com: 0.167D-03-0.677D-02-0.942D-03 0.155D-01 0.153D+00 0.208D+00

Coeff-Com: 0.631D+00

Coeff: 0.167D-03-0.677D-02-0.942D-03 0.155D-01 0.153D+00 0.208D+00

Coeff: 0.631D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=1.79D-08 MaxDP=6.38D-07 DE=-2.24D-09 OVMax= 2.36D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.62D-08 CP: 1.00D+00 1.04D+00 7.74D-01 7.49D-01 9.19D-01

CP: 6.96D-01 9.20D-01

E= -1359.18269581542 Delta-E= -0.000000000061 Rises=F Damp=F

DIIS: error= 3.57D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.18269581542 IErMin= 8 ErrMin= 3.57D-07

ErrMax= 3.57D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.40D-10 BMatP= 3.30D-10

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

Coeff-Com: 0.429D-04-0.972D-03-0.139D-02-0.146D-02 0.732D-02 0.292D-01

Coeff-Com: 0.401D+00 0.567D+00

Coeff: 0.429D-04-0.972D-03-0.139D-02-0.146D-02 0.732D-02 0.292D-01

Coeff: 0.401D+00 0.567D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=8.61D-09 MaxDP=3.87D-07 DE=-6.09D-11 OVMax= 1.37D-06

Error on total polarization charges = 0.06719

SCF Done: E(UB3LYP) = -1359.18269582 A.U. after 8 cycles

NFock= 8 Conv=0.86D-08 -V/T= 1.9682

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7631 S= 0.5065

<L.S>= 0.000000000000E+00

KE= 1.403845530051D+03 PE=-9.372146830084D+03 EE= 3.557787391839D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.26

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7631, after 0.7501

Leave Link 502 at Wed Jul 31 02:54:28 2019, MaxMem= 4294967296 cpu: 757.2

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 636

NBasis= 636 NAE= 111 NBE= 110 NFC= 0 NFV= 0

NROrb= 636 NOA= 111 NOB= 110 NVA= 525 NVB= 526

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.14750036D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.38325571D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.14750818D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.88283713D-01

Leave Link 801 at Wed Jul 31 02:54:29 2019, MaxMem= 4294967296 cpu: 0.4

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 45.

Will process 46 centers per pass.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16169 LenP2D= 44682.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 11 by ecpmxn.

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

Leave Link 1101 at Wed Jul 31 02:54:32 2019, MaxMem= 4294967296 cpu: 44.4

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Wed Jul 31 02:54:32 2019, MaxMem= 4294967296 cpu: 1.1

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 45.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966832.

G2DrvN: will do 46 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

G2PCM: DoFxE=T DoFxN=T DoGrad=T DoDP/DQ/DG/TGxP=FFFF NFrqRd= 0 IEInf=0 SqF1=F DoCFld=F IF1Alg=4.

GePol: Maximum number of non-zero 1st derivatives = 255

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Wed Jul 31 02:56:29 2019, MaxMem= 4294967296 cpu: 1870.3

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=111111111111111111111111111111111111111111111

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Using symmetry in CPHF.

Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.

Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.

NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 4294965570 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 0.

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

IRaf= 650000000 NMat= 42 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

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

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

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

NMat0= 42 NMatS0= 42 NMatT0= 0 NMatD0= 42 NMtDS0= 0 NMtDT0= 0

Integrals replicated using symmetry in FoFCou.

There are 42 degrees of freedom in the 1st order CPHF. IDoFFX=4 NUNeed= 42.

42 vectors produced by pass 0 Test12= 2.77D-13 2.38D-09 XBig12= 8.07D+03 5.92D+01.

AX will form 42 AO Fock derivatives at one time.

42 vectors produced by pass 1 Test12= 2.77D-13 2.38D-09 XBig12= 1.08D+03 6.87D+00.

42 vectors produced by pass 2 Test12= 2.77D-13 2.38D-09 XBig12= 2.83D+02 5.66D+00.

42 vectors produced by pass 3 Test12= 2.77D-13 2.38D-09 XBig12= 8.33D+01 2.11D+00.

42 vectors produced by pass 4 Test12= 2.77D-13 2.38D-09 XBig12= 9.13D+00 5.12D-01.

42 vectors produced by pass 5 Test12= 2.77D-13 2.38D-09 XBig12= 3.12D-01 6.12D-02.

42 vectors produced by pass 6 Test12= 2.77D-13 2.38D-09 XBig12= 1.25D-02 9.54D-03.

42 vectors produced by pass 7 Test12= 2.77D-13 2.38D-09 XBig12= 2.59D-04 1.43D-03.

37 vectors produced by pass 8 Test12= 2.77D-13 2.38D-09 XBig12= 4.97D-06 1.69D-04.

23 vectors produced by pass 9 Test12= 2.77D-13 2.38D-09 XBig12= 6.89D-08 2.30D-05.

8 vectors produced by pass 10 Test12= 2.77D-13 2.38D-09 XBig12= 9.02D-10 2.52D-06.

2 vectors produced by pass 11 Test12= 2.77D-13 2.38D-09 XBig12= 9.74D-12 1.94D-07.

2 vectors produced by pass 12 Test12= 2.77D-13 2.38D-09 XBig12= 1.35D-13 3.28D-08.

1 vectors produced by pass 13 Test12= 2.77D-13 2.38D-09 XBig12= 2.11D-15 2.41D-09.

InvSVY: IOpt=1 It= 1 EMax= 5.68D-14

Solved reduced A of dimension 409 with 42 vectors.

FullF1: Do perturbations 1 to 42.

Isotropic polarizability for W= 0.000000 1007.34 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Wed Jul 31 03:49:20 2019, MaxMem= 4294967296 cpu: 50737.5

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16169 LenP2D= 44682.

LDataN: DoStor=T MaxTD1= 7 Len= 274

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 255

Leave Link 701 at Wed Jul 31 03:49:54 2019, MaxMem= 4294967296 cpu: 549.9

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

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

Leave Link 702 at Wed Jul 31 03:49:54 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

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

wScrn= 0.000000 ICntrl= 100127 IOpCl= 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 Wed Jul 31 03:51:45 2019, MaxMem= 4294967296 cpu: 1770.9

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

Dipole =-4.07729406D-14-4.72524797D-13-1.45294107D-02

Polarizability= 1.65483017D+03-1.96788718D-06 1.18004369D+03

9.18144319D-06-4.53342334D-07 1.87131294D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000007912 0.000114008 0.000000486

2 6 -0.000021392 0.000052594 0.000001703

3 7 0.000432346 0.000000000 -0.000187780

4 6 -0.000021392 -0.000052594 0.000001703

5 6 0.000007912 -0.000114008 0.000000486

6 6 -0.000040097 -0.000022061 0.000000099

7 6 0.000045116 -0.000029285 0.000002326

8 7 -0.000000000 0.000298144 -0.000150862

9 6 -0.000045116 -0.000029285 0.000002326

10 6 0.000099862 0.000023154 0.000000424

11 6 -0.000099862 0.000023154 0.000000424

12 6 -0.000040097 0.000022061 0.000000099

13 6 0.000045116 0.000029285 0.000002326

14 6 -0.000099862 -0.000023154 0.000000424

15 6 0.000099862 -0.000023154 0.000000424

16 6 -0.000045116 0.000029285 0.000002326

17 7 0.000000000 -0.000298144 -0.000150862

18 6 0.000040097 0.000022061 0.000000099

19 6 0.000021392 0.000052594 0.000001703

20 6 -0.000007912 0.000114008 0.000000486

21 6 -0.000007912 -0.000114008 0.000000486

22 6 0.000021392 -0.000052594 0.000001703

23 7 -0.000432346 0.000000000 -0.000187780

24 1 0.000005947 0.000005618 0.000000155

25 1 0.000005947 -0.000005618 0.000000155

26 1 0.000002782 0.000004356 0.000000195

27 1 -0.000002782 0.000004356 0.000000195

28 1 -0.000002782 -0.000004356 0.000000195

29 1 0.000002782 -0.000004356 0.000000195

30 1 -0.000005947 0.000005618 0.000000155

31 1 -0.000005947 -0.000005618 0.000000155

32 30 -0.000000000 0.000000000 0.000656798

33 6 0.000040097 -0.000022061 0.000000099

34 6 0.000009330 0.000007665 -0.000000146

35 6 -0.000009330 -0.000007665 -0.000000146

36 6 0.000006819 0.000005286 -0.000000215

37 6 -0.000006819 -0.000005286 -0.000000215

38 6 -0.000009330 0.000007665 -0.000000146

39 6 -0.000006819 0.000005286 -0.000000215

40 6 0.000009330 -0.000007665 -0.000000146

41 6 0.000006819 -0.000005286 -0.000000215

42 1 -0.000012083 -0.000004301 0.000000093

43 1 -0.000012083 0.000004301 0.000000093

44 1 0.000012083 0.000004301 0.000000093

45 1 0.000012083 -0.000004301 0.000000093

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

Cartesian Forces: Max 0.000656798 RMS 0.000095379

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

Leave Link 716 at Wed Jul 31 03:51:45 2019, MaxMem= 4294967296 cpu: 0.8

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000279449 RMS 0.000045048

Search for a local minimum.

Step number 8 out of a maximum of 270

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

RMS Force = .45048D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -1.05D-04 DEPred=-9.60D-05 R= 1.10D+00

TightC=F SS= 1.41D+00 RLast= 1.31D-01 DXNew= 2.1213D-01 3.9274D-01

Trust test= 1.10D+00 RLast= 1.31D-01 DXMaxT set to 2.12D-01

ITU= 1 1 -1 0 0 -1 0 0

Eigenvalues --- 0.00151 0.00335 0.00452 0.00551 0.00655

Eigenvalues --- 0.00957 0.01116 0.01121 0.01163 0.01231

Eigenvalues --- 0.01241 0.01277 0.01295 0.01344 0.01385

Eigenvalues --- 0.01506 0.01521 0.01551 0.01867 0.01921

Eigenvalues --- 0.01943 0.01964 0.01981 0.02004 0.02023

Eigenvalues --- 0.02089 0.02101 0.02122 0.02123 0.02538

Eigenvalues --- 0.03001 0.03171 0.03195 0.03654 0.04003

Eigenvalues --- 0.04121 0.04123 0.04136 0.04137 0.04146

Eigenvalues --- 0.04359 0.04359 0.06247 0.06297 0.08267

Eigenvalues --- 0.08278 0.08294 0.08563 0.08843 0.08877

Eigenvalues --- 0.08955 0.09220 0.09275 0.09570 0.09610

Eigenvalues --- 0.09627 0.09656 0.09995 0.10408 0.10411

Eigenvalues --- 0.10442 0.10496 0.12293 0.13213 0.13551

Eigenvalues --- 0.13583 0.16015 0.16898 0.16961 0.19287

Eigenvalues --- 0.19798 0.20064 0.20080 0.20345 0.20621

Eigenvalues --- 0.20663 0.20836 0.21610 0.21810 0.21876

Eigenvalues --- 0.21942 0.25999 0.26177 0.27686 0.27930

Eigenvalues --- 0.28029 0.29422 0.29974 0.31686 0.32484

Eigenvalues --- 0.32762 0.32772 0.33604 0.35666 0.35681

Eigenvalues --- 0.35843 0.36113 0.36431 0.37024 0.37099

Eigenvalues --- 0.37155 0.37327 0.37389 0.37556 0.37837

Eigenvalues --- 0.38030 0.38349 0.38790 0.39214 0.40226

Eigenvalues --- 0.40229 0.40232 0.40232 0.41167 0.41278

Eigenvalues --- 0.41873 0.42413 0.45348 0.46039 0.46379

Eigenvalues --- 0.46597 0.50200 0.50207 0.52640 0.53052

Eigenvalues --- 1.03354 1.04102 1.04435 1.04669

En-DIIS/RFO-DIIS IScMMF= 0 using points: 8 7 6 5 4

RFO step: Lambda=-2.03972164D-06.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 7.31D-04 SmlDif= 1.00D-05

RMS Error= 0.1875808066D-03 NUsed= 5 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.42251 1.59443 -1.05259 0.03075 0.00489

Iteration 1 RMS(Cart)= 0.00066231 RMS(Int)= 0.00004569

Iteration 2 RMS(Cart)= 0.00000151 RMS(Int)= 0.00004568

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00004568

ITry= 1 IFail=0 DXMaxC= 8.70D-03 DCOld= 1.00D+10 DXMaxT= 2.12D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.08D-04 for atom 37.

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

(Linear) (Quad) (Total)

R1 2.74740 -0.00002 -0.00007 -0.00003 -0.00012 2.74728

R2 2.56785 0.00008 0.00016 0.00003 0.00009 2.56794

R3 2.04153 -0.00000 -0.00000 -0.00000 -0.00001 2.04152

R4 2.59161 0.00007 0.00012 0.00007 0.00021 2.59182

R5 2.65494 -0.00007 -0.00010 0.00003 -0.00013 2.65481

R6 2.59161 0.00007 0.00012 0.00007 0.00021 2.59182

R7 3.96380 -0.00028 -0.00062 -0.00062 -0.00117 3.96262

R8 2.74740 -0.00002 -0.00007 -0.00003 -0.00012 2.74728

R9 2.65494 -0.00007 -0.00010 0.00003 -0.00013 2.65481

R10 2.04153 -0.00000 -0.00000 -0.00000 -0.00001 2.04152

R11 2.72016 -0.00004 -0.00001 0.00001 -0.00011 2.72004

R12 2.69155 -0.00001 -0.00004 -0.00001 -0.00003 2.69152

R13 2.59136 0.00002 0.00009 -0.00005 0.00008 2.59144

R14 2.69694 -0.00004 -0.00015 0.00001 -0.00013 2.69681

R15 2.59136 0.00002 0.00009 -0.00006 0.00008 2.59144

R16 3.97151 -0.00017 -0.00112 0.00048 -0.00058 3.97093

R17 2.69694 -0.00004 -0.00015 0.00001 -0.00013 2.69681

R18 2.72016 -0.00004 -0.00001 0.00001 -0.00011 2.72004

R19 2.61500 0.00005 0.00017 0.00003 0.00010 2.61510

R20 2.04177 -0.00000 -0.00001 0.00000 -0.00001 2.04176

R21 2.04177 -0.00000 -0.00001 0.00000 -0.00001 2.04176

R22 2.72016 -0.00004 -0.00001 0.00001 -0.00011 2.72004

R23 2.69155 -0.00001 -0.00004 -0.00001 -0.00003 2.69152

R24 2.69694 -0.00004 -0.00015 0.00001 -0.00013 2.69681

R25 2.59136 0.00002 0.00009 -0.00005 0.00008 2.59144

R26 2.61500 0.00005 0.00017 0.00003 0.00010 2.61510

R27 2.04177 -0.00000 -0.00001 0.00000 -0.00001 2.04176

R28 2.69694 -0.00004 -0.00015 0.00001 -0.00013 2.69681

R29 2.04177 -0.00000 -0.00001 0.00000 -0.00001 2.04176

R30 2.59136 0.00002 0.00009 -0.00005 0.00008 2.59144

R31 2.72016 -0.00004 -0.00001 0.00001 -0.00011 2.72004

R32 3.97151 -0.00017 -0.00112 0.00052 -0.00058 3.97093

R33 2.65494 -0.00007 -0.00010 0.00003 -0.00013 2.65481

R34 2.69155 -0.00001 -0.00004 -0.00001 -0.00003 2.69152

R35 2.74740 -0.00002 -0.00007 -0.00003 -0.00012 2.74728

R36 2.59161 0.00007 0.00012 0.00007 0.00021 2.59182

R37 2.56785 0.00008 0.00016 0.00003 0.00009 2.56794

R38 2.04153 -0.00000 -0.00000 -0.00000 -0.00001 2.04152

R39 2.74740 -0.00002 -0.00007 -0.00003 -0.00012 2.74728

R40 2.04153 -0.00000 -0.00000 -0.00000 -0.00001 2.04152

R41 2.59161 0.00007 0.00012 0.00007 0.00021 2.59182

R42 2.65494 -0.00007 -0.00010 0.00003 -0.00013 2.65481

R43 3.96380 -0.00028 -0.00062 -0.00058 -0.00117 3.96262

R44 2.69155 -0.00001 -0.00004 -0.00001 -0.00003 2.69152

R45 2.28358 -0.00001 -0.00001 -0.00000 -0.00001 2.28357

R46 2.28358 -0.00001 -0.00001 -0.00000 -0.00001 2.28357

R47 2.01601 -0.00001 -0.00002 -0.00001 -0.00002 2.01599

R48 2.01601 -0.00001 -0.00002 -0.00001 -0.00002 2.01599

R49 2.28358 -0.00001 -0.00001 -0.00000 -0.00001 2.28357

R50 2.01601 -0.00001 -0.00002 -0.00001 -0.00002 2.01599

R51 2.28358 -0.00001 -0.00001 -0.00000 -0.00001 2.28357

R52 2.01601 -0.00001 -0.00002 -0.00001 -0.00002 2.01599

A1 1.87116 -0.00001 -0.00002 0.00000 -0.00002 1.87114

A2 2.18753 -0.00000 -0.00004 -0.00003 -0.00006 2.18747

A3 2.22449 0.00001 0.00006 0.00002 0.00008 2.22457

A4 1.89866 0.00004 0.00007 0.00002 0.00017 1.89882

A5 2.18526 -0.00005 -0.00003 -0.00014 -0.00022 2.18504

A6 2.19926 0.00001 -0.00004 0.00011 0.00006 2.19932

A7 1.88514 -0.00006 -0.00011 -0.00005 -0.00029 1.88485

A8 2.19902 0.00003 0.00011 0.00004 0.00014 2.19917

A9 2.19902 0.00003 0.00011 0.00001 0.00014 2.19917

A10 1.89866 0.00004 0.00007 0.00002 0.00017 1.89882

A11 2.19926 0.00001 -0.00004 0.00012 0.00006 2.19932

A12 2.18526 -0.00005 -0.00003 -0.00014 -0.00022 2.18504

A13 1.87116 -0.00001 -0.00002 0.00000 -0.00002 1.87114

A14 2.22449 0.00001 0.00006 0.00002 0.00008 2.22457

A15 2.18753 -0.00000 -0.00004 -0.00003 -0.00006 2.18747

A16 2.21378 -0.00006 -0.00018 -0.00002 -0.00027 2.21351

A17 2.04219 0.00001 0.00002 0.00002 0.00010 2.04229

A18 2.02721 0.00005 0.00016 0.00000 0.00017 2.02738

A19 2.18164 -0.00001 0.00007 -0.00013 -0.00007 2.18157

A20 2.19493 -0.00004 -0.00020 0.00010 -0.00013 2.19480

A21 1.90662 0.00005 0.00013 0.00003 0.00020 1.90682

A22 1.87945 -0.00007 -0.00018 -0.00001 -0.00028 1.87917

A23 2.20187 0.00003 0.00012 -0.00001 0.00014 2.20201

A24 2.20187 0.00003 0.00012 0.00002 0.00014 2.20201

A25 1.90662 0.00005 0.00013 0.00003 0.00020 1.90682

A26 2.18164 -0.00001 0.00007 -0.00013 -0.00007 2.18157

A27 2.19493 -0.00004 -0.00020 0.00010 -0.00013 2.19480

A28 1.86605 -0.00002 -0.00004 -0.00003 -0.00006 1.86599

A29 2.19643 0.00000 -0.00002 0.00001 -0.00002 2.19640

A30 2.22071 0.00001 0.00006 0.00002 0.00008 2.22080

A31 1.86605 -0.00002 -0.00004 -0.00003 -0.00006 1.86599

A32 2.19643 0.00000 -0.00002 0.00001 -0.00002 2.19640

A33 2.22071 0.00001 0.00006 0.00002 0.00008 2.22080

A34 2.21378 -0.00006 -0.00018 -0.00002 -0.00027 2.21351

A35 2.04219 0.00001 0.00002 0.00002 0.00010 2.04229

A36 2.02721 0.00005 0.00016 0.00000 0.00017 2.02738

A37 2.19493 -0.00004 -0.00020 0.00009 -0.00013 2.19480

A38 2.18164 -0.00001 0.00007 -0.00012 -0.00007 2.18157

A39 1.90662 0.00005 0.00013 0.00003 0.00020 1.90682

A40 1.86605 -0.00002 -0.00004 -0.00003 -0.00006 1.86599

A41 2.19643 0.00000 -0.00002 0.00001 -0.00002 2.19640

A42 2.22071 0.00001 0.00006 0.00002 0.00008 2.22080

A43 1.86605 -0.00002 -0.00004 -0.00003 -0.00006 1.86599

A44 2.22071 0.00001 0.00006 0.00002 0.00008 2.22080

A45 2.19643 0.00000 -0.00002 0.00001 -0.00002 2.19640

A46 1.90662 0.00005 0.00013 0.00003 0.00020 1.90682

A47 2.19493 -0.00004 -0.00020 0.00009 -0.00013 2.19480

A48 2.18164 -0.00001 0.00007 -0.00013 -0.00007 2.18157

A49 1.87945 -0.00007 -0.00018 -0.00001 -0.00028 1.87917

A50 2.20187 0.00003 0.00012 -0.00000 0.00014 2.20201

A51 2.20187 0.00003 0.00012 0.00002 0.00014 2.20201

A52 2.21378 -0.00006 -0.00018 -0.00003 -0.00027 2.21351

A53 2.02721 0.00005 0.00016 0.00001 0.00017 2.02738

A54 2.04219 0.00001 0.00002 0.00002 0.00010 2.04229

A55 2.18526 -0.00005 -0.00003 -0.00014 -0.00022 2.18504

A56 2.19926 0.00001 -0.00004 0.00012 0.00006 2.19932

A57 1.89866 0.00004 0.00007 0.00003 0.00017 1.89882

A58 1.87116 -0.00001 -0.00002 0.00000 -0.00002 1.87114

A59 2.18753 -0.00000 -0.00004 -0.00003 -0.00006 2.18747

A60 2.22449 0.00001 0.00006 0.00003 0.00008 2.22457

A61 1.87116 -0.00001 -0.00002 0.00000 -0.00002 1.87114

A62 2.22449 0.00001 0.00006 0.00003 0.00008 2.22457

A63 2.18753 -0.00000 -0.00004 -0.00003 -0.00006 2.18747

A64 1.89866 0.00004 0.00007 0.00003 0.00017 1.89882

A65 2.18526 -0.00005 -0.00003 -0.00015 -0.00022 2.18504

A66 2.19926 0.00001 -0.00004 0.00012 0.00006 2.19932

A67 1.88514 -0.00006 -0.00011 -0.00006 -0.00029 1.88485

A68 2.19902 0.00003 0.00011 0.00004 0.00014 2.19917

A69 2.19902 0.00003 0.00011 0.00002 0.00014 2.19917

A70 1.57079 0.00000 0.00020 0.00002 0.00001 1.57080

A71 1.57079 0.00000 0.00020 0.00000 0.00001 1.57080

A72 1.57079 0.00000 0.00020 -0.00000 0.00001 1.57080

A73 1.57079 0.00000 0.00020 -0.00002 0.00001 1.57080

A74 2.21378 -0.00006 -0.00018 -0.00002 -0.00027 2.21351

A75 2.02721 0.00005 0.00016 0.00000 0.00017 2.02738

A76 2.04219 0.00001 0.00002 0.00002 0.00010 2.04229

A77 3.14157 0.00000 0.00040 -0.00002 0.00002 3.14159

A78 3.14157 0.00000 0.00040 -0.00002 0.00002 3.14159

A79 3.12422 -0.00000 0.00003 -0.00004 -0.00000 3.12421

A80 3.15897 0.00000 -0.00004 0.00004 0.00000 3.15897

A81 3.14732 -0.00001 -0.00016 -0.00003 -0.00012 3.14720

A82 3.14732 -0.00001 -0.00016 -0.00003 -0.00012 3.14720

A83 3.15897 0.00000 -0.00004 0.00004 0.00000 3.15897

A84 3.14732 -0.00001 -0.00016 -0.00003 -0.00012 3.14720

A85 3.12422 -0.00000 0.00003 -0.00004 -0.00000 3.12421

A86 3.14732 -0.00001 -0.00016 -0.00003 -0.00012 3.14720

A87 3.13523 0.00015 0.00415 -0.00019 0.00396 3.13919

A88 3.14717 -0.00013 -0.00348 -0.00013 -0.00360 3.14357

A89 3.14162 -0.00000 0.00007 -0.00008 -0.00001 3.14161

A90 3.14155 0.00000 -0.00005 0.00008 0.00002 3.14157

A91 3.14160 0.00000 -0.00004 0.00004 -0.00000 3.14160

A92 3.14160 0.00000 -0.00004 0.00004 -0.00000 3.14160

A93 3.14164 -0.00000 0.00005 -0.00008 -0.00002 3.14161

A94 3.14158 -0.00000 0.00004 -0.00004 0.00000 3.14159

A95 3.14157 0.00000 -0.00007 0.00008 0.00001 3.14158

A96 3.14158 -0.00000 0.00004 -0.00004 0.00000 3.14159

D1 -0.00009 -0.00001 0.00008 -0.00004 0.00004 -0.00005

D2 -3.14154 -0.00002 0.00006 -0.00013 -0.00007 3.14157

D3 3.14139 -0.00000 0.00016 -0.00004 0.00012 3.14151

D4 -0.00006 -0.00001 0.00014 -0.00013 0.00001 -0.00006

D5 -0.00000 0.00000 0.00000 -0.00000 -0.00000 -0.00000

D6 3.14148 0.00001 0.00008 -0.00000 0.00008 3.14156

D7 -3.14148 -0.00001 -0.00008 0.00000 -0.00008 -3.14156

D8 -0.00000 -0.00000 -0.00000 0.00000 0.00000 0.00000

D9 0.00015 0.00002 -0.00013 0.00006 -0.00006 0.00009

D10 3.13831 0.00004 0.00199 0.00003 0.00203 3.14034

D11 -3.14159 0.00002 -0.00011 0.00016 0.00005 -3.14153

D12 -0.00342 0.00004 0.00201 0.00012 0.00214 -0.00128

D13 3.14116 0.00004 0.00033 -0.00003 0.00031 3.14147

D14 -0.00013 0.00000 0.00016 -0.00003 0.00013 -0.00001

D15 -0.00027 0.00003 0.00031 -0.00014 0.00018 -0.00009

D16 -3.14156 -0.00000 0.00013 -0.00014 -0.00001 -3.14157

D17 -0.00015 -0.00002 0.00013 -0.00006 0.00006 -0.00009

D18 3.14159 -0.00002 0.00011 -0.00016 -0.00005 3.14153

D19 -3.13831 -0.00004 -0.00199 -0.00003 -0.00203 -3.14034

D20 0.00342 -0.00004 -0.00201 -0.00013 -0.00214 0.00128

D21 3.14082 0.00006 0.00050 0.00009 0.00057 3.14139

D22 0.00480 -0.00008 -0.00298 -0.00005 -0.00303 0.00178

D23 -0.00480 0.00008 0.00298 0.00005 0.00303 -0.00178

D24 -3.14082 -0.00006 -0.00050 -0.00009 -0.00057 -3.14139

D25 0.00009 0.00001 -0.00008 0.00004 -0.00004 0.00005

D26 -3.14139 0.00000 -0.00016 0.00004 -0.00012 -3.14151

D27 3.14154 0.00002 -0.00006 0.00013 0.00007 -3.14157

D28 0.00006 0.00001 -0.00014 0.00013 -0.00001 0.00006

D29 0.00027 -0.00003 -0.00031 0.00014 -0.00018 0.00009

D30 3.14156 0.00000 -0.00013 0.00014 0.00001 3.14157

D31 -3.14116 -0.00004 -0.00033 0.00003 -0.00031 -3.14147

D32 0.00013 -0.00000 -0.00016 0.00003 -0.00013 0.00001

D33 -0.00053 0.00003 0.00037 -0.00006 0.00031 -0.00022

D34 3.14053 0.00004 0.00075 -0.00013 0.00062 3.14115

D35 3.14136 -0.00001 0.00019 -0.00006 0.00013 3.14149

D36 -0.00077 0.00001 0.00057 -0.00013 0.00044 -0.00033

D37 3.14103 0.00003 0.00045 -0.00015 0.00030 3.14134

D38 -0.00294 0.00005 0.00191 -0.00002 0.00190 -0.00105

D39 -0.00010 0.00002 0.00012 -0.00008 0.00004 -0.00006

D40 3.13911 0.00004 0.00159 0.00004 0.00163 3.14074

D41 -3.14107 -0.00002 -0.00040 0.00011 -0.00029 -3.14136

D42 0.00030 -0.00001 -0.00022 0.00007 -0.00016 0.00014

D43 0.00006 -0.00001 -0.00008 0.00005 -0.00002 0.00004

D44 3.14143 -0.00000 0.00010 0.00000 0.00011 3.14154

D45 0.00010 -0.00002 -0.00012 0.00008 -0.00004 0.00006

D46 -3.14103 -0.00003 -0.00045 0.00015 -0.00030 -3.14134

D47 -3.13911 -0.00004 -0.00159 -0.00004 -0.00163 -3.14074

D48 0.00294 -0.00005 -0.00191 0.00002 -0.00190 0.00105

D49 0.00459 -0.00008 -0.00294 0.00002 -0.00292 0.00167

D50 3.13982 0.00007 0.00121 -0.00017 0.00104 3.14085

D51 -3.13982 -0.00007 -0.00121 0.00017 -0.00104 -3.14085

D52 -0.00459 0.00008 0.00294 -0.00002 0.00292 -0.00167

D53 -0.00006 0.00001 0.00008 -0.00005 0.00002 -0.00004

D54 -3.14143 0.00000 -0.00010 -0.00000 -0.00011 -3.14154

D55 3.14107 0.00002 0.00040 -0.00011 0.00029 3.14136

D56 -0.00030 0.00001 0.00022 -0.00007 0.00016 -0.00014

D57 0.00053 -0.00003 -0.00037 0.00006 -0.00031 0.00022

D58 -3.14136 0.00001 -0.00019 0.00006 -0.00013 -3.14149

D59 -3.14053 -0.00004 -0.00075 0.00013 -0.00062 -3.14115

D60 0.00077 -0.00001 -0.00057 0.00013 -0.00044 0.00033

D61 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D62 -3.14136 -0.00001 -0.00018 0.00005 -0.00013 -3.14150

D63 3.14136 0.00001 0.00018 -0.00005 0.00013 3.14150

D64 -0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D65 -3.14053 -0.00004 -0.00075 0.00013 -0.00062 -3.14115

D66 0.00053 -0.00003 -0.00037 0.00006 -0.00031 0.00022

D67 0.00077 -0.00001 -0.00057 0.00013 -0.00044 0.00033

D68 -3.14136 0.00001 -0.00019 0.00006 -0.00013 -3.14149

D69 3.14107 0.00002 0.00040 -0.00011 0.00029 3.14136

D70 -0.00030 0.00001 0.00022 -0.00007 0.00016 -0.00014

D71 -0.00006 0.00001 0.00008 -0.00005 0.00002 -0.00004

D72 -3.14143 0.00000 -0.00010 -0.00000 -0.00011 -3.14154

D73 -3.14103 -0.00003 -0.00045 0.00015 -0.00030 -3.14134

D74 0.00294 -0.00005 -0.00191 0.00002 -0.00190 0.00105

D75 0.00010 -0.00002 -0.00012 0.00008 -0.00004 0.00006

D76 -3.13911 -0.00004 -0.00159 -0.00004 -0.00163 -3.14074

D77 0.00000 -0.00000 -0.00000 -0.00000 0.00000 0.00000

D78 -3.14136 -0.00001 -0.00018 0.00005 -0.00013 -3.14150

D79 3.14136 0.00001 0.00018 -0.00005 0.00013 3.14150

D80 -0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D81 0.00006 -0.00001 -0.00008 0.00005 -0.00002 0.00004

D82 -3.14107 -0.00002 -0.00040 0.00011 -0.00029 -3.14136

D83 3.14143 -0.00000 0.00010 0.00000 0.00011 3.14154

D84 0.00030 -0.00001 -0.00022 0.00007 -0.00016 0.00014

D85 -0.00010 0.00002 0.00012 -0.00008 0.00004 -0.00006

D86 3.13911 0.00004 0.00159 0.00004 0.00163 3.14074

D87 3.14103 0.00003 0.00045 -0.00015 0.00030 3.14134

D88 -0.00294 0.00005 0.00191 -0.00002 0.00190 -0.00105

D89 3.14053 0.00004 0.00075 -0.00013 0.00062 3.14115

D90 -0.00077 0.00001 0.00057 -0.00013 0.00044 -0.00033

D91 -0.00053 0.00003 0.00037 -0.00006 0.00031 -0.00022

D92 3.14136 -0.00001 0.00019 -0.00006 0.00013 3.14149

D93 -0.00459 0.00008 0.00294 -0.00002 0.00292 -0.00167

D94 -3.13982 -0.00007 -0.00121 0.00017 -0.00104 -3.14085

D95 3.13982 0.00007 0.00121 -0.00017 0.00104 3.14085

D96 0.00459 -0.00008 -0.00294 0.00002 -0.00292 0.00167

D97 -3.14116 -0.00004 -0.00033 0.00003 -0.00031 -3.14147

D98 0.00027 -0.00003 -0.00031 0.00014 -0.00018 0.00009

D99 0.00013 -0.00000 -0.00016 0.00003 -0.00013 0.00001

D100 3.14156 0.00000 -0.00013 0.00014 0.00001 3.14157

D101 3.14154 0.00002 -0.00006 0.00013 0.00007 -3.14157

D102 0.00006 0.00001 -0.00014 0.00013 -0.00001 0.00006

D103 0.00009 0.00001 -0.00008 0.00004 -0.00004 0.00005

D104 -3.14139 0.00000 -0.00016 0.00004 -0.00012 -3.14151

D105 3.14159 -0.00002 0.00011 -0.00016 -0.00005 3.14153

D106 0.00342 -0.00004 -0.00201 -0.00012 -0.00214 0.00128

D107 -0.00015 -0.00002 0.00013 -0.00006 0.00006 -0.00009

D108 -3.13831 -0.00004 -0.00199 -0.00003 -0.00203 -3.14034

D109 -0.00000 -0.00000 0.00000 0.00000 -0.00000 -0.00000

D110 -3.14148 -0.00001 -0.00008 0.00000 -0.00008 -3.14156

D111 3.14148 0.00001 0.00008 -0.00000 0.00008 3.14156

D112 0.00000 0.00000 -0.00000 -0.00000 -0.00000 -0.00000

D113 -0.00009 -0.00001 0.00008 -0.00004 0.00004 -0.00005

D114 -3.14154 -0.00002 0.00006 -0.00013 -0.00007 3.14157

D115 3.14139 -0.00000 0.00016 -0.00004 0.00012 3.14151

D116 -0.00006 -0.00001 0.00014 -0.00013 0.00001 -0.00006

D117 0.00015 0.00002 -0.00013 0.00006 -0.00006 0.00009

D118 3.13831 0.00004 0.00199 0.00003 0.00203 3.14034

D119 -3.14159 0.00002 -0.00011 0.00016 0.00005 -3.14153

D120 -0.00342 0.00004 0.00201 0.00013 0.00214 -0.00128

D121 3.14116 0.00004 0.00033 -0.00003 0.00031 3.14147

D122 -0.00013 0.00000 0.00016 -0.00003 0.00013 -0.00001

D123 -0.00027 0.00003 0.00031 -0.00014 0.00018 -0.00009

D124 -3.14156 -0.00000 0.00013 -0.00014 -0.00001 -3.14157

D125 -3.14082 -0.00006 -0.00050 -0.00009 -0.00057 -3.14139

D126 -0.00480 0.00008 0.00298 0.00005 0.00303 -0.00178

D127 0.00480 -0.00008 -0.00298 -0.00005 -0.00303 0.00178

D128 3.14082 0.00006 0.00050 0.00009 0.00057 3.14139

Item Value Threshold Converged?

Maximum Force 0.000279 0.000450 YES

RMS Force 0.000045 0.000300 YES

Maximum Displacement 0.008699 0.001800 NO

RMS Displacement 0.000665 0.001200 YES

Predicted change in Energy=-4.258367D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Wed Jul 31 03:51:45 2019, MaxMem= 4294967296 cpu: 1.1

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -4.291872 0.679448 -0.024175

2 6 0 -2.903152 1.109552 -0.024460

3 7 0 -2.096927 0.000000 -0.024556

4 6 0 -2.903152 -1.109552 -0.024460

5 6 0 -4.291872 -0.679448 -0.024175

6 6 0 -2.469369 -2.445770 -0.024579

7 6 0 -1.107097 -2.910577 -0.024719

8 7 0 -0.000000 -2.101324 -0.025003

9 6 0 1.107097 -2.910577 -0.024719

10 6 0 0.691927 -4.275940 -0.024324

11 6 0 -0.691927 -4.275940 -0.024324

12 6 0 -2.469369 2.445770 -0.024579

13 6 0 -1.107097 2.910577 -0.024719

14 6 0 -0.691927 4.275940 -0.024324

15 6 0 0.691927 4.275940 -0.024324

16 6 0 1.107097 2.910577 -0.024719

17 7 0 0.000000 2.101324 -0.025003

18 6 0 2.469369 2.445770 -0.024579

19 6 0 2.903152 1.109552 -0.024460

20 6 0 4.291872 0.679448 -0.024175

21 6 0 4.291872 -0.679448 -0.024175

22 6 0 2.903152 -1.109552 -0.024460

23 7 0 2.096927 -0.000000 -0.024556

24 1 0 -5.149425 1.336488 -0.023974

25 1 0 -5.149425 -1.336488 -0.023974

26 1 0 1.345804 -5.136073 -0.023995

27 1 0 -1.345804 -5.136073 -0.023995

28 1 0 -1.345804 5.136073 -0.023995

29 1 0 1.345804 5.136073 -0.023995

30 1 0 5.149425 1.336488 -0.023974

31 1 0 5.149425 -1.336488 -0.023974

32 30 0 -0.000000 -0.000000 -0.027080

33 6 0 2.469369 -2.445770 -0.024579

34 6 0 3.476496 -3.452897 -0.024413

35 6 0 -3.476496 3.452897 -0.024413

36 6 0 4.315998 -4.322095 -0.024252

37 6 0 -4.315998 4.322095 -0.024252

38 6 0 -3.476496 -3.452897 -0.024413

39 6 0 -4.315998 -4.322095 -0.024252

40 6 0 3.476496 3.452897 -0.024413

41 6 0 4.315998 4.322095 -0.024252

42 1 0 5.061421 5.085273 -0.024105

43 1 0 5.061421 -5.085273 -0.024105

44 1 0 -5.061421 -5.085273 -0.024105

45 1 0 -5.061421 5.085273 -0.024105

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.453799 0.000000

3 N 2.297701 1.371533 0.000000

4 C 2.264743 2.219104 1.371533 0.000000

5 C 1.358895 2.264743 2.297701 1.453799 0.000000

6 C 3.617803 3.581687 2.473965 1.404865 2.537993

7 C 4.799069 4.403095 3.074284 2.543522 3.888538

8 N 5.113986 4.328743 2.968613 3.067882 4.521271

9 C 6.483606 5.678339 4.328652 4.396111 5.841815

10 C 7.028095 6.475192 5.105034 4.790679 6.145975

11 C 6.124987 5.821773 4.500855 3.862063 5.088650

12 C 2.537993 1.404865 2.473965 3.581687 3.617803

13 C 3.888538 2.543522 3.074284 4.403095 4.799069

14 C 5.088650 3.862063 4.500855 5.821773 6.124987

15 C 6.145975 4.790679 5.105034 6.475192 7.028095

16 C 5.841815 4.396111 4.328652 5.678339 6.483606

17 N 4.521271 3.067882 2.968613 4.328743 5.113986

18 C 6.988152 5.536195 5.180044 6.442383 7.448581

19 C 7.207867 5.806304 5.121708 6.215914 7.414100

20 C 8.583743 7.207867 6.424827 7.414100 8.690641

21 C 8.690641 7.414100 6.424827 7.207867 8.583743

22 C 7.414100 6.215914 5.121708 5.806304 7.207867

23 N 6.424827 5.121708 4.193854 5.121708 6.424827

24 H 1.080324 2.257708 3.332258 3.320972 2.190752

25 H 2.190752 3.320972 3.332258 2.257708 1.080324

26 H 8.099609 7.553903 6.183174 5.853759 7.186438

27 H 6.519171 6.436860 5.190706 4.317199 5.342361

28 H 5.342361 4.317199 5.190706 6.436860 6.519171

29 H 7.186438 5.853759 6.183174 7.553903 8.099609

30 H 9.464132 8.055774 7.368570 8.415885 9.654123

31 H 9.654123 8.415885 7.368570 8.055774 9.464132

32 Zn 4.345321 3.107958 2.096929 3.107958 4.345321

33 C 7.448581 6.442383 5.180044 5.536195 6.988152

34 C 8.799080 7.843204 6.556336 6.796409 8.248609

35 C 2.890823 2.412465 3.718293 4.598332 4.212019

36 C 9.955443 9.034318 7.733441 7.901680 9.346887

37 C 3.642727 3.509496 4.858475 5.612390 5.001601

38 C 4.212019 4.598332 3.718293 2.412465 2.890823

39 C 5.001601 5.612390 4.858475 3.509496 3.642727

40 C 8.248609 6.796409 6.556336 7.843204 8.799080

41 C 9.346887 7.901680 7.733441 9.034318 9.955443

42 H 10.339022 8.901729 8.780772 10.090108 10.987087

43 H 10.987087 10.090108 8.780772 8.901729 10.339022

44 H 5.815859 6.560030 5.886275 4.523769 4.472528

45 H 4.472528 4.523769 5.886275 6.560030 5.815859

6 7 8 9 10

6 C 0.000000

7 C 1.439385 0.000000

8 N 2.493276 1.371333 0.000000

9 C 3.606544 2.214194 1.371333 0.000000

10 C 3.652850 2.258474 2.282043 1.427089 0.000000

11 C 2.551240 1.427089 2.282043 2.258474 1.383853

12 C 4.891540 5.526865 5.174345 6.440618 7.428000

13 C 5.526865 5.821154 5.132720 6.228041 7.408274

14 C 6.952747 7.198500 6.414691 7.408274 8.663124

15 C 7.428000 7.408274 6.414691 7.198500 8.551881

16 C 6.440618 6.228041 5.132720 5.821154 7.198500

17 N 5.174345 5.132720 4.202647 5.132720 6.414691

18 C 6.951136 6.440618 5.174345 5.526865 6.952747

19 C 6.442383 5.678339 4.328743 4.403095 5.821773

20 C 7.448581 6.483606 5.113986 4.799069 6.124987

21 C 6.988152 5.841815 4.521271 3.888538 5.088650

22 C 5.536195 4.396111 3.067882 2.543522 3.862063

23 N 5.180044 4.328652 2.968613 3.074284 4.500855

24 H 4.635534 5.863274 6.191537 7.561854 8.100663

25 H 2.900553 4.337992 5.205916 6.451498 6.539249

26 H 4.668327 3.312032 3.319773 2.238261 1.080455

27 H 2.915498 2.238261 3.319773 3.312032 2.211826

28 H 7.664642 8.050190 7.361460 8.412211 9.630075

29 H 8.487631 8.412211 7.361460 8.050190 9.434699

30 H 8.505969 7.561854 6.191537 5.863274 7.167192

31 H 7.699126 6.451498 5.205916 4.337992 5.339445

32 Zn 3.475569 3.114021 2.101325 3.114021 4.331563

33 C 4.938738 3.606544 2.493276 1.439385 2.551240

34 C 6.030557 4.615565 3.729983 2.430671 2.903658

35 C 5.984026 6.790276 6.552510 7.842393 8.781268

36 C 7.040014 5.603779 4.853830 3.505628 3.624365

37 C 7.015271 7.912559 7.738743 9.039995 9.950152

38 C 1.424293 2.430671 3.729983 4.615565 4.248900

39 C 2.632610 3.505628 4.853830 5.603779 5.008137

40 C 8.375415 7.842393 6.552510 6.790276 8.215153

41 C 9.583590 9.039995 7.738743 7.912559 9.330600

42 H 10.650325 10.098725 8.790060 8.920219 10.330770

43 H 7.979961 6.540636 5.875537 4.512868 4.443816

44 H 3.699421 4.512868 5.875537 6.540636 5.809994

45 H 7.964631 8.920219 8.790060 10.098725 10.987872

11 12 13 14 15

11 C 0.000000

12 C 6.952747 0.000000

13 C 7.198500 1.439385 0.000000

14 C 8.551881 2.551240 1.427089 0.000000

15 C 8.663124 3.652850 2.258474 1.383853 0.000000

16 C 7.408274 3.606544 2.214194 2.258474 1.427089

17 N 6.414691 2.493276 1.371333 2.282043 2.282043

18 C 7.428000 4.938738 3.606544 3.652850 2.551240

19 C 6.475192 5.536195 4.396111 4.790679 3.862063

20 C 7.028095 6.988152 5.841815 6.145975 5.088650

21 C 6.145975 7.448581 6.483606 7.028095 6.124987

22 C 4.790679 6.442383 5.678339 6.475192 5.821773

23 N 5.105034 5.180044 4.328652 5.105034 4.500855

24 H 7.167192 2.900553 4.337992 5.339445 6.539249

25 H 5.339445 4.635534 5.863274 7.167192 8.100663

26 H 2.211826 8.487631 8.412211 9.630075 9.434699

27 H 1.080455 7.664642 8.050190 9.434699 9.630075

28 H 9.434699 2.915498 2.238261 1.080455 2.211826

29 H 9.630075 4.668327 3.312032 2.211826 1.080455

30 H 8.100663 7.699126 6.451498 6.539249 5.339445

31 H 6.539249 8.505969 7.561854 8.100663 7.167192

32 Zn 4.331563 3.475569 3.114021 4.331563 4.331563

33 C 3.652850 6.951136 6.440618 7.428000 6.952747

34 C 4.248900 8.375415 7.842393 8.781268 8.215153

35 C 8.215153 1.424293 2.430671 2.903658 4.248900

36 C 5.008137 9.583590 9.039995 9.950152 9.330600

37 C 9.330600 2.632610 3.505628 3.624365 5.008137

38 C 2.903658 5.984026 6.790276 8.215153 8.781268

39 C 3.624365 7.015271 7.912559 9.330600 9.950152

40 C 8.781268 6.030557 4.615565 4.248900 2.903658

41 C 9.950152 7.040014 5.603779 5.008137 3.624365

42 H 10.987872 7.979961 6.540636 5.809994 4.443816

43 H 5.809994 10.650325 10.098725 10.987872 10.330770

44 H 4.443816 7.964631 8.920219 10.330770 10.987872

45 H 10.330770 3.699421 4.512868 4.443816 5.809994

16 17 18 19 20

16 C 0.000000

17 N 1.371333 0.000000

18 C 1.439385 2.493276 0.000000

19 C 2.543522 3.067882 1.404865 0.000000

20 C 3.888538 4.521271 2.537993 1.453799 0.000000

21 C 4.799069 5.113986 3.617803 2.264743 1.358895

22 C 4.403095 4.328743 3.581687 2.219104 2.264743

23 N 3.074284 2.968613 2.473965 1.371533 2.297701

24 H 6.451498 5.205916 7.699126 8.055774 9.464132

25 H 7.561854 6.191537 8.505969 8.415885 9.654123

26 H 8.050190 7.361460 7.664642 6.436860 6.519171

27 H 8.412211 7.361460 8.487631 7.553903 8.099609

28 H 3.312032 3.319773 4.668327 5.853759 7.186438

29 H 2.238261 3.319773 2.915498 4.317199 5.342361

30 H 4.337992 5.205916 2.900553 2.257708 1.080324

31 H 5.863274 6.191537 4.635534 3.320972 2.190752

32 Zn 3.114021 2.101325 3.475569 3.107958 4.345321

33 C 5.526865 5.174345 4.891540 3.581687 3.617803

34 C 6.790276 6.552510 5.984026 4.598332 4.212019

35 C 4.615565 3.729983 6.030557 6.796409 8.248609

36 C 7.912559 7.738743 7.015271 5.612390 5.001601

37 C 5.603779 4.853830 7.040014 7.901680 9.346887

38 C 7.842393 6.552510 8.375415 7.843204 8.799080

39 C 9.039995 7.738743 9.583590 9.034318 9.955443

40 C 2.430671 3.729983 1.424293 2.412465 2.890823

41 C 3.505628 4.853830 2.632610 3.509496 3.642727

42 H 4.512868 5.875537 3.699421 4.523769 4.472528

43 H 8.920219 8.790060 7.964631 6.560030 5.815859

44 H 10.098725 8.790060 10.650325 10.090108 10.987087

45 H 6.540636 5.875537 7.979961 8.901729 10.339022

21 22 23 24 25

21 C 0.000000

22 C 1.453799 0.000000

23 N 2.297701 1.371533 0.000000

24 H 9.654123 8.415885 7.368570 0.000000

25 H 9.464132 8.055774 7.368570 2.672976 0.000000

26 H 5.342361 4.317199 5.190706 9.169626 7.524948

27 H 7.186438 5.853759 6.183174 7.507435 5.376280

28 H 8.099609 7.553903 6.183174 5.376280 7.507435

29 H 6.519171 6.436860 5.190706 7.524948 9.169626

30 H 2.190752 3.320972 3.332258 10.298851 10.640072

31 H 1.080324 2.257708 3.332258 10.640072 10.298851

32 Zn 4.345321 3.107958 2.096929 5.320037 5.320037

33 C 2.537993 1.404865 2.473965 8.505969 7.699126

34 C 2.890823 2.412465 3.718293 9.866343 8.881763

35 C 8.799080 7.843204 6.556336 2.697754 5.073154

36 C 3.642727 3.509496 4.858475 11.027865 9.925124

37 C 9.955443 9.034318 7.733441 3.099750 5.719629

38 C 8.248609 6.796409 6.556336 5.073154 2.697754

39 C 9.346887 7.901680 7.733441 5.719629 3.099750

40 C 4.212019 4.598332 3.718293 8.881763 9.866343

41 C 5.001601 5.612390 4.858475 9.925124 11.027865

42 H 5.815859 6.560030 5.886275 10.877260 12.062355

43 H 4.472528 4.523769 5.886275 12.062355 10.877260

44 H 10.339022 8.901729 8.780772 6.422364 3.749818

45 H 10.987087 10.090108 8.780772 3.749818 6.422364

26 27 28 29 30

26 H 0.000000

27 H 2.691607 0.000000

28 H 10.618933 10.272146 0.000000

29 H 10.272146 10.618933 2.691607 0.000000

30 H 7.507435 9.169626 7.524948 5.376280 0.000000

31 H 5.376280 7.524948 9.169626 7.507435 2.672976

32 Zn 5.309467 5.309467 5.309467 5.309467 5.320037

33 C 2.915498 4.668327 8.487631 7.664642 4.635534

34 C 2.715315 5.107608 9.850126 8.849308 5.073154

35 C 9.850126 8.849308 2.715315 5.107608 8.881763

36 C 3.079710 5.720014 11.023290 9.913576 5.719629

37 C 11.023290 9.913576 3.079710 5.720014 9.925124

38 C 5.107608 2.715315 8.849308 9.850126 9.866343

39 C 5.720014 3.079710 9.913576 11.023290 11.027865

40 C 8.849308 9.850126 5.107608 2.715315 2.697754

41 C 9.913576 11.023290 5.720014 3.079710 3.099750

42 H 10.875740 12.063517 6.407426 3.715965 3.749818

43 H 3.715965 6.407426 12.063517 10.875740 6.422364

44 H 6.407426 3.715965 10.875740 12.063517 12.062355

45 H 12.063517 10.875740 3.715965 6.407426 10.877260

31 32 33 34 35

31 H 0.000000

32 Zn 5.320037 0.000000

33 C 2.900553 3.475569 0.000000

34 C 2.697754 4.899850 1.424293 0.000000

35 C 9.866343 4.899850 8.375415 9.799698 0.000000

36 C 3.099750 6.108056 2.632610 1.208416 11.007882

37 C 11.027865 6.108056 9.583590 11.007882 1.208416

38 C 8.881763 4.899850 6.030557 6.952993 6.905793

39 C 9.925124 6.108056 7.040014 7.840821 7.820182

40 C 5.073154 4.899850 5.984026 6.905793 6.952993

41 C 5.719629 6.108056 7.015271 7.820182 7.840821

42 H 6.422364 7.174817 7.964631 8.684027 8.692565

43 H 3.749818 7.174817 3.699421 2.275223 12.074617

44 H 10.877260 7.174817 7.979961 8.692565 8.684027

45 H 12.062355 7.174817 10.650325 12.074617 2.275223

36 37 38 39 40

36 C 0.000000

37 C 12.216111 0.000000

38 C 7.840821 7.820182 0.000000

39 C 8.631996 8.644190 1.208416 0.000000

40 C 7.820182 7.840821 9.799698 11.007882 0.000000

41 C 8.644190 8.631996 11.007882 12.216111 1.208416

42 H 9.436855 9.408423 12.074617 13.282867 2.275223

43 H 1.066816 13.282867 8.692565 9.408423 8.684027

44 H 9.408423 9.436855 2.275223 1.066816 12.074617

45 H 13.282867 1.066816 8.684027 9.436855 8.692565

41 42 43 44 45

41 C 0.000000

42 H 1.066816 0.000000

43 H 9.436855 10.170547 0.000000

44 H 13.282867 14.349633 10.122842 0.000000

45 H 9.408423 10.122842 14.349633 10.170547 0.000000

Stoichiometry C28H12N4Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C28H12)]

Deg. of freedom 34

Full point group C2V NOp 4

RotChk: IX=2 Diff= 1.24D-13

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.679448 4.291872 0.000601

2 6 0 1.109552 2.903152 0.000316

3 7 0 0.000000 2.096927 0.000220

4 6 0 -1.109552 2.903152 0.000316

5 6 0 -0.679448 4.291872 0.000601

6 6 0 -2.445770 2.469369 0.000197

7 6 0 -2.910577 1.107097 0.000057

8 7 0 -2.101324 -0.000000 -0.000227

9 6 0 -2.910577 -1.107097 0.000057

10 6 0 -4.275940 -0.691927 0.000451

11 6 0 -4.275940 0.691927 0.000451

12 6 0 2.445770 2.469369 0.000197

13 6 0 2.910577 1.107097 0.000057

14 6 0 4.275940 0.691927 0.000451

15 6 0 4.275940 -0.691927 0.000451

16 6 0 2.910577 -1.107097 0.000057

17 7 0 2.101324 0.000000 -0.000227

18 6 0 2.445770 -2.469369 0.000197

19 6 0 1.109552 -2.903152 0.000316

20 6 0 0.679448 -4.291872 0.000601

21 6 0 -0.679448 -4.291872 0.000601

22 6 0 -1.109552 -2.903152 0.000316

23 7 0 0.000000 -2.096927 0.000220

24 1 0 1.336488 5.149425 0.000802

25 1 0 -1.336488 5.149425 0.000802

26 1 0 -5.136073 -1.345804 0.000781

27 1 0 -5.136073 1.345804 0.000781

28 1 0 5.136073 1.345804 0.000781

29 1 0 5.136073 -1.345804 0.000781

30 1 0 1.336488 -5.149425 0.000802

31 1 0 -1.336488 -5.149425 0.000802

32 30 0 0.000000 0.000000 -0.002304

33 6 0 -2.445770 -2.469369 0.000197

34 6 0 -3.452897 -3.476496 0.000363

35 6 0 3.452897 3.476496 0.000363

36 6 0 -4.322095 -4.315998 0.000524

37 6 0 4.322095 4.315998 0.000524

38 6 0 -3.452897 3.476496 0.000363

39 6 0 -4.322095 4.315998 0.000524

40 6 0 3.452897 -3.476496 0.000363

41 6 0 4.322095 -4.315998 0.000524

42 1 0 5.085273 -5.061421 0.000671

43 1 0 -5.085273 -5.061421 0.000671

44 1 0 -5.085273 5.061421 0.000671

45 1 0 5.085273 5.061421 0.000671

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

Rotational constants (GHZ): 0.1459357 0.1453026 0.0728092

Leave Link 202 at Wed Jul 31 03:51:45 2019, MaxMem= 4294967296 cpu: 0.2

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

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

Pseudo-potential data read from rwf file.

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

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

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

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

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

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

111 alpha electrons 110 beta electrons

nuclear repulsion energy 3051.5911609237 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= 13 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= -0.1303219889 Hartrees.

Nuclear repulsion after empirical dispersion term = 3051.4608389348 Hartrees.

No density basis found on file 724.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

2nd derivatives : Analytical E(r).r(xy)/FMM algorithm (CHGder, D2EAlg=3).

Cavity 2nd derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3878

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.59D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 80

GePol: Fraction of low-weight points (<1% of avg) = 2.06%

GePol: Cavity surface area = 416.536 Ang\*\*2

GePol: Cavity volume = 421.091 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0083855923 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3051.4692245271 Hartrees.

Leave Link 301 at Wed Jul 31 03:51:45 2019, MaxMem= 4294967296 cpu: 1.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16169 LenP2D= 44682.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.48D-05 NBF= 172 148 158 158

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

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Wed Jul 31 03:51:46 2019, MaxMem= 4294967296 cpu: 10.9

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

DipDrv: MaxL=1.

Leave Link 303 at Wed Jul 31 03:51:46 2019, MaxMem= 4294967296 cpu: 1.3

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

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

B after Tr= -0.000000 0.000000 0.000000

Rot= 1.000000 -0.000000 -0.000000 -0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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The electronic state of the initial guess is 2-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7631 S= 0.5065

Leave Link 401 at Wed Jul 31 03:51:47 2019, MaxMem= 4294967296 cpu: 22.9

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1387497 IEndB= 1387497 NGot= 4294967296 MDV= 4294047352

LenX= 4294047352 LenY= 4293596440

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= 650000000 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= 45116652.

Iteration 1 A\*A^-1 deviation from unit magnitude is 4.88D-15 for 3876.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.77D-15 for 3859 539.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.11D-15 for 3876.

Iteration 1 A^-1\*A deviation from orthogonality is 2.52D-14 for 3834 3688.

E= -1359.18269777012

DIIS: error= 8.22D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.18269777012 IErMin= 1 ErrMin= 8.22D-05

ErrMax= 8.22D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.95D-06 BMatP= 7.95D-06

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

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.388 Goal= None Shift= 0.000

Gap= 0.438 Goal= None Shift= 0.000

RMSDP=8.57D-06 MaxDP=4.42D-04 OVMax= 3.61D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 8.56D-06 CP: 1.00D+00

E= -1359.18270005176 Delta-E= -0.000002281638 Rises=F Damp=F

DIIS: error= 1.24D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.18270005176 IErMin= 2 ErrMin= 1.24D-05

ErrMax= 1.24D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.15D-07 BMatP= 7.95D-06

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

Coeff-Com: -0.127D-01 0.101D+01

Coeff: -0.127D-01 0.101D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=8.22D-07 MaxDP=1.90D-05 DE=-2.28D-06 OVMax= 6.44D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 7.69D-07 CP: 1.00D+00 1.03D+00

E= -1359.18270006669 Delta-E= -0.000000014931 Rises=F Damp=F

DIIS: error= 1.68D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.18270006669 IErMin= 2 ErrMin= 1.24D-05

ErrMax= 1.68D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.32D-07 BMatP= 1.15D-07

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

Coeff-Com: -0.161D-01 0.534D+00 0.482D+00

Coeff: -0.161D-01 0.534D+00 0.482D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=3.34D-07 MaxDP=2.00D-05 DE=-1.49D-08 OVMax= 6.20D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.18D-07 CP: 1.00D+00 1.04D+00 6.74D-01

E= -1359.18270008858 Delta-E= -0.000000021884 Rises=F Damp=F

DIIS: error= 4.40D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.18270008858 IErMin= 4 ErrMin= 4.40D-06

ErrMax= 4.40D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.51D-08 BMatP= 1.15D-07

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

Coeff-Com: -0.712D-02 0.147D+00 0.268D+00 0.591D+00

Coeff: -0.712D-02 0.147D+00 0.268D+00 0.591D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=9.98D-08 MaxDP=7.16D-06 DE=-2.19D-08 OVMax= 1.82D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 8.12D-08 CP: 1.00D+00 1.04D+00 6.87D-01 7.37D-01

E= -1359.18270009162 Delta-E= -0.000000003046 Rises=F Damp=F

DIIS: error= 1.84D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.18270009162 IErMin= 5 ErrMin= 1.84D-06

ErrMax= 1.84D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.27D-09 BMatP= 1.51D-08

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

Coeff-Com: -0.194D-02 0.239D-01 0.909D-01 0.298D+00 0.589D+00

Coeff: -0.194D-02 0.239D-01 0.909D-01 0.298D+00 0.589D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=3.12D-08 MaxDP=1.60D-06 DE=-3.05D-09 OVMax= 4.72D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.63D-08 CP: 1.00D+00 1.04D+00 6.87D-01 8.01D-01 8.86D-01

E= -1359.18270009180 Delta-E= -0.000000000180 Rises=F Damp=F

DIIS: error= 6.38D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.18270009180 IErMin= 6 ErrMin= 6.38D-07

ErrMax= 6.38D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.63D-10 BMatP= 1.27D-09

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

Coeff-Com: 0.174D-03-0.141D-01 0.666D-03 0.480D-01 0.302D+00 0.663D+00

Coeff: 0.174D-03-0.141D-01 0.666D-03 0.480D-01 0.302D+00 0.663D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=1.23D-08 MaxDP=3.63D-07 DE=-1.80D-10 OVMax= 1.99D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 6.74D-09 CP: 1.00D+00 1.04D+00 6.95D-01 8.07D-01 9.13D-01

CP: 6.98D-01

E= -1359.18270009183 Delta-E= -0.000000000026 Rises=F Damp=F

DIIS: error= 7.52D-08 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.18270009183 IErMin= 7 ErrMin= 7.52D-08

ErrMax= 7.52D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.14D-11 BMatP= 1.63D-10

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

Coeff-Com: 0.176D-03-0.865D-02-0.282D-02 0.136D-01 0.137D+00 0.348D+00

Coeff-Com: 0.512D+00

Coeff: 0.176D-03-0.865D-02-0.282D-02 0.136D-01 0.137D+00 0.348D+00

Coeff: 0.512D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=3.38D-09 MaxDP=1.36D-07 DE=-2.64D-11 OVMax= 7.68D-07

Error on total polarization charges = 0.06719

SCF Done: E(UB3LYP) = -1359.18270009 A.U. after 7 cycles

NFock= 7 Conv=0.34D-08 -V/T= 1.9682

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7631 S= 0.5065

<L.S>= 0.000000000000E+00

KE= 1.403847075524D+03 PE=-9.372427584664D+03 EE= 3.557928584521D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.26

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7631, after 0.7501

Leave Link 502 at Wed Jul 31 03:52:32 2019, MaxMem= 4294967296 cpu: 671.9

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 636

NBasis= 636 NAE= 111 NBE= 110 NFC= 0 NFV= 0

NROrb= 636 NOA= 111 NOB= 110 NVA= 525 NVB= 526

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.15010491D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.38333412D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.14957148D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.88292791D-01

Leave Link 801 at Wed Jul 31 03:52:32 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 45.

Will process 46 centers per pass.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16169 LenP2D= 44682.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 11 by ecpmxn.

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

Leave Link 1101 at Wed Jul 31 03:52:35 2019, MaxMem= 4294967296 cpu: 44.5

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Wed Jul 31 03:52:35 2019, MaxMem= 4294967296 cpu: 1.0

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 45.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966832.

G2DrvN: will do 46 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

G2PCM: DoFxE=T DoFxN=T DoGrad=T DoDP/DQ/DG/TGxP=FFFF NFrqRd= 0 IEInf=0 SqF1=F DoCFld=F IF1Alg=4.

GePol: Maximum number of non-zero 1st derivatives = 255

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Wed Jul 31 03:54:32 2019, MaxMem= 4294967296 cpu: 1872.4

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=111111111111111111111111111111111111111111111

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Using symmetry in CPHF.

Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.

Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.

NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 4294965570 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 0.

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

IRaf= 650000000 NMat= 42 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

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

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

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

NMat0= 42 NMatS0= 42 NMatT0= 0 NMatD0= 42 NMtDS0= 0 NMtDT0= 0

Integrals replicated using symmetry in FoFCou.

There are 42 degrees of freedom in the 1st order CPHF. IDoFFX=4 NUNeed= 42.

42 vectors produced by pass 0 Test12= 2.77D-13 2.38D-09 XBig12= 8.07D+03 5.92D+01.

AX will form 42 AO Fock derivatives at one time.

42 vectors produced by pass 1 Test12= 2.77D-13 2.38D-09 XBig12= 1.08D+03 6.87D+00.

42 vectors produced by pass 2 Test12= 2.77D-13 2.38D-09 XBig12= 2.83D+02 5.66D+00.

42 vectors produced by pass 3 Test12= 2.77D-13 2.38D-09 XBig12= 8.40D+01 2.10D+00.

42 vectors produced by pass 4 Test12= 2.77D-13 2.38D-09 XBig12= 9.36D+00 5.38D-01.

42 vectors produced by pass 5 Test12= 2.77D-13 2.38D-09 XBig12= 3.13D-01 6.47D-02.

42 vectors produced by pass 6 Test12= 2.77D-13 2.38D-09 XBig12= 1.26D-02 9.63D-03.

42 vectors produced by pass 7 Test12= 2.77D-13 2.38D-09 XBig12= 2.62D-04 1.43D-03.

35 vectors produced by pass 8 Test12= 2.77D-13 2.38D-09 XBig12= 5.03D-06 1.71D-04.

25 vectors produced by pass 9 Test12= 2.77D-13 2.38D-09 XBig12= 7.11D-08 2.34D-05.

7 vectors produced by pass 10 Test12= 2.77D-13 2.38D-09 XBig12= 9.30D-10 2.59D-06.

2 vectors produced by pass 11 Test12= 2.77D-13 2.38D-09 XBig12= 9.97D-12 2.05D-07.

2 vectors produced by pass 12 Test12= 2.77D-13 2.38D-09 XBig12= 1.39D-13 3.06D-08.

InvSVY: IOpt=1 It= 1 EMax= 7.11D-14

Solved reduced A of dimension 407 with 42 vectors.

FullF1: Do perturbations 1 to 42.

Isotropic polarizability for W= 0.000000 1007.20 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Wed Jul 31 04:45:34 2019, MaxMem= 4294967296 cpu: 48996.9

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16169 LenP2D= 44682.

LDataN: DoStor=T MaxTD1= 7 Len= 274

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 255

Leave Link 701 at Wed Jul 31 04:46:09 2019, MaxMem= 4294967296 cpu: 553.3

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

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

Leave Link 702 at Wed Jul 31 04:46:09 2019, MaxMem= 4294967296 cpu: 0.4

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

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

wScrn= 0.000000 ICntrl= 100127 IOpCl= 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 Wed Jul 31 04:47:59 2019, MaxMem= 4294967296 cpu: 1763.8

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

Dipole = 2.41612286D-13 2.06779038D-14-5.28673721D-03

Polarizability= 1.65458678D+03-1.84776227D-05 1.17988472D+03

8.40738939D-06-3.02769304D-06 1.87128383D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000003074 0.000042271 0.000000139

2 6 -0.000008019 0.000019737 0.000000812

3 7 0.000148873 0.000000000 -0.000072600

4 6 -0.000008019 -0.000019737 0.000000812

5 6 0.000003074 -0.000042271 0.000000139

6 6 -0.000014862 -0.000008327 -0.000000144

7 6 0.000016400 -0.000011142 0.000000673

8 7 0.000000000 0.000093553 -0.000049469

9 6 -0.000016400 -0.000011142 0.000000673

10 6 0.000036891 0.000008900 0.000000147

11 6 -0.000036891 0.000008900 0.000000147

12 6 -0.000014862 0.000008327 -0.000000144

13 6 0.000016400 0.000011142 0.000000673

14 6 -0.000036891 -0.000008900 0.000000147

15 6 0.000036891 -0.000008900 0.000000147

16 6 -0.000016400 0.000011142 0.000000673

17 7 0.000000000 -0.000093553 -0.000049469

18 6 0.000014862 0.000008327 -0.000000144

19 6 0.000008019 0.000019737 0.000000812

20 6 -0.000003074 0.000042271 0.000000139

21 6 -0.000003074 -0.000042271 0.000000139

22 6 0.000008019 -0.000019737 0.000000812

23 7 -0.000148873 -0.000000000 -0.000072600

24 1 0.000002238 0.000002108 0.000000071

25 1 0.000002238 -0.000002108 0.000000071

26 1 0.000001054 0.000001646 0.000000092

27 1 -0.000001054 0.000001646 0.000000092

28 1 -0.000001054 -0.000001646 0.000000092

29 1 0.000001054 -0.000001646 0.000000092

30 1 -0.000002238 0.000002108 0.000000071

31 1 -0.000002238 -0.000002108 0.000000071

32 30 -0.000000000 0.000000000 0.000237114

33 6 0.000014862 -0.000008327 -0.000000144

34 6 0.000003504 0.000002738 0.000000120

35 6 -0.000003504 -0.000002738 0.000000120

36 6 0.000002500 0.000001940 -0.000000111

37 6 -0.000002500 -0.000001940 -0.000000111

38 6 -0.000003504 0.000002738 0.000000120

39 6 -0.000002500 0.000001940 -0.000000111

40 6 0.000003504 -0.000002738 0.000000120

41 6 0.000002500 -0.000001940 -0.000000111

42 1 -0.000004617 -0.000001732 -0.000000044

43 1 -0.000004617 0.000001732 -0.000000044

44 1 0.000004617 0.000001732 -0.000000044

45 1 0.000004617 -0.000001732 -0.000000044

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

Cartesian Forces: Max 0.000237114 RMS 0.000033473

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

Leave Link 716 at Wed Jul 31 04:47:59 2019, MaxMem= 4294967296 cpu: 0.8

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000096000 RMS 0.000015647

Search for a local minimum.

Step number 9 out of a maximum of 270

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

RMS Force = .15647D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -4.28D-06 DEPred=-4.26D-06 R= 1.00D+00

TightC=F SS= 1.41D+00 RLast= 1.32D-02 DXNew= 3.5676D-01 3.9660D-02

Trust test= 1.00D+00 RLast= 1.32D-02 DXMaxT set to 2.12D-01

ITU= 1 1 1 -1 0 0 -1 0 0

Eigenvalues --- 0.00150 0.00335 0.00452 0.00551 0.00654

Eigenvalues --- 0.00957 0.01116 0.01121 0.01163 0.01231

Eigenvalues --- 0.01239 0.01277 0.01293 0.01344 0.01382

Eigenvalues --- 0.01506 0.01521 0.01550 0.01862 0.01921

Eigenvalues --- 0.01942 0.01965 0.01975 0.02004 0.02020

Eigenvalues --- 0.02089 0.02100 0.02121 0.02123 0.02524

Eigenvalues --- 0.03000 0.03165 0.03195 0.03650 0.04003

Eigenvalues --- 0.04121 0.04123 0.04135 0.04137 0.04146

Eigenvalues --- 0.04358 0.04359 0.06243 0.06295 0.08267

Eigenvalues --- 0.08277 0.08293 0.08561 0.08842 0.08876

Eigenvalues --- 0.08959 0.09215 0.09272 0.09571 0.09610

Eigenvalues --- 0.09627 0.09656 0.09998 0.10408 0.10411

Eigenvalues --- 0.10442 0.10496 0.12305 0.13214 0.13554

Eigenvalues --- 0.13583 0.16014 0.16901 0.16962 0.19289

Eigenvalues --- 0.19802 0.20061 0.20084 0.20348 0.20622

Eigenvalues --- 0.20663 0.20834 0.21612 0.21813 0.21879

Eigenvalues --- 0.21945 0.26000 0.26183 0.27688 0.27939

Eigenvalues --- 0.28029 0.29424 0.29978 0.31686 0.32488

Eigenvalues --- 0.32763 0.32784 0.33602 0.35665 0.35682

Eigenvalues --- 0.35843 0.36112 0.36433 0.37025 0.37099

Eigenvalues --- 0.37156 0.37328 0.37390 0.37558 0.37834

Eigenvalues --- 0.38034 0.38344 0.38794 0.39213 0.40228

Eigenvalues --- 0.40231 0.40234 0.40234 0.41172 0.41283

Eigenvalues --- 0.41883 0.42421 0.45359 0.46055 0.46392

Eigenvalues --- 0.46611 0.50197 0.50204 0.52626 0.53039

Eigenvalues --- 1.03358 1.04106 1.04439 1.04672

En-DIIS/RFO-DIIS IScMMF= 0 using points: 9 8 7 6 5

RFO step: Lambda=-2.57674034D-07.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= -2.17D-04 SmlDif= 1.00D-05

RMS Error= 0.6825203087D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.49087 -0.48859 -0.04887 0.04162 0.00497

Iteration 1 RMS(Cart)= 0.00040457 RMS(Int)= 0.00000227

Iteration 2 RMS(Cart)= 0.00000058 RMS(Int)= 0.00000225

ITry= 1 IFail=0 DXMaxC= 5.23D-03 DCOld= 1.00D+10 DXMaxT= 2.12D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.02D-05 for atom 37.

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

(Linear) (Quad) (Total)

R1 2.74728 -0.00001 -0.00007 -0.00001 -0.00007 2.74721

R2 2.56794 0.00003 0.00003 0.00003 0.00006 2.56800

R3 2.04152 -0.00000 -0.00000 -0.00000 -0.00000 2.04151

R4 2.59182 0.00003 0.00011 0.00001 0.00013 2.59195

R5 2.65481 -0.00002 -0.00008 0.00000 -0.00007 2.65474

R6 2.59182 0.00003 0.00011 0.00001 0.00013 2.59195

R7 3.96262 -0.00010 -0.00066 -0.00003 -0.00069 3.96193

R8 2.74728 -0.00001 -0.00007 -0.00001 -0.00007 2.74721

R9 2.65481 -0.00002 -0.00008 0.00000 -0.00007 2.65474

R10 2.04152 -0.00000 -0.00000 -0.00000 -0.00000 2.04151

R11 2.72004 -0.00001 -0.00008 0.00001 -0.00006 2.71998

R12 2.69152 -0.00000 -0.00001 -0.00000 -0.00002 2.69150

R13 2.59144 0.00001 0.00005 -0.00001 0.00004 2.59148

R14 2.69681 -0.00002 -0.00007 -0.00001 -0.00007 2.69673

R15 2.59144 0.00001 0.00005 -0.00001 0.00004 2.59148

R16 3.97093 -0.00005 -0.00031 0.00007 -0.00025 3.97068

R17 2.69681 -0.00002 -0.00007 -0.00001 -0.00007 2.69673

R18 2.72004 -0.00001 -0.00008 0.00001 -0.00006 2.71998

R19 2.61510 0.00002 0.00003 0.00003 0.00007 2.61517

R20 2.04176 -0.00000 -0.00000 -0.00000 -0.00000 2.04176

R21 2.04176 -0.00000 -0.00000 -0.00000 -0.00000 2.04176

R22 2.72004 -0.00001 -0.00008 0.00001 -0.00006 2.71998

R23 2.69152 -0.00000 -0.00001 -0.00000 -0.00002 2.69150

R24 2.69681 -0.00002 -0.00007 -0.00001 -0.00007 2.69673

R25 2.59144 0.00001 0.00005 -0.00001 0.00004 2.59148

R26 2.61510 0.00002 0.00003 0.00003 0.00007 2.61517

R27 2.04176 -0.00000 -0.00000 -0.00000 -0.00000 2.04176

R28 2.69681 -0.00002 -0.00007 -0.00001 -0.00007 2.69673

R29 2.04176 -0.00000 -0.00000 -0.00000 -0.00000 2.04176

R30 2.59144 0.00001 0.00005 -0.00001 0.00004 2.59148

R31 2.72004 -0.00001 -0.00008 0.00001 -0.00006 2.71998

R32 3.97093 -0.00005 -0.00031 0.00006 -0.00025 3.97068

R33 2.65481 -0.00002 -0.00008 0.00000 -0.00007 2.65474

R34 2.69152 -0.00000 -0.00001 -0.00000 -0.00002 2.69150

R35 2.74728 -0.00001 -0.00007 -0.00001 -0.00007 2.74721

R36 2.59182 0.00003 0.00011 0.00001 0.00013 2.59195

R37 2.56794 0.00003 0.00003 0.00003 0.00006 2.56800

R38 2.04152 -0.00000 -0.00000 -0.00000 -0.00000 2.04151

R39 2.74728 -0.00001 -0.00007 -0.00001 -0.00007 2.74721

R40 2.04152 -0.00000 -0.00000 -0.00000 -0.00000 2.04151

R41 2.59182 0.00003 0.00011 0.00001 0.00013 2.59195

R42 2.65481 -0.00002 -0.00008 0.00000 -0.00007 2.65474

R43 3.96262 -0.00010 -0.00066 -0.00003 -0.00069 3.96193

R44 2.69152 -0.00000 -0.00001 -0.00000 -0.00002 2.69150

R45 2.28357 -0.00000 -0.00001 -0.00000 -0.00001 2.28357

R46 2.28357 -0.00000 -0.00001 -0.00000 -0.00001 2.28357

R47 2.01599 -0.00000 -0.00001 -0.00000 -0.00001 2.01598

R48 2.01599 -0.00000 -0.00001 -0.00000 -0.00001 2.01598

R49 2.28357 -0.00000 -0.00001 -0.00000 -0.00001 2.28357

R50 2.01599 -0.00000 -0.00001 -0.00000 -0.00001 2.01598

R51 2.28357 -0.00000 -0.00001 -0.00000 -0.00001 2.28357

R52 2.01599 -0.00000 -0.00001 -0.00000 -0.00001 2.01598

A1 1.87114 -0.00000 -0.00001 0.00000 -0.00001 1.87113

A2 2.18747 -0.00000 -0.00003 -0.00001 -0.00004 2.18744

A3 2.22457 0.00000 0.00004 0.00000 0.00005 2.22462

A4 1.89882 0.00001 0.00010 -0.00000 0.00009 1.89891

A5 2.18504 -0.00002 -0.00013 -0.00001 -0.00013 2.18491

A6 2.19932 0.00000 0.00003 0.00001 0.00004 2.19937

A7 1.88485 -0.00002 -0.00017 0.00000 -0.00016 1.88469

A8 2.19917 0.00001 0.00008 -0.00000 0.00008 2.19925

A9 2.19917 0.00001 0.00008 -0.00000 0.00008 2.19925

A10 1.89882 0.00001 0.00010 -0.00000 0.00009 1.89891

A11 2.19932 0.00000 0.00003 0.00001 0.00004 2.19937

A12 2.18504 -0.00002 -0.00013 -0.00001 -0.00013 2.18491

A13 1.87114 -0.00000 -0.00001 0.00000 -0.00001 1.87113

A14 2.22457 0.00000 0.00004 0.00000 0.00005 2.22462

A15 2.18747 -0.00000 -0.00003 -0.00001 -0.00004 2.18744

A16 2.21351 -0.00002 -0.00015 -0.00000 -0.00015 2.21336

A17 2.04229 0.00000 0.00006 -0.00001 0.00005 2.04235

A18 2.02738 0.00002 0.00009 0.00001 0.00010 2.02748

A19 2.18157 -0.00000 -0.00004 -0.00001 -0.00005 2.18152

A20 2.19480 -0.00001 -0.00007 0.00000 -0.00006 2.19474

A21 1.90682 0.00002 0.00011 0.00000 0.00011 1.90693

A22 1.87917 -0.00002 -0.00016 0.00000 -0.00015 1.87903

A23 2.20201 0.00001 0.00008 -0.00000 0.00007 2.20208

A24 2.20201 0.00001 0.00008 -0.00000 0.00007 2.20208

A25 1.90682 0.00002 0.00011 0.00000 0.00011 1.90693

A26 2.18157 -0.00000 -0.00004 -0.00001 -0.00005 2.18152

A27 2.19480 -0.00001 -0.00007 0.00000 -0.00006 2.19474

A28 1.86599 -0.00001 -0.00003 -0.00001 -0.00004 1.86595

A29 2.19640 0.00000 -0.00001 0.00000 -0.00001 2.19639

A30 2.22080 0.00001 0.00004 0.00000 0.00005 2.22084

A31 1.86599 -0.00001 -0.00003 -0.00001 -0.00004 1.86595

A32 2.19640 0.00000 -0.00001 0.00000 -0.00001 2.19639

A33 2.22080 0.00001 0.00004 0.00000 0.00005 2.22084

A34 2.21351 -0.00002 -0.00015 -0.00000 -0.00015 2.21336

A35 2.04229 0.00000 0.00006 -0.00001 0.00005 2.04235

A36 2.02738 0.00002 0.00009 0.00001 0.00010 2.02748

A37 2.19480 -0.00001 -0.00007 0.00000 -0.00006 2.19474

A38 2.18157 -0.00000 -0.00004 -0.00001 -0.00005 2.18152

A39 1.90682 0.00002 0.00011 0.00000 0.00011 1.90693

A40 1.86599 -0.00001 -0.00003 -0.00001 -0.00004 1.86595

A41 2.19640 0.00000 -0.00001 0.00000 -0.00001 2.19639

A42 2.22080 0.00001 0.00004 0.00000 0.00005 2.22084

A43 1.86599 -0.00001 -0.00003 -0.00001 -0.00004 1.86595

A44 2.22080 0.00001 0.00004 0.00000 0.00005 2.22084

A45 2.19640 0.00000 -0.00001 0.00000 -0.00001 2.19639

A46 1.90682 0.00002 0.00011 0.00000 0.00011 1.90693

A47 2.19480 -0.00001 -0.00007 0.00000 -0.00006 2.19474

A48 2.18157 -0.00000 -0.00004 -0.00001 -0.00005 2.18152

A49 1.87917 -0.00002 -0.00016 0.00000 -0.00015 1.87903

A50 2.20201 0.00001 0.00008 -0.00000 0.00007 2.20208

A51 2.20201 0.00001 0.00008 -0.00000 0.00007 2.20208

A52 2.21351 -0.00002 -0.00015 -0.00000 -0.00015 2.21336

A53 2.02738 0.00002 0.00009 0.00001 0.00010 2.02748

A54 2.04229 0.00000 0.00006 -0.00001 0.00005 2.04235

A55 2.18504 -0.00002 -0.00013 -0.00001 -0.00013 2.18491

A56 2.19932 0.00000 0.00003 0.00001 0.00004 2.19937

A57 1.89882 0.00001 0.00010 -0.00000 0.00009 1.89891

A58 1.87114 -0.00000 -0.00001 0.00000 -0.00001 1.87113

A59 2.18747 -0.00000 -0.00003 -0.00001 -0.00004 2.18744

A60 2.22457 0.00000 0.00004 0.00000 0.00005 2.22462

A61 1.87114 -0.00000 -0.00001 0.00000 -0.00001 1.87113

A62 2.22457 0.00000 0.00004 0.00000 0.00005 2.22462

A63 2.18747 -0.00000 -0.00003 -0.00001 -0.00004 2.18744

A64 1.89882 0.00001 0.00010 -0.00000 0.00009 1.89891

A65 2.18504 -0.00002 -0.00013 -0.00001 -0.00013 2.18491

A66 2.19932 0.00000 0.00003 0.00001 0.00004 2.19937

A67 1.88485 -0.00002 -0.00017 0.00000 -0.00016 1.88469

A68 2.19917 0.00001 0.00008 -0.00000 0.00008 2.19925

A69 2.19917 0.00001 0.00008 -0.00000 0.00008 2.19925

A70 1.57080 0.00000 -0.00001 -0.00000 0.00000 1.57080

A71 1.57080 0.00000 -0.00001 -0.00000 0.00000 1.57080

A72 1.57080 0.00000 -0.00001 -0.00000 0.00000 1.57080

A73 1.57080 0.00000 -0.00001 0.00000 0.00000 1.57080

A74 2.21351 -0.00002 -0.00015 -0.00000 -0.00015 2.21336

A75 2.02738 0.00002 0.00009 0.00001 0.00010 2.02748

A76 2.04229 0.00000 0.00006 -0.00001 0.00005 2.04235

A77 3.14159 0.00000 -0.00002 0.00000 0.00000 3.14159

A78 3.14159 0.00000 -0.00002 0.00000 0.00000 3.14159

A79 3.12421 -0.00000 -0.00000 -0.00000 -0.00001 3.12421

A80 3.15897 0.00000 0.00000 0.00000 0.00001 3.15898

A81 3.14720 -0.00000 -0.00005 -0.00002 -0.00007 3.14713

A82 3.14720 -0.00000 -0.00005 -0.00002 -0.00007 3.14713

A83 3.15897 0.00000 0.00000 0.00000 0.00001 3.15898

A84 3.14720 -0.00000 -0.00005 -0.00002 -0.00007 3.14713

A85 3.12421 -0.00000 -0.00000 -0.00000 -0.00001 3.12421

A86 3.14720 -0.00000 -0.00005 -0.00002 -0.00007 3.14713

A87 3.13919 0.00005 0.00241 0.00007 0.00248 3.14167

A88 3.14357 -0.00005 -0.00214 0.00009 -0.00205 3.14152

A89 3.14161 -0.00000 -0.00001 -0.00001 -0.00001 3.14159

A90 3.14157 0.00000 0.00001 0.00001 0.00002 3.14159

A91 3.14160 -0.00000 -0.00000 -0.00000 -0.00001 3.14159

A92 3.14160 -0.00000 -0.00000 -0.00000 -0.00001 3.14159

A93 3.14161 -0.00000 -0.00001 -0.00001 -0.00002 3.14159

A94 3.14159 0.00000 0.00000 0.00000 0.00001 3.14159

A95 3.14158 0.00000 0.00001 0.00001 0.00001 3.14159

A96 3.14159 0.00000 0.00000 0.00000 0.00001 3.14159

D1 -0.00005 -0.00000 0.00003 0.00003 0.00005 -0.00000

D2 3.14157 -0.00000 -0.00003 0.00005 0.00002 3.14159

D3 3.14151 -0.00000 0.00007 0.00001 0.00008 -3.14159

D4 -0.00006 -0.00000 0.00001 0.00004 0.00005 -0.00000

D5 0.00000 0.00000 0.00000 0.00000 -0.00000 0.00000

D6 3.14156 0.00000 0.00005 -0.00002 0.00003 -3.14159

D7 -3.14156 -0.00000 -0.00005 0.00002 -0.00003 3.14159

D8 -0.00000 -0.00000 -0.00000 -0.00000 0.00000 0.00000

D9 0.00009 0.00000 -0.00004 -0.00004 -0.00009 0.00000

D10 3.14034 0.00001 0.00123 0.00006 0.00129 -3.14155

D11 -3.14153 0.00001 0.00002 -0.00007 -0.00005 -3.14159

D12 -0.00128 0.00002 0.00129 0.00003 0.00132 0.00004

D13 3.14147 0.00001 0.00018 -0.00005 0.00013 -3.14158

D14 -0.00001 0.00000 0.00006 -0.00005 0.00001 0.00000

D15 -0.00009 0.00001 0.00011 -0.00002 0.00009 0.00000

D16 -3.14157 -0.00000 -0.00001 -0.00002 -0.00003 3.14159

D17 -0.00009 -0.00000 0.00004 0.00004 0.00009 -0.00000

D18 3.14153 -0.00001 -0.00002 0.00007 0.00005 3.14159

D19 -3.14034 -0.00001 -0.00123 -0.00006 -0.00129 3.14155

D20 0.00128 -0.00002 -0.00129 -0.00003 -0.00132 -0.00004

D21 3.14139 0.00002 0.00032 -0.00011 0.00022 -3.14158

D22 0.00178 -0.00003 -0.00182 -0.00002 -0.00184 -0.00006

D23 -0.00178 0.00003 0.00182 0.00002 0.00184 0.00006

D24 -3.14139 -0.00002 -0.00032 0.00011 -0.00022 3.14158

D25 0.00005 0.00000 -0.00003 -0.00003 -0.00005 0.00000

D26 -3.14151 0.00000 -0.00007 -0.00001 -0.00008 3.14159

D27 -3.14157 0.00000 0.00003 -0.00005 -0.00002 -3.14159

D28 0.00006 0.00000 -0.00001 -0.00004 -0.00005 0.00000

D29 0.00009 -0.00001 -0.00011 0.00002 -0.00009 -0.00000

D30 3.14157 0.00000 0.00001 0.00002 0.00003 -3.14159

D31 -3.14147 -0.00001 -0.00018 0.00005 -0.00013 3.14158

D32 0.00001 -0.00000 -0.00006 0.00005 -0.00001 -0.00000

D33 -0.00022 0.00001 0.00020 0.00002 0.00022 0.00000

D34 3.14115 0.00001 0.00040 0.00005 0.00045 -3.14158

D35 3.14149 -0.00000 0.00008 0.00002 0.00010 -3.14159

D36 -0.00033 0.00000 0.00028 0.00005 0.00033 0.00000

D37 3.14134 0.00001 0.00021 0.00005 0.00026 -3.14159

D38 -0.00105 0.00002 0.00112 -0.00003 0.00109 0.00004

D39 -0.00006 0.00001 0.00004 0.00002 0.00006 -0.00000

D40 3.14074 0.00001 0.00095 -0.00006 0.00089 -3.14156

D41 -3.14136 -0.00001 -0.00019 -0.00004 -0.00024 3.14159

D42 0.00014 -0.00000 -0.00011 -0.00004 -0.00014 -0.00000

D43 0.00004 -0.00001 -0.00002 -0.00002 -0.00004 0.00000

D44 3.14154 -0.00000 0.00006 -0.00001 0.00006 -3.14159

D45 0.00006 -0.00001 -0.00004 -0.00002 -0.00006 0.00000

D46 -3.14134 -0.00001 -0.00021 -0.00005 -0.00026 3.14159

D47 -3.14074 -0.00001 -0.00095 0.00006 -0.00089 3.14156

D48 0.00105 -0.00002 -0.00112 0.00003 -0.00109 -0.00004

D49 0.00167 -0.00003 -0.00174 0.00001 -0.00173 -0.00006

D50 3.14085 0.00003 0.00066 0.00009 0.00075 -3.14158

D51 -3.14085 -0.00003 -0.00066 -0.00009 -0.00075 3.14158

D52 -0.00167 0.00003 0.00174 -0.00001 0.00173 0.00006

D53 -0.00004 0.00001 0.00002 0.00002 0.00004 -0.00000

D54 -3.14154 0.00000 -0.00006 0.00001 -0.00006 3.14159

D55 3.14136 0.00001 0.00019 0.00004 0.00024 -3.14159

D56 -0.00014 0.00000 0.00011 0.00004 0.00014 0.00000

D57 0.00022 -0.00001 -0.00020 -0.00002 -0.00022 -0.00000

D58 -3.14149 0.00000 -0.00008 -0.00002 -0.00010 3.14159

D59 -3.14115 -0.00001 -0.00040 -0.00005 -0.00045 3.14158

D60 0.00033 -0.00000 -0.00028 -0.00005 -0.00033 -0.00000

D61 -0.00000 0.00000 -0.00000 -0.00000 0.00000 0.00000

D62 -3.14150 -0.00001 -0.00009 -0.00001 -0.00010 3.14159

D63 3.14150 0.00001 0.00009 0.00001 0.00010 -3.14159

D64 0.00000 0.00000 0.00000 0.00000 -0.00000 -0.00000

D65 -3.14115 -0.00001 -0.00040 -0.00005 -0.00045 3.14158

D66 0.00022 -0.00001 -0.00020 -0.00002 -0.00022 -0.00000

D67 0.00033 -0.00000 -0.00028 -0.00005 -0.00033 -0.00000

D68 -3.14149 0.00000 -0.00008 -0.00002 -0.00010 3.14159

D69 3.14136 0.00001 0.00019 0.00004 0.00024 -3.14159

D70 -0.00014 0.00000 0.00011 0.00004 0.00014 0.00000

D71 -0.00004 0.00001 0.00002 0.00002 0.00004 -0.00000

D72 -3.14154 0.00000 -0.00006 0.00001 -0.00006 3.14159

D73 -3.14134 -0.00001 -0.00021 -0.00005 -0.00026 3.14159

D74 0.00105 -0.00002 -0.00112 0.00003 -0.00109 -0.00004

D75 0.00006 -0.00001 -0.00004 -0.00002 -0.00006 0.00000

D76 -3.14074 -0.00001 -0.00095 0.00006 -0.00089 3.14156

D77 -0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D78 -3.14150 -0.00001 -0.00009 -0.00001 -0.00010 3.14159

D79 3.14150 0.00001 0.00009 0.00001 0.00010 -3.14159

D80 0.00000 -0.00000 -0.00000 -0.00000 -0.00000 0.00000

D81 0.00004 -0.00001 -0.00002 -0.00002 -0.00004 0.00000

D82 -3.14136 -0.00001 -0.00019 -0.00004 -0.00024 3.14159

D83 3.14154 -0.00000 0.00006 -0.00001 0.00006 -3.14159

D84 0.00014 -0.00000 -0.00011 -0.00004 -0.00014 -0.00000

D85 -0.00006 0.00001 0.00004 0.00002 0.00006 -0.00000

D86 3.14074 0.00001 0.00095 -0.00006 0.00089 -3.14156

D87 3.14134 0.00001 0.00021 0.00005 0.00026 -3.14159

D88 -0.00105 0.00002 0.00112 -0.00003 0.00109 0.00004

D89 3.14115 0.00001 0.00040 0.00005 0.00045 -3.14158

D90 -0.00033 0.00000 0.00028 0.00005 0.00033 0.00000

D91 -0.00022 0.00001 0.00020 0.00002 0.00022 0.00000

D92 3.14149 -0.00000 0.00008 0.00002 0.00010 -3.14159

D93 -0.00167 0.00003 0.00174 -0.00001 0.00173 0.00006

D94 -3.14085 -0.00003 -0.00066 -0.00009 -0.00075 3.14158

D95 3.14085 0.00003 0.00066 0.00009 0.00075 -3.14158

D96 0.00167 -0.00003 -0.00174 0.00001 -0.00173 -0.00006

D97 -3.14147 -0.00001 -0.00018 0.00005 -0.00013 3.14158

D98 0.00009 -0.00001 -0.00011 0.00002 -0.00009 -0.00000

D99 0.00001 -0.00000 -0.00006 0.00005 -0.00001 -0.00000

D100 3.14157 0.00000 0.00001 0.00002 0.00003 -3.14159

D101 -3.14157 0.00000 0.00003 -0.00005 -0.00002 -3.14159

D102 0.00006 0.00000 -0.00001 -0.00004 -0.00005 0.00000

D103 0.00005 0.00000 -0.00003 -0.00003 -0.00005 0.00000

D104 -3.14151 0.00000 -0.00007 -0.00001 -0.00008 3.14159

D105 3.14153 -0.00001 -0.00002 0.00007 0.00005 3.14159

D106 0.00128 -0.00002 -0.00129 -0.00003 -0.00132 -0.00004

D107 -0.00009 -0.00000 0.00004 0.00004 0.00009 -0.00000

D108 -3.14034 -0.00001 -0.00123 -0.00006 -0.00129 3.14155

D109 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D110 -3.14156 -0.00000 -0.00005 0.00002 -0.00003 3.14159

D111 3.14156 0.00000 0.00005 -0.00002 0.00003 -3.14159

D112 -0.00000 0.00000 -0.00000 0.00000 0.00000 0.00000

D113 -0.00005 -0.00000 0.00003 0.00003 0.00005 -0.00000

D114 3.14157 -0.00000 -0.00003 0.00005 0.00002 3.14159

D115 3.14151 -0.00000 0.00007 0.00001 0.00008 -3.14159

D116 -0.00006 -0.00000 0.00001 0.00004 0.00005 -0.00000

D117 0.00009 0.00000 -0.00004 -0.00004 -0.00009 0.00000

D118 3.14034 0.00001 0.00123 0.00006 0.00129 -3.14155

D119 -3.14153 0.00001 0.00002 -0.00007 -0.00005 -3.14159

D120 -0.00128 0.00002 0.00129 0.00003 0.00132 0.00004

D121 3.14147 0.00001 0.00018 -0.00005 0.00013 -3.14158

D122 -0.00001 0.00000 0.00006 -0.00005 0.00001 0.00000

D123 -0.00009 0.00001 0.00011 -0.00002 0.00009 0.00000

D124 -3.14157 -0.00000 -0.00001 -0.00002 -0.00003 3.14159

D125 -3.14139 -0.00002 -0.00032 0.00011 -0.00022 3.14158

D126 -0.00178 0.00003 0.00182 0.00002 0.00184 0.00006

D127 0.00178 -0.00003 -0.00182 -0.00002 -0.00184 -0.00006

D128 3.14139 0.00002 0.00032 -0.00011 0.00022 -3.14158

Item Value Threshold Converged?

Maximum Force 0.000096 0.000450 YES

RMS Force 0.000016 0.000300 YES

Maximum Displacement 0.005228 0.001800 NO

RMS Displacement 0.000405 0.001200 YES

Predicted change in Energy=-6.414535D-07

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Wed Jul 31 04:47:59 2019, MaxMem= 4294967296 cpu: 1.1

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

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -4.291603 0.679463 -0.024405

2 6 0 -2.902914 1.109543 -0.024397

3 7 0 -2.096563 0.000000 -0.024391

4 6 0 -2.902914 -1.109543 -0.024397

5 6 0 -4.291603 -0.679463 -0.024405

6 6 0 -2.469308 -2.445779 -0.024399

7 6 0 -1.107053 -2.910541 -0.024400

8 7 0 -0.000000 -2.101194 -0.024394

9 6 0 1.107053 -2.910541 -0.024400

10 6 0 0.691944 -4.275881 -0.024411

11 6 0 -0.691944 -4.275881 -0.024411

12 6 0 -2.469308 2.445779 -0.024399

13 6 0 -1.107053 2.910541 -0.024400

14 6 0 -0.691944 4.275881 -0.024411

15 6 0 0.691944 4.275881 -0.024411

16 6 0 1.107053 2.910541 -0.024400

17 7 0 0.000000 2.101194 -0.024394

18 6 0 2.469308 2.445779 -0.024399

19 6 0 2.902914 1.109543 -0.024397

20 6 0 4.291603 0.679463 -0.024405

21 6 0 4.291603 -0.679463 -0.024405

22 6 0 2.902914 -1.109543 -0.024397

23 7 0 2.096563 -0.000000 -0.024391

24 1 0 -5.149124 1.336543 -0.024412

25 1 0 -5.149124 -1.336543 -0.024412

26 1 0 1.345862 -5.135981 -0.024419

27 1 0 -1.345862 -5.135981 -0.024419

28 1 0 -1.345862 5.135981 -0.024419

29 1 0 1.345862 5.135981 -0.024419

30 1 0 5.149124 1.336543 -0.024412

31 1 0 5.149124 -1.336543 -0.024412

32 30 0 -0.000000 0.000000 -0.024313

33 6 0 2.469308 -2.445779 -0.024399

34 6 0 3.476498 -3.452829 -0.024405

35 6 0 -3.476498 3.452829 -0.024405

36 6 0 4.316051 -4.321973 -0.024411

37 6 0 -4.316051 4.321973 -0.024411

38 6 0 -3.476498 -3.452829 -0.024405

39 6 0 -4.316051 -4.321973 -0.024411

40 6 0 3.476498 3.452829 -0.024405

41 6 0 4.316051 4.321973 -0.024411

42 1 0 5.061461 5.085155 -0.024416

43 1 0 5.061461 -5.085155 -0.024416

44 1 0 -5.061461 -5.085155 -0.024416

45 1 0 -5.061461 5.085155 -0.024416

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.453762 0.000000

3 N 2.297797 1.371600 0.000000

4 C 2.264729 2.219085 1.371600 0.000000

5 C 1.358926 2.264729 2.297797 1.453762 0.000000

6 C 3.617720 3.581665 2.474020 1.404828 2.537840

7 C 4.798904 4.402975 3.074146 2.543366 3.888324

8 N 5.113698 4.328480 2.968264 3.067619 4.520970

9 C 6.483334 5.678108 4.328326 4.395843 5.841506

10 C 7.027886 6.475014 5.104796 4.790481 6.145728

11 C 6.124784 5.821613 4.500680 3.861876 5.088395

12 C 2.537840 1.404828 2.474020 3.581665 3.617720

13 C 3.888324 2.543366 3.074146 4.402975 4.798904

14 C 5.088395 3.861876 4.500680 5.821613 6.124784

15 C 6.145728 4.790481 5.104796 6.475014 7.027886

16 C 5.841506 4.395843 4.328326 5.678108 6.483334

17 N 4.520970 3.067619 2.968264 4.328480 5.113698

18 C 6.987831 5.535910 5.179673 6.442133 7.448292

19 C 7.207361 5.805829 5.121119 6.215464 7.413611

20 C 8.583206 7.207361 6.424200 7.413611 8.690115

21 C 8.690115 7.413611 6.424200 7.207361 8.583206

22 C 7.413611 6.215464 5.121119 5.805829 7.207361

23 N 6.424200 5.121119 4.193127 5.121119 6.424200

24 H 1.080322 2.257650 3.332337 3.320962 2.190804

25 H 2.190804 3.320962 3.332337 2.257650 1.080322

26 H 8.099407 7.553718 6.182927 5.853572 7.186206

27 H 6.518956 6.436690 5.190554 4.317015 5.342092

28 H 5.342092 4.317015 5.190554 6.436690 6.518956

29 H 7.186206 5.853572 6.182927 7.553718 8.099407

30 H 9.463565 8.055237 7.367925 8.415382 9.653580

31 H 9.653580 8.415382 7.367925 8.055237 9.463565

32 Zn 4.345058 3.107732 2.096563 3.107732 4.345058

33 C 7.448292 6.442133 5.179673 5.535910 6.987831

34 C 8.798820 7.842967 6.555992 6.796167 8.248330

35 C 2.890667 2.412465 3.718366 4.598286 4.211916

36 C 9.955203 9.034092 7.733115 7.901466 9.346635

37 C 3.642591 3.509510 4.858557 5.612336 5.001496

38 C 4.211916 4.598286 3.718366 2.412465 2.890667

39 C 5.001496 5.612336 4.858557 3.509510 3.642591

40 C 8.248330 6.796167 6.555992 7.842967 8.798820

41 C 9.346635 7.901466 7.733115 9.034092 9.955203

42 H 10.338759 8.901504 8.780440 10.089874 10.986839

43 H 10.986839 10.089874 8.780440 8.901504 10.338759

44 H 5.815798 6.560000 5.886376 4.523806 4.472449

45 H 4.472449 4.523806 5.886376 6.560000 5.815798

6 7 8 9 10

6 C 0.000000

7 C 1.439354 0.000000

8 N 2.493235 1.371353 0.000000

9 C 3.606433 2.214107 1.371353 0.000000

10 C 3.652778 2.258439 2.282116 1.427050 0.000000

11 C 2.551136 1.427050 2.282116 2.258439 1.383889

12 C 4.891558 5.526834 5.174209 6.440537 7.427936

13 C 5.526834 5.821081 5.132548 6.227941 7.408175

14 C 6.952678 7.198401 6.414505 7.408175 8.663013

15 C 7.427936 7.408175 6.414505 7.198401 8.551763

16 C 6.440537 6.227941 5.132548 5.821081 7.198401

17 N 5.174209 5.132548 4.202387 5.132548 6.414505

18 C 6.951062 6.440537 5.174209 5.526834 6.952678

19 C 6.442133 5.678108 4.328480 4.402975 5.821613

20 C 7.448292 6.483334 5.113698 4.798904 6.124784

21 C 6.987831 5.841506 4.520970 3.888324 5.088395

22 C 5.535910 4.395843 3.067619 2.543366 3.861876

23 N 5.179673 4.328326 2.968264 3.074146 4.500680

24 H 4.635447 5.863109 6.191244 7.561578 8.100456

25 H 2.900313 4.337718 5.205590 6.451141 6.538944

26 H 4.668266 3.312005 3.319831 2.238217 1.080453

27 H 2.915359 2.238217 3.319831 3.312005 2.211883

28 H 7.664543 8.050064 7.361253 8.412093 9.629943

29 H 8.487556 8.412093 7.361253 8.050064 9.434551

30 H 8.505672 7.561578 6.191244 5.863109 7.166991

31 H 7.698760 6.451141 5.205590 4.337718 5.339116

32 Zn 3.475531 3.113971 2.101194 3.113971 4.331507

33 C 4.938615 3.606433 2.493235 1.439354 2.551136

34 C 6.030485 4.615519 3.730007 2.430708 2.903645

35 C 5.983979 6.790194 6.552343 7.842284 8.781166

36 C 7.039971 5.603767 4.853880 3.505682 3.624400

37 C 7.015192 7.912453 7.738563 9.039873 9.950031

38 C 1.424283 2.430708 3.730007 4.615519 4.248920

39 C 2.632596 3.505682 4.853880 5.603767 5.008207

40 C 8.375331 7.842284 6.552343 6.790194 8.215029

41 C 9.583504 9.039873 7.738563 7.912453 9.330447

42 H 10.650232 10.098600 8.789881 8.920117 10.330619

43 H 7.979899 6.540606 5.875578 4.512903 4.443827

44 H 3.699401 4.512903 5.875578 6.540606 5.810043

45 H 7.964561 8.920117 8.789881 10.098600 10.987751

11 12 13 14 15

11 C 0.000000

12 C 6.952678 0.000000

13 C 7.198401 1.439354 0.000000

14 C 8.551763 2.551136 1.427050 0.000000

15 C 8.663013 3.652778 2.258439 1.383889 0.000000

16 C 7.408175 3.606433 2.214107 2.258439 1.427050

17 N 6.414505 2.493235 1.371353 2.282116 2.282116

18 C 7.427936 4.938615 3.606433 3.652778 2.551136

19 C 6.475014 5.535910 4.395843 4.790481 3.861876

20 C 7.027886 6.987831 5.841506 6.145728 5.088395

21 C 6.145728 7.448292 6.483334 7.027886 6.124784

22 C 4.790481 6.442133 5.678108 6.475014 5.821613

23 N 5.104796 5.179673 4.328326 5.104796 4.500680

24 H 7.166991 2.900313 4.337718 5.339116 6.538944

25 H 5.339116 4.635447 5.863109 7.166991 8.100456

26 H 2.211883 8.487556 8.412093 9.629943 9.434551

27 H 1.080453 7.664543 8.050064 9.434551 9.629943

28 H 9.434551 2.915359 2.238217 1.080453 2.211883

29 H 9.629943 4.668266 3.312005 2.211883 1.080453

30 H 8.100456 7.698760 6.451141 6.538944 5.339116

31 H 6.538944 8.505672 7.561578 8.100456 7.166991

32 Zn 4.331507 3.475531 3.113971 4.331507 4.331507

33 C 3.652778 6.951062 6.440537 7.427936 6.952678

34 C 4.248920 8.375331 7.842284 8.781166 8.215029

35 C 8.215029 1.424283 2.430708 2.903645 4.248920

36 C 5.008207 9.583504 9.039873 9.950031 9.330447

37 C 9.330447 2.632596 3.505682 3.624400 5.008207

38 C 2.903645 5.983979 6.790194 8.215029 8.781166

39 C 3.624400 7.015192 7.912453 9.330447 9.950031

40 C 8.781166 6.030485 4.615519 4.248920 2.903645

41 C 9.950031 7.039971 5.603767 5.008207 3.624400

42 H 10.987751 7.979899 6.540606 5.810043 4.443827

43 H 5.810043 10.650232 10.098600 10.987751 10.330619

44 H 4.443827 7.964561 8.920117 10.330619 10.987751

45 H 10.330619 3.699401 4.512903 4.443827 5.810043

16 17 18 19 20

16 C 0.000000

17 N 1.371353 0.000000

18 C 1.439354 2.493235 0.000000

19 C 2.543366 3.067619 1.404828 0.000000

20 C 3.888324 4.520970 2.537840 1.453762 0.000000

21 C 4.798904 5.113698 3.617720 2.264729 1.358926

22 C 4.402975 4.328480 3.581665 2.219085 2.264729

23 N 3.074146 2.968264 2.474020 1.371600 2.297797

24 H 6.451141 5.205590 7.698760 8.055237 9.463565

25 H 7.561578 6.191244 8.505672 8.415382 9.653580

26 H 8.050064 7.361253 7.664543 6.436690 6.518956

27 H 8.412093 7.361253 8.487556 7.553718 8.099407

28 H 3.312005 3.319831 4.668266 5.853572 7.186206

29 H 2.238217 3.319831 2.915359 4.317015 5.342092

30 H 4.337718 5.205590 2.900313 2.257650 1.080322

31 H 5.863109 6.191244 4.635447 3.320962 2.190804

32 Zn 3.113971 2.101194 3.475531 3.107732 4.345058

33 C 5.526834 5.174209 4.891558 3.581665 3.617720

34 C 6.790194 6.552343 5.983979 4.598286 4.211916

35 C 4.615519 3.730007 6.030485 6.796167 8.248330

36 C 7.912453 7.738563 7.015192 5.612336 5.001496

37 C 5.603767 4.853880 7.039971 7.901466 9.346635

38 C 7.842284 6.552343 8.375331 7.842967 8.798820

39 C 9.039873 7.738563 9.583504 9.034092 9.955203

40 C 2.430708 3.730007 1.424283 2.412465 2.890667

41 C 3.505682 4.853880 2.632596 3.509510 3.642591

42 H 4.512903 5.875578 3.699401 4.523806 4.472449

43 H 8.920117 8.789881 7.964561 6.560000 5.815798

44 H 10.098600 8.789881 10.650232 10.089874 10.986839

45 H 6.540606 5.875578 7.979899 8.901504 10.338759

21 22 23 24 25

21 C 0.000000

22 C 1.453762 0.000000

23 N 2.297797 1.371600 0.000000

24 H 9.653580 8.415382 7.367925 0.000000

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26 H 5.342092 4.317015 5.190554 9.169427 7.524664

27 H 7.186206 5.853572 6.182927 7.507221 5.375921

28 H 8.099407 7.553718 6.182927 5.375921 7.507221

29 H 6.518956 6.436690 5.190554 7.524664 9.169427

30 H 2.190804 3.320962 3.332337 10.298247 10.639515

31 H 1.080322 2.257650 3.332337 10.639515 10.298247

32 Zn 4.345058 3.107732 2.096563 5.319758 5.319758

33 C 2.537840 1.404828 2.474020 8.505672 7.698760

34 C 2.890667 2.412465 3.718366 9.866074 8.881442

35 C 8.798820 7.842967 6.555992 2.697470 5.073042

36 C 3.642591 3.509510 4.858557 11.027616 9.924833

37 C 9.955203 9.034092 7.733115 3.099484 5.719511

38 C 8.248330 6.796167 6.555992 5.073042 2.697470

39 C 9.346635 7.901466 7.733115 5.719511 3.099484

40 C 4.211916 4.598286 3.718366 8.881442 9.866074

41 C 5.001496 5.612336 4.858557 9.924833 11.027616

42 H 5.815798 6.560000 5.886376 10.876954 12.062100

43 H 4.472449 4.523806 5.886376 12.062100 10.876954

44 H 10.338759 8.901504 8.780440 6.422296 3.749637

45 H 10.986839 10.089874 8.780440 3.749637 6.422296

26 27 28 29 30

26 H 0.000000

27 H 2.691723 0.000000

28 H 10.618784 10.271962 0.000000

29 H 10.271962 10.618784 2.691723 0.000000

30 H 7.507221 9.169427 7.524664 5.375921 0.000000

31 H 5.375921 7.524664 9.169427 7.507221 2.673086

32 Zn 5.309392 5.309392 5.309392 5.309392 5.319758

33 C 2.915359 4.668266 8.487556 7.664543 4.635447

34 C 2.715255 5.107656 9.850015 8.849139 5.073042

35 C 9.850015 8.849139 2.715255 5.107656 8.881442

36 C 3.079713 5.720128 11.023164 9.913370 5.719511

37 C 11.023164 9.913370 3.079713 5.720128 9.924833

38 C 5.107656 2.715255 8.849139 9.850015 9.866074

39 C 5.720128 3.079713 9.913370 11.023164 11.027616

40 C 8.849139 9.850015 5.107656 2.715255 2.697470

41 C 9.913370 11.023164 5.720128 3.079713 3.099484

42 H 10.875537 12.063391 6.407524 3.715947 3.749637

43 H 3.715947 6.407524 12.063391 10.875537 6.422296

44 H 6.407524 3.715947 10.875537 12.063391 12.062100

45 H 12.063391 10.875537 3.715947 6.407524 10.876954

31 32 33 34 35

31 H 0.000000

32 Zn 5.319758 0.000000

33 C 2.900313 3.475531 0.000000

34 C 2.697470 4.899802 1.424283 0.000000

35 C 9.866074 4.899802 8.375331 9.799605 0.000000

36 C 3.099484 6.108006 2.632596 1.208412 11.007786

37 C 11.027616 6.108006 9.583504 11.007786 1.208412

38 C 8.881442 4.899802 6.030485 6.952995 6.905658

39 C 9.924833 6.108006 7.039971 7.840869 7.819999

40 C 5.073042 4.899802 5.983979 6.905658 6.952995

41 C 5.719511 6.108006 7.015192 7.819999 7.840869

42 H 6.422296 7.174761 7.964561 8.683852 8.692596

43 H 3.749637 7.174761 3.699401 2.275214 12.074515

44 H 10.876954 7.174761 7.979899 8.692596 8.683852

45 H 12.062100 7.174761 10.650232 12.074515 2.275214

36 37 38 39 40

36 C 0.000000

37 C 12.216013 0.000000

38 C 7.840869 7.819999 0.000000

39 C 8.632102 8.643945 1.208412 0.000000

40 C 7.819999 7.840869 9.799605 11.007786 0.000000

41 C 8.643945 8.632102 11.007786 12.216013 1.208412

42 H 9.436614 9.408516 12.074515 13.282763 2.275214

43 H 1.066810 13.282763 8.692596 9.408516 8.683852

44 H 9.408516 9.436614 2.275214 1.066810 12.074515

45 H 13.282763 1.066810 8.683852 9.436614 8.692596

41 42 43 44 45

41 C 0.000000

42 H 1.066810 0.000000

43 H 9.436614 10.170310 0.000000

44 H 13.282763 14.349522 10.122923 0.000000

45 H 9.408516 10.122923 14.349522 10.170310 0.000000

Stoichiometry C28H12N4Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C28H12)]

Deg. of freedom 34

Full point group C2V NOp 4

RotChk: IX=0 Diff= 2.35D-14

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 0.679463 4.291603 -0.000014

2 6 0 1.109543 2.902914 -0.000005

3 7 0 0.000000 2.096563 0.000000

4 6 0 -1.109543 2.902914 -0.000005

5 6 0 -0.679463 4.291603 -0.000014

6 6 0 -2.445779 2.469308 -0.000007

7 6 0 -2.910541 1.107053 -0.000008

8 7 0 -2.101194 0.000000 -0.000002

9 6 0 -2.910541 -1.107053 -0.000008

10 6 0 -4.275881 -0.691944 -0.000019

11 6 0 -4.275881 0.691944 -0.000019

12 6 0 2.445779 2.469308 -0.000007

13 6 0 2.910541 1.107053 -0.000008

14 6 0 4.275881 0.691944 -0.000019

15 6 0 4.275881 -0.691944 -0.000019

16 6 0 2.910541 -1.107053 -0.000008

17 7 0 2.101194 -0.000000 -0.000002

18 6 0 2.445779 -2.469308 -0.000007

19 6 0 1.109543 -2.902914 -0.000005

20 6 0 0.679463 -4.291603 -0.000014

21 6 0 -0.679463 -4.291603 -0.000014

22 6 0 -1.109543 -2.902914 -0.000005

23 7 0 -0.000000 -2.096563 0.000000

24 1 0 1.336543 5.149124 -0.000021

25 1 0 -1.336543 5.149124 -0.000021

26 1 0 -5.135981 -1.345862 -0.000028

27 1 0 -5.135981 1.345862 -0.000028

28 1 0 5.135981 1.345862 -0.000028

29 1 0 5.135981 -1.345862 -0.000028

30 1 0 1.336543 -5.149124 -0.000021

31 1 0 -1.336543 -5.149124 -0.000021

32 30 0 0.000000 0.000000 0.000079

33 6 0 -2.445779 -2.469308 -0.000007

34 6 0 -3.452829 -3.476498 -0.000013

35 6 0 3.452829 3.476498 -0.000013

36 6 0 -4.321973 -4.316051 -0.000019

37 6 0 4.321973 4.316051 -0.000019

38 6 0 -3.452829 3.476498 -0.000013

39 6 0 -4.321973 4.316051 -0.000019

40 6 0 3.452829 -3.476498 -0.000013

41 6 0 4.321973 -4.316051 -0.000019

42 1 0 5.085155 -5.061461 -0.000025

43 1 0 -5.085155 -5.061461 -0.000025

44 1 0 -5.085155 5.061461 -0.000025

45 1 0 5.085155 5.061461 -0.000025

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

Rotational constants (GHZ): 0.1459412 0.1453120 0.0728130

Leave Link 202 at Wed Jul 31 04:47:59 2019, MaxMem= 4294967296 cpu: 0.1

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

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

Pseudo-potential data read from rwf file.

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

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

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

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

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

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

111 alpha electrons 110 beta electrons

nuclear repulsion energy 3051.6645072271 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= 13 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= -0.1303254608 Hartrees.

Nuclear repulsion after empirical dispersion term = 3051.5341817663 Hartrees.

No density basis found on file 724.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

2nd derivatives : Analytical E(r).r(xy)/FMM algorithm (CHGder, D2EAlg=3).

Cavity 2nd derivative terms included.

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

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

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

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

GePol: Number of points = 3878

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.61D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 76

GePol: Fraction of low-weight points (<1% of avg) = 1.96%

GePol: Cavity surface area = 416.523 Ang\*\*2

GePol: Cavity volume = 421.083 Ang\*\*3

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

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

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

PCM non-electrostatic energy = 0.0083855474 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3051.5425673138 Hartrees.

Leave Link 301 at Wed Jul 31 04:47:59 2019, MaxMem= 4294967296 cpu: 1.9

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16169 LenP2D= 44682.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.48D-05 NBF= 172 148 158 158

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

Precomputing XC quadrature grid using

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

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

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

Leave Link 302 at Wed Jul 31 04:48:00 2019, MaxMem= 4294967296 cpu: 10.7

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

DipDrv: MaxL=1.

Leave Link 303 at Wed Jul 31 04:48:00 2019, MaxMem= 4294967296 cpu: 1.4

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

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

B after Tr= 0.000000 -0.000000 -0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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The electronic state of the initial guess is 2-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7631 S= 0.5065

Leave Link 401 at Wed Jul 31 04:48:01 2019, MaxMem= 4294967296 cpu: 22.3

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1387497 IEndB= 1387497 NGot= 4294967296 MDV= 4294047352

LenX= 4294047352 LenY= 4293596440

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= 650000000 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= 45116652.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.22D-15 for 3870.

Iteration 1 A\*A^-1 deviation from orthogonality is 7.11D-15 for 3861 541.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.77D-15 for 3870.

Iteration 1 A^-1\*A deviation from orthogonality is 1.20D-14 for 3747 3689.

E= -1359.18269984839

DIIS: error= 5.11D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.18269984839 IErMin= 1 ErrMin= 5.11D-05

ErrMax= 5.11D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.98D-06 BMatP= 2.98D-06

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

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.388 Goal= None Shift= 0.000

Gap= 0.438 Goal= None Shift= 0.000

RMSDP=5.18D-06 MaxDP=2.74D-04 OVMax= 2.23D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.18D-06 CP: 1.00D+00

E= -1359.18270072215 Delta-E= -0.000000873757 Rises=F Damp=F

DIIS: error= 6.16D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.18270072215 IErMin= 2 ErrMin= 6.16D-06

ErrMax= 6.16D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.03D-08 BMatP= 2.98D-06

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

Coeff-Com: -0.160D-01 0.102D+01

Coeff: -0.160D-01 0.102D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=4.91D-07 MaxDP=1.22D-05 DE=-8.74D-07 OVMax= 4.00D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.56D-07 CP: 1.00D+00 1.03D+00

E= -1359.18270072817 Delta-E= -0.000000006021 Rises=F Damp=F

DIIS: error= 8.23D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.18270072817 IErMin= 2 ErrMin= 6.16D-06

ErrMax= 8.23D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.50D-08 BMatP= 4.03D-08

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

Coeff-Com: -0.170D-01 0.533D+00 0.484D+00

Coeff: -0.170D-01 0.533D+00 0.484D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=1.97D-07 MaxDP=1.29D-05 DE=-6.02D-09 OVMax= 3.93D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.33D-07 CP: 1.00D+00 1.04D+00 6.84D-01

E= -1359.18270073586 Delta-E= -0.000000007695 Rises=F Damp=F

DIIS: error= 2.85D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.18270073586 IErMin= 4 ErrMin= 2.85D-06

ErrMax= 2.85D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.89D-09 BMatP= 4.03D-08

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

Coeff-Com: -0.714D-02 0.142D+00 0.278D+00 0.587D+00

Coeff: -0.714D-02 0.142D+00 0.278D+00 0.587D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=6.12D-08 MaxDP=4.59D-06 DE=-7.70D-09 OVMax= 1.15D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 5.04D-08 CP: 1.00D+00 1.04D+00 6.97D-01 7.42D-01

E= -1359.18270073709 Delta-E= -0.000000001230 Rises=F Damp=F

DIIS: error= 1.01D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.18270073709 IErMin= 5 ErrMin= 1.01D-06

ErrMax= 1.01D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.01D-10 BMatP= 5.89D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.180D-02 0.198D-01 0.909D-01 0.282D+00 0.609D+00

Coeff: -0.180D-02 0.198D-01 0.909D-01 0.282D+00 0.609D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=1.84D-08 MaxDP=8.85D-07 DE=-1.23D-09 OVMax= 2.96D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.56D-08 CP: 1.00D+00 1.04D+00 7.00D-01 8.00D-01 8.88D-01

E= -1359.18270073717 Delta-E= -0.000000000076 Rises=F Damp=F

DIIS: error= 3.82D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.18270073717 IErMin= 6 ErrMin= 3.82D-07

ErrMax= 3.82D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.13D-11 BMatP= 4.01D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.196D-03-0.146D-01 0.213D-02 0.505D-01 0.336D+00 0.626D+00

Coeff: 0.196D-03-0.146D-01 0.213D-02 0.505D-01 0.336D+00 0.626D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=7.73D-09 MaxDP=2.17D-07 DE=-7.64D-11 OVMax= 1.33D-06

Error on total polarization charges = 0.06719

SCF Done: E(UB3LYP) = -1359.18270074 A.U. after 6 cycles

NFock= 6 Conv=0.77D-08 -V/T= 1.9682

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7631 S= 0.5065

<L.S>= 0.000000000000E+00

KE= 1.403847868853D+03 PE=-9.372576959242D+03 EE= 3.558003822338D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.26

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 0.7631, after 0.7501

Leave Link 502 at Wed Jul 31 04:48:41 2019, MaxMem= 4294967296 cpu: 595.3

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 636

NBasis= 636 NAE= 111 NBE= 110 NFC= 0 NFV= 0

NROrb= 636 NOA= 111 NOB= 110 NVA= 525 NVB= 526

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.15076479D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.38338309D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.15049510D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.88296892D-01

Leave Link 801 at Wed Jul 31 04:48:41 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 45.

Will process 46 centers per pass.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16169 LenP2D= 44682.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 11 by ecpmxn.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Wed Jul 31 04:48:44 2019, MaxMem= 4294967296 cpu: 44.8

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Wed Jul 31 04:48:44 2019, MaxMem= 4294967296 cpu: 1.1

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 45.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966832.

G2DrvN: will do 46 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

G2PCM: DoFxE=T DoFxN=T DoGrad=T DoDP/DQ/DG/TGxP=FFFF NFrqRd= 0 IEInf=0 SqF1=F DoCFld=F IF1Alg=4.

GePol: Maximum number of non-zero 1st derivatives = 255

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Wed Jul 31 04:50:41 2019, MaxMem= 4294967296 cpu: 1869.4

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=111111111111111111111111111111111111111111111

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Using symmetry in CPHF.

Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.

Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.

NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 4294965570 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 0.

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 650000000 NMat= 42 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 42 NMatS0= 42 NMatT0= 0 NMatD0= 42 NMtDS0= 0 NMtDT0= 0

Integrals replicated using symmetry in FoFCou.

There are 42 degrees of freedom in the 1st order CPHF. IDoFFX=4 NUNeed= 42.

42 vectors produced by pass 0 Test12= 2.77D-13 2.38D-09 XBig12= 8.07D+03 5.92D+01.

AX will form 42 AO Fock derivatives at one time.

42 vectors produced by pass 1 Test12= 2.77D-13 2.38D-09 XBig12= 1.08D+03 6.87D+00.

42 vectors produced by pass 2 Test12= 2.77D-13 2.38D-09 XBig12= 2.83D+02 5.66D+00.

42 vectors produced by pass 3 Test12= 2.77D-13 2.38D-09 XBig12= 8.41D+01 2.10D+00.

42 vectors produced by pass 4 Test12= 2.77D-13 2.38D-09 XBig12= 9.55D+00 5.63D-01.

42 vectors produced by pass 5 Test12= 2.77D-13 2.38D-09 XBig12= 3.14D-01 7.10D-02.

42 vectors produced by pass 6 Test12= 2.77D-13 2.38D-09 XBig12= 1.26D-02 9.65D-03.

42 vectors produced by pass 7 Test12= 2.77D-13 2.38D-09 XBig12= 2.65D-04 1.44D-03.

35 vectors produced by pass 8 Test12= 2.77D-13 2.38D-09 XBig12= 5.11D-06 1.74D-04.

24 vectors produced by pass 9 Test12= 2.77D-13 2.38D-09 XBig12= 7.04D-08 2.24D-05.

10 vectors produced by pass 10 Test12= 2.77D-13 2.38D-09 XBig12= 9.27D-10 2.64D-06.

2 vectors produced by pass 11 Test12= 2.77D-13 2.38D-09 XBig12= 9.79D-12 1.96D-07.

2 vectors produced by pass 12 Test12= 2.77D-13 2.38D-09 XBig12= 1.30D-13 2.87D-08.

2 vectors produced by pass 13 Test12= 2.77D-13 2.38D-09 XBig12= 3.54D-15 2.60D-09.

InvSVY: IOpt=1 It= 1 EMax= 7.11D-14

Solved reduced A of dimension 411 with 42 vectors.

FullF1: Do perturbations 1 to 42.

Isotropic polarizability for W= 0.000000 1007.13 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Wed Jul 31 05:36:31 2019, MaxMem= 4294967296 cpu: 44004.3

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16169 LenP2D= 44682.

LDataN: DoStor=T MaxTD1= 7 Len= 274

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 255

Leave Link 701 at Wed Jul 31 05:37:06 2019, MaxMem= 4294967296 cpu: 550.0

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Wed Jul 31 05:37:06 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

Compute integral second derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 100127 IOpCl= 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 Wed Jul 31 05:38:56 2019, MaxMem= 4294967296 cpu: 1759.8

(Enter /home/kira/g09/l716.exe)

Dipole = 4.10796397D-13-5.43079470D-13 1.92607280D-04

Polarizability= 1.65446918D+03-1.46225991D-05 1.17979773D+03

5.99577530D-08 4.08497230D-07 1.87126946D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000000063 -0.000002223 0.000000002

2 6 0.000000504 -0.000000985 -0.000000040

3 7 -0.000007341 -0.000000000 0.000001959

4 6 0.000000504 0.000000985 -0.000000040

5 6 -0.000000063 0.000002223 0.000000002

6 6 0.000000577 0.000000585 -0.000000005

7 6 -0.000000924 0.000000285 -0.000000047

8 7 0.000000000 -0.000004908 0.000002340

9 6 0.000000924 0.000000285 -0.000000047

10 6 -0.000001883 -0.000000442 0.000000000

11 6 0.000001883 -0.000000442 0.000000000

12 6 0.000000577 -0.000000585 -0.000000005

13 6 -0.000000924 -0.000000285 -0.000000047

14 6 0.000001883 0.000000442 0.000000000

15 6 -0.000001883 0.000000442 0.000000000

16 6 0.000000924 -0.000000285 -0.000000047

17 7 0.000000000 0.000004908 0.000002340

18 6 -0.000000577 -0.000000585 -0.000000005

19 6 -0.000000504 -0.000000985 -0.000000040

20 6 0.000000063 -0.000002223 0.000000002

21 6 0.000000063 0.000002223 0.000000002

22 6 -0.000000504 0.000000985 -0.000000040

23 7 0.000007341 0.000000000 0.000001959

24 1 -0.000000114 -0.000000113 -0.000000006

25 1 -0.000000114 0.000000113 -0.000000006

26 1 -0.000000048 -0.000000061 -0.000000006

27 1 0.000000048 -0.000000061 -0.000000006

28 1 0.000000048 0.000000061 -0.000000006

29 1 -0.000000048 0.000000061 -0.000000006

30 1 0.000000114 -0.000000113 -0.000000006

31 1 0.000000114 0.000000113 -0.000000006

32 30 -0.000000000 -0.000000000 -0.000008213

33 6 -0.000000577 0.000000585 -0.000000005

34 6 -0.000000172 -0.000000177 0.000000003

35 6 0.000000172 0.000000177 0.000000003

36 6 -0.000000149 -0.000000079 0.000000003

37 6 0.000000149 0.000000079 0.000000003

38 6 0.000000172 -0.000000177 0.000000003

39 6 0.000000149 -0.000000079 0.000000003

40 6 -0.000000172 0.000000177 0.000000003

41 6 -0.000000149 0.000000079 0.000000003

42 1 0.000000232 0.000000090 -0.000000000

43 1 0.000000232 -0.000000090 -0.000000000

44 1 -0.000000232 -0.000000090 -0.000000000

45 1 -0.000000232 0.000000090 -0.000000000

-------------------------------------------------------------------

Cartesian Forces: Max 0.000008213 RMS 0.000001463

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Wed Jul 31 05:38:56 2019, MaxMem= 4294967296 cpu: 0.8

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000004527 RMS 0.000000709

Search for a local minimum.

Step number 10 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .70854D-06 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -6.45D-07 DEPred=-6.41D-07 R= 1.01D+00

Trust test= 1.01D+00 RLast= 8.00D-03 DXMaxT set to 2.12D-01

ITU= 0 1 1 1 -1 0 0 -1 0 0

Eigenvalues --- 0.00149 0.00336 0.00452 0.00551 0.00653

Eigenvalues --- 0.00957 0.01115 0.01121 0.01162 0.01231

Eigenvalues --- 0.01238 0.01277 0.01292 0.01344 0.01381

Eigenvalues --- 0.01506 0.01521 0.01550 0.01859 0.01921

Eigenvalues --- 0.01942 0.01965 0.01973 0.02005 0.02018

Eigenvalues --- 0.02089 0.02100 0.02120 0.02123 0.02513

Eigenvalues --- 0.03000 0.03163 0.03195 0.03647 0.04002

Eigenvalues --- 0.04121 0.04122 0.04135 0.04136 0.04146

Eigenvalues --- 0.04358 0.04359 0.06241 0.06295 0.08266

Eigenvalues --- 0.08277 0.08293 0.08561 0.08841 0.08875

Eigenvalues --- 0.08962 0.09213 0.09270 0.09571 0.09610

Eigenvalues --- 0.09627 0.09656 0.09998 0.10408 0.10411

Eigenvalues --- 0.10442 0.10496 0.12312 0.13214 0.13555

Eigenvalues --- 0.13583 0.16014 0.16903 0.16963 0.19290

Eigenvalues --- 0.19804 0.20059 0.20086 0.20350 0.20623

Eigenvalues --- 0.20663 0.20832 0.21613 0.21814 0.21881

Eigenvalues --- 0.21947 0.26000 0.26186 0.27688 0.27944

Eigenvalues --- 0.28029 0.29425 0.29980 0.31686 0.32490

Eigenvalues --- 0.32764 0.32791 0.33601 0.35666 0.35683

Eigenvalues --- 0.35843 0.36111 0.36435 0.37025 0.37100

Eigenvalues --- 0.37157 0.37328 0.37390 0.37559 0.37832

Eigenvalues --- 0.38036 0.38341 0.38797 0.39213 0.40229

Eigenvalues --- 0.40233 0.40235 0.40236 0.41174 0.41286

Eigenvalues --- 0.41887 0.42425 0.45365 0.46064 0.46399

Eigenvalues --- 0.46618 0.50195 0.50201 0.52617 0.53031

Eigenvalues --- 1.03361 1.04108 1.04441 1.04674

En-DIIS/RFO-DIIS IScMMF= 0 using points: 10 9 8 7 6

RFO step: Lambda=-4.22697003D-10.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 1.43D-04 SmlDif= 1.00D-05

RMS Error= 0.2596386991D-05 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.03064 -0.07344 0.04229 0.00047 0.00004

Iteration 1 RMS(Cart)= 0.00001325 RMS(Int)= 0.00000010

Iteration 2 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000010

ITry= 1 IFail=0 DXMaxC= 1.66D-04 DCOld= 1.00D+10 DXMaxT= 2.12D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 4.55D-07 for atom 37.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.74721 0.00000 0.00000 0.00000 0.00000 2.74722

R2 2.56800 -0.00000 -0.00000 -0.00000 -0.00000 2.56800

R3 2.04151 0.00000 0.00000 0.00000 0.00000 2.04151

R4 2.59195 -0.00000 -0.00000 -0.00000 -0.00001 2.59194

R5 2.65474 0.00000 0.00000 -0.00000 0.00000 2.65474

R6 2.59195 -0.00000 -0.00000 -0.00000 -0.00001 2.59194

R7 3.96193 0.00000 0.00003 0.00000 0.00003 3.96196

R8 2.74721 0.00000 0.00000 0.00000 0.00000 2.74722

R9 2.65474 0.00000 0.00000 -0.00000 0.00000 2.65474

R10 2.04151 0.00000 0.00000 0.00000 0.00000 2.04151

R11 2.71998 0.00000 0.00000 -0.00000 0.00000 2.71999

R12 2.69150 0.00000 0.00000 0.00000 0.00000 2.69151

R13 2.59148 -0.00000 -0.00000 0.00000 -0.00000 2.59148

R14 2.69673 0.00000 0.00000 0.00000 0.00000 2.69674

R15 2.59148 -0.00000 -0.00000 0.00000 -0.00000 2.59148

R16 3.97068 0.00000 0.00002 -0.00000 0.00001 3.97069

R17 2.69673 0.00000 0.00000 0.00000 0.00000 2.69674

R18 2.71998 0.00000 0.00000 -0.00000 0.00000 2.71999

R19 2.61517 -0.00000 -0.00000 -0.00000 -0.00000 2.61517

R20 2.04176 0.00000 0.00000 -0.00000 0.00000 2.04176

R21 2.04176 0.00000 0.00000 -0.00000 0.00000 2.04176

R22 2.71998 0.00000 0.00000 -0.00000 0.00000 2.71999

R23 2.69150 0.00000 0.00000 0.00000 0.00000 2.69151

R24 2.69673 0.00000 0.00000 0.00000 0.00000 2.69674

R25 2.59148 -0.00000 -0.00000 0.00000 -0.00000 2.59148

R26 2.61517 -0.00000 -0.00000 -0.00000 -0.00000 2.61517

R27 2.04176 0.00000 0.00000 -0.00000 0.00000 2.04176

R28 2.69673 0.00000 0.00000 0.00000 0.00000 2.69674

R29 2.04176 0.00000 0.00000 -0.00000 0.00000 2.04176

R30 2.59148 -0.00000 -0.00000 0.00000 -0.00000 2.59148

R31 2.71998 0.00000 0.00000 -0.00000 0.00000 2.71999

R32 3.97068 0.00000 0.00002 -0.00000 0.00001 3.97069

R33 2.65474 0.00000 0.00000 -0.00000 0.00000 2.65474

R34 2.69150 0.00000 0.00000 0.00000 0.00000 2.69151

R35 2.74721 0.00000 0.00000 0.00000 0.00000 2.74722

R36 2.59195 -0.00000 -0.00000 -0.00000 -0.00001 2.59194

R37 2.56800 -0.00000 -0.00000 -0.00000 -0.00000 2.56800

R38 2.04151 0.00000 0.00000 0.00000 0.00000 2.04151

R39 2.74721 0.00000 0.00000 0.00000 0.00000 2.74722

R40 2.04151 0.00000 0.00000 0.00000 0.00000 2.04151

R41 2.59195 -0.00000 -0.00000 -0.00000 -0.00001 2.59194

R42 2.65474 0.00000 0.00000 -0.00000 0.00000 2.65474

R43 3.96193 0.00000 0.00003 0.00000 0.00003 3.96196

R44 2.69150 0.00000 0.00000 0.00000 0.00000 2.69151

R45 2.28357 0.00000 0.00000 0.00000 0.00000 2.28357

R46 2.28357 0.00000 0.00000 0.00000 0.00000 2.28357

R47 2.01598 0.00000 0.00000 0.00000 0.00000 2.01598

R48 2.01598 0.00000 0.00000 0.00000 0.00000 2.01598

R49 2.28357 0.00000 0.00000 0.00000 0.00000 2.28357

R50 2.01598 0.00000 0.00000 0.00000 0.00000 2.01598

R51 2.28357 0.00000 0.00000 0.00000 0.00000 2.28357

R52 2.01598 0.00000 0.00000 0.00000 0.00000 2.01598

A1 1.87113 0.00000 0.00000 -0.00000 0.00000 1.87113

A2 2.18744 0.00000 0.00000 0.00000 0.00000 2.18744

A3 2.22462 -0.00000 -0.00000 -0.00000 -0.00000 2.22462

A4 1.89891 -0.00000 -0.00000 0.00000 -0.00000 1.89891

A5 2.18491 0.00000 0.00000 0.00000 0.00001 2.18491

A6 2.19937 -0.00000 -0.00000 -0.00000 -0.00000 2.19936

A7 1.88469 0.00000 0.00001 -0.00000 0.00001 1.88470

A8 2.19925 -0.00000 -0.00000 -0.00000 -0.00000 2.19924

A9 2.19925 -0.00000 -0.00000 0.00000 -0.00000 2.19924

A10 1.89891 -0.00000 -0.00000 0.00000 -0.00000 1.89891

A11 2.19937 -0.00000 -0.00000 -0.00000 -0.00000 2.19936

A12 2.18491 0.00000 0.00000 0.00000 0.00001 2.18491

A13 1.87113 0.00000 0.00000 -0.00000 0.00000 1.87113

A14 2.22462 -0.00000 -0.00000 -0.00000 -0.00000 2.22462

A15 2.18744 0.00000 0.00000 0.00000 0.00000 2.18744

A16 2.21336 0.00000 0.00001 0.00000 0.00001 2.21337

A17 2.04235 -0.00000 -0.00000 0.00000 -0.00000 2.04234

A18 2.02748 -0.00000 -0.00000 -0.00000 -0.00000 2.02747

A19 2.18152 0.00000 0.00000 -0.00000 0.00000 2.18152

A20 2.19474 0.00000 0.00000 0.00000 0.00000 2.19474

A21 1.90693 -0.00000 -0.00000 -0.00000 -0.00000 1.90692

A22 1.87903 0.00000 0.00001 -0.00000 0.00001 1.87903

A23 2.20208 -0.00000 -0.00000 0.00000 -0.00000 2.20208

A24 2.20208 -0.00000 -0.00000 0.00000 -0.00000 2.20208

A25 1.90693 -0.00000 -0.00000 -0.00000 -0.00000 1.90692

A26 2.18152 0.00000 0.00000 -0.00000 0.00000 2.18152

A27 2.19474 0.00000 0.00000 0.00000 0.00000 2.19474

A28 1.86595 0.00000 0.00000 0.00000 0.00000 1.86595

A29 2.19639 -0.00000 0.00000 -0.00000 0.00000 2.19639

A30 2.22084 -0.00000 -0.00000 -0.00000 -0.00000 2.22084

A31 1.86595 0.00000 0.00000 0.00000 0.00000 1.86595

A32 2.19639 -0.00000 0.00000 -0.00000 0.00000 2.19639

A33 2.22084 -0.00000 -0.00000 -0.00000 -0.00000 2.22084

A34 2.21336 0.00000 0.00001 0.00000 0.00001 2.21337

A35 2.04235 -0.00000 -0.00000 0.00000 -0.00000 2.04234

A36 2.02748 -0.00000 -0.00000 -0.00000 -0.00000 2.02747

A37 2.19474 0.00000 0.00000 0.00000 0.00000 2.19474

A38 2.18152 0.00000 0.00000 -0.00000 0.00000 2.18152

A39 1.90693 -0.00000 -0.00000 -0.00000 -0.00000 1.90692

A40 1.86595 0.00000 0.00000 0.00000 0.00000 1.86595

A41 2.19639 -0.00000 0.00000 -0.00000 0.00000 2.19639

A42 2.22084 -0.00000 -0.00000 -0.00000 -0.00000 2.22084

A43 1.86595 0.00000 0.00000 0.00000 0.00000 1.86595

A44 2.22084 -0.00000 -0.00000 -0.00000 -0.00000 2.22084

A45 2.19639 -0.00000 0.00000 -0.00000 0.00000 2.19639

A46 1.90693 -0.00000 -0.00000 -0.00000 -0.00000 1.90692

A47 2.19474 0.00000 0.00000 0.00000 0.00000 2.19474

A48 2.18152 0.00000 0.00000 -0.00000 0.00000 2.18152

A49 1.87903 0.00000 0.00001 -0.00000 0.00001 1.87903

A50 2.20208 -0.00000 -0.00000 0.00000 -0.00000 2.20208

A51 2.20208 -0.00000 -0.00000 0.00000 -0.00000 2.20208

A52 2.21336 0.00000 0.00001 0.00000 0.00001 2.21337

A53 2.02748 -0.00000 -0.00000 -0.00000 -0.00000 2.02747

A54 2.04235 -0.00000 -0.00000 0.00000 -0.00000 2.04234

A55 2.18491 0.00000 0.00000 0.00000 0.00001 2.18491

A56 2.19937 -0.00000 -0.00000 -0.00000 -0.00000 2.19936

A57 1.89891 -0.00000 -0.00000 0.00000 -0.00000 1.89891

A58 1.87113 0.00000 0.00000 -0.00000 0.00000 1.87113

A59 2.18744 0.00000 0.00000 0.00000 0.00000 2.18744

A60 2.22462 -0.00000 -0.00000 -0.00000 -0.00000 2.22462

A61 1.87113 0.00000 0.00000 -0.00000 0.00000 1.87113

A62 2.22462 -0.00000 -0.00000 -0.00000 -0.00000 2.22462

A63 2.18744 0.00000 0.00000 0.00000 0.00000 2.18744

A64 1.89891 -0.00000 -0.00000 0.00000 -0.00000 1.89891

A65 2.18491 0.00000 0.00000 0.00000 0.00001 2.18491

A66 2.19937 -0.00000 -0.00000 -0.00000 -0.00000 2.19936

A67 1.88469 0.00000 0.00001 -0.00000 0.00001 1.88470

A68 2.19925 -0.00000 -0.00000 -0.00000 -0.00000 2.19924

A69 2.19925 -0.00000 -0.00000 0.00000 -0.00000 2.19924

A70 1.57080 0.00000 -0.00000 -0.00000 0.00000 1.57080

A71 1.57080 0.00000 -0.00000 -0.00000 0.00000 1.57080

A72 1.57080 0.00000 -0.00000 0.00000 0.00000 1.57080

A73 1.57080 0.00000 -0.00000 0.00000 0.00000 1.57080

A74 2.21336 0.00000 0.00001 0.00000 0.00001 2.21337

A75 2.02748 -0.00000 -0.00000 -0.00000 -0.00000 2.02747

A76 2.04235 -0.00000 -0.00000 0.00000 -0.00000 2.04234

A77 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

A78 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

A79 3.12421 0.00000 0.00000 -0.00000 -0.00000 3.12421

A80 3.15898 -0.00000 -0.00000 0.00000 0.00000 3.15898

A81 3.14713 0.00000 0.00000 0.00000 0.00000 3.14713

A82 3.14713 0.00000 0.00000 0.00000 0.00000 3.14713

A83 3.15898 -0.00000 -0.00000 0.00000 0.00000 3.15898

A84 3.14713 0.00000 0.00000 0.00000 0.00000 3.14713

A85 3.12421 0.00000 0.00000 -0.00000 -0.00000 3.12421

A86 3.14713 0.00000 0.00000 0.00000 0.00000 3.14713

A87 3.14167 -0.00000 -0.00007 0.00000 -0.00007 3.14160

A88 3.14152 0.00000 0.00007 0.00000 0.00007 3.14159

A89 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

A90 3.14159 -0.00000 -0.00000 -0.00000 -0.00000 3.14159

A91 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

A92 3.14159 -0.00000 -0.00000 0.00000 0.00000 3.14159

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 -3.14155 -0.00000 -0.00004 0.00000 -0.00004 -3.14159

D11 -3.14159 -0.00000 -0.00000 -0.00000 -0.00000 3.14159

D12 0.00004 -0.00000 -0.00004 -0.00000 -0.00004 0.00000

D13 -3.14158 -0.00000 -0.00001 -0.00000 -0.00001 3.14159

D14 0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000

D15 0.00000 -0.00000 -0.00000 0.00000 -0.00000 -0.00000

D16 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

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 3.14155 0.00000 0.00004 -0.00000 0.00004 3.14159

D20 -0.00004 0.00000 0.00004 0.00000 0.00004 -0.00000

D21 -3.14158 -0.00000 -0.00001 -0.00000 -0.00002 3.14159

D22 -0.00006 0.00000 0.00006 0.00000 0.00006 -0.00000

D23 0.00006 -0.00000 -0.00006 -0.00000 -0.00006 0.00000

D24 3.14158 0.00000 0.00001 0.00000 0.00002 -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 -0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D30 -3.14159 -0.00000 0.00000 -0.00000 -0.00000 -3.14159

D31 3.14158 0.00000 0.00001 0.00000 0.00001 -3.14159

D32 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D33 0.00000 -0.00000 -0.00000 0.00000 -0.00000 -0.00000

D34 -3.14158 -0.00000 -0.00001 0.00000 -0.00001 3.14159

D35 -3.14159 0.00000 -0.00000 0.00000 -0.00000 3.14159

D36 0.00000 -0.00000 -0.00001 0.00000 -0.00000 -0.00000

D37 -3.14159 -0.00000 -0.00000 0.00000 -0.00000 -3.14159

D38 0.00004 -0.00000 -0.00004 -0.00000 -0.00004 0.00000

D39 -0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D40 -3.14156 -0.00000 -0.00003 -0.00000 -0.00004 -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 3.14156 0.00000 0.00003 0.00000 0.00004 3.14159

D48 -0.00004 0.00000 0.00004 0.00000 0.00004 -0.00000

D49 -0.00006 0.00000 0.00006 0.00000 0.00006 -0.00000

D50 -3.14158 -0.00000 -0.00002 0.00000 -0.00001 -3.14159

D51 3.14158 0.00000 0.00002 -0.00000 0.00001 3.14159

D52 0.00006 -0.00000 -0.00006 -0.00000 -0.00006 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 3.14158 0.00000 0.00001 -0.00000 0.00001 -3.14159

D60 -0.00000 0.00000 0.00001 -0.00000 0.00000 0.00000

D61 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D62 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D63 -3.14159 -0.00000 -0.00000 0.00000 -0.00000 3.14159

D64 0.00000 -0.00000 0.00000 0.00000 -0.00000 0.00000

D65 3.14158 0.00000 0.00001 -0.00000 0.00001 -3.14159

D66 -0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D67 -0.00000 0.00000 0.00001 -0.00000 0.00000 0.00000

D68 3.14159 -0.00000 0.00000 -0.00000 0.00000 -3.14159

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 -0.00004 0.00000 0.00004 0.00000 0.00004 -0.00000

D75 0.00000 0.00000 -0.00000 -0.00000 -0.00000 -0.00000

D76 3.14156 0.00000 0.00003 0.00000 0.00004 3.14159

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 -3.14159 -0.00000 -0.00000 0.00000 -0.00000 3.14159

D80 0.00000 0.00000 0.00000 -0.00000 -0.00000 0.00000

D81 0.00000 0.00000 -0.00000 -0.00000 -0.00000 -0.00000

D82 3.14159 0.00000 0.00000 -0.00000 0.00000 3.14159

D83 -3.14159 0.00000 -0.00000 0.00000 -0.00000 3.14159

D84 -0.00000 0.00000 0.00000 -0.00000 0.00000 -0.00000

D85 -0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D86 -3.14156 -0.00000 -0.00003 -0.00000 -0.00004 -3.14159

D87 -3.14159 -0.00000 -0.00000 0.00000 -0.00000 -3.14159

D88 0.00004 -0.00000 -0.00004 -0.00000 -0.00004 0.00000

D89 -3.14158 -0.00000 -0.00001 0.00000 -0.00001 3.14159

D90 0.00000 -0.00000 -0.00001 0.00000 -0.00000 -0.00000

D91 0.00000 -0.00000 -0.00000 0.00000 -0.00000 -0.00000

D92 -3.14159 0.00000 -0.00000 0.00000 -0.00000 3.14159

D93 0.00006 -0.00000 -0.00006 -0.00000 -0.00006 0.00000

D94 3.14158 0.00000 0.00002 -0.00000 0.00001 3.14159

D95 -3.14158 -0.00000 -0.00002 0.00000 -0.00001 -3.14159

D96 -0.00006 0.00000 0.00006 0.00000 0.00006 -0.00000

D97 3.14158 0.00000 0.00001 0.00000 0.00001 -3.14159

D98 -0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D99 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D100 -3.14159 -0.00000 0.00000 -0.00000 -0.00000 -3.14159

D101 -3.14159 -0.00000 -0.00000 -0.00000 -0.00000 3.14159

D102 0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000

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 -0.00004 0.00000 0.00004 0.00000 0.00004 -0.00000

D107 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D108 3.14155 0.00000 0.00004 -0.00000 0.00004 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 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D114 3.14159 0.00000 0.00000 0.00000 0.00000 -3.14159

D115 -3.14159 0.00000 -0.00000 0.00000 -0.00000 -3.14159

D116 -0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D117 0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000

D118 -3.14155 -0.00000 -0.00004 0.00000 -0.00004 -3.14159

D119 -3.14159 -0.00000 -0.00000 -0.00000 -0.00000 3.14159

D120 0.00004 -0.00000 -0.00004 -0.00000 -0.00004 0.00000

D121 -3.14158 -0.00000 -0.00001 -0.00000 -0.00001 3.14159

D122 0.00000 -0.00000 -0.00000 -0.00000 -0.00000 -0.00000

D123 0.00000 -0.00000 -0.00000 0.00000 -0.00000 -0.00000

D124 3.14159 0.00000 -0.00000 0.00000 0.00000 3.14159

D125 3.14158 0.00000 0.00001 0.00000 0.00002 -3.14159

D126 0.00006 -0.00000 -0.00006 -0.00000 -0.00006 0.00000

D127 -0.00006 0.00000 0.00006 0.00000 0.00006 -0.00000

D128 -3.14158 -0.00000 -0.00001 -0.00000 -0.00002 3.14159

Item Value Threshold Converged?

Maximum Force 0.000005 0.000450 YES

RMS Force 0.000001 0.000300 YES

Maximum Displacement 0.000166 0.001800 YES

RMS Displacement 0.000013 0.001200 YES

Predicted change in Energy=-9.259935D-10

Optimization completed.

-- Stationary point found.

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! Optimized Parameters !

! (Angstroms and Degrees) !

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! Name Definition Value Derivative Info. !

--------------------------------------------------------------------------------

! R1 R(1,2) 1.4538 -DE/DX = 0.0 !

! R2 R(1,5) 1.3589 -DE/DX = 0.0 !

! R3 R(1,24) 1.0803 -DE/DX = 0.0 !

! R4 R(2,3) 1.3716 -DE/DX = 0.0 !

! R5 R(2,12) 1.4048 -DE/DX = 0.0 !

! R6 R(3,4) 1.3716 -DE/DX = 0.0 !

! R7 R(3,32) 2.0966 -DE/DX = 0.0 !

! R8 R(4,5) 1.4538 -DE/DX = 0.0 !

! R9 R(4,6) 1.4048 -DE/DX = 0.0 !

! R10 R(5,25) 1.0803 -DE/DX = 0.0 !

! R11 R(6,7) 1.4394 -DE/DX = 0.0 !

! R12 R(6,38) 1.4243 -DE/DX = 0.0 !

! R13 R(7,8) 1.3714 -DE/DX = 0.0 !

! R14 R(7,11) 1.427 -DE/DX = 0.0 !

! R15 R(8,9) 1.3714 -DE/DX = 0.0 !

! R16 R(8,32) 2.1012 -DE/DX = 0.0 !

! R17 R(9,10) 1.427 -DE/DX = 0.0 !

! R18 R(9,33) 1.4394 -DE/DX = 0.0 !

! R19 R(10,11) 1.3839 -DE/DX = 0.0 !

! R20 R(10,26) 1.0805 -DE/DX = 0.0 !

! R21 R(11,27) 1.0805 -DE/DX = 0.0 !

! R22 R(12,13) 1.4394 -DE/DX = 0.0 !

! R23 R(12,35) 1.4243 -DE/DX = 0.0 !

! R24 R(13,14) 1.427 -DE/DX = 0.0 !

! R25 R(13,17) 1.3714 -DE/DX = 0.0 !

! R26 R(14,15) 1.3839 -DE/DX = 0.0 !

! R27 R(14,28) 1.0805 -DE/DX = 0.0 !

! R28 R(15,16) 1.427 -DE/DX = 0.0 !

! R29 R(15,29) 1.0805 -DE/DX = 0.0 !

! R30 R(16,17) 1.3714 -DE/DX = 0.0 !

! R31 R(16,18) 1.4394 -DE/DX = 0.0 !

! R32 R(17,32) 2.1012 -DE/DX = 0.0 !

! R33 R(18,19) 1.4048 -DE/DX = 0.0 !

! R34 R(18,40) 1.4243 -DE/DX = 0.0 !

! R35 R(19,20) 1.4538 -DE/DX = 0.0 !

! R36 R(19,23) 1.3716 -DE/DX = 0.0 !

! R37 R(20,21) 1.3589 -DE/DX = 0.0 !

! R38 R(20,30) 1.0803 -DE/DX = 0.0 !

! R39 R(21,22) 1.4538 -DE/DX = 0.0 !

! R40 R(21,31) 1.0803 -DE/DX = 0.0 !

! R41 R(22,23) 1.3716 -DE/DX = 0.0 !

! R42 R(22,33) 1.4048 -DE/DX = 0.0 !

! R43 R(23,32) 2.0966 -DE/DX = 0.0 !

! R44 R(33,34) 1.4243 -DE/DX = 0.0 !

! R45 R(34,36) 1.2084 -DE/DX = 0.0 !

! R46 R(35,37) 1.2084 -DE/DX = 0.0 !

! R47 R(36,43) 1.0668 -DE/DX = 0.0 !

! R48 R(37,45) 1.0668 -DE/DX = 0.0 !

! R49 R(38,39) 1.2084 -DE/DX = 0.0 !

! R50 R(39,44) 1.0668 -DE/DX = 0.0 !

! R51 R(40,41) 1.2084 -DE/DX = 0.0 !

! R52 R(41,42) 1.0668 -DE/DX = 0.0 !

! A1 A(2,1,5) 107.2079 -DE/DX = 0.0 !

! A2 A(2,1,24) 125.3308 -DE/DX = 0.0 !

! A3 A(5,1,24) 127.4613 -DE/DX = 0.0 !

! A4 A(1,2,3) 108.7996 -DE/DX = 0.0 !

! A5 A(1,2,12) 125.186 -DE/DX = 0.0 !

! A6 A(3,2,12) 126.0144 -DE/DX = 0.0 !

! A7 A(2,3,4) 107.9851 -DE/DX = 0.0 !

! A8 A(2,3,32) 126.0075 -DE/DX = 0.0 !

! A9 A(4,3,32) 126.0075 -DE/DX = 0.0 !

! A10 A(3,4,5) 108.7996 -DE/DX = 0.0 !

! A11 A(3,4,6) 126.0144 -DE/DX = 0.0 !

! A12 A(5,4,6) 125.186 -DE/DX = 0.0 !

! A13 A(1,5,4) 107.2079 -DE/DX = 0.0 !

! A14 A(1,5,25) 127.4613 -DE/DX = 0.0 !

! A15 A(4,5,25) 125.3308 -DE/DX = 0.0 !

! A16 A(4,6,7) 126.8163 -DE/DX = 0.0 !

! A17 A(4,6,38) 117.0178 -DE/DX = 0.0 !

! A18 A(7,6,38) 116.1658 -DE/DX = 0.0 !

! A19 A(6,7,8) 124.992 -DE/DX = 0.0 !

! A20 A(6,7,11) 125.7492 -DE/DX = 0.0 !

! A21 A(8,7,11) 109.2588 -DE/DX = 0.0 !

! A22 A(7,8,9) 107.6603 -DE/DX = 0.0 !

! A23 A(7,8,32) 126.1699 -DE/DX = 0.0 !

! A24 A(9,8,32) 126.1699 -DE/DX = 0.0 !

! A25 A(8,9,10) 109.2588 -DE/DX = 0.0 !

! A26 A(8,9,33) 124.992 -DE/DX = 0.0 !

! A27 A(10,9,33) 125.7492 -DE/DX = 0.0 !

! A28 A(9,10,11) 106.911 -DE/DX = 0.0 !

! A29 A(9,10,26) 125.8439 -DE/DX = 0.0 !

! A30 A(11,10,26) 127.245 -DE/DX = 0.0 !

! A31 A(7,11,10) 106.911 -DE/DX = 0.0 !

! A32 A(7,11,27) 125.8439 -DE/DX = 0.0 !

! A33 A(10,11,27) 127.245 -DE/DX = 0.0 !

! A34 A(2,12,13) 126.8163 -DE/DX = 0.0 !

! A35 A(2,12,35) 117.0178 -DE/DX = 0.0 !

! A36 A(13,12,35) 116.1658 -DE/DX = 0.0 !

! A37 A(12,13,14) 125.7492 -DE/DX = 0.0 !

! A38 A(12,13,17) 124.992 -DE/DX = 0.0 !

! A39 A(14,13,17) 109.2588 -DE/DX = 0.0 !

! A40 A(13,14,15) 106.911 -DE/DX = 0.0 !

! A41 A(13,14,28) 125.8439 -DE/DX = 0.0 !

! A42 A(15,14,28) 127.245 -DE/DX = 0.0 !

! A43 A(14,15,16) 106.911 -DE/DX = 0.0 !

! A44 A(14,15,29) 127.245 -DE/DX = 0.0 !

! A45 A(16,15,29) 125.8439 -DE/DX = 0.0 !

! A46 A(15,16,17) 109.2588 -DE/DX = 0.0 !

! A47 A(15,16,18) 125.7492 -DE/DX = 0.0 !

! A48 A(17,16,18) 124.992 -DE/DX = 0.0 !

! A49 A(13,17,16) 107.6603 -DE/DX = 0.0 !

! A50 A(13,17,32) 126.1699 -DE/DX = 0.0 !

! A51 A(16,17,32) 126.1699 -DE/DX = 0.0 !

! A52 A(16,18,19) 126.8163 -DE/DX = 0.0 !

! A53 A(16,18,40) 116.1658 -DE/DX = 0.0 !

! A54 A(19,18,40) 117.0178 -DE/DX = 0.0 !

! A55 A(18,19,20) 125.186 -DE/DX = 0.0 !

! A56 A(18,19,23) 126.0144 -DE/DX = 0.0 !

! A57 A(20,19,23) 108.7996 -DE/DX = 0.0 !

! A58 A(19,20,21) 107.2079 -DE/DX = 0.0 !

! A59 A(19,20,30) 125.3308 -DE/DX = 0.0 !

! A60 A(21,20,30) 127.4613 -DE/DX = 0.0 !

! A61 A(20,21,22) 107.2079 -DE/DX = 0.0 !

! A62 A(20,21,31) 127.4613 -DE/DX = 0.0 !

! A63 A(22,21,31) 125.3308 -DE/DX = 0.0 !

! A64 A(21,22,23) 108.7996 -DE/DX = 0.0 !

! A65 A(21,22,33) 125.186 -DE/DX = 0.0 !

! A66 A(23,22,33) 126.0144 -DE/DX = 0.0 !

! A67 A(19,23,22) 107.9851 -DE/DX = 0.0 !

! A68 A(19,23,32) 126.0075 -DE/DX = 0.0 !

! A69 A(22,23,32) 126.0075 -DE/DX = 0.0 !

! A70 A(3,32,8) 90.0 -DE/DX = 0.0 !

! A71 A(3,32,17) 90.0 -DE/DX = 0.0 !

! A72 A(8,32,23) 90.0 -DE/DX = 0.0 !

! A73 A(17,32,23) 90.0 -DE/DX = 0.0 !

! A74 A(9,33,22) 126.8163 -DE/DX = 0.0 !

! A75 A(9,33,34) 116.1658 -DE/DX = 0.0 !

! A76 A(22,33,34) 117.0178 -DE/DX = 0.0 !

! A77 L(3,32,23,17,-1) 180.0 -DE/DX = 0.0 !

! A78 L(8,32,17,23,-1) 180.0 -DE/DX = 0.0 !

! A79 L(33,34,36,26,-1) 179.0039 -DE/DX = 0.0 !

! A80 L(12,35,37,24,-1) 180.9961 -DE/DX = 0.0 !

! A81 L(34,36,43,26,-1) 180.3172 -DE/DX = 0.0 !

! A82 L(35,37,45,28,-1) 180.3172 -DE/DX = 0.0 !

! A83 L(6,38,39,25,-1) 180.9961 -DE/DX = 0.0 !

! A84 L(38,39,44,27,-1) 180.3172 -DE/DX = 0.0 !

! A85 L(18,40,41,29,-1) 179.0039 -DE/DX = 0.0 !

! A86 L(40,41,42,29,-1) 180.3172 -DE/DX = 0.0 !

! A87 L(3,32,23,17,-2) 180.0043 -DE/DX = 0.0 !

! A88 L(8,32,17,23,-2) 179.9956 -DE/DX = 0.0 !

! A89 L(33,34,36,26,-2) 180.0 -DE/DX = 0.0 !

! A90 L(12,35,37,24,-2) 180.0 -DE/DX = 0.0 !

! A91 L(34,36,43,26,-2) 180.0 -DE/DX = 0.0 !

! A92 L(35,37,45,28,-2) 180.0 -DE/DX = 0.0 !

! A93 L(6,38,39,25,-2) 180.0 -DE/DX = 0.0 !

! A94 L(38,39,44,27,-2) 180.0 -DE/DX = 0.0 !

! A95 L(18,40,41,29,-2) 180.0 -DE/DX = 0.0 !

! A96 L(40,41,42,29,-2) 180.0 -DE/DX = 0.0 !

! D1 D(5,1,2,3) 0.0 -DE/DX = 0.0 !

! D2 D(5,1,2,12) -180.0002 -DE/DX = 0.0 !

! D3 D(24,1,2,3) -179.9999 -DE/DX = 0.0 !

! D4 D(24,1,2,12) -0.0001 -DE/DX = 0.0 !

! D5 D(2,1,5,4) 0.0 -DE/DX = 0.0 !

! D6 D(2,1,5,25) 180.0001 -DE/DX = 0.0 !

! D7 D(24,1,5,4) -180.0001 -DE/DX = 0.0 !

! D8 D(24,1,5,25) 0.0 -DE/DX = 0.0 !

! D9 D(1,2,3,4) 0.0 -DE/DX = 0.0 !

! D10 D(1,2,3,32) -179.9978 -DE/DX = 0.0 !

! D11 D(12,2,3,4) 180.0003 -DE/DX = 0.0 !

! D12 D(12,2,3,32) 0.0024 -DE/DX = 0.0 !

! D13 D(1,2,12,13) 180.0004 -DE/DX = 0.0 !

! D14 D(1,2,12,35) 0.0003 -DE/DX = 0.0 !

! D15 D(3,2,12,13) 0.0002 -DE/DX = 0.0 !

! D16 D(3,2,12,35) 180.0 -DE/DX = 0.0 !

! D17 D(2,3,4,5) 0.0 -DE/DX = 0.0 !

! D18 D(2,3,4,6) -180.0003 -DE/DX = 0.0 !

! D19 D(32,3,4,5) 179.9978 -DE/DX = 0.0 !

! D20 D(32,3,4,6) -0.0024 -DE/DX = 0.0 !

! D21 D(2,3,32,8) 180.0009 -DE/DX = 0.0 !

! D22 D(2,3,32,17) -0.0035 -DE/DX = 0.0 !

! D23 D(4,3,32,8) 0.0035 -DE/DX = 0.0 !

! D24 D(4,3,32,17) -180.0009 -DE/DX = 0.0 !

! D25 D(3,4,5,1) 0.0 -DE/DX = 0.0 !

! D26 D(3,4,5,25) 179.9999 -DE/DX = 0.0 !

! D27 D(6,4,5,1) 180.0002 -DE/DX = 0.0 !

! D28 D(6,4,5,25) 0.0001 -DE/DX = 0.0 !

! D29 D(3,4,6,7) -0.0002 -DE/DX = 0.0 !

! D30 D(3,4,6,38) -180.0 -DE/DX = 0.0 !

! D31 D(5,4,6,7) -180.0004 -DE/DX = 0.0 !

! D32 D(5,4,6,38) -0.0003 -DE/DX = 0.0 !

! D33 D(4,6,7,8) 0.0002 -DE/DX = 0.0 !

! D34 D(4,6,7,11) 180.0004 -DE/DX = 0.0 !

! D35 D(38,6,7,8) 180.0 -DE/DX = 0.0 !

! D36 D(38,6,7,11) 0.0002 -DE/DX = 0.0 !

! D37 D(6,7,8,9) -179.9999 -DE/DX = 0.0 !

! D38 D(6,7,8,32) 0.0023 -DE/DX = 0.0 !

! D39 D(11,7,8,9) -0.0001 -DE/DX = 0.0 !

! D40 D(11,7,8,32) -179.9978 -DE/DX = 0.0 !

! D41 D(6,7,11,10) 179.9998 -DE/DX = 0.0 !

! D42 D(6,7,11,27) -0.0001 -DE/DX = 0.0 !

! D43 D(8,7,11,10) 0.0 -DE/DX = 0.0 !

! D44 D(8,7,11,27) 180.0001 -DE/DX = 0.0 !

! D45 D(7,8,9,10) 0.0001 -DE/DX = 0.0 !

! D46 D(7,8,9,33) 179.9999 -DE/DX = 0.0 !

! D47 D(32,8,9,10) 179.9978 -DE/DX = 0.0 !

! D48 D(32,8,9,33) -0.0023 -DE/DX = 0.0 !

! D49 D(7,8,32,3) -0.0034 -DE/DX = 0.0 !

! D50 D(7,8,32,23) -179.9992 -DE/DX = 0.0 !

! D51 D(9,8,32,3) 179.9992 -DE/DX = 0.0 !

! D52 D(9,8,32,23) 0.0034 -DE/DX = 0.0 !

! D53 D(8,9,10,11) 0.0 -DE/DX = 0.0 !

! D54 D(8,9,10,26) -180.0001 -DE/DX = 0.0 !

! D55 D(33,9,10,11) -179.9998 -DE/DX = 0.0 !

! D56 D(33,9,10,26) 0.0001 -DE/DX = 0.0 !

! D57 D(8,9,33,22) -0.0002 -DE/DX = 0.0 !

! D58 D(8,9,33,34) -180.0 -DE/DX = 0.0 !

! D59 D(10,9,33,22) -180.0004 -DE/DX = 0.0 !

! D60 D(10,9,33,34) -0.0002 -DE/DX = 0.0 !

! D61 D(9,10,11,7) 0.0 -DE/DX = 0.0 !

! D62 D(9,10,11,27) 179.9999 -DE/DX = 0.0 !

! D63 D(26,10,11,7) 180.0001 -DE/DX = 0.0 !

! D64 D(26,10,11,27) 0.0 -DE/DX = 0.0 !

! D65 D(2,12,13,14) -180.0004 -DE/DX = 0.0 !

! D66 D(2,12,13,17) -0.0002 -DE/DX = 0.0 !

! D67 D(35,12,13,14) -0.0002 -DE/DX = 0.0 !

! D68 D(35,12,13,17) -180.0 -DE/DX = 0.0 !

! D69 D(12,13,14,15) -179.9998 -DE/DX = 0.0 !

! D70 D(12,13,14,28) 0.0001 -DE/DX = 0.0 !

! D71 D(17,13,14,15) 0.0 -DE/DX = 0.0 !

! D72 D(17,13,14,28) -180.0001 -DE/DX = 0.0 !

! D73 D(12,13,17,16) 179.9999 -DE/DX = 0.0 !

! D74 D(12,13,17,32) -0.0023 -DE/DX = 0.0 !

! D75 D(14,13,17,16) 0.0001 -DE/DX = 0.0 !

! D76 D(14,13,17,32) 179.9978 -DE/DX = 0.0 !

! D77 D(13,14,15,16) 0.0 -DE/DX = 0.0 !

! D78 D(13,14,15,29) 179.9999 -DE/DX = 0.0 !

! D79 D(28,14,15,16) 180.0001 -DE/DX = 0.0 !

! D80 D(28,14,15,29) 0.0 -DE/DX = 0.0 !

! D81 D(14,15,16,17) 0.0 -DE/DX = 0.0 !

! D82 D(14,15,16,18) 179.9998 -DE/DX = 0.0 !

! D83 D(29,15,16,17) 180.0001 -DE/DX = 0.0 !

! D84 D(29,15,16,18) -0.0001 -DE/DX = 0.0 !

! D85 D(15,16,17,13) -0.0001 -DE/DX = 0.0 !

! D86 D(15,16,17,32) -179.9978 -DE/DX = 0.0 !

! D87 D(18,16,17,13) -179.9999 -DE/DX = 0.0 !

! D88 D(18,16,17,32) 0.0023 -DE/DX = 0.0 !

! D89 D(15,16,18,19) 180.0004 -DE/DX = 0.0 !

! D90 D(15,16,18,40) 0.0002 -DE/DX = 0.0 !

! D91 D(17,16,18,19) 0.0002 -DE/DX = 0.0 !

! D92 D(17,16,18,40) 180.0 -DE/DX = 0.0 !

! D93 D(13,17,32,3) 0.0034 -DE/DX = 0.0 !

! D94 D(13,17,32,23) 179.9992 -DE/DX = 0.0 !

! D95 D(16,17,32,3) -179.9992 -DE/DX = 0.0 !

! D96 D(16,17,32,23) -0.0034 -DE/DX = 0.0 !

! D97 D(16,18,19,20) -180.0004 -DE/DX = 0.0 !

! D98 D(16,18,19,23) -0.0002 -DE/DX = 0.0 !

! D99 D(40,18,19,20) -0.0003 -DE/DX = 0.0 !

! D100 D(40,18,19,23) -180.0 -DE/DX = 0.0 !

! D101 D(18,19,20,21) 180.0002 -DE/DX = 0.0 !

! D102 D(18,19,20,30) 0.0001 -DE/DX = 0.0 !

! D103 D(23,19,20,21) 0.0 -DE/DX = 0.0 !

! D104 D(23,19,20,30) 179.9999 -DE/DX = 0.0 !

! D105 D(18,19,23,22) -180.0003 -DE/DX = 0.0 !

! D106 D(18,19,23,32) -0.0024 -DE/DX = 0.0 !

! D107 D(20,19,23,22) 0.0 -DE/DX = 0.0 !

! D108 D(20,19,23,32) 179.9978 -DE/DX = 0.0 !

! D109 D(19,20,21,22) 0.0 -DE/DX = 0.0 !

! D110 D(19,20,21,31) -180.0001 -DE/DX = 0.0 !

! D111 D(30,20,21,22) 180.0001 -DE/DX = 0.0 !

! D112 D(30,20,21,31) 0.0 -DE/DX = 0.0 !

! D113 D(20,21,22,23) 0.0 -DE/DX = 0.0 !

! D114 D(20,21,22,33) -180.0002 -DE/DX = 0.0 !

! D115 D(31,21,22,23) -179.9999 -DE/DX = 0.0 !

! D116 D(31,21,22,33) -0.0001 -DE/DX = 0.0 !

! D117 D(21,22,23,19) 0.0 -DE/DX = 0.0 !

! D118 D(21,22,23,32) -179.9978 -DE/DX = 0.0 !

! D119 D(33,22,23,19) 180.0003 -DE/DX = 0.0 !

! D120 D(33,22,23,32) 0.0024 -DE/DX = 0.0 !

! D121 D(21,22,33,9) 180.0004 -DE/DX = 0.0 !

! D122 D(21,22,33,34) 0.0003 -DE/DX = 0.0 !

! D123 D(23,22,33,9) 0.0002 -DE/DX = 0.0 !

! D124 D(23,22,33,34) 180.0 -DE/DX = 0.0 !

! D125 D(19,23,32,8) -180.0009 -DE/DX = 0.0 !

! D126 D(19,23,32,17) 0.0035 -DE/DX = 0.0 !

! D127 D(22,23,32,8) -0.0035 -DE/DX = 0.0 !

! D128 D(22,23,32,17) 180.0009 -DE/DX = 0.0 !

--------------------------------------------------------------------------------

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Largest change from initial coordinates is atom 32 0.050 Angstoms.

Leave Link 103 at Wed Jul 31 05:38:56 2019, MaxMem= 4294967296 cpu: 1.1

(Enter /home/kira/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -4.291603 0.679463 -0.024405

2 6 0 -2.902914 1.109543 -0.024397

3 7 0 -2.096563 0.000000 -0.024391

4 6 0 -2.902914 -1.109543 -0.024397

5 6 0 -4.291603 -0.679463 -0.024405

6 6 0 -2.469308 -2.445779 -0.024399

7 6 0 -1.107053 -2.910541 -0.024400

8 7 0 -0.000000 -2.101194 -0.024394

9 6 0 1.107053 -2.910541 -0.024400

10 6 0 0.691944 -4.275881 -0.024411

11 6 0 -0.691944 -4.275881 -0.024411

12 6 0 -2.469308 2.445779 -0.024399

13 6 0 -1.107053 2.910541 -0.024400

14 6 0 -0.691944 4.275881 -0.024411

15 6 0 0.691944 4.275881 -0.024411

16 6 0 1.107053 2.910541 -0.024400

17 7 0 0.000000 2.101194 -0.024394

18 6 0 2.469308 2.445779 -0.024399

19 6 0 2.902914 1.109543 -0.024397

20 6 0 4.291603 0.679463 -0.024405

21 6 0 4.291603 -0.679463 -0.024405

22 6 0 2.902914 -1.109543 -0.024397

23 7 0 2.096563 -0.000000 -0.024391

24 1 0 -5.149124 1.336543 -0.024412

25 1 0 -5.149124 -1.336543 -0.024412

26 1 0 1.345862 -5.135981 -0.024419

27 1 0 -1.345862 -5.135981 -0.024419

28 1 0 -1.345862 5.135981 -0.024419

29 1 0 1.345862 5.135981 -0.024419

30 1 0 5.149124 1.336543 -0.024412

31 1 0 5.149124 -1.336543 -0.024412

32 30 0 -0.000000 0.000000 -0.024313

33 6 0 2.469308 -2.445779 -0.024399

34 6 0 3.476498 -3.452829 -0.024405

35 6 0 -3.476498 3.452829 -0.024405

36 6 0 4.316051 -4.321973 -0.024411

37 6 0 -4.316051 4.321973 -0.024411

38 6 0 -3.476498 -3.452829 -0.024405

39 6 0 -4.316051 -4.321973 -0.024411

40 6 0 3.476498 3.452829 -0.024405

41 6 0 4.316051 4.321973 -0.024411

42 1 0 5.061461 5.085155 -0.024416

43 1 0 5.061461 -5.085155 -0.024416

44 1 0 -5.061461 -5.085155 -0.024416

45 1 0 -5.061461 5.085155 -0.024416

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.453762 0.000000

3 N 2.297797 1.371600 0.000000

4 C 2.264729 2.219085 1.371600 0.000000

5 C 1.358926 2.264729 2.297797 1.453762 0.000000

6 C 3.617720 3.581665 2.474020 1.404828 2.537840

7 C 4.798904 4.402975 3.074146 2.543366 3.888324

8 N 5.113698 4.328480 2.968264 3.067619 4.520970

9 C 6.483334 5.678108 4.328326 4.395843 5.841506

10 C 7.027886 6.475014 5.104796 4.790481 6.145728

11 C 6.124784 5.821613 4.500680 3.861876 5.088395

12 C 2.537840 1.404828 2.474020 3.581665 3.617720

13 C 3.888324 2.543366 3.074146 4.402975 4.798904

14 C 5.088395 3.861876 4.500680 5.821613 6.124784

15 C 6.145728 4.790481 5.104796 6.475014 7.027886

16 C 5.841506 4.395843 4.328326 5.678108 6.483334

17 N 4.520970 3.067619 2.968264 4.328480 5.113698

18 C 6.987831 5.535910 5.179673 6.442133 7.448292

19 C 7.207361 5.805829 5.121119 6.215464 7.413611

20 C 8.583206 7.207361 6.424200 7.413611 8.690115

21 C 8.690115 7.413611 6.424200 7.207361 8.583206

22 C 7.413611 6.215464 5.121119 5.805829 7.207361

23 N 6.424200 5.121119 4.193127 5.121119 6.424200

24 H 1.080322 2.257650 3.332337 3.320962 2.190804

25 H 2.190804 3.320962 3.332337 2.257650 1.080322

26 H 8.099407 7.553718 6.182927 5.853572 7.186206

27 H 6.518956 6.436690 5.190554 4.317015 5.342092

28 H 5.342092 4.317015 5.190554 6.436690 6.518956

29 H 7.186206 5.853572 6.182927 7.553718 8.099407

30 H 9.463565 8.055237 7.367925 8.415382 9.653580

31 H 9.653580 8.415382 7.367925 8.055237 9.463565

32 Zn 4.345058 3.107732 2.096563 3.107732 4.345058

33 C 7.448292 6.442133 5.179673 5.535910 6.987831

34 C 8.798820 7.842967 6.555992 6.796167 8.248330

35 C 2.890667 2.412465 3.718366 4.598286 4.211916

36 C 9.955203 9.034092 7.733115 7.901466 9.346635

37 C 3.642591 3.509510 4.858557 5.612336 5.001496

38 C 4.211916 4.598286 3.718366 2.412465 2.890667

39 C 5.001496 5.612336 4.858557 3.509510 3.642591

40 C 8.248330 6.796167 6.555992 7.842967 8.798820

41 C 9.346635 7.901466 7.733115 9.034092 9.955203

42 H 10.338759 8.901504 8.780440 10.089874 10.986839

43 H 10.986839 10.089874 8.780440 8.901504 10.338759

44 H 5.815798 6.560000 5.886376 4.523806 4.472449

45 H 4.472449 4.523806 5.886376 6.560000 5.815798

6 7 8 9 10

6 C 0.000000

7 C 1.439354 0.000000

8 N 2.493235 1.371353 0.000000

9 C 3.606433 2.214107 1.371353 0.000000

10 C 3.652778 2.258439 2.282116 1.427050 0.000000

11 C 2.551136 1.427050 2.282116 2.258439 1.383889

12 C 4.891558 5.526834 5.174209 6.440537 7.427936

13 C 5.526834 5.821081 5.132548 6.227941 7.408175

14 C 6.952678 7.198401 6.414505 7.408175 8.663013

15 C 7.427936 7.408175 6.414505 7.198401 8.551763

16 C 6.440537 6.227941 5.132548 5.821081 7.198401

17 N 5.174209 5.132548 4.202387 5.132548 6.414505

18 C 6.951062 6.440537 5.174209 5.526834 6.952678

19 C 6.442133 5.678108 4.328480 4.402975 5.821613

20 C 7.448292 6.483334 5.113698 4.798904 6.124784

21 C 6.987831 5.841506 4.520970 3.888324 5.088395

22 C 5.535910 4.395843 3.067619 2.543366 3.861876

23 N 5.179673 4.328326 2.968264 3.074146 4.500680

24 H 4.635447 5.863109 6.191244 7.561578 8.100456

25 H 2.900313 4.337718 5.205590 6.451141 6.538944

26 H 4.668266 3.312005 3.319831 2.238217 1.080453

27 H 2.915359 2.238217 3.319831 3.312005 2.211883

28 H 7.664543 8.050064 7.361253 8.412093 9.629943

29 H 8.487556 8.412093 7.361253 8.050064 9.434551

30 H 8.505672 7.561578 6.191244 5.863109 7.166991

31 H 7.698760 6.451141 5.205590 4.337718 5.339116

32 Zn 3.475531 3.113971 2.101194 3.113971 4.331507

33 C 4.938615 3.606433 2.493235 1.439354 2.551136

34 C 6.030485 4.615519 3.730007 2.430708 2.903645

35 C 5.983979 6.790194 6.552343 7.842284 8.781166

36 C 7.039971 5.603767 4.853880 3.505682 3.624400

37 C 7.015192 7.912453 7.738563 9.039873 9.950031

38 C 1.424283 2.430708 3.730007 4.615519 4.248920

39 C 2.632596 3.505682 4.853880 5.603767 5.008207

40 C 8.375331 7.842284 6.552343 6.790194 8.215029

41 C 9.583504 9.039873 7.738563 7.912453 9.330447

42 H 10.650232 10.098600 8.789881 8.920117 10.330619

43 H 7.979899 6.540606 5.875578 4.512903 4.443827

44 H 3.699401 4.512903 5.875578 6.540606 5.810043

45 H 7.964561 8.920117 8.789881 10.098600 10.987751

11 12 13 14 15

11 C 0.000000

12 C 6.952678 0.000000

13 C 7.198401 1.439354 0.000000

14 C 8.551763 2.551136 1.427050 0.000000

15 C 8.663013 3.652778 2.258439 1.383889 0.000000

16 C 7.408175 3.606433 2.214107 2.258439 1.427050

17 N 6.414505 2.493235 1.371353 2.282116 2.282116

18 C 7.427936 4.938615 3.606433 3.652778 2.551136

19 C 6.475014 5.535910 4.395843 4.790481 3.861876

20 C 7.027886 6.987831 5.841506 6.145728 5.088395

21 C 6.145728 7.448292 6.483334 7.027886 6.124784

22 C 4.790481 6.442133 5.678108 6.475014 5.821613

23 N 5.104796 5.179673 4.328326 5.104796 4.500680

24 H 7.166991 2.900313 4.337718 5.339116 6.538944

25 H 5.339116 4.635447 5.863109 7.166991 8.100456

26 H 2.211883 8.487556 8.412093 9.629943 9.434551

27 H 1.080453 7.664543 8.050064 9.434551 9.629943

28 H 9.434551 2.915359 2.238217 1.080453 2.211883

29 H 9.629943 4.668266 3.312005 2.211883 1.080453

30 H 8.100456 7.698760 6.451141 6.538944 5.339116

31 H 6.538944 8.505672 7.561578 8.100456 7.166991

32 Zn 4.331507 3.475531 3.113971 4.331507 4.331507

33 C 3.652778 6.951062 6.440537 7.427936 6.952678

34 C 4.248920 8.375331 7.842284 8.781166 8.215029

35 C 8.215029 1.424283 2.430708 2.903645 4.248920

36 C 5.008207 9.583504 9.039873 9.950031 9.330447

37 C 9.330447 2.632596 3.505682 3.624400 5.008207

38 C 2.903645 5.983979 6.790194 8.215029 8.781166

39 C 3.624400 7.015192 7.912453 9.330447 9.950031

40 C 8.781166 6.030485 4.615519 4.248920 2.903645

41 C 9.950031 7.039971 5.603767 5.008207 3.624400

42 H 10.987751 7.979899 6.540606 5.810043 4.443827

43 H 5.810043 10.650232 10.098600 10.987751 10.330619

44 H 4.443827 7.964561 8.920117 10.330619 10.987751

45 H 10.330619 3.699401 4.512903 4.443827 5.810043

16 17 18 19 20

16 C 0.000000

17 N 1.371353 0.000000

18 C 1.439354 2.493235 0.000000

19 C 2.543366 3.067619 1.404828 0.000000

20 C 3.888324 4.520970 2.537840 1.453762 0.000000

21 C 4.798904 5.113698 3.617720 2.264729 1.358926

22 C 4.402975 4.328480 3.581665 2.219085 2.264729

23 N 3.074146 2.968264 2.474020 1.371600 2.297797

24 H 6.451141 5.205590 7.698760 8.055237 9.463565

25 H 7.561578 6.191244 8.505672 8.415382 9.653580

26 H 8.050064 7.361253 7.664543 6.436690 6.518956

27 H 8.412093 7.361253 8.487556 7.553718 8.099407

28 H 3.312005 3.319831 4.668266 5.853572 7.186206

29 H 2.238217 3.319831 2.915359 4.317015 5.342092

30 H 4.337718 5.205590 2.900313 2.257650 1.080322

31 H 5.863109 6.191244 4.635447 3.320962 2.190804

32 Zn 3.113971 2.101194 3.475531 3.107732 4.345058

33 C 5.526834 5.174209 4.891558 3.581665 3.617720

34 C 6.790194 6.552343 5.983979 4.598286 4.211916

35 C 4.615519 3.730007 6.030485 6.796167 8.248330

36 C 7.912453 7.738563 7.015192 5.612336 5.001496

37 C 5.603767 4.853880 7.039971 7.901466 9.346635

38 C 7.842284 6.552343 8.375331 7.842967 8.798820

39 C 9.039873 7.738563 9.583504 9.034092 9.955203

40 C 2.430708 3.730007 1.424283 2.412465 2.890667

41 C 3.505682 4.853880 2.632596 3.509510 3.642591

42 H 4.512903 5.875578 3.699401 4.523806 4.472449

43 H 8.920117 8.789881 7.964561 6.560000 5.815798

44 H 10.098600 8.789881 10.650232 10.089874 10.986839

45 H 6.540606 5.875578 7.979899 8.901504 10.338759

21 22 23 24 25

21 C 0.000000

22 C 1.453762 0.000000

23 N 2.297797 1.371600 0.000000

24 H 9.653580 8.415382 7.367925 0.000000

25 H 9.463565 8.055237 7.367925 2.673086 0.000000

26 H 5.342092 4.317015 5.190554 9.169427 7.524664

27 H 7.186206 5.853572 6.182927 7.507221 5.375921

28 H 8.099407 7.553718 6.182927 5.375921 7.507221

29 H 6.518956 6.436690 5.190554 7.524664 9.169427

30 H 2.190804 3.320962 3.332337 10.298247 10.639515

31 H 1.080322 2.257650 3.332337 10.639515 10.298247

32 Zn 4.345058 3.107732 2.096563 5.319758 5.319758

33 C 2.537840 1.404828 2.474020 8.505672 7.698760

34 C 2.890667 2.412465 3.718366 9.866074 8.881442

35 C 8.798820 7.842967 6.555992 2.697470 5.073042

36 C 3.642591 3.509510 4.858557 11.027616 9.924833

37 C 9.955203 9.034092 7.733115 3.099484 5.719511

38 C 8.248330 6.796167 6.555992 5.073042 2.697470

39 C 9.346635 7.901466 7.733115 5.719511 3.099484

40 C 4.211916 4.598286 3.718366 8.881442 9.866074

41 C 5.001496 5.612336 4.858557 9.924833 11.027616

42 H 5.815798 6.560000 5.886376 10.876954 12.062100

43 H 4.472449 4.523806 5.886376 12.062100 10.876954

44 H 10.338759 8.901504 8.780440 6.422296 3.749637

45 H 10.986839 10.089874 8.780440 3.749637 6.422296

26 27 28 29 30

26 H 0.000000

27 H 2.691723 0.000000

28 H 10.618784 10.271962 0.000000

29 H 10.271962 10.618784 2.691723 0.000000

30 H 7.507221 9.169427 7.524664 5.375921 0.000000

31 H 5.375921 7.524664 9.169427 7.507221 2.673086

32 Zn 5.309392 5.309392 5.309392 5.309392 5.319758

33 C 2.915359 4.668266 8.487556 7.664543 4.635447

34 C 2.715255 5.107656 9.850015 8.849139 5.073042

35 C 9.850015 8.849139 2.715255 5.107656 8.881442

36 C 3.079713 5.720128 11.023164 9.913370 5.719511

37 C 11.023164 9.913370 3.079713 5.720128 9.924833

38 C 5.107656 2.715255 8.849139 9.850015 9.866074

39 C 5.720128 3.079713 9.913370 11.023164 11.027616

40 C 8.849139 9.850015 5.107656 2.715255 2.697470

41 C 9.913370 11.023164 5.720128 3.079713 3.099484

42 H 10.875537 12.063391 6.407524 3.715947 3.749637

43 H 3.715947 6.407524 12.063391 10.875537 6.422296

44 H 6.407524 3.715947 10.875537 12.063391 12.062100

45 H 12.063391 10.875537 3.715947 6.407524 10.876954

31 32 33 34 35

31 H 0.000000

32 Zn 5.319758 0.000000

33 C 2.900313 3.475531 0.000000

34 C 2.697470 4.899802 1.424283 0.000000

35 C 9.866074 4.899802 8.375331 9.799605 0.000000

36 C 3.099484 6.108006 2.632596 1.208412 11.007786

37 C 11.027616 6.108006 9.583504 11.007786 1.208412

38 C 8.881442 4.899802 6.030485 6.952995 6.905658

39 C 9.924833 6.108006 7.039971 7.840869 7.819999

40 C 5.073042 4.899802 5.983979 6.905658 6.952995

41 C 5.719511 6.108006 7.015192 7.819999 7.840869

42 H 6.422296 7.174761 7.964561 8.683852 8.692596

43 H 3.749637 7.174761 3.699401 2.275214 12.074515

44 H 10.876954 7.174761 7.979899 8.692596 8.683852

45 H 12.062100 7.174761 10.650232 12.074515 2.275214

36 37 38 39 40

36 C 0.000000

37 C 12.216013 0.000000

38 C 7.840869 7.819999 0.000000

39 C 8.632102 8.643945 1.208412 0.000000

40 C 7.819999 7.840869 9.799605 11.007786 0.000000

41 C 8.643945 8.632102 11.007786 12.216013 1.208412

42 H 9.436614 9.408516 12.074515 13.282763 2.275214

43 H 1.066810 13.282763 8.692596 9.408516 8.683852

44 H 9.408516 9.436614 2.275214 1.066810 12.074515

45 H 13.282763 1.066810 8.683852 9.436614 8.692596

41 42 43 44 45

41 C 0.000000

42 H 1.066810 0.000000

43 H 9.436614 10.170310 0.000000

44 H 13.282763 14.349522 10.122923 0.000000

45 H 9.408516 10.122923 14.349522 10.170310 0.000000

Stoichiometry C28H12N4Zn(1-,2)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C28H12)]

Deg. of freedom 34

Full point group C2V NOp 4

RotChk: IX=0 Diff= 8.72D-14

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 0.679463 4.291603 -0.000014

2 6 0 1.109543 2.902914 -0.000005

3 7 0 0.000000 2.096563 0.000000

4 6 0 -1.109543 2.902914 -0.000005

5 6 0 -0.679463 4.291603 -0.000014

6 6 0 -2.445779 2.469308 -0.000007

7 6 0 -2.910541 1.107053 -0.000008

8 7 0 -2.101194 0.000000 -0.000002

9 6 0 -2.910541 -1.107053 -0.000008

10 6 0 -4.275881 -0.691944 -0.000019

11 6 0 -4.275881 0.691944 -0.000019

12 6 0 2.445779 2.469308 -0.000007

13 6 0 2.910541 1.107053 -0.000008

14 6 0 4.275881 0.691944 -0.000019

15 6 0 4.275881 -0.691944 -0.000019

16 6 0 2.910541 -1.107053 -0.000008

17 7 0 2.101194 -0.000000 -0.000002

18 6 0 2.445779 -2.469308 -0.000007

19 6 0 1.109543 -2.902914 -0.000005

20 6 0 0.679463 -4.291603 -0.000014

21 6 0 -0.679463 -4.291603 -0.000014

22 6 0 -1.109543 -2.902914 -0.000005

23 7 0 -0.000000 -2.096563 0.000000

24 1 0 1.336543 5.149124 -0.000021

25 1 0 -1.336543 5.149124 -0.000021

26 1 0 -5.135981 -1.345862 -0.000028

27 1 0 -5.135981 1.345862 -0.000028

28 1 0 5.135981 1.345862 -0.000028

29 1 0 5.135981 -1.345862 -0.000028

30 1 0 1.336543 -5.149124 -0.000021

31 1 0 -1.336543 -5.149124 -0.000021

32 30 0 0.000000 0.000000 0.000079

33 6 0 -2.445779 -2.469308 -0.000007

34 6 0 -3.452829 -3.476498 -0.000013

35 6 0 3.452829 3.476498 -0.000013

36 6 0 -4.321973 -4.316051 -0.000019

37 6 0 4.321973 4.316051 -0.000019

38 6 0 -3.452829 3.476498 -0.000013

39 6 0 -4.321973 4.316051 -0.000019

40 6 0 3.452829 -3.476498 -0.000013

41 6 0 4.321973 -4.316051 -0.000019

42 1 0 5.085155 -5.061461 -0.000025

43 1 0 -5.085155 -5.061461 -0.000025

44 1 0 -5.085155 5.061461 -0.000025

45 1 0 5.085155 5.061461 -0.000025

---------------------------------------------------------------------

Rotational constants (GHZ): 0.1459412 0.1453120 0.0728130

Leave Link 202 at Wed Jul 31 05:38:56 2019, MaxMem= 4294967296 cpu: 0.1

(Enter /home/kira/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 1 IROHF=0.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Population analysis using the SCF density.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Orbital symmetries:

Alpha Orbitals:

Occupied (B2) (A1) (B1) (A1) (B2) (A1) (A2) (B1) (A2) (B1)

(B2) (A1) (B1) (A1) (A2) (B2) (A2) (B1) (B2) (A1)

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(B2) (A1) (A1) (B1) (B2)

Beta Orbitals:

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(B2) (A1) (B1) (A1) (A2) (B2) (A2) (B1) (B2) (A1)

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The electronic state is 2-B2.

Alpha occ. eigenvalues -- -14.29443 -14.29443 -14.29391 -14.29391 -10.20559

Alpha occ. eigenvalues -- -10.20558 -10.20558 -10.20558 -10.19628 -10.19628

Alpha occ. eigenvalues -- -10.19628 -10.19628 -10.19530 -10.19530 -10.19530

Alpha occ. eigenvalues -- -10.19530 -10.17453 -10.17453 -10.17453 -10.17453

Alpha occ. eigenvalues -- -10.16597 -10.16597 -10.16529 -10.16529 -10.16024

Alpha occ. eigenvalues -- -10.16024 -10.16024 -10.16023 -10.15210 -10.15210

Alpha occ. eigenvalues -- -10.15154 -10.15154 -0.95528 -0.94923 -0.94398

Alpha occ. eigenvalues -- -0.93748 -0.83320 -0.81539 -0.81243 -0.79546

Alpha occ. eigenvalues -- -0.76265 -0.76131 -0.75308 -0.74891 -0.74176

Alpha occ. eigenvalues -- -0.73443 -0.73410 -0.71625 -0.71321 -0.66483

Alpha occ. eigenvalues -- -0.65787 -0.61276 -0.58788 -0.58130 -0.57696

Alpha occ. eigenvalues -- -0.57296 -0.56531 -0.55817 -0.54728 -0.54696

Alpha occ. eigenvalues -- -0.54459 -0.54123 -0.53957 -0.53855 -0.53435

Alpha occ. eigenvalues -- -0.51771 -0.51270 -0.51250 -0.50807 -0.50185

Alpha occ. eigenvalues -- -0.50106 -0.49074 -0.47956 -0.44193 -0.43312

Alpha occ. eigenvalues -- -0.43311 -0.42809 -0.41668 -0.41501 -0.41485

Alpha occ. eigenvalues -- -0.41128 -0.39928 -0.39726 -0.38756 -0.38465

Alpha occ. eigenvalues -- -0.37247 -0.37174 -0.36799 -0.36704 -0.36303

Alpha occ. eigenvalues -- -0.36124 -0.33149 -0.32938 -0.31475 -0.30909

Alpha occ. eigenvalues -- -0.30634 -0.28641 -0.28293 -0.28255 -0.27936

Alpha occ. eigenvalues -- -0.26598 -0.25980 -0.25702 -0.25642 -0.25190

Alpha occ. eigenvalues -- -0.24240 -0.23911 -0.23516 -0.20393 -0.19168

Alpha occ. eigenvalues -- -0.12988

Alpha virt. eigenvalues -- -0.09155 -0.05420 0.03213 0.03719 0.03963

Alpha virt. eigenvalues -- 0.04103 0.04422 0.04481 0.04633 0.05014

Alpha virt. eigenvalues -- 0.05082 0.05243 0.06000 0.06100 0.06122

Alpha virt. eigenvalues -- 0.06218 0.06256 0.07571 0.08225 0.08787

Alpha virt. eigenvalues -- 0.08822 0.08856 0.10090 0.10194 0.10302

Alpha virt. eigenvalues -- 0.10375 0.11887 0.12833 0.13021 0.14031

Alpha virt. eigenvalues -- 0.15145 0.16750 0.17439 0.17462 0.17559

Alpha virt. eigenvalues -- 0.18239 0.19377 0.20125 0.21017 0.23004

Alpha virt. eigenvalues -- 0.23896 0.24375 0.24865 0.25091 0.25471

Alpha virt. eigenvalues -- 0.25639 0.25770 0.26781 0.26846 0.27420

Alpha virt. eigenvalues -- 0.27539 0.27700 0.29025 0.30662 0.31118

Alpha virt. eigenvalues -- 0.31886 0.32225 0.33366 0.33483 0.33934

Alpha virt. eigenvalues -- 0.36160 0.36307 0.36389 0.36475 0.36487

Alpha virt. eigenvalues -- 0.36880 0.37166 0.37277 0.37364 0.37608

Alpha virt. eigenvalues -- 0.37698 0.39102 0.39489 0.40321 0.40862

Alpha virt. eigenvalues -- 0.41297 0.41298 0.41626 0.42222 0.42378

Alpha virt. eigenvalues -- 0.42497 0.43421 0.43599 0.44090 0.44698

Alpha virt. eigenvalues -- 0.44989 0.45022 0.45085 0.45519 0.45927

Alpha virt. eigenvalues -- 0.45977 0.46496 0.48226 0.48437 0.48771

Alpha virt. eigenvalues -- 0.49145 0.49631 0.49741 0.50194 0.50397

Alpha virt. eigenvalues -- 0.51797 0.52100 0.52342 0.52528 0.52737

Alpha virt. eigenvalues -- 0.53045 0.53179 0.53294 0.55786 0.57336

Alpha virt. eigenvalues -- 0.57428 0.57833 0.58047 0.58337 0.58345

Alpha virt. eigenvalues -- 0.58401 0.58665 0.58685 0.59434 0.59647

Alpha virt. eigenvalues -- 0.61905 0.62806 0.63086 0.63199 0.63531

Alpha virt. eigenvalues -- 0.63738 0.63999 0.64473 0.64758 0.64831

Alpha virt. eigenvalues -- 0.65585 0.65652 0.65962 0.66154 0.66355

Alpha virt. eigenvalues -- 0.69210 0.69369 0.69752 0.69890 0.71159

Alpha virt. eigenvalues -- 0.71181 0.71425 0.71526 0.72670 0.72701

Alpha virt. eigenvalues -- 0.74544 0.74963 0.75167 0.75277 0.75450

Alpha virt. eigenvalues -- 0.75750 0.75761 0.76211 0.76214 0.76425

Alpha virt. eigenvalues -- 0.78121 0.78672 0.79924 0.82194 0.82205

Alpha virt. eigenvalues -- 0.82834 0.82839 0.84036 0.84997 0.85430

Alpha virt. eigenvalues -- 0.86509 0.86678 0.87249 0.89241 0.90858

Alpha virt. eigenvalues -- 0.91278 0.92000 0.92105 0.93599 0.93675

Alpha virt. eigenvalues -- 0.95748 0.96311 0.97133 0.97902 0.98581

Alpha virt. eigenvalues -- 0.98823 1.00380 1.01720 1.01915 1.02032

Alpha virt. eigenvalues -- 1.02196 1.02584 1.02929 1.03039 1.04851

Alpha virt. eigenvalues -- 1.06745 1.07287 1.08307 1.08417 1.08571

Alpha virt. eigenvalues -- 1.08656 1.09379 1.09415 1.12536 1.13299

Alpha virt. eigenvalues -- 1.13332 1.13770 1.13937 1.14058 1.14178

Alpha virt. eigenvalues -- 1.14851 1.15013 1.15145 1.16090 1.16753

Alpha virt. eigenvalues -- 1.17582 1.17857 1.18418 1.18553 1.19406

Alpha virt. eigenvalues -- 1.19678 1.20134 1.20408 1.20414 1.22080

Alpha virt. eigenvalues -- 1.22556 1.22760 1.22942 1.23066 1.24943

Alpha virt. eigenvalues -- 1.25948 1.26083 1.26110 1.27336 1.27431

Alpha virt. eigenvalues -- 1.27600 1.28499 1.29199 1.30696 1.32968

Alpha virt. eigenvalues -- 1.33132 1.34687 1.34959 1.35448 1.38195

Alpha virt. eigenvalues -- 1.43886 1.46404 1.46521 1.48898 1.48957

Alpha virt. eigenvalues -- 1.49036 1.49089 1.50471 1.53708 1.53795

Alpha virt. eigenvalues -- 1.53958 1.56167 1.56304 1.56310 1.56314

Alpha virt. eigenvalues -- 1.56315 1.56398 1.58417 1.58715 1.58771

Alpha virt. eigenvalues -- 1.58957 1.59647 1.59972 1.60182 1.60650

Alpha virt. eigenvalues -- 1.61603 1.61988 1.62190 1.63431 1.63746

Alpha virt. eigenvalues -- 1.64437 1.65993 1.66008 1.66111 1.66484

Alpha virt. eigenvalues -- 1.67126 1.67430 1.71269 1.71367 1.73066

Alpha virt. eigenvalues -- 1.74386 1.75067 1.76770 1.77832 1.77867

Alpha virt. eigenvalues -- 1.77879 1.79982 1.80348 1.80805 1.81094

Alpha virt. eigenvalues -- 1.81097 1.81591 1.82066 1.82334 1.84774

Alpha virt. eigenvalues -- 1.85701 1.87144 1.88245 1.88942 1.89047

Alpha virt. eigenvalues -- 1.89857 1.89920 1.89926 1.91099 1.91276

Alpha virt. eigenvalues -- 1.91635 1.92196 1.94306 1.95671 1.95693

Alpha virt. eigenvalues -- 1.95761 1.95973 1.96182 1.96872 1.97382

Alpha virt. eigenvalues -- 1.98323 1.98496 2.00585 2.00809 2.02197

Alpha virt. eigenvalues -- 2.04230 2.04579 2.05216 2.05540 2.05945

Alpha virt. eigenvalues -- 2.10334 2.11059 2.13042 2.13245 2.15093

Alpha virt. eigenvalues -- 2.19020 2.20702 2.27596 2.27736 2.28698

Alpha virt. eigenvalues -- 2.29172 2.29692 2.32587 2.32621 2.34617

Alpha virt. eigenvalues -- 2.34881 2.35576 2.37019 2.37394 2.37520

Alpha virt. eigenvalues -- 2.38145 2.38577 2.41617 2.41699 2.41943

Alpha virt. eigenvalues -- 2.42084 2.42302 2.42582 2.44562 2.46761

Alpha virt. eigenvalues -- 2.49421 2.49442 2.50402 2.50692 2.53253

Alpha virt. eigenvalues -- 2.54573 2.55022 2.55062 2.57159 2.57525

Alpha virt. eigenvalues -- 2.58142 2.58539 2.58939 2.59116 2.59275

Alpha virt. eigenvalues -- 2.60938 2.61679 2.62914 2.63801 2.63862

Alpha virt. eigenvalues -- 2.65747 2.65897 2.66166 2.67886 2.68413

Alpha virt. eigenvalues -- 2.72131 2.72281 2.74661 2.77992 2.78679

Alpha virt. eigenvalues -- 2.79110 2.81405 2.82153 2.83698 2.84290

Alpha virt. eigenvalues -- 2.84451 2.85676 2.88066 2.88520 2.89489

Alpha virt. eigenvalues -- 2.89517 2.89532 2.89554 2.92878 2.96401

Alpha virt. eigenvalues -- 2.96511 2.96923 2.97142 2.97387 2.98468

Alpha virt. eigenvalues -- 2.98726 2.99749 2.99853 3.00833 3.01695

Alpha virt. eigenvalues -- 3.02653 3.03708 3.05243 3.05327 3.05708

Alpha virt. eigenvalues -- 3.05821 3.06729 3.06974 3.08331 3.09243

Alpha virt. eigenvalues -- 3.09585 3.09859 3.10614 3.18089 3.18350

Alpha virt. eigenvalues -- 3.19989 3.20152 3.20537 3.22036 3.22398

Alpha virt. eigenvalues -- 3.24282 3.26386 3.26724 3.27624 3.29313

Alpha virt. eigenvalues -- 3.31311 3.31462 3.32110 3.32149 3.33495

Alpha virt. eigenvalues -- 3.33503 3.35064 3.36254 3.36801 3.38906

Alpha virt. eigenvalues -- 3.39045 3.45993 3.49545 3.53020 3.53187

Alpha virt. eigenvalues -- 3.53971 3.57428 3.57970 3.58446 3.59267

Alpha virt. eigenvalues -- 3.60698 3.64367 3.66547 3.66607 3.83091

Alpha virt. eigenvalues -- 3.83334 3.84354 3.85293 3.85978 3.86382

Alpha virt. eigenvalues -- 3.87240 3.91215 3.93768 3.95741 3.97901

Alpha virt. eigenvalues -- 4.01016 4.12862 4.22258 4.22840 4.33772

Alpha virt. eigenvalues -- 4.34191 4.48025 4.53207 4.53767 4.62354

Alpha virt. eigenvalues -- 4.67379 4.67664 4.67765 5.15793 5.20391

Alpha virt. eigenvalues -- 5.20676 5.32503 7.77723 7.77790 7.88521

Alpha virt. eigenvalues -- 7.94219 8.14181 11.11736 23.27992 23.33199

Alpha virt. eigenvalues -- 23.33485 23.36237 23.53113 23.55307 23.58478

Alpha virt. eigenvalues -- 23.59339 23.76509 23.77980 23.78986 23.80931

Alpha virt. eigenvalues -- 23.89735 23.90942 23.97434 23.97791 24.02111

Alpha virt. eigenvalues -- 24.02399 24.04575 24.04635 24.11375 24.11378

Alpha virt. eigenvalues -- 24.14647 24.14860 24.94431 24.94489 24.94803

Alpha virt. eigenvalues -- 24.94815 35.63760 35.65222 35.66541 35.66565

Beta occ. eigenvalues -- -14.29437 -14.29436 -14.29283 -14.29282 -10.20595

Beta occ. eigenvalues -- -10.20595 -10.20594 -10.20594 -10.19487 -10.19487

Beta occ. eigenvalues -- -10.19487 -10.19487 -10.19413 -10.19412 -10.19412

Beta occ. eigenvalues -- -10.19412 -10.17486 -10.17486 -10.17486 -10.17486

Beta occ. eigenvalues -- -10.16603 -10.16603 -10.16535 -10.16535 -10.15957

Beta occ. eigenvalues -- -10.15957 -10.15957 -10.15957 -10.15115 -10.15115

Beta occ. eigenvalues -- -10.15057 -10.15057 -0.95375 -0.94781 -0.94232

Beta occ. eigenvalues -- -0.93598 -0.83067 -0.81332 -0.80977 -0.79347

Beta occ. eigenvalues -- -0.76183 -0.76052 -0.75130 -0.74683 -0.74083

Beta occ. eigenvalues -- -0.73335 -0.73244 -0.71417 -0.71109 -0.66076

Beta occ. eigenvalues -- -0.65735 -0.61073 -0.58660 -0.58033 -0.57661

Beta occ. eigenvalues -- -0.57139 -0.56490 -0.55796 -0.54697 -0.54691

Beta occ. eigenvalues -- -0.54450 -0.54008 -0.53871 -0.53718 -0.53335

Beta occ. eigenvalues -- -0.51718 -0.51205 -0.51182 -0.50708 -0.50105

Beta occ. eigenvalues -- -0.50018 -0.49013 -0.47865 -0.44089 -0.43222

Beta occ. eigenvalues -- -0.43216 -0.42363 -0.41575 -0.41431 -0.41175

Beta occ. eigenvalues -- -0.40501 -0.39875 -0.39670 -0.38400 -0.38300

Beta occ. eigenvalues -- -0.37168 -0.37036 -0.36716 -0.36674 -0.36064

Beta occ. eigenvalues -- -0.35700 -0.32660 -0.32494 -0.31129 -0.30775

Beta occ. eigenvalues -- -0.30607 -0.28612 -0.28258 -0.28221 -0.27899

Beta occ. eigenvalues -- -0.26181 -0.25517 -0.25292 -0.25264 -0.25099

Beta occ. eigenvalues -- -0.23481 -0.23447 -0.23202 -0.19418 -0.17973

Beta virt. eigenvalues -- -0.09143 -0.08982 -0.04234 0.03304 0.03753

Beta virt. eigenvalues -- 0.03999 0.04129 0.04658 0.04734 0.05062

Beta virt. eigenvalues -- 0.05230 0.05271 0.05403 0.06121 0.06230

Beta virt. eigenvalues -- 0.06251 0.06579 0.06956 0.08098 0.08248

Beta virt. eigenvalues -- 0.08811 0.08854 0.08888 0.10107 0.10208

Beta virt. eigenvalues -- 0.10337 0.10415 0.11911 0.12836 0.13082

Beta virt. eigenvalues -- 0.14066 0.15537 0.16806 0.18053 0.18111

Beta virt. eigenvalues -- 0.18160 0.18309 0.19423 0.20194 0.21120

Beta virt. eigenvalues -- 0.23279 0.24060 0.24485 0.24937 0.25154

Beta virt. eigenvalues -- 0.25549 0.25690 0.25859 0.26848 0.26970

Beta virt. eigenvalues -- 0.27585 0.27661 0.27807 0.29101 0.30851

Beta virt. eigenvalues -- 0.31200 0.31970 0.32302 0.33424 0.33533

Beta virt. eigenvalues -- 0.33999 0.36326 0.36475 0.36518 0.36661

Beta virt. eigenvalues -- 0.36726 0.37055 0.37219 0.37407 0.37517

Beta virt. eigenvalues -- 0.37639 0.37860 0.39216 0.39641 0.40462

Beta virt. eigenvalues -- 0.41035 0.41313 0.41550 0.41862 0.42322

Beta virt. eigenvalues -- 0.42635 0.42691 0.43599 0.43679 0.44190

Beta virt. eigenvalues -- 0.44909 0.45121 0.45226 0.45305 0.45606

Beta virt. eigenvalues -- 0.46023 0.46246 0.46595 0.48342 0.48686

Beta virt. eigenvalues -- 0.48968 0.49326 0.49903 0.49951 0.50293

Beta virt. eigenvalues -- 0.50493 0.51932 0.52159 0.52524 0.52592

Beta virt. eigenvalues -- 0.52968 0.53168 0.53254 0.53360 0.55955

Beta virt. eigenvalues -- 0.57492 0.57557 0.57918 0.58121 0.58420

Beta virt. eigenvalues -- 0.58522 0.58667 0.58738 0.58790 0.59558

Beta virt. eigenvalues -- 0.59695 0.61989 0.62824 0.63252 0.63402

Beta virt. eigenvalues -- 0.63603 0.63793 0.64023 0.64551 0.64842

Beta virt. eigenvalues -- 0.64909 0.65678 0.65690 0.66051 0.66340

Beta virt. eigenvalues -- 0.66371 0.69224 0.69486 0.69770 0.69965

Beta virt. eigenvalues -- 0.71255 0.71264 0.71612 0.71820 0.72754

Beta virt. eigenvalues -- 0.72758 0.74594 0.75222 0.75337 0.75364

Beta virt. eigenvalues -- 0.75496 0.75817 0.75852 0.76294 0.76327

Beta virt. eigenvalues -- 0.76519 0.78181 0.78896 0.80270 0.82216

Beta virt. eigenvalues -- 0.82327 0.82875 0.82899 0.84133 0.85035

Beta virt. eigenvalues -- 0.85561 0.86592 0.86719 0.87429 0.89332

Beta virt. eigenvalues -- 0.90944 0.91327 0.92142 0.92219 0.93698

Beta virt. eigenvalues -- 0.93720 0.95816 0.96441 0.97192 0.98188

Beta virt. eigenvalues -- 0.98790 0.98843 1.00473 1.01860 1.02157

Beta virt. eigenvalues -- 1.02300 1.02392 1.02626 1.03002 1.03183

Beta virt. eigenvalues -- 1.04905 1.07051 1.07443 1.08643 1.08724

Beta virt. eigenvalues -- 1.08843 1.08925 1.09429 1.09493 1.12658

Beta virt. eigenvalues -- 1.13375 1.13378 1.14013 1.14158 1.14175

Beta virt. eigenvalues -- 1.14272 1.15007 1.15138 1.15398 1.16210

Beta virt. eigenvalues -- 1.16843 1.17658 1.18069 1.18539 1.18778

Beta virt. eigenvalues -- 1.19550 1.19719 1.20239 1.20495 1.20734

Beta virt. eigenvalues -- 1.22179 1.22825 1.22836 1.23016 1.23121

Beta virt. eigenvalues -- 1.24977 1.26027 1.26217 1.26233 1.27451

Beta virt. eigenvalues -- 1.27511 1.27728 1.28800 1.29311 1.30878

Beta virt. eigenvalues -- 1.33238 1.33316 1.34817 1.35093 1.35572

Beta virt. eigenvalues -- 1.38255 1.44002 1.46495 1.46582 1.49063

Beta virt. eigenvalues -- 1.49169 1.49233 1.49321 1.50727 1.53857

Beta virt. eigenvalues -- 1.53874 1.54000 1.56311 1.56412 1.56430

Beta virt. eigenvalues -- 1.56437 1.56438 1.56443 1.58709 1.58824

Beta virt. eigenvalues -- 1.58845 1.59128 1.59762 1.60029 1.60230

Beta virt. eigenvalues -- 1.60781 1.61808 1.62214 1.62255 1.63603

Beta virt. eigenvalues -- 1.63826 1.64775 1.66043 1.66076 1.66237

Beta virt. eigenvalues -- 1.66524 1.67288 1.67650 1.71302 1.71508

Beta virt. eigenvalues -- 1.73168 1.74543 1.75164 1.77011 1.77922

Beta virt. eigenvalues -- 1.77957 1.77975 1.80283 1.80577 1.80843

Beta virt. eigenvalues -- 1.81154 1.81380 1.81685 1.82263 1.82340

Beta virt. eigenvalues -- 1.84801 1.85951 1.87222 1.88533 1.89105

Beta virt. eigenvalues -- 1.89133 1.90146 1.90151 1.90281 1.91272

Beta virt. eigenvalues -- 1.91494 1.91931 1.92267 1.94581 1.95903

Beta virt. eigenvalues -- 1.95975 1.96022 1.96129 1.96365 1.97081

Beta virt. eigenvalues -- 1.97660 1.98508 1.98511 2.00664 2.00858

Beta virt. eigenvalues -- 2.02460 2.04384 2.04797 2.05438 2.05654

Beta virt. eigenvalues -- 2.06429 2.10430 2.11127 2.13076 2.13582

Beta virt. eigenvalues -- 2.15120 2.19143 2.20764 2.27904 2.28044

Beta virt. eigenvalues -- 2.28790 2.29186 2.29917 2.32835 2.32877

Beta virt. eigenvalues -- 2.34863 2.34974 2.35613 2.37268 2.37474

Beta virt. eigenvalues -- 2.37752 2.38504 2.38613 2.41621 2.41729

Beta virt. eigenvalues -- 2.41986 2.42110 2.42428 2.42661 2.44650

Beta virt. eigenvalues -- 2.47063 2.49443 2.49613 2.50466 2.50824

Beta virt. eigenvalues -- 2.53543 2.54837 2.55298 2.55309 2.57268

Beta virt. eigenvalues -- 2.57866 2.58241 2.58774 2.59064 2.59147

Beta virt. eigenvalues -- 2.59653 2.61011 2.61850 2.62970 2.64052

Beta virt. eigenvalues -- 2.64176 2.65753 2.65933 2.66464 2.68128

Beta virt. eigenvalues -- 2.68587 2.72187 2.72326 2.74736 2.78254

Beta virt. eigenvalues -- 2.78881 2.79321 2.81585 2.82387 2.83910

Beta virt. eigenvalues -- 2.84337 2.84824 2.86048 2.88106 2.88574

Beta virt. eigenvalues -- 2.89625 2.89635 2.89649 2.89665 2.92934

Beta virt. eigenvalues -- 2.96603 2.96682 2.96991 2.97203 2.97933

Beta virt. eigenvalues -- 2.98722 2.99039 2.99740 2.99837 3.00853

Beta virt. eigenvalues -- 3.02046 3.02712 3.03720 3.05674 3.05763

Beta virt. eigenvalues -- 3.05867 3.05901 3.06783 3.07049 3.08403

Beta virt. eigenvalues -- 3.09656 3.09780 3.09906 3.10666 3.18102

Beta virt. eigenvalues -- 3.18382 3.20015 3.20197 3.20616 3.22068

Beta virt. eigenvalues -- 3.22430 3.24372 3.26477 3.26785 3.27678

Beta virt. eigenvalues -- 3.29379 3.31390 3.31507 3.32167 3.32192

Beta virt. eigenvalues -- 3.33538 3.33573 3.35132 3.36284 3.36890

Beta virt. eigenvalues -- 3.39011 3.39081 3.46080 3.49622 3.53073

Beta virt. eigenvalues -- 3.53227 3.54018 3.57430 3.58031 3.58452

Beta virt. eigenvalues -- 3.59430 3.60834 3.64441 3.66598 3.66689

Beta virt. eigenvalues -- 3.83194 3.83505 3.84352 3.85351 3.86274

Beta virt. eigenvalues -- 3.86641 3.87510 3.91496 3.93870 3.95882

Beta virt. eigenvalues -- 3.98021 4.01141 4.13028 4.22416 4.23013

Beta virt. eigenvalues -- 4.33929 4.34328 4.48102 4.53259 4.54001

Beta virt. eigenvalues -- 4.62485 4.67556 4.67821 4.67842 5.15897

Beta virt. eigenvalues -- 5.20503 5.20771 5.32613 7.77722 7.77816

Beta virt. eigenvalues -- 7.88520 7.94222 8.14185 11.11745 23.28034

Beta virt. eigenvalues -- 23.33233 23.33526 23.36273 23.53144 23.55309

Beta virt. eigenvalues -- 23.58588 23.59416 23.76586 23.78069 23.79046

Beta virt. eigenvalues -- 23.81003 23.89829 23.91039 23.97536 23.97900

Beta virt. eigenvalues -- 24.02197 24.02497 24.04637 24.04704 24.11484

Beta virt. eigenvalues -- 24.11490 24.14640 24.14857 24.94443 24.94502

Beta virt. eigenvalues -- 24.94816 24.94828 35.63805 35.65299 35.66495

Beta virt. eigenvalues -- 35.66734

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 5.169664 0.393327 -0.076885 -0.066234 0.543032 0.012578

2 C 0.393327 4.884226 0.433279 -0.143062 -0.066234 -0.000663

3 N -0.076885 0.433279 6.973606 0.433279 -0.076885 -0.028648

4 C -0.066234 -0.143062 0.433279 4.884226 0.393327 0.429525

5 C 0.543032 -0.066234 -0.076885 0.393327 5.169664 -0.072828

6 C 0.012578 -0.000663 -0.028648 0.429525 -0.072828 5.249313

7 C -0.001110 -0.000419 -0.015658 -0.106838 0.012395 0.389760

8 N 0.000051 0.000356 -0.013107 -0.018537 -0.000323 -0.021553

9 C -0.000005 0.000001 0.000275 -0.000301 0.000041 0.000288

10 C 0.000001 -0.000005 0.000042 -0.001183 -0.000005 0.013914

11 C -0.000006 0.000045 -0.000242 0.013483 -0.000171 -0.077771

12 C -0.072828 0.429525 -0.028648 -0.000663 0.012578 -0.002102

13 C 0.012395 -0.106838 -0.015658 -0.000419 -0.001110 0.000175

14 C -0.000171 0.013483 -0.000242 0.000045 -0.000006 0.000001

15 C -0.000005 -0.001183 0.000042 -0.000005 0.000001 -0.000000

16 C 0.000041 -0.000301 0.000275 0.000001 -0.000005 0.000001

17 N -0.000323 -0.018537 -0.013107 0.000356 0.000051 -0.000153

18 C 0.000001 0.000191 -0.000145 0.000001 -0.000000 0.000002

19 C -0.000000 -0.000059 0.000157 -0.000004 0.000000 0.000001

20 C -0.000000 -0.000000 0.000001 0.000000 0.000000 -0.000000

21 C 0.000000 0.000000 0.000001 -0.000000 -0.000000 0.000001

22 C 0.000000 -0.000004 0.000157 -0.000059 -0.000000 0.000191

23 N 0.000001 0.000157 -0.001575 0.000157 0.000001 -0.000145

24 H 0.387538 -0.038845 0.005449 0.005823 -0.034650 -0.000199

25 H -0.034650 0.005823 0.005449 -0.038845 0.387538 -0.005436

26 H 0.000000 0.000000 0.000002 0.000010 0.000000 -0.000193

27 H -0.000000 0.000001 0.000000 -0.000040 0.000004 -0.005466

28 H 0.000004 -0.000040 0.000000 0.000001 -0.000000 0.000000

29 H 0.000000 0.000010 0.000002 0.000000 0.000000 0.000000

30 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

31 H 0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.000000

32 Zn 0.002578 -0.014175 0.133189 -0.014175 0.002578 -0.011504

33 C -0.000000 0.000001 -0.000145 0.000191 0.000001 -0.002062

34 C -0.000000 0.000000 -0.000000 0.000002 0.000000 -0.000046

35 C -0.014561 -0.077932 0.003691 -0.000482 0.002545 -0.000051

36 C -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000002

37 C -0.000181 -0.005852 -0.000058 -0.000046 0.000352 -0.000002

38 C 0.002545 -0.000482 0.003691 -0.077932 -0.014561 0.547984

39 C 0.000352 -0.000046 -0.000058 -0.005852 -0.000181 -0.108518

40 C 0.000000 0.000002 -0.000000 0.000000 -0.000000 0.000000

41 C 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

42 H 0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000

43 H -0.000000 0.000000 0.000000 0.000000 0.000000 -0.000000

44 H 0.000002 -0.000000 0.000001 -0.000076 0.000099 0.001954

45 H 0.000099 -0.000076 0.000001 -0.000000 0.000002 -0.000000

7 8 9 10 11 12

1 C -0.001110 0.000051 -0.000005 0.000001 -0.000006 -0.072828

2 C -0.000419 0.000356 0.000001 -0.000005 0.000045 0.429525

3 N -0.015658 -0.013107 0.000275 0.000042 -0.000242 -0.028648

4 C -0.106838 -0.018537 -0.000301 -0.001183 0.013483 -0.000663

5 C 0.012395 -0.000323 0.000041 -0.000005 -0.000171 0.012578

6 C 0.389760 -0.021553 0.000288 0.013914 -0.077771 -0.002102

7 C 4.896946 0.440188 -0.153596 -0.072302 0.444994 0.000175

8 N 0.440188 6.943734 0.440188 -0.084049 -0.084049 -0.000153

9 C -0.153596 0.440188 4.896946 0.444994 -0.072302 0.000001

10 C -0.072302 -0.084049 0.444994 5.216909 0.497364 -0.000000

11 C 0.444994 -0.084049 -0.072302 0.497364 5.216909 0.000001

12 C 0.000175 -0.000153 0.000001 -0.000000 0.000001 5.249313

13 C -0.000050 0.000148 -0.000004 0.000000 -0.000000 0.389760

14 C -0.000000 0.000002 0.000000 0.000000 -0.000000 -0.077771

15 C 0.000000 0.000002 -0.000000 -0.000000 0.000000 0.013914

16 C -0.000004 0.000148 -0.000050 -0.000000 0.000000 0.000288

17 N 0.000148 -0.001459 0.000148 0.000002 0.000002 -0.021553

18 C 0.000001 -0.000153 0.000175 0.000001 -0.000000 -0.002062

19 C 0.000001 0.000356 -0.000419 0.000045 -0.000005 0.000191

20 C -0.000005 0.000051 -0.001110 -0.000006 0.000001 0.000001

21 C 0.000041 -0.000323 0.012395 -0.000171 -0.000005 -0.000000

22 C -0.000301 -0.018537 -0.106838 0.013483 -0.001183 0.000001

23 N 0.000275 -0.013107 -0.015658 -0.000242 0.000042 -0.000145

24 H 0.000008 0.000002 0.000000 0.000000 0.000000 -0.005436

25 H 0.000006 -0.000001 0.000001 -0.000000 0.000002 -0.000199

26 H 0.005525 0.005921 -0.040423 0.389923 -0.036009 0.000000

27 H -0.040423 0.005921 0.005525 -0.036009 0.389923 0.000000

28 H -0.000000 0.000000 -0.000000 0.000000 -0.000000 -0.005466

29 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000193

30 H 0.000000 0.000002 0.000008 0.000000 0.000000 0.000000

31 H 0.000001 -0.000001 0.000006 0.000002 -0.000000 0.000000

32 Zn -0.013668 0.135437 -0.013668 0.002395 0.002395 -0.011504

33 C 0.000288 -0.021553 0.389760 -0.077771 0.013914 0.000002

34 C -0.000398 0.003805 -0.075014 -0.015778 0.002356 0.000000

35 C 0.000002 -0.000000 0.000000 -0.000000 0.000000 0.547984

36 C -0.000047 -0.000060 -0.004798 -0.000350 0.000311 0.000000

37 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.108518

38 C -0.075014 0.003805 -0.000398 0.002356 -0.015778 -0.000051

39 C -0.004798 -0.000060 -0.000047 0.000311 -0.000350 -0.000002

40 C 0.000000 -0.000000 0.000002 0.000000 -0.000000 -0.000046

41 C -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000002

42 H 0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

43 H 0.000000 0.000001 -0.000009 0.000088 0.000001 0.000000

44 H -0.000009 0.000001 0.000000 0.000001 0.000088 -0.000000

45 H 0.000000 0.000000 0.000000 -0.000000 0.000000 0.001954

13 14 15 16 17 18

1 C 0.012395 -0.000171 -0.000005 0.000041 -0.000323 0.000001

2 C -0.106838 0.013483 -0.001183 -0.000301 -0.018537 0.000191

3 N -0.015658 -0.000242 0.000042 0.000275 -0.013107 -0.000145

4 C -0.000419 0.000045 -0.000005 0.000001 0.000356 0.000001

5 C -0.001110 -0.000006 0.000001 -0.000005 0.000051 -0.000000

6 C 0.000175 0.000001 -0.000000 0.000001 -0.000153 0.000002

7 C -0.000050 -0.000000 0.000000 -0.000004 0.000148 0.000001

8 N 0.000148 0.000002 0.000002 0.000148 -0.001459 -0.000153

9 C -0.000004 0.000000 -0.000000 -0.000050 0.000148 0.000175

10 C 0.000000 0.000000 -0.000000 -0.000000 0.000002 0.000001

11 C -0.000000 -0.000000 0.000000 0.000000 0.000002 -0.000000

12 C 0.389760 -0.077771 0.013914 0.000288 -0.021553 -0.002062

13 C 4.896946 0.444994 -0.072302 -0.153596 0.440188 0.000288

14 C 0.444994 5.216909 0.497364 -0.072302 -0.084049 0.013914

15 C -0.072302 0.497364 5.216909 0.444994 -0.084049 -0.077771

16 C -0.153596 -0.072302 0.444994 4.896946 0.440188 0.389760

17 N 0.440188 -0.084049 -0.084049 0.440188 6.943734 -0.021553

18 C 0.000288 0.013914 -0.077771 0.389760 -0.021553 5.249313

19 C -0.000301 -0.001183 0.013483 -0.106838 -0.018537 0.429525

20 C 0.000041 -0.000005 -0.000171 0.012395 -0.000323 -0.072828

21 C -0.000005 0.000001 -0.000006 -0.001110 0.000051 0.012578

22 C 0.000001 -0.000005 0.000045 -0.000419 0.000356 -0.000663

23 N 0.000275 0.000042 -0.000242 -0.015658 -0.013107 -0.028648

24 H 0.000006 0.000002 -0.000000 0.000001 -0.000001 0.000000

25 H 0.000008 0.000000 0.000000 0.000000 0.000002 0.000000

26 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

27 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

28 H -0.040423 0.389923 -0.036009 0.005525 0.005921 -0.000193

29 H 0.005525 -0.036009 0.389923 -0.040423 0.005921 -0.005466

30 H 0.000001 -0.000000 0.000002 0.000006 -0.000001 -0.005436

31 H 0.000000 0.000000 0.000000 0.000008 0.000002 -0.000199

32 Zn -0.013668 0.002395 0.002395 -0.013668 0.135437 -0.011504

33 C 0.000001 -0.000000 0.000001 0.000175 -0.000153 -0.002102

34 C 0.000000 -0.000000 0.000000 0.000002 -0.000000 -0.000051

35 C -0.075014 -0.015778 0.002356 -0.000398 0.003805 -0.000046

36 C -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000002

37 C -0.004798 -0.000350 0.000311 -0.000047 -0.000060 -0.000002

38 C 0.000002 0.000000 -0.000000 0.000000 -0.000000 0.000000

39 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

40 C -0.000398 0.002356 -0.015778 -0.075014 0.003805 0.547984

41 C -0.000047 0.000311 -0.000350 -0.004798 -0.000060 -0.108518

42 H 0.000000 0.000001 0.000088 -0.000009 0.000001 0.001954

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 -0.000009 0.000088 0.000001 0.000000 0.000001 -0.000000

19 20 21 22 23 24

1 C -0.000000 -0.000000 0.000000 0.000000 0.000001 0.387538

2 C -0.000059 -0.000000 0.000000 -0.000004 0.000157 -0.038845

3 N 0.000157 0.000001 0.000001 0.000157 -0.001575 0.005449

4 C -0.000004 0.000000 -0.000000 -0.000059 0.000157 0.005823

5 C 0.000000 0.000000 -0.000000 -0.000000 0.000001 -0.034650

6 C 0.000001 -0.000000 0.000001 0.000191 -0.000145 -0.000199

7 C 0.000001 -0.000005 0.000041 -0.000301 0.000275 0.000008

8 N 0.000356 0.000051 -0.000323 -0.018537 -0.013107 0.000002

9 C -0.000419 -0.001110 0.012395 -0.106838 -0.015658 0.000000

10 C 0.000045 -0.000006 -0.000171 0.013483 -0.000242 0.000000

11 C -0.000005 0.000001 -0.000005 -0.001183 0.000042 0.000000

12 C 0.000191 0.000001 -0.000000 0.000001 -0.000145 -0.005436

13 C -0.000301 0.000041 -0.000005 0.000001 0.000275 0.000006

14 C -0.001183 -0.000005 0.000001 -0.000005 0.000042 0.000002

15 C 0.013483 -0.000171 -0.000006 0.000045 -0.000242 -0.000000

16 C -0.106838 0.012395 -0.001110 -0.000419 -0.015658 0.000001

17 N -0.018537 -0.000323 0.000051 0.000356 -0.013107 -0.000001

18 C 0.429525 -0.072828 0.012578 -0.000663 -0.028648 0.000000

19 C 4.884226 0.393327 -0.066234 -0.143062 0.433279 -0.000000

20 C 0.393327 5.169664 0.543032 -0.066234 -0.076885 -0.000000

21 C -0.066234 0.543032 5.169664 0.393327 -0.076885 0.000000

22 C -0.143062 -0.066234 0.393327 4.884226 0.433279 -0.000000

23 N 0.433279 -0.076885 -0.076885 0.433279 6.973606 0.000000

24 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.440325

25 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.002320

26 H 0.000001 -0.000000 0.000004 -0.000040 0.000000 -0.000000

27 H 0.000000 0.000000 0.000000 0.000010 0.000002 -0.000000

28 H 0.000010 0.000000 0.000000 0.000000 0.000002 -0.000008

29 H -0.000040 0.000004 -0.000000 0.000001 0.000000 -0.000000

30 H -0.038845 0.387538 -0.034650 0.005823 0.005449 -0.000000

31 H 0.005823 -0.034650 0.387538 -0.038845 0.005449 -0.000000

32 Zn -0.014175 0.002578 0.002578 -0.014175 0.133189 -0.000457

33 C -0.000663 0.012578 -0.072828 0.429525 -0.028648 0.000000

34 C -0.000482 0.002545 -0.014561 -0.077932 0.003691 -0.000000

35 C 0.000002 0.000000 -0.000000 0.000000 -0.000000 0.007373

36 C -0.000046 0.000352 -0.000181 -0.005852 -0.000058 -0.000000

37 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.004019

38 C 0.000000 -0.000000 0.000000 0.000002 -0.000000 -0.000086

39 C -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000008

40 C -0.077932 -0.014561 0.002545 -0.000482 0.003691 -0.000000

41 C -0.005852 -0.000181 0.000352 -0.000046 -0.000058 -0.000000

42 H -0.000076 0.000099 0.000002 -0.000000 0.000001 -0.000000

43 H -0.000000 0.000002 0.000099 -0.000076 0.000001 -0.000000

44 H 0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000

45 H 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000073

25 26 27 28 29 30

1 C -0.034650 0.000000 -0.000000 0.000004 0.000000 -0.000000

2 C 0.005823 0.000000 0.000001 -0.000040 0.000010 -0.000000

3 N 0.005449 0.000002 0.000000 0.000000 0.000002 0.000000

4 C -0.038845 0.000010 -0.000040 0.000001 0.000000 -0.000000

5 C 0.387538 0.000000 0.000004 -0.000000 0.000000 0.000000

6 C -0.005436 -0.000193 -0.005466 0.000000 0.000000 0.000000

7 C 0.000006 0.005525 -0.040423 -0.000000 -0.000000 0.000000

8 N -0.000001 0.005921 0.005921 0.000000 0.000000 0.000002

9 C 0.000001 -0.040423 0.005525 -0.000000 -0.000000 0.000008

10 C -0.000000 0.389923 -0.036009 0.000000 -0.000000 0.000000

11 C 0.000002 -0.036009 0.389923 -0.000000 0.000000 0.000000

12 C -0.000199 0.000000 0.000000 -0.005466 -0.000193 0.000000

13 C 0.000008 -0.000000 -0.000000 -0.040423 0.005525 0.000001

14 C 0.000000 0.000000 -0.000000 0.389923 -0.036009 -0.000000

15 C 0.000000 -0.000000 0.000000 -0.036009 0.389923 0.000002

16 C 0.000000 -0.000000 -0.000000 0.005525 -0.040423 0.000006

17 N 0.000002 0.000000 0.000000 0.005921 0.005921 -0.000001

18 C 0.000000 0.000000 0.000000 -0.000193 -0.005466 -0.005436

19 C -0.000000 0.000001 0.000000 0.000010 -0.000040 -0.038845

20 C 0.000000 -0.000000 0.000000 0.000000 0.000004 0.387538

21 C -0.000000 0.000004 0.000000 0.000000 -0.000000 -0.034650

22 C -0.000000 -0.000040 0.000010 0.000000 0.000001 0.005823

23 N 0.000000 0.000000 0.000002 0.000002 0.000000 0.005449

24 H -0.002320 -0.000000 -0.000000 -0.000008 -0.000000 -0.000000

25 H 0.440325 -0.000000 -0.000008 -0.000000 -0.000000 -0.000000

26 H -0.000000 0.454615 -0.001956 -0.000000 -0.000000 -0.000000

27 H -0.000008 -0.001956 0.454615 -0.000000 -0.000000 -0.000000

28 H -0.000000 -0.000000 -0.000000 0.454615 -0.001956 -0.000000

29 H -0.000000 -0.000000 -0.000000 -0.001956 0.454615 -0.000008

30 H -0.000000 -0.000000 -0.000000 -0.000000 -0.000008 0.440325

31 H -0.000000 -0.000008 -0.000000 -0.000000 -0.000000 -0.002320

32 Zn -0.000457 -0.000502 -0.000502 -0.000502 -0.000502 -0.000457

33 C 0.000000 -0.005466 -0.000193 0.000000 0.000000 -0.000199

34 C -0.000000 0.006929 -0.000087 -0.000000 -0.000000 -0.000086

35 C -0.000086 -0.000000 -0.000000 0.006929 -0.000087 -0.000000

36 C -0.000000 0.003684 -0.000010 -0.000000 -0.000000 -0.000008

37 C -0.000008 -0.000000 -0.000000 0.003684 -0.000010 -0.000000

38 C 0.007373 -0.000087 0.006929 -0.000000 -0.000000 -0.000000

39 C 0.004019 -0.000010 0.003684 -0.000000 -0.000000 -0.000000

40 C -0.000000 -0.000000 -0.000000 -0.000087 0.006929 0.007373

41 C -0.000000 -0.000000 -0.000000 -0.000010 0.003684 0.004019

42 H -0.000000 -0.000000 -0.000000 -0.000000 0.000060 0.000073

43 H -0.000000 0.000060 -0.000000 -0.000000 -0.000000 -0.000000

44 H 0.000073 -0.000000 0.000060 -0.000000 -0.000000 -0.000000

45 H -0.000000 -0.000000 -0.000000 0.000060 -0.000000 -0.000000

31 32 33 34 35 36

1 C 0.000000 0.002578 -0.000000 -0.000000 -0.014561 -0.000000

2 C -0.000000 -0.014175 0.000001 0.000000 -0.077932 -0.000000

3 N 0.000000 0.133189 -0.000145 -0.000000 0.003691 0.000000

4 C -0.000000 -0.014175 0.000191 0.000002 -0.000482 0.000000

5 C -0.000000 0.002578 0.000001 0.000000 0.002545 0.000000

6 C 0.000000 -0.011504 -0.002062 -0.000046 -0.000051 -0.000002

7 C 0.000001 -0.013668 0.000288 -0.000398 0.000002 -0.000047

8 N -0.000001 0.135437 -0.021553 0.003805 -0.000000 -0.000060

9 C 0.000006 -0.013668 0.389760 -0.075014 0.000000 -0.004798

10 C 0.000002 0.002395 -0.077771 -0.015778 -0.000000 -0.000350

11 C -0.000000 0.002395 0.013914 0.002356 0.000000 0.000311

12 C 0.000000 -0.011504 0.000002 0.000000 0.547984 0.000000

13 C 0.000000 -0.013668 0.000001 0.000000 -0.075014 -0.000000

14 C 0.000000 0.002395 -0.000000 -0.000000 -0.015778 -0.000000

15 C 0.000000 0.002395 0.000001 0.000000 0.002356 0.000000

16 C 0.000008 -0.013668 0.000175 0.000002 -0.000398 0.000000

17 N 0.000002 0.135437 -0.000153 -0.000000 0.003805 0.000000

18 C -0.000199 -0.011504 -0.002102 -0.000051 -0.000046 -0.000002

19 C 0.005823 -0.014175 -0.000663 -0.000482 0.000002 -0.000046

20 C -0.034650 0.002578 0.012578 0.002545 0.000000 0.000352

21 C 0.387538 0.002578 -0.072828 -0.014561 -0.000000 -0.000181

22 C -0.038845 -0.014175 0.429525 -0.077932 0.000000 -0.005852

23 N 0.005449 0.133189 -0.028648 0.003691 -0.000000 -0.000058

24 H -0.000000 -0.000457 0.000000 -0.000000 0.007373 -0.000000

25 H -0.000000 -0.000457 0.000000 -0.000000 -0.000086 -0.000000

26 H -0.000008 -0.000502 -0.005466 0.006929 -0.000000 0.003684

27 H -0.000000 -0.000502 -0.000193 -0.000087 -0.000000 -0.000010

28 H -0.000000 -0.000502 0.000000 -0.000000 0.006929 -0.000000

29 H -0.000000 -0.000502 0.000000 -0.000000 -0.000087 -0.000000

30 H -0.002320 -0.000457 -0.000199 -0.000086 -0.000000 -0.000008

31 H 0.440325 -0.000457 -0.005436 0.007373 -0.000000 0.004019

32 Zn -0.000457 10.245367 -0.011504 -0.000916 -0.000916 -0.000081

33 C -0.005436 -0.011504 5.249313 0.547984 0.000000 -0.108518

34 C 0.007373 -0.000916 0.547984 4.806397 0.000000 0.850981

35 C -0.000000 -0.000916 0.000000 0.000000 4.806397 0.000000

36 C 0.004019 -0.000081 -0.108518 0.850981 0.000000 5.227627

37 C -0.000000 -0.000081 0.000000 0.000000 0.850981 0.000000

38 C -0.000000 -0.000916 -0.000046 -0.000001 -0.000001 -0.000000

39 C -0.000000 -0.000081 -0.000002 -0.000000 -0.000000 -0.000000

40 C -0.000086 -0.000916 -0.000051 -0.000001 -0.000001 -0.000000

41 C -0.000008 -0.000081 -0.000002 -0.000000 -0.000000 -0.000000

42 H -0.000000 -0.000005 -0.000000 -0.000000 -0.000000 0.000000

43 H 0.000073 -0.000005 0.001954 -0.019853 0.000000 0.372588

44 H -0.000000 -0.000005 -0.000000 -0.000000 -0.000000 0.000000

45 H -0.000000 -0.000005 0.000000 0.000000 -0.019853 0.000000

37 38 39 40 41 42

1 C -0.000181 0.002545 0.000352 0.000000 0.000000 0.000000

2 C -0.005852 -0.000482 -0.000046 0.000002 0.000000 0.000000

3 N -0.000058 0.003691 -0.000058 -0.000000 0.000000 0.000000

4 C -0.000046 -0.077932 -0.005852 0.000000 -0.000000 0.000000

5 C 0.000352 -0.014561 -0.000181 -0.000000 -0.000000 -0.000000

6 C -0.000002 0.547984 -0.108518 0.000000 0.000000 0.000000

7 C 0.000000 -0.075014 -0.004798 0.000000 -0.000000 0.000000

8 N 0.000000 0.003805 -0.000060 -0.000000 0.000000 0.000000

9 C -0.000000 -0.000398 -0.000047 0.000002 0.000000 0.000000

10 C -0.000000 0.002356 0.000311 0.000000 0.000000 0.000000

11 C 0.000000 -0.015778 -0.000350 -0.000000 -0.000000 -0.000000

12 C -0.108518 -0.000051 -0.000002 -0.000046 -0.000002 -0.000000

13 C -0.004798 0.000002 0.000000 -0.000398 -0.000047 0.000000

14 C -0.000350 0.000000 0.000000 0.002356 0.000311 0.000001

15 C 0.000311 -0.000000 -0.000000 -0.015778 -0.000350 0.000088

16 C -0.000047 0.000000 -0.000000 -0.075014 -0.004798 -0.000009

17 N -0.000060 -0.000000 0.000000 0.003805 -0.000060 0.000001

18 C -0.000002 0.000000 0.000000 0.547984 -0.108518 0.001954

19 C 0.000000 0.000000 -0.000000 -0.077932 -0.005852 -0.000076

20 C 0.000000 -0.000000 -0.000000 -0.014561 -0.000181 0.000099

21 C -0.000000 0.000000 0.000000 0.002545 0.000352 0.000002

22 C -0.000000 0.000002 0.000000 -0.000482 -0.000046 -0.000000

23 N 0.000000 -0.000000 0.000000 0.003691 -0.000058 0.000001

24 H 0.004019 -0.000086 -0.000008 -0.000000 -0.000000 -0.000000

25 H -0.000008 0.007373 0.004019 -0.000000 -0.000000 -0.000000

26 H -0.000000 -0.000087 -0.000010 -0.000000 -0.000000 -0.000000

27 H -0.000000 0.006929 0.003684 -0.000000 -0.000000 -0.000000

28 H 0.003684 -0.000000 -0.000000 -0.000087 -0.000010 -0.000000

29 H -0.000010 -0.000000 -0.000000 0.006929 0.003684 0.000060

30 H -0.000000 -0.000000 -0.000000 0.007373 0.004019 0.000073

31 H -0.000000 -0.000000 -0.000000 -0.000086 -0.000008 -0.000000

32 Zn -0.000081 -0.000916 -0.000081 -0.000916 -0.000081 -0.000005

33 C 0.000000 -0.000046 -0.000002 -0.000051 -0.000002 -0.000000

34 C 0.000000 -0.000001 -0.000000 -0.000001 -0.000000 -0.000000

35 C 0.850981 -0.000001 -0.000000 -0.000001 -0.000000 -0.000000

36 C 0.000000 -0.000000 -0.000000 -0.000000 -0.000000 0.000000

37 C 5.227627 -0.000000 -0.000000 -0.000000 -0.000000 0.000000

38 C -0.000000 4.806397 0.850981 0.000000 0.000000 0.000000

39 C -0.000000 0.850981 5.227627 0.000000 0.000000 0.000000

40 C -0.000000 0.000000 0.000000 4.806397 0.850981 -0.019853

41 C -0.000000 0.000000 0.000000 0.850981 5.227627 0.372588

42 H 0.000000 0.000000 0.000000 -0.019853 0.372588 0.355112

43 H 0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

44 H 0.000000 -0.019853 0.372588 0.000000 0.000000 0.000000

45 H 0.372588 -0.000000 0.000000 -0.000000 0.000000 0.000000

43 44 45

1 C -0.000000 0.000002 0.000099

2 C 0.000000 -0.000000 -0.000076

3 N 0.000000 0.000001 0.000001

4 C 0.000000 -0.000076 -0.000000

5 C 0.000000 0.000099 0.000002

6 C -0.000000 0.001954 -0.000000

7 C 0.000000 -0.000009 0.000000

8 N 0.000001 0.000001 0.000000

9 C -0.000009 0.000000 0.000000

10 C 0.000088 0.000001 -0.000000

11 C 0.000001 0.000088 0.000000

12 C 0.000000 -0.000000 0.001954

13 C 0.000000 0.000000 -0.000009

14 C -0.000000 0.000000 0.000088

15 C 0.000000 -0.000000 0.000001

16 C 0.000000 0.000000 0.000000

17 N 0.000000 0.000000 0.000001

18 C -0.000000 0.000000 -0.000000

19 C -0.000000 0.000000 0.000000

20 C 0.000002 -0.000000 0.000000

21 C 0.000099 0.000000 -0.000000

22 C -0.000076 0.000000 0.000000

23 N 0.000001 0.000000 0.000000

24 H -0.000000 -0.000000 0.000073

25 H -0.000000 0.000073 -0.000000

26 H 0.000060 -0.000000 -0.000000

27 H -0.000000 0.000060 -0.000000

28 H -0.000000 -0.000000 0.000060

29 H -0.000000 -0.000000 -0.000000

30 H -0.000000 -0.000000 -0.000000

31 H 0.000073 -0.000000 -0.000000

32 Zn -0.000005 -0.000005 -0.000005

33 C 0.001954 -0.000000 0.000000

34 C -0.019853 -0.000000 0.000000

35 C 0.000000 -0.000000 -0.019853

36 C 0.372588 0.000000 0.000000

37 C 0.000000 0.000000 0.372588

38 C -0.000000 -0.019853 -0.000000

39 C 0.000000 0.372588 0.000000

40 C -0.000000 0.000000 -0.000000

41 C 0.000000 0.000000 0.000000

42 H 0.000000 0.000000 0.000000

43 H 0.355112 0.000000 0.000000

44 H 0.000000 0.355112 0.000000

45 H 0.000000 0.000000 0.355112

Atomic-Atomic Spin Densities.

1 2 3 4 5 6

1 C -0.007116 -0.005352 0.002072 0.000444 0.008154 -0.000626

2 C -0.005352 -0.029423 -0.012045 0.004032 0.000444 0.000621

3 N 0.002072 -0.012045 0.104471 -0.012045 0.002072 -0.005472

4 C 0.000444 0.004032 -0.012045 -0.029423 -0.005352 0.022705

5 C 0.008154 0.000444 0.002072 -0.005352 -0.007116 -0.001029

6 C -0.000626 0.000621 -0.005472 0.022705 -0.001029 0.114691

7 C 0.000016 -0.000068 0.001851 -0.002873 0.000273 -0.037915

8 N 0.000000 0.000005 -0.000037 0.000324 -0.000001 0.000398

9 C -0.000000 0.000002 -0.000083 0.000077 -0.000000 0.000781

10 C -0.000000 0.000000 -0.000010 0.000039 -0.000000 0.000885

11 C 0.000000 -0.000002 0.000058 -0.000680 0.000012 -0.007408

12 C -0.001029 0.022705 -0.005472 0.000621 -0.000626 0.000097

13 C 0.000273 -0.002873 0.001851 -0.000068 0.000016 -0.000007

14 C 0.000012 -0.000680 0.000058 -0.000002 0.000000 -0.000000

15 C -0.000000 0.000039 -0.000010 0.000000 -0.000000 0.000000

16 C -0.000000 0.000077 -0.000083 0.000002 -0.000000 0.000000

17 N -0.000001 0.000324 -0.000037 0.000005 0.000000 0.000000

18 C 0.000000 -0.000009 0.000011 -0.000000 0.000000 -0.000000

19 C 0.000000 0.000001 0.000001 -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 0.000000 -0.000000 0.000001 0.000001 0.000000 -0.000009

23 N -0.000000 0.000001 -0.000037 0.000001 -0.000000 0.000011

24 H -0.000214 0.000228 -0.000006 -0.000044 0.000128 -0.000008

25 H 0.000128 -0.000044 -0.000006 0.000228 -0.000214 0.000019

26 H 0.000000 -0.000000 -0.000000 -0.000001 -0.000000 0.000003

27 H -0.000000 0.000000 -0.000000 0.000014 0.000000 0.000304

28 H 0.000000 0.000014 -0.000000 0.000000 -0.000000 0.000000

29 H -0.000000 -0.000001 -0.000000 -0.000000 0.000000 -0.000000

30 H 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000

31 H 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000

32 Zn 0.000017 0.000052 -0.001939 0.000052 0.000017 0.000078

33 C 0.000000 -0.000000 0.000011 -0.000009 0.000000 -0.000026

34 C 0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

35 C 0.000106 -0.000729 -0.000051 0.000015 -0.000074 0.000002

36 C -0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

37 C 0.000203 -0.000595 0.000016 0.000000 0.000001 0.000000

38 C -0.000074 0.000015 -0.000051 -0.000729 0.000106 0.004853

39 C 0.000001 0.000000 0.000016 -0.000595 0.000203 -0.002986

40 C 0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

41 C -0.000000 -0.000000 -0.000000 0.000000 -0.000000 0.000000

42 H 0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.000000

43 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 -0.000000

44 H -0.000000 0.000000 0.000000 -0.000005 0.000001 -0.000005

45 H 0.000001 -0.000005 0.000000 0.000000 -0.000000 0.000000

7 8 9 10 11 12

1 C 0.000016 0.000000 -0.000000 -0.000000 0.000000 -0.001029

2 C -0.000068 0.000005 0.000002 0.000000 -0.000002 0.022705

3 N 0.001851 -0.000037 -0.000083 -0.000010 0.000058 -0.005472

4 C -0.002873 0.000324 0.000077 0.000039 -0.000680 0.000621

5 C 0.000273 -0.000001 -0.000000 -0.000000 0.000012 -0.000626

6 C -0.037915 0.000398 0.000781 0.000885 -0.007408 0.000097

7 C 0.100767 0.002651 -0.011606 -0.011044 0.032487 -0.000007

8 N 0.002651 -0.029982 0.002651 -0.000303 -0.000303 0.000000

9 C -0.011606 0.002651 0.100767 0.032487 -0.011044 0.000000

10 C -0.011044 -0.000303 0.032487 0.083613 -0.034193 0.000000

11 C 0.032487 -0.000303 -0.011044 -0.034193 0.083613 -0.000000

12 C -0.000007 0.000000 0.000000 0.000000 -0.000000 0.114691

13 C 0.000002 0.000001 -0.000001 -0.000000 0.000000 -0.037915

14 C 0.000000 -0.000000 -0.000000 -0.000000 0.000000 -0.007408

15 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 0.000885

16 C -0.000001 0.000001 0.000002 0.000000 -0.000000 0.000781

17 N 0.000001 -0.000006 0.000001 -0.000000 -0.000000 0.000398

18 C 0.000000 0.000000 -0.000007 -0.000000 0.000000 -0.000026

19 C 0.000002 0.000005 -0.000068 -0.000002 0.000000 -0.000009

20 C -0.000000 0.000000 0.000016 0.000000 -0.000000 0.000000

21 C -0.000000 -0.000001 0.000273 0.000012 -0.000000 0.000000

22 C 0.000077 0.000324 -0.002873 -0.000680 0.000039 -0.000000

23 N -0.000083 -0.000037 0.001851 0.000058 -0.000010 0.000011

24 H 0.000000 -0.000000 -0.000000 0.000000 -0.000000 0.000019

25 H -0.000005 0.000000 0.000000 -0.000000 0.000000 -0.000008

26 H 0.000022 -0.000029 -0.000481 0.000203 0.000152 -0.000000

27 H -0.000481 -0.000029 0.000022 0.000152 0.000203 0.000000

28 H -0.000000 0.000000 0.000000 0.000000 -0.000000 0.000304

29 H 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000003

30 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

31 H 0.000000 0.000000 -0.000005 0.000000 -0.000000 0.000000

32 Zn 0.000258 0.000067 0.000258 -0.000037 -0.000037 0.000078

33 C 0.000781 0.000398 -0.037915 -0.007408 0.000885 -0.000000

34 C -0.000019 -0.000081 0.000235 0.000133 0.000074 0.000000

35 C -0.000000 0.000000 0.000000 -0.000000 -0.000000 0.004853

36 C -0.000006 -0.000000 0.001136 0.000622 -0.000023 0.000000

37 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.002986

38 C 0.000235 -0.000081 -0.000019 0.000074 0.000133 0.000002

39 C 0.001136 -0.000000 -0.000006 -0.000023 0.000622 0.000000

40 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

41 C -0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000

42 H 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

43 H -0.000000 -0.000000 0.000002 0.000000 0.000000 0.000000

44 H 0.000002 -0.000000 -0.000000 0.000000 0.000000 0.000000

45 H -0.000000 0.000000 0.000000 -0.000000 -0.000000 -0.000005

13 14 15 16 17 18

1 C 0.000273 0.000012 -0.000000 -0.000000 -0.000001 0.000000

2 C -0.002873 -0.000680 0.000039 0.000077 0.000324 -0.000009

3 N 0.001851 0.000058 -0.000010 -0.000083 -0.000037 0.000011

4 C -0.000068 -0.000002 0.000000 0.000002 0.000005 -0.000000

5 C 0.000016 0.000000 -0.000000 -0.000000 0.000000 0.000000

6 C -0.000007 -0.000000 0.000000 0.000000 0.000000 -0.000000

7 C 0.000002 0.000000 -0.000000 -0.000001 0.000001 0.000000

8 N 0.000001 -0.000000 -0.000000 0.000001 -0.000006 0.000000

9 C -0.000001 -0.000000 0.000000 0.000002 0.000001 -0.000007

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 C -0.037915 -0.007408 0.000885 0.000781 0.000398 -0.000026

13 C 0.100767 0.032487 -0.011044 -0.011606 0.002651 0.000781

14 C 0.032487 0.083613 -0.034193 -0.011044 -0.000303 0.000885

15 C -0.011044 -0.034193 0.083613 0.032487 -0.000303 -0.007408

16 C -0.011606 -0.011044 0.032487 0.100767 0.002651 -0.037915

17 N 0.002651 -0.000303 -0.000303 0.002651 -0.029982 0.000398

18 C 0.000781 0.000885 -0.007408 -0.037915 0.000398 0.114691

19 C 0.000077 0.000039 -0.000680 -0.002873 0.000324 0.022705

20 C -0.000000 -0.000000 0.000012 0.000273 -0.000001 -0.001029

21 C -0.000000 -0.000000 0.000000 0.000016 0.000000 -0.000626

22 C 0.000002 0.000000 -0.000002 -0.000068 0.000005 0.000621

23 N -0.000083 -0.000010 0.000058 0.001851 -0.000037 -0.005472

24 H -0.000005 0.000000 -0.000000 0.000000 0.000000 0.000000

25 H 0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.000000

26 H 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

27 H -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000

28 H -0.000481 0.000203 0.000152 0.000022 -0.000029 0.000003

29 H 0.000022 0.000152 0.000203 -0.000481 -0.000029 0.000304

30 H 0.000000 -0.000000 0.000000 -0.000005 0.000000 0.000019

31 H -0.000000 0.000000 -0.000000 0.000000 -0.000000 -0.000008

32 Zn 0.000258 -0.000037 -0.000037 0.000258 0.000067 0.000078

33 C 0.000000 0.000000 -0.000000 -0.000007 0.000000 0.000097

34 C 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000002

35 C 0.000235 0.000133 0.000074 -0.000019 -0.000081 0.000000

36 C -0.000000 -0.000000 0.000000 0.000000 0.000000 0.000000

37 C 0.001136 0.000622 -0.000023 -0.000006 -0.000000 0.000000

38 C -0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000000

39 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

40 C -0.000019 0.000074 0.000133 0.000235 -0.000081 0.004853

41 C -0.000006 -0.000023 0.000622 0.001136 -0.000000 -0.002986

42 H -0.000000 0.000000 0.000000 0.000002 -0.000000 -0.000005

43 H 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000000

44 H -0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000000

45 H 0.000002 0.000000 0.000000 -0.000000 -0.000000 -0.000000

19 20 21 22 23 24

1 C 0.000000 -0.000000 -0.000000 0.000000 -0.000000 -0.000214

2 C 0.000001 0.000000 0.000000 -0.000000 0.000001 0.000228

3 N 0.000001 -0.000000 -0.000000 0.000001 -0.000037 -0.000006

4 C -0.000000 0.000000 0.000000 0.000001 0.000001 -0.000044

5 C 0.000000 -0.000000 -0.000000 0.000000 -0.000000 0.000128

6 C -0.000000 0.000000 0.000000 -0.000009 0.000011 -0.000008

7 C 0.000002 -0.000000 -0.000000 0.000077 -0.000083 0.000000

8 N 0.000005 0.000000 -0.000001 0.000324 -0.000037 -0.000000

9 C -0.000068 0.000016 0.000273 -0.002873 0.001851 -0.000000

10 C -0.000002 0.000000 0.000012 -0.000680 0.000058 0.000000

11 C 0.000000 -0.000000 -0.000000 0.000039 -0.000010 -0.000000

12 C -0.000009 0.000000 0.000000 -0.000000 0.000011 0.000019

13 C 0.000077 -0.000000 -0.000000 0.000002 -0.000083 -0.000005

14 C 0.000039 -0.000000 -0.000000 0.000000 -0.000010 0.000000

15 C -0.000680 0.000012 0.000000 -0.000002 0.000058 -0.000000

16 C -0.002873 0.000273 0.000016 -0.000068 0.001851 0.000000

17 N 0.000324 -0.000001 0.000000 0.000005 -0.000037 0.000000

18 C 0.022705 -0.001029 -0.000626 0.000621 -0.005472 0.000000

19 C -0.029423 -0.005352 0.000444 0.004032 -0.012045 0.000000

20 C -0.005352 -0.007116 0.008154 0.000444 0.002072 0.000000

21 C 0.000444 0.008154 -0.007116 -0.005352 0.002072 0.000000

22 C 0.004032 0.000444 -0.005352 -0.029423 -0.012045 0.000000

23 N -0.012045 0.002072 0.002072 -0.012045 0.104471 -0.000000

24 H 0.000000 0.000000 0.000000 0.000000 -0.000000 0.000183

25 H 0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000007

26 H 0.000000 -0.000000 0.000000 0.000014 -0.000000 0.000000

27 H -0.000000 0.000000 -0.000000 -0.000001 -0.000000 0.000000

28 H -0.000001 -0.000000 0.000000 -0.000000 -0.000000 0.000000

29 H 0.000014 0.000000 -0.000000 0.000000 -0.000000 -0.000000

30 H 0.000228 -0.000214 0.000128 -0.000044 -0.000006 0.000000

31 H -0.000044 0.000128 -0.000214 0.000228 -0.000006 0.000000

32 Zn 0.000052 0.000017 0.000017 0.000052 -0.001939 -0.000000

33 C 0.000621 -0.000626 -0.001029 0.022705 -0.005472 0.000000

34 C 0.000015 -0.000074 0.000106 -0.000729 -0.000051 0.000000

35 C -0.000000 0.000000 0.000000 -0.000000 0.000000 0.000016

36 C 0.000000 0.000001 0.000203 -0.000595 0.000016 0.000000

37 C -0.000000 -0.000000 -0.000000 0.000000 -0.000000 0.000067

38 C -0.000000 0.000000 0.000000 -0.000000 0.000000 -0.000000

39 C 0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000

40 C -0.000729 0.000106 -0.000074 0.000015 -0.000051 0.000000

41 C -0.000595 0.000203 0.000001 0.000000 0.000016 0.000000

42 H -0.000005 0.000001 -0.000000 0.000000 0.000000 0.000000

43 H 0.000000 -0.000000 0.000001 -0.000005 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 0.000002

25 26 27 28 29 30

1 C 0.000128 0.000000 -0.000000 0.000000 -0.000000 0.000000

2 C -0.000044 -0.000000 0.000000 0.000014 -0.000001 0.000000

3 N -0.000006 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000

4 C 0.000228 -0.000001 0.000014 0.000000 -0.000000 0.000000

5 C -0.000214 -0.000000 0.000000 -0.000000 0.000000 0.000000

6 C 0.000019 0.000003 0.000304 0.000000 -0.000000 0.000000

7 C -0.000005 0.000022 -0.000481 -0.000000 0.000000 -0.000000

8 N 0.000000 -0.000029 -0.000029 0.000000 0.000000 -0.000000

9 C 0.000000 -0.000481 0.000022 0.000000 -0.000000 0.000000

10 C -0.000000 0.000203 0.000152 0.000000 -0.000000 -0.000000

11 C 0.000000 0.000152 0.000203 -0.000000 0.000000 0.000000

12 C -0.000008 -0.000000 0.000000 0.000304 0.000003 0.000000

13 C 0.000000 0.000000 -0.000000 -0.000481 0.000022 0.000000

14 C -0.000000 0.000000 -0.000000 0.000203 0.000152 -0.000000

15 C 0.000000 -0.000000 0.000000 0.000152 0.000203 0.000000

16 C -0.000000 -0.000000 0.000000 0.000022 -0.000481 -0.000005

17 N -0.000000 0.000000 0.000000 -0.000029 -0.000029 0.000000

18 C 0.000000 0.000000 -0.000000 0.000003 0.000304 0.000019

19 C 0.000000 0.000000 -0.000000 -0.000001 0.000014 0.000228

20 C 0.000000 -0.000000 0.000000 -0.000000 0.000000 -0.000214

21 C 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000128

22 C 0.000000 0.000014 -0.000001 -0.000000 0.000000 -0.000044

23 N -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000006

24 H -0.000007 0.000000 0.000000 0.000000 -0.000000 0.000000

25 H 0.000183 -0.000000 0.000000 0.000000 0.000000 0.000000

26 H -0.000000 -0.004236 0.000077 0.000000 -0.000000 0.000000

27 H 0.000000 0.000077 -0.004236 -0.000000 0.000000 0.000000

28 H 0.000000 0.000000 -0.000000 -0.004236 0.000077 -0.000000

29 H 0.000000 -0.000000 0.000000 0.000077 -0.004236 0.000000

30 H 0.000000 0.000000 0.000000 -0.000000 0.000000 0.000183

31 H 0.000000 0.000000 -0.000000 0.000000 0.000000 -0.000007

32 Zn -0.000000 -0.000003 -0.000003 -0.000003 -0.000003 -0.000000

33 C 0.000000 0.000304 0.000003 -0.000000 0.000000 -0.000008

34 C 0.000000 -0.000204 0.000003 -0.000000 -0.000000 -0.000000

35 C -0.000000 -0.000000 -0.000000 -0.000204 0.000003 0.000000

36 C 0.000000 -0.000145 0.000000 -0.000000 -0.000000 -0.000000

37 C -0.000000 -0.000000 -0.000000 -0.000145 0.000000 0.000000

38 C 0.000016 0.000003 -0.000204 -0.000000 -0.000000 0.000000

39 C 0.000067 0.000000 -0.000145 -0.000000 -0.000000 0.000000

40 C 0.000000 -0.000000 -0.000000 0.000003 -0.000204 0.000016

41 C 0.000000 -0.000000 -0.000000 0.000000 -0.000145 0.000067

42 H 0.000000 -0.000000 -0.000000 0.000000 -0.000006 0.000002

43 H 0.000000 -0.000006 0.000000 -0.000000 -0.000000 -0.000000

44 H 0.000002 0.000000 -0.000006 -0.000000 -0.000000 0.000000

45 H -0.000000 -0.000000 -0.000000 -0.000006 0.000000 0.000000

31 32 33 34 35 36

1 C 0.000000 0.000017 0.000000 0.000000 0.000106 -0.000000

2 C 0.000000 0.000052 -0.000000 -0.000000 -0.000729 0.000000

3 N -0.000000 -0.001939 0.000011 0.000000 -0.000051 -0.000000

4 C 0.000000 0.000052 -0.000009 -0.000000 0.000015 -0.000000

5 C 0.000000 0.000017 0.000000 0.000000 -0.000074 -0.000000

6 C 0.000000 0.000078 -0.000026 0.000000 0.000002 0.000000

7 C 0.000000 0.000258 0.000781 -0.000019 -0.000000 -0.000006

8 N 0.000000 0.000067 0.000398 -0.000081 0.000000 -0.000000

9 C -0.000005 0.000258 -0.037915 0.000235 0.000000 0.001136

10 C 0.000000 -0.000037 -0.007408 0.000133 -0.000000 0.000622

11 C -0.000000 -0.000037 0.000885 0.000074 -0.000000 -0.000023

12 C 0.000000 0.000078 -0.000000 0.000000 0.004853 0.000000

13 C -0.000000 0.000258 0.000000 0.000000 0.000235 -0.000000

14 C 0.000000 -0.000037 0.000000 -0.000000 0.000133 -0.000000

15 C -0.000000 -0.000037 -0.000000 -0.000000 0.000074 0.000000

16 C 0.000000 0.000258 -0.000007 -0.000000 -0.000019 0.000000

17 N -0.000000 0.000067 0.000000 0.000000 -0.000081 0.000000

18 C -0.000008 0.000078 0.000097 0.000002 0.000000 0.000000

19 C -0.000044 0.000052 0.000621 0.000015 -0.000000 0.000000

20 C 0.000128 0.000017 -0.000626 -0.000074 0.000000 0.000001

21 C -0.000214 0.000017 -0.001029 0.000106 0.000000 0.000203

22 C 0.000228 0.000052 0.022705 -0.000729 -0.000000 -0.000595

23 N -0.000006 -0.001939 -0.005472 -0.000051 0.000000 0.000016

24 H 0.000000 -0.000000 0.000000 0.000000 0.000016 0.000000

25 H 0.000000 -0.000000 0.000000 0.000000 -0.000000 0.000000

26 H 0.000000 -0.000003 0.000304 -0.000204 -0.000000 -0.000145

27 H -0.000000 -0.000003 0.000003 0.000003 -0.000000 0.000000

28 H 0.000000 -0.000003 -0.000000 -0.000000 -0.000204 -0.000000

29 H 0.000000 -0.000003 0.000000 -0.000000 0.000003 -0.000000

30 H -0.000007 -0.000000 -0.000008 -0.000000 0.000000 -0.000000

31 H 0.000183 -0.000000 0.000019 0.000016 0.000000 0.000067

32 Zn -0.000000 -0.001616 0.000078 -0.000020 -0.000020 -0.000005

33 C 0.000019 0.000078 0.114691 0.004853 0.000000 -0.002986

34 C 0.000016 -0.000020 0.004853 -0.029882 0.000000 -0.000995

35 C 0.000000 -0.000020 0.000000 0.000000 -0.029882 0.000000

36 C 0.000067 -0.000005 -0.002986 -0.000995 0.000000 0.056824

37 C 0.000000 -0.000005 0.000000 0.000000 -0.000995 -0.000000

38 C 0.000000 -0.000020 0.000000 0.000000 0.000000 0.000000

39 C 0.000000 -0.000005 0.000000 0.000000 0.000000 -0.000000

40 C -0.000000 -0.000020 0.000002 0.000000 0.000000 0.000000

41 C -0.000000 -0.000005 0.000000 0.000000 0.000000 0.000000

42 H -0.000000 -0.000000 0.000000 0.000000 0.000000 0.000000

43 H 0.000002 -0.000000 -0.000005 -0.000234 -0.000000 -0.000245

44 H 0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000000

45 H 0.000000 -0.000000 0.000000 -0.000000 -0.000234 -0.000000

37 38 39 40 41 42

1 C 0.000203 -0.000074 0.000001 0.000000 -0.000000 0.000000

2 C -0.000595 0.000015 0.000000 -0.000000 -0.000000 -0.000000

3 N 0.000016 -0.000051 0.000016 0.000000 -0.000000 0.000000

4 C 0.000000 -0.000729 -0.000595 -0.000000 0.000000 -0.000000

5 C 0.000001 0.000106 0.000203 0.000000 -0.000000 -0.000000

6 C 0.000000 0.004853 -0.002986 0.000000 0.000000 0.000000

7 C 0.000000 0.000235 0.001136 0.000000 -0.000000 0.000000

8 N 0.000000 -0.000081 -0.000000 0.000000 0.000000 0.000000

9 C -0.000000 -0.000019 -0.000006 -0.000000 0.000000 -0.000000

10 C -0.000000 0.000074 -0.000023 -0.000000 0.000000 -0.000000

11 C 0.000000 0.000133 0.000622 -0.000000 -0.000000 -0.000000

12 C -0.002986 0.000002 0.000000 0.000000 0.000000 -0.000000

13 C 0.001136 -0.000000 0.000000 -0.000019 -0.000006 -0.000000

14 C 0.000622 -0.000000 0.000000 0.000074 -0.000023 0.000000

15 C -0.000023 -0.000000 -0.000000 0.000133 0.000622 0.000000

16 C -0.000006 0.000000 -0.000000 0.000235 0.001136 0.000002

17 N -0.000000 0.000000 0.000000 -0.000081 -0.000000 -0.000000

18 C 0.000000 0.000000 0.000000 0.004853 -0.002986 -0.000005

19 C -0.000000 -0.000000 0.000000 -0.000729 -0.000595 -0.000005

20 C -0.000000 0.000000 -0.000000 0.000106 0.000203 0.000001

21 C -0.000000 0.000000 -0.000000 -0.000074 0.000001 -0.000000

22 C 0.000000 -0.000000 -0.000000 0.000015 0.000000 0.000000

23 N -0.000000 0.000000 -0.000000 -0.000051 0.000016 0.000000

24 H 0.000067 -0.000000 -0.000000 0.000000 0.000000 0.000000

25 H -0.000000 0.000016 0.000067 0.000000 0.000000 0.000000

26 H -0.000000 0.000003 0.000000 -0.000000 -0.000000 -0.000000

27 H -0.000000 -0.000204 -0.000145 -0.000000 -0.000000 -0.000000

28 H -0.000145 -0.000000 -0.000000 0.000003 0.000000 0.000000

29 H 0.000000 -0.000000 -0.000000 -0.000204 -0.000145 -0.000006

30 H 0.000000 0.000000 0.000000 0.000016 0.000067 0.000002

31 H 0.000000 0.000000 0.000000 -0.000000 -0.000000 -0.000000

32 Zn -0.000005 -0.000020 -0.000005 -0.000020 -0.000005 -0.000000

33 C 0.000000 0.000000 0.000000 0.000002 0.000000 0.000000

34 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 C -0.000995 0.000000 0.000000 0.000000 0.000000 0.000000

36 C -0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000

37 C 0.056824 0.000000 0.000000 0.000000 -0.000000 0.000000

38 C 0.000000 -0.029882 -0.000995 0.000000 0.000000 -0.000000

39 C 0.000000 -0.000995 0.056824 0.000000 -0.000000 -0.000000

40 C 0.000000 0.000000 0.000000 -0.029882 -0.000995 -0.000234

41 C -0.000000 0.000000 -0.000000 -0.000995 0.056824 -0.000245

42 H 0.000000 -0.000000 -0.000000 -0.000234 -0.000245 -0.001809

43 H -0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

44 H 0.000000 -0.000234 -0.000245 -0.000000 -0.000000 -0.000000

45 H -0.000245 0.000000 0.000000 0.000000 0.000000 -0.000000

43 44 45

1 C -0.000000 -0.000000 0.000001

2 C -0.000000 0.000000 -0.000005

3 N 0.000000 0.000000 0.000000

4 C -0.000000 -0.000005 0.000000

5 C 0.000000 0.000001 -0.000000

6 C -0.000000 -0.000005 0.000000

7 C -0.000000 0.000002 -0.000000

8 N -0.000000 -0.000000 0.000000

9 C 0.000002 -0.000000 0.000000

10 C 0.000000 0.000000 -0.000000

11 C 0.000000 0.000000 -0.000000

12 C 0.000000 0.000000 -0.000005

13 C 0.000000 -0.000000 0.000002

14 C -0.000000 -0.000000 0.000000

15 C -0.000000 -0.000000 0.000000

16 C -0.000000 0.000000 -0.000000

17 N 0.000000 0.000000 -0.000000

18 C 0.000000 0.000000 -0.000000

19 C 0.000000 -0.000000 -0.000000

20 C -0.000000 -0.000000 0.000000

21 C 0.000001 0.000000 -0.000000

22 C -0.000005 -0.000000 -0.000000

23 N 0.000000 0.000000 0.000000

24 H 0.000000 -0.000000 0.000002

25 H 0.000000 0.000002 -0.000000

26 H -0.000006 0.000000 -0.000000

27 H 0.000000 -0.000006 -0.000000

28 H -0.000000 -0.000000 -0.000006

29 H -0.000000 -0.000000 0.000000

30 H -0.000000 0.000000 0.000000

31 H 0.000002 0.000000 0.000000

32 Zn -0.000000 -0.000000 -0.000000

33 C -0.000005 -0.000000 0.000000

34 C -0.000234 0.000000 -0.000000

35 C -0.000000 0.000000 -0.000234

36 C -0.000245 0.000000 -0.000000

37 C -0.000000 0.000000 -0.000245

38 C 0.000000 -0.000234 0.000000

39 C 0.000000 -0.000245 0.000000

40 C 0.000000 -0.000000 0.000000

41 C 0.000000 -0.000000 0.000000

42 H 0.000000 -0.000000 -0.000000

43 H -0.001809 -0.000000 -0.000000

44 H -0.000000 -0.001809 0.000000

45 H -0.000000 0.000000 -0.001809

Mulliken charges and spin densities:

1 2

1 C -0.257250 -0.002986

2 C 0.314325 -0.023266

3 N -0.721532 0.075103

4 C 0.314325 -0.023266

5 C -0.257250 -0.002986

6 C -0.308344 0.089957

7 C 0.293888 0.076453

8 N -0.703091 -0.024067

9 C 0.293888 0.076453

10 C -0.293961 0.064578

11 C -0.293961 0.064578

12 C -0.308344 0.089957

13 C 0.293888 0.076453

14 C -0.293961 0.064578

15 C -0.293961 0.064578

16 C 0.293888 0.076453

17 N -0.703091 -0.024067

18 C -0.308344 0.089957

19 C 0.314325 -0.023266

20 C -0.257250 -0.002986

21 C -0.257250 -0.002986

22 C 0.314325 -0.023266

23 N -0.721532 0.075103

24 H 0.231394 0.000359

25 H 0.231394 0.000359

26 H 0.218024 -0.004327

27 H 0.218024 -0.004327

28 H 0.218024 -0.004327

29 H 0.218024 -0.004327

30 H 0.231394 0.000359

31 H 0.231394 0.000359

32 Zn 1.362713 -0.004005

33 C -0.308344 0.089957

34 C -0.026860 -0.026854

35 C -0.026860 -0.026854

36 C -0.339547 0.053869

37 C -0.339547 0.053869

38 C -0.026860 -0.026854

39 C -0.339547 0.053869

40 C -0.026860 -0.026854

41 C -0.339547 0.053869

42 H 0.289964 -0.002299

43 H 0.289964 -0.002299

44 H 0.289964 -0.002299

45 H 0.289964 -0.002299

Sum of Mulliken charges = -1.00000 1.00000

Mulliken charges and spin densities with hydrogens summed into heavy atoms:

1 2

1 C -0.025856 -0.002627

2 C 0.314325 -0.023266

3 N -0.721532 0.075103

4 C 0.314325 -0.023266

5 C -0.025856 -0.002627

6 C -0.308344 0.089957

7 C 0.293888 0.076453

8 N -0.703091 -0.024067

9 C 0.293888 0.076453

10 C -0.075936 0.060251

11 C -0.075936 0.060251

12 C -0.308344 0.089957

13 C 0.293888 0.076453

14 C -0.075936 0.060251

15 C -0.075936 0.060251

16 C 0.293888 0.076453

17 N -0.703091 -0.024067

18 C -0.308344 0.089957

19 C 0.314325 -0.023266

20 C -0.025856 -0.002627

21 C -0.025856 -0.002627

22 C 0.314325 -0.023266

23 N -0.721532 0.075103

32 Zn 1.362713 -0.004005

33 C -0.308344 0.089957

34 C -0.026860 -0.026854

35 C -0.026860 -0.026854

36 C -0.049583 0.051570

37 C -0.049583 0.051570

38 C -0.026860 -0.026854

39 C -0.049583 0.051570

40 C -0.026860 -0.026854

41 C -0.049583 0.051570

APT charges:

1

1 C 0.169817

2 C 0.450416

3 N -1.304183

4 C 0.450416

5 C 0.169815

6 C -0.239344

7 C -0.477646

8 N -0.597424

9 C -0.477646

10 C 0.262518

11 C 0.262519

12 C -0.239344

13 C -0.477646

14 C 0.262519

15 C 0.262519

16 C -0.477646

17 N -0.597423

18 C -0.239342

19 C 0.450414

20 C 0.169816

21 C 0.169816

22 C 0.450416

23 N -1.304182

24 H 0.079790

25 H 0.079789

26 H 0.070089

27 H 0.070089

28 H 0.070088

29 H 0.070089

30 H 0.079790

31 H 0.079789

32 Zn 1.353532

33 C -0.239342

34 C 0.747878

35 C 0.747880

36 C -1.026095

37 C -1.026095

38 C 0.747878

39 C -1.026094

40 C 0.747879

41 C -1.026096

42 H 0.324997

43 H 0.324996

44 H 0.324997

45 H 0.324996

Sum of APT charges = -1.00000

APT charges with hydrogens summed into heavy atoms:

1

1 C 0.249607

2 C 0.450416

3 N -1.304183

4 C 0.450416

5 C 0.249605

6 C -0.239344

7 C -0.477646

8 N -0.597424

9 C -0.477646

10 C 0.332607

11 C 0.332608

12 C -0.239344

13 C -0.477646

14 C 0.332608

15 C 0.332608

16 C -0.477646

17 N -0.597423

18 C -0.239342

19 C 0.450414

20 C 0.249605

21 C 0.249605

22 C 0.450416

23 N -1.304182

32 Zn 1.353532

33 C -0.239342

34 C 0.747878

35 C 0.747880

36 C -0.701098

37 C -0.701099

38 C 0.747878

39 C -0.701097

40 C 0.747879

41 C -0.701099

Electronic spatial extent (au): <R\*\*2>= 13621.9831

Charge= -1.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0000 Y= -0.0000 Z= 0.0005 Tot= 0.0005

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -218.4580 YY= -200.1387 ZZ= -205.5079

XY= -0.0000 XZ= 0.0000 YZ= 0.0000

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= -10.4232 YY= 7.8962 ZZ= 2.5270

XY= -0.0000 XZ= 0.0000 YZ= 0.0000

Octapole moment (field-independent basis, Debye-Ang\*\*2):

XXX= 0.0000 YYY= 0.0000 ZZZ= 0.0054 XYY= -0.0000

XXY= -0.0000 XXZ= -0.0001 XZZ= -0.0000 YZZ= 0.0000

YYZ= -0.0002 XYZ= 0.0000

Hexadecapole moment (field-independent basis, Debye-Ang\*\*3):

XXXX= -9165.5323 YYYY= -8826.2430 ZZZZ= -233.4921 XXXY= 0.0000

XXXZ= -0.0000 YYYX= -0.0000 YYYZ= 0.0000 ZZZX= -0.0000

ZZZY= -0.0000 XXYY= -2389.7137 XXZZ= -1868.1743 YYZZ= -1855.5303

XXYZ= -0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 3.051542567314D+03 E-N=-9.372576931971D+03 KE= 1.403847868853D+03

Symmetry A1 KE= 4.231245044903D+02

Symmetry A2 KE= 2.908940071178D+02

Symmetry B1 KE= 3.441803913717D+02

Symmetry B2 KE= 3.456489658734D+02

Exact polarizability:1654.469 -0.0001179.798 0.000 0.000 187.127

Approx polarizability:1784.920 -0.0001191.061 0.000 -0.000 219.921

Isotropic Fermi Contact Couplings

Atom a.u. MegaHertz Gauss 10(-4) cm-1

1 C(13) -0.00009 -0.10384 -0.03705 -0.03464

2 C(13) -0.00642 -7.22270 -2.57724 -2.40923

3 N(14) 0.00898 2.90121 1.03522 0.96774

4 C(13) -0.00642 -7.22270 -2.57724 -2.40923

5 C(13) -0.00009 -0.10384 -0.03705 -0.03464

6 C(13) 0.00378 4.25313 1.51762 1.41869

7 C(13) 0.00076 0.85826 0.30625 0.28629

8 N(14) -0.00567 -1.83162 -0.65357 -0.61096

9 C(13) 0.00076 0.85826 0.30625 0.28629

10 C(13) -0.00003 -0.02876 -0.01026 -0.00959

11 C(13) -0.00003 -0.02876 -0.01026 -0.00959

12 C(13) 0.00378 4.25313 1.51762 1.41869

13 C(13) 0.00076 0.85826 0.30625 0.28629

14 C(13) -0.00003 -0.02876 -0.01026 -0.00959

15 C(13) -0.00003 -0.02876 -0.01026 -0.00959

16 C(13) 0.00076 0.85826 0.30625 0.28629

17 N(14) -0.00567 -1.83162 -0.65357 -0.61096

18 C(13) 0.00378 4.25313 1.51762 1.41869

19 C(13) -0.00642 -7.22270 -2.57724 -2.40923

20 C(13) -0.00009 -0.10384 -0.03705 -0.03464

21 C(13) -0.00009 -0.10384 -0.03705 -0.03464

22 C(13) -0.00642 -7.22270 -2.57724 -2.40923

23 N(14) 0.00898 2.90121 1.03522 0.96774

24 H(1) 0.00008 0.37176 0.13265 0.12401

25 H(1) 0.00008 0.37176 0.13265 0.12401

26 H(1) -0.00122 -5.43511 -1.93938 -1.81296

27 H(1) -0.00122 -5.43511 -1.93938 -1.81296

28 H(1) -0.00122 -5.43511 -1.93938 -1.81296

29 H(1) -0.00122 -5.43511 -1.93938 -1.81296

30 H(1) 0.00008 0.37176 0.13265 0.12401

31 H(1) 0.00008 0.37176 0.13265 0.12401

32 Zn(67) 0.00000 0.00000 0.00000 0.00000

33 C(13) 0.00378 4.25313 1.51762 1.41869

34 C(13) -0.00676 -7.59495 -2.71007 -2.53340

35 C(13) -0.00676 -7.59495 -2.71007 -2.53340

36 C(13) 0.00271 3.05020 1.08839 1.01744

37 C(13) 0.00271 3.05020 1.08839 1.01744

38 C(13) -0.00676 -7.59495 -2.71007 -2.53340

39 C(13) 0.00271 3.05020 1.08839 1.01744

40 C(13) -0.00676 -7.59495 -2.71007 -2.53340

41 C(13) 0.00271 3.05020 1.08839 1.01744

42 H(1) -0.00087 -3.89801 -1.39091 -1.30024

43 H(1) -0.00087 -3.89801 -1.39091 -1.30024

44 H(1) -0.00087 -3.89801 -1.39091 -1.30024

45 H(1) -0.00087 -3.89801 -1.39091 -1.30024

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Center ---- Spin Dipole Couplings ----

3XX-RR 3YY-RR 3ZZ-RR

--------------------------------------------------------

1 Atom 0.003471 0.003897 -0.007368

2 Atom 0.015531 0.006645 -0.022176

3 Atom -0.086856 -0.091141 0.177997

4 Atom 0.015531 0.006645 -0.022176

5 Atom 0.003471 0.003897 -0.007368

6 Atom -0.060699 -0.059668 0.120367

7 Atom -0.050746 -0.050768 0.101514

8 Atom 0.019896 0.020027 -0.039923

9 Atom -0.050746 -0.050768 0.101514

10 Atom -0.042672 -0.043114 0.085786

11 Atom -0.042672 -0.043114 0.085786

12 Atom -0.060699 -0.059668 0.120367

13 Atom -0.050746 -0.050768 0.101514

14 Atom -0.042672 -0.043114 0.085786

15 Atom -0.042672 -0.043114 0.085786

16 Atom -0.050746 -0.050768 0.101514

17 Atom 0.019896 0.020027 -0.039923

18 Atom -0.060699 -0.059668 0.120367

19 Atom 0.015531 0.006645 -0.022176

20 Atom 0.003471 0.003897 -0.007368

21 Atom 0.003471 0.003897 -0.007368

22 Atom 0.015531 0.006645 -0.022176

23 Atom -0.086856 -0.091141 0.177997

24 Atom 0.000408 0.000713 -0.001122

25 Atom 0.000408 0.000713 -0.001122

26 Atom 0.004680 -0.002457 -0.002223

27 Atom 0.004680 -0.002457 -0.002223

28 Atom 0.004680 -0.002457 -0.002223

29 Atom 0.004680 -0.002457 -0.002223

30 Atom 0.000408 0.000713 -0.001122

31 Atom 0.000408 0.000713 -0.001122

32 Atom -0.008739 0.008239 0.000499

33 Atom -0.060699 -0.059668 0.120367

34 Atom 0.007174 0.007950 -0.015124

35 Atom 0.007174 0.007950 -0.015124

36 Atom -0.025433 -0.024109 0.049542

37 Atom -0.025433 -0.024109 0.049542

38 Atom 0.007174 0.007950 -0.015124

39 Atom -0.025433 -0.024109 0.049542

40 Atom 0.007174 0.007950 -0.015124

41 Atom -0.025433 -0.024109 0.049542

42 Atom 0.000166 0.000607 -0.000773

43 Atom 0.000166 0.000607 -0.000773

44 Atom 0.000166 0.000607 -0.000773

45 Atom 0.000166 0.000607 -0.000773

--------------------------------------------------------

XY XZ YZ

--------------------------------------------------------

1 Atom -0.000552 -0.000000 0.000000

2 Atom 0.000966 -0.000000 -0.000000

3 Atom -0.000000 0.000000 0.000003

4 Atom -0.000966 0.000000 -0.000000

5 Atom 0.000552 0.000000 0.000000

6 Atom 0.001452 -0.000001 0.000000

7 Atom 0.003289 -0.000001 -0.000000

8 Atom 0.000000 0.000001 -0.000000

9 Atom -0.003289 -0.000001 0.000000

10 Atom 0.000273 -0.000001 0.000000

11 Atom -0.000273 -0.000001 -0.000000

12 Atom -0.001452 0.000001 0.000000

13 Atom -0.003289 0.000001 -0.000000

14 Atom 0.000273 0.000001 -0.000000

15 Atom -0.000273 0.000001 0.000000

16 Atom 0.003289 0.000001 0.000000

17 Atom 0.000000 -0.000001 0.000000

18 Atom 0.001452 0.000001 -0.000000

19 Atom -0.000966 -0.000000 0.000000

20 Atom 0.000552 -0.000000 -0.000000

21 Atom -0.000552 0.000000 -0.000000

22 Atom 0.000966 0.000000 0.000000

23 Atom -0.000000 0.000000 -0.000003

24 Atom -0.000722 -0.000000 -0.000000

25 Atom 0.000722 0.000000 -0.000000

26 Atom 0.005998 0.000000 0.000000

27 Atom -0.005998 0.000000 -0.000000

28 Atom 0.005998 -0.000000 -0.000000

29 Atom -0.005998 -0.000000 0.000000

30 Atom 0.000722 -0.000000 0.000000

31 Atom -0.000722 0.000000 0.000000

32 Atom -0.000000 0.000000 0.000000

33 Atom -0.001452 -0.000001 -0.000000

34 Atom 0.008904 0.000001 -0.000000

35 Atom 0.008904 -0.000001 0.000000

36 Atom -0.002787 -0.000001 0.000000

37 Atom -0.002787 0.000001 -0.000000

38 Atom -0.008904 0.000001 0.000000

39 Atom 0.002787 -0.000001 -0.000000

40 Atom -0.008904 -0.000001 -0.000000

41 Atom 0.002787 0.000001 0.000000

42 Atom -0.003919 0.000000 0.000000

43 Atom 0.003919 -0.000000 0.000000

44 Atom -0.003919 -0.000000 -0.000000

45 Atom 0.003919 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 -0.0074 -0.989 -0.353 -0.330 0.0000 -0.0000 1.0000

1 C(13) Bbb 0.0031 0.415 0.148 0.138 0.8247 0.5655 -0.0000

Bcc 0.0043 0.574 0.205 0.191 -0.5655 0.8247 0.0000

Baa -0.0222 -2.976 -1.062 -0.993 0.0000 0.0000 1.0000

2 C(13) Bbb 0.0065 0.878 0.313 0.293 -0.1068 0.9943 -0.0000

Bcc 0.0156 2.098 0.749 0.700 0.9943 0.1068 -0.0000

Baa -0.0911 -3.515 -1.254 -1.173 0.0000 1.0000 -0.0000

3 N(14) Bbb -0.0869 -3.350 -1.195 -1.117 1.0000 -0.0000 0.0000

Bcc 0.1780 6.865 2.450 2.290 0.0000 0.0000 1.0000

Baa -0.0222 -2.976 -1.062 -0.993 -0.0000 0.0000 1.0000

4 C(13) Bbb 0.0065 0.878 0.313 0.293 0.1068 0.9943 -0.0000

Bcc 0.0156 2.098 0.749 0.700 0.9943 -0.1068 0.0000

Baa -0.0074 -0.989 -0.353 -0.330 -0.0000 -0.0000 1.0000

5 C(13) Bbb 0.0031 0.415 0.148 0.138 0.8247 -0.5655 0.0000

Bcc 0.0043 0.574 0.205 0.191 0.5655 0.8247 0.0000

Baa -0.0617 -8.283 -2.956 -2.763 0.8168 -0.5769 0.0000

6 C(13) Bbb -0.0586 -7.869 -2.808 -2.625 0.5769 0.8168 0.0000

Bcc 0.1204 16.152 5.763 5.388 -0.0000 0.0000 1.0000

Baa -0.0540 -7.252 -2.588 -2.419 -0.7059 0.7083 -0.0000

7 C(13) Bbb -0.0475 -6.370 -2.273 -2.125 0.7083 0.7059 0.0000

Bcc 0.1015 13.622 4.861 4.544 -0.0000 -0.0000 1.0000

Baa -0.0399 -1.540 -0.549 -0.514 -0.0000 0.0000 1.0000

8 N(14) Bbb 0.0199 0.767 0.274 0.256 1.0000 -0.0000 0.0000

Bcc 0.0200 0.772 0.276 0.258 0.0000 1.0000 0.0000

Baa -0.0540 -7.252 -2.588 -2.419 0.7059 0.7083 0.0000

9 C(13) Bbb -0.0475 -6.370 -2.273 -2.125 0.7083 -0.7059 0.0000

Bcc 0.1015 13.622 4.861 4.544 -0.0000 0.0000 1.0000

Baa -0.0432 -5.803 -2.071 -1.936 -0.4306 0.9025 -0.0000

10 C(13) Bbb -0.0425 -5.709 -2.037 -1.904 0.9025 0.4306 0.0000

Bcc 0.0858 11.512 4.108 3.840 -0.0000 0.0000 1.0000

Baa -0.0432 -5.803 -2.071 -1.936 0.4306 0.9025 0.0000

11 C(13) Bbb -0.0425 -5.709 -2.037 -1.904 0.9025 -0.4306 0.0000

Bcc 0.0858 11.512 4.108 3.840 -0.0000 -0.0000 1.0000

Baa -0.0617 -8.283 -2.956 -2.763 0.8168 0.5769 -0.0000

12 C(13) Bbb -0.0586 -7.869 -2.808 -2.625 -0.5769 0.8168 0.0000

Bcc 0.1204 16.152 5.763 5.388 0.0000 0.0000 1.0000

Baa -0.0540 -7.252 -2.588 -2.419 0.7059 0.7083 -0.0000

13 C(13) Bbb -0.0475 -6.370 -2.273 -2.125 0.7083 -0.7059 -0.0000

Bcc 0.1015 13.622 4.861 4.544 0.0000 -0.0000 1.0000

Baa -0.0432 -5.803 -2.071 -1.936 -0.4306 0.9025 0.0000

14 C(13) Bbb -0.0425 -5.709 -2.037 -1.904 0.9025 0.4306 -0.0000

Bcc 0.0858 11.512 4.108 3.840 0.0000 -0.0000 1.0000

Baa -0.0432 -5.803 -2.071 -1.936 0.4306 0.9025 -0.0000

15 C(13) Bbb -0.0425 -5.709 -2.037 -1.904 0.9025 -0.4306 -0.0000

Bcc 0.0858 11.512 4.108 3.840 0.0000 0.0000 1.0000

Baa -0.0540 -7.252 -2.588 -2.419 -0.7059 0.7083 0.0000

16 C(13) Bbb -0.0475 -6.370 -2.273 -2.125 0.7083 0.7059 -0.0000

Bcc 0.1015 13.622 4.861 4.544 0.0000 0.0000 1.0000

Baa -0.0399 -1.540 -0.549 -0.514 0.0000 -0.0000 1.0000

17 N(14) Bbb 0.0199 0.767 0.274 0.256 1.0000 -0.0000 -0.0000

Bcc 0.0200 0.772 0.276 0.258 0.0000 1.0000 -0.0000

Baa -0.0617 -8.283 -2.956 -2.763 0.8168 -0.5769 -0.0000

18 C(13) Bbb -0.0586 -7.869 -2.808 -2.625 0.5769 0.8168 -0.0000

Bcc 0.1204 16.152 5.763 5.388 0.0000 -0.0000 1.0000

Baa -0.0222 -2.976 -1.062 -0.993 0.0000 -0.0000 1.0000

19 C(13) Bbb 0.0065 0.878 0.313 0.293 0.1068 0.9943 0.0000

Bcc 0.0156 2.098 0.749 0.700 0.9943 -0.1068 -0.0000

Baa -0.0074 -0.989 -0.353 -0.330 0.0000 0.0000 1.0000

20 C(13) Bbb 0.0031 0.415 0.148 0.138 0.8247 -0.5655 -0.0000

Bcc 0.0043 0.574 0.205 0.191 0.5655 0.8247 -0.0000

Baa -0.0074 -0.989 -0.353 -0.330 -0.0000 0.0000 1.0000

21 C(13) Bbb 0.0031 0.415 0.148 0.138 0.8247 0.5655 0.0000

Bcc 0.0043 0.574 0.205 0.191 -0.5655 0.8247 -0.0000

Baa -0.0222 -2.976 -1.062 -0.993 -0.0000 -0.0000 1.0000

22 C(13) Bbb 0.0065 0.878 0.313 0.293 -0.1068 0.9943 0.0000

Bcc 0.0156 2.098 0.749 0.700 0.9943 0.1068 0.0000

Baa -0.0911 -3.515 -1.254 -1.173 -0.0000 1.0000 0.0000

23 N(14) Bbb -0.0869 -3.350 -1.195 -1.117 1.0000 0.0000 0.0000

Bcc 0.1780 6.865 2.450 2.290 0.0000 -0.0000 1.0000

Baa -0.0011 -0.599 -0.214 -0.200 0.0000 0.0000 1.0000

24 H(1) Bbb -0.0002 -0.095 -0.034 -0.032 0.7768 0.6298 -0.0000

Bcc 0.0013 0.693 0.247 0.231 -0.6298 0.7768 -0.0000

Baa -0.0011 -0.599 -0.214 -0.200 -0.0000 0.0000 1.0000

25 H(1) Bbb -0.0002 -0.095 -0.034 -0.032 0.7768 -0.6298 0.0000

Bcc 0.0013 0.693 0.247 0.231 0.6298 0.7768 -0.0000

Baa -0.0059 -3.131 -1.117 -1.044 -0.4943 0.8693 -0.0000

26 H(1) Bbb -0.0022 -1.186 -0.423 -0.396 -0.0000 0.0000 1.0000

Bcc 0.0081 4.317 1.540 1.440 0.8693 0.4943 0.0000

Baa -0.0059 -3.131 -1.117 -1.044 0.4943 0.8693 0.0000

27 H(1) Bbb -0.0022 -1.186 -0.423 -0.396 -0.0000 -0.0000 1.0000

Bcc 0.0081 4.317 1.540 1.440 0.8693 -0.4943 0.0000

Baa -0.0059 -3.131 -1.117 -1.044 -0.4943 0.8693 0.0000

28 H(1) Bbb -0.0022 -1.186 -0.423 -0.396 0.0000 -0.0000 1.0000

Bcc 0.0081 4.317 1.540 1.440 0.8693 0.4943 -0.0000

Baa -0.0059 -3.131 -1.117 -1.044 0.4943 0.8693 -0.0000

29 H(1) Bbb -0.0022 -1.186 -0.423 -0.396 0.0000 0.0000 1.0000

Bcc 0.0081 4.317 1.540 1.440 0.8693 -0.4943 -0.0000

Baa -0.0011 -0.599 -0.214 -0.200 0.0000 -0.0000 1.0000

30 H(1) Bbb -0.0002 -0.095 -0.034 -0.032 0.7768 -0.6298 -0.0000

Bcc 0.0013 0.693 0.247 0.231 0.6298 0.7768 0.0000

Baa -0.0011 -0.599 -0.214 -0.200 -0.0000 -0.0000 1.0000

31 H(1) Bbb -0.0002 -0.095 -0.034 -0.032 0.7768 0.6298 0.0000

Bcc 0.0013 0.693 0.247 0.231 -0.6298 0.7768 0.0000

Baa -0.0087 -0.292 -0.104 -0.098 1.0000 0.0000 -0.0000

32 Zn(67) Bbb 0.0005 0.017 0.006 0.006 0.0000 0.0000 1.0000

Bcc 0.0082 0.276 0.098 0.092 -0.0000 1.0000 -0.0000

Baa -0.0617 -8.283 -2.956 -2.763 0.8168 0.5769 0.0000

33 C(13) Bbb -0.0586 -7.869 -2.808 -2.625 -0.5769 0.8168 -0.0000

Bcc 0.1204 16.152 5.763 5.388 -0.0000 -0.0000 1.0000

Baa -0.0151 -2.030 -0.724 -0.677 -0.0000 0.0000 1.0000

34 C(13) Bbb -0.0014 -0.181 -0.065 -0.060 0.7223 -0.6916 0.0000

Bcc 0.0165 2.211 0.789 0.737 0.6916 0.7223 0.0000

Baa -0.0151 -2.030 -0.724 -0.677 0.0000 -0.0000 1.0000

35 C(13) Bbb -0.0014 -0.181 -0.065 -0.060 0.7223 -0.6916 -0.0000

Bcc 0.0165 2.211 0.789 0.737 0.6916 0.7223 -0.0000

Baa -0.0276 -3.708 -1.323 -1.237 0.7846 0.6200 0.0000

36 C(13) Bbb -0.0219 -2.940 -1.049 -0.981 -0.6200 0.7846 -0.0000

Bcc 0.0495 6.648 2.372 2.218 -0.0000 0.0000 1.0000

Baa -0.0276 -3.708 -1.323 -1.237 0.7846 0.6200 -0.0000

37 C(13) Bbb -0.0219 -2.940 -1.049 -0.981 -0.6200 0.7846 0.0000

Bcc 0.0495 6.648 2.372 2.218 0.0000 -0.0000 1.0000

Baa -0.0151 -2.030 -0.724 -0.677 -0.0000 -0.0000 1.0000

38 C(13) Bbb -0.0014 -0.181 -0.065 -0.060 0.7223 0.6916 0.0000

Bcc 0.0165 2.211 0.789 0.737 -0.6916 0.7223 -0.0000

Baa -0.0276 -3.708 -1.323 -1.237 0.7846 -0.6200 0.0000

39 C(13) Bbb -0.0219 -2.940 -1.049 -0.981 0.6200 0.7846 0.0000

Bcc 0.0495 6.648 2.372 2.218 -0.0000 -0.0000 1.0000

Baa -0.0151 -2.030 -0.724 -0.677 0.0000 0.0000 1.0000

40 C(13) Bbb -0.0014 -0.181 -0.065 -0.060 0.7223 0.6916 -0.0000

Bcc 0.0165 2.211 0.789 0.737 -0.6916 0.7223 0.0000

Baa -0.0276 -3.708 -1.323 -1.237 0.7846 -0.6200 -0.0000

41 C(13) Bbb -0.0219 -2.940 -1.049 -0.981 0.6200 0.7846 -0.0000

Bcc 0.0495 6.648 2.372 2.218 0.0000 0.0000 1.0000

Baa -0.0035 -1.888 -0.674 -0.630 0.7267 0.6870 -0.0000

42 H(1) Bbb -0.0008 -0.412 -0.147 -0.138 0.0000 0.0000 1.0000

Bcc 0.0043 2.301 0.821 0.767 -0.6870 0.7267 0.0000

Baa -0.0035 -1.888 -0.674 -0.630 0.7267 -0.6870 0.0000

43 H(1) Bbb -0.0008 -0.412 -0.147 -0.138 -0.0000 0.0000 1.0000

Bcc 0.0043 2.301 0.821 0.767 0.6870 0.7267 0.0000

Baa -0.0035 -1.888 -0.674 -0.630 0.7267 0.6870 0.0000

44 H(1) Bbb -0.0008 -0.412 -0.147 -0.138 -0.0000 -0.0000 1.0000

Bcc 0.0043 2.301 0.821 0.767 -0.6870 0.7267 -0.0000

Baa -0.0035 -1.888 -0.674 -0.630 0.7267 -0.6870 -0.0000

45 H(1) Bbb -0.0008 -0.412 -0.147 -0.138 0.0000 -0.0000 1.0000

Bcc 0.0043 2.301 0.821 0.767 0.6870 0.7267 -0.0000

---------------------------------------------------------------------------------

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Wed Jul 31 05:38:58 2019, MaxMem= 4294967296 cpu: 31.6

(Enter /home/kira/g09/l716.exe)

Rotating derivatives to standard orientation.

Dipole = 4.10796397D-13-5.43079470D-13 1.92607280D-04

Polarizability= 1.65446918D+03-1.46225698D-05 1.17979773D+03

5.99577530D-08 4.08497230D-07 1.87126946D+02

Full mass-weighted force constant matrix:

Low frequencies --- -0.0007 0.0007 0.0007 8.5283 11.9875 12.9890

Low frequencies --- 15.3205 39.9794 49.8576

Diagonal vibrational polarizability:

172.1283003 50.9553981 145.8967396

Harmonic frequencies (cm\*\*-1), IR intensities (KM/Mole), Raman scattering

activities (A\*\*4/AMU), depolarization ratios for plane and unpolarized

incident light, reduced masses (AMU), force constants (mDyne/A),

and normal coordinates:

1 2 3

A2 A1 A1

Frequencies -- 12.9890 39.9794 49.8576

Red. masses -- 6.2069 5.9479 5.2955

Frc consts -- 0.0006 0.0056 0.0078

IR Inten -- 0.0000 1.9871 0.0243

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.03 0.00 0.00 0.04 -0.00 -0.00 -0.17

2 6 0.00 0.00 0.05 0.00 0.00 -0.04 0.00 -0.00 -0.08

3 7 0.00 0.00 -0.00 0.00 0.00 -0.10 -0.00 -0.00 -0.05

4 6 0.00 -0.00 -0.05 -0.00 0.00 -0.04 -0.00 -0.00 -0.08

5 6 0.00 -0.00 -0.03 -0.00 0.00 0.04 0.00 -0.00 -0.17

6 6 0.00 -0.00 -0.09 -0.00 0.00 -0.02 -0.00 -0.00 -0.01

7 6 0.00 -0.00 -0.05 -0.00 0.00 -0.07 -0.00 0.00 0.07

8 7 -0.00 -0.00 -0.00 -0.00 -0.00 -0.09 -0.00 0.00 -0.02

9 6 -0.00 -0.00 0.05 -0.00 -0.00 -0.07 -0.00 -0.00 0.07

10 6 -0.00 -0.00 0.03 -0.00 -0.00 -0.05 -0.00 -0.00 0.22

11 6 0.00 -0.00 -0.03 -0.00 0.00 -0.05 -0.00 0.00 0.22

12 6 0.00 0.00 0.09 0.00 0.00 -0.02 0.00 -0.00 -0.01

13 6 0.00 0.00 0.05 0.00 0.00 -0.07 0.00 0.00 0.07

14 6 0.00 0.00 0.03 0.00 0.00 -0.05 0.00 0.00 0.22

15 6 -0.00 0.00 -0.03 0.00 -0.00 -0.05 0.00 -0.00 0.22

16 6 -0.00 0.00 -0.05 0.00 -0.00 -0.07 0.00 -0.00 0.07

17 7 -0.00 0.00 -0.00 0.00 0.00 -0.09 0.00 -0.00 -0.02

18 6 -0.00 0.00 -0.09 0.00 -0.00 -0.02 0.00 0.00 -0.01

19 6 -0.00 0.00 -0.05 0.00 -0.00 -0.04 0.00 0.00 -0.08

20 6 -0.00 0.00 -0.03 0.00 -0.00 0.04 -0.00 0.00 -0.17

21 6 -0.00 -0.00 0.03 -0.00 -0.00 0.04 0.00 0.00 -0.17

22 6 -0.00 -0.00 0.05 -0.00 -0.00 -0.04 -0.00 0.00 -0.08

23 7 -0.00 -0.00 -0.00 -0.00 -0.00 -0.10 0.00 0.00 -0.05

24 1 0.00 0.00 0.07 -0.00 0.00 0.09 -0.00 -0.00 -0.22

25 1 0.00 -0.00 -0.07 0.00 0.00 0.09 0.00 -0.00 -0.22

26 1 -0.00 -0.00 0.06 -0.00 0.00 -0.03 -0.00 0.00 0.32

27 1 0.00 -0.00 -0.06 -0.00 -0.00 -0.03 -0.00 -0.00 0.32

28 1 0.00 0.00 0.06 0.00 -0.00 -0.03 0.00 -0.00 0.32

29 1 -0.00 0.00 -0.06 0.00 0.00 -0.03 0.00 0.00 0.32

30 1 -0.00 0.00 -0.07 -0.00 -0.00 0.09 -0.00 0.00 -0.22

31 1 -0.00 -0.00 0.07 0.00 -0.00 0.09 0.00 0.00 -0.22

32 30 -0.00 -0.00 -0.00 0.00 0.00 -0.11 -0.00 -0.00 -0.04

33 6 -0.00 -0.00 0.09 -0.00 -0.00 -0.02 -0.00 0.00 -0.01

34 6 -0.00 -0.00 0.18 -0.00 -0.00 0.10 -0.00 -0.00 0.01

35 6 0.00 0.00 0.18 0.00 0.00 0.10 0.00 0.00 0.01

36 6 -0.00 -0.00 0.27 -0.00 0.00 0.25 0.00 -0.00 0.04

37 6 0.00 0.00 0.27 0.00 -0.00 0.25 -0.00 0.00 0.04

38 6 0.00 -0.00 -0.18 -0.00 0.00 0.10 -0.00 0.00 0.01

39 6 0.00 -0.00 -0.27 -0.00 -0.00 0.25 0.00 0.00 0.04

40 6 -0.00 0.00 -0.18 0.00 -0.00 0.10 0.00 -0.00 0.01

41 6 -0.00 0.00 -0.27 0.00 0.00 0.25 -0.00 -0.00 0.04

42 1 -0.00 -0.00 -0.35 0.00 0.00 0.38 -0.00 -0.00 0.06

43 1 -0.00 0.00 0.35 -0.00 0.00 0.38 0.00 -0.00 0.06

44 1 0.00 0.00 -0.35 -0.00 -0.00 0.38 0.00 0.00 0.06

45 1 0.00 -0.00 0.35 0.00 -0.00 0.38 -0.00 0.00 0.06

4 5 6

B1 B2 A1

Frequencies -- 60.4494 65.9576 90.0270

Red. masses -- 4.9670 5.0610 5.5969

Frc consts -- 0.0107 0.0130 0.0267

IR Inten -- 0.0000 0.0000 0.3311

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.00 -0.01 -0.00 0.00 0.18 -0.00 -0.00 -0.19

2 6 0.00 -0.00 -0.00 -0.00 0.00 0.09 -0.00 -0.00 -0.03

3 7 0.00 -0.00 0.00 0.00 0.00 0.06 0.00 -0.00 0.06

4 6 0.00 0.00 0.00 0.00 0.00 0.09 0.00 -0.00 -0.03

5 6 0.00 0.00 0.01 0.00 0.00 0.18 0.00 -0.00 -0.19

6 6 0.00 0.00 -0.01 0.00 0.00 0.03 0.00 -0.00 -0.00

7 6 0.00 0.00 -0.08 0.00 0.00 0.01 0.00 -0.00 0.00

8 7 0.00 0.00 -0.03 -0.00 -0.00 -0.00 0.00 -0.00 0.09

9 6 0.00 -0.00 -0.08 -0.00 0.00 -0.01 0.00 0.00 0.00

10 6 0.00 -0.00 -0.19 -0.00 0.00 0.00 0.00 0.00 -0.14

11 6 0.00 0.00 -0.19 0.00 0.00 -0.00 0.00 -0.00 -0.14

12 6 0.00 -0.00 0.01 -0.00 0.00 0.03 -0.00 -0.00 -0.00

13 6 0.00 -0.00 0.08 -0.00 0.00 0.01 -0.00 -0.00 0.00

14 6 0.00 -0.00 0.19 -0.00 0.00 -0.00 -0.00 -0.00 -0.14

15 6 0.00 0.00 0.19 0.00 0.00 0.00 -0.00 0.00 -0.14

16 6 0.00 0.00 0.08 0.00 0.00 -0.01 -0.00 0.00 0.00

17 7 0.00 0.00 0.03 -0.00 -0.00 0.00 -0.00 0.00 0.09

18 6 0.00 0.00 0.01 0.00 0.00 -0.03 -0.00 0.00 -0.00

19 6 0.00 0.00 -0.00 0.00 0.00 -0.09 -0.00 0.00 -0.03

20 6 0.00 0.00 -0.01 0.00 0.00 -0.18 -0.00 0.00 -0.19

21 6 0.00 -0.00 0.01 -0.00 0.00 -0.18 0.00 0.00 -0.19

22 6 0.00 -0.00 0.00 -0.00 0.00 -0.09 0.00 0.00 -0.03

23 7 0.00 -0.00 -0.00 0.00 0.00 -0.06 -0.00 0.00 0.06

24 1 0.00 -0.00 -0.02 -0.00 0.00 0.23 0.00 -0.00 -0.31

25 1 0.00 0.00 0.02 0.00 0.00 0.23 -0.00 -0.00 -0.31

26 1 0.00 -0.00 -0.27 -0.00 0.00 -0.00 0.00 -0.00 -0.24

27 1 0.00 0.00 -0.27 0.00 0.00 0.00 0.00 0.00 -0.24

28 1 0.00 -0.00 0.27 -0.00 0.00 0.00 -0.00 0.00 -0.24

29 1 0.00 0.00 0.27 0.00 0.00 -0.00 -0.00 -0.00 -0.24

30 1 0.00 0.00 -0.02 0.00 0.00 -0.23 0.00 0.00 -0.31

31 1 0.00 -0.00 0.02 -0.00 0.00 -0.23 -0.00 0.00 -0.31

32 30 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.15

33 6 0.00 -0.00 -0.01 -0.00 0.00 -0.03 0.00 0.00 -0.00

34 6 -0.00 0.00 0.07 -0.00 0.00 0.07 0.00 0.00 0.02

35 6 -0.00 0.00 -0.07 -0.00 0.00 -0.07 -0.00 -0.00 0.02

36 6 -0.00 0.00 0.20 -0.00 0.00 0.21 0.00 0.00 0.09

37 6 -0.00 0.00 -0.20 -0.00 0.00 -0.21 -0.00 -0.00 0.09

38 6 -0.00 -0.00 0.07 0.00 0.00 -0.07 0.00 -0.00 0.02

39 6 -0.00 -0.00 0.20 0.00 0.00 -0.21 0.00 -0.00 0.09

40 6 -0.00 -0.00 -0.07 0.00 0.00 0.07 -0.00 0.00 0.02

41 6 -0.00 -0.00 -0.20 0.00 0.00 0.21 -0.00 0.00 0.09

42 1 -0.00 -0.00 -0.30 0.00 0.00 0.32 -0.00 -0.00 0.15

43 1 -0.00 0.00 0.30 -0.00 0.00 0.32 0.00 -0.00 0.15

44 1 -0.00 -0.00 0.30 0.00 0.00 -0.32 0.00 0.00 0.15

45 1 -0.00 0.00 -0.30 -0.00 0.00 -0.32 -0.00 0.00 0.15

7 8 9

A1 B1 B2

Frequencies -- 111.1235 113.7220 113.9180

Red. masses -- 4.2468 4.3782 4.3701

Frc consts -- 0.0309 0.0334 0.0334

IR Inten -- 0.0000 6.4213 1.4086

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.01 -0.00 -0.01 -0.00 -0.00 0.00 0.04 0.00

2 6 0.00 0.01 0.00 -0.02 0.00 0.00 0.00 0.04 -0.00

3 7 0.00 0.01 0.00 -0.02 -0.00 0.00 -0.00 0.04 -0.00

4 6 -0.00 0.01 0.00 -0.02 -0.00 -0.00 -0.00 0.04 -0.00

5 6 -0.00 0.01 -0.00 -0.01 0.00 0.00 -0.00 0.04 0.00

6 6 0.00 0.00 -0.00 -0.02 0.00 -0.00 -0.00 0.02 -0.00

7 6 0.01 -0.00 -0.00 -0.03 0.00 -0.00 0.00 0.02 -0.00

8 7 0.01 -0.00 -0.00 -0.04 -0.00 -0.00 -0.00 0.02 0.00

9 6 0.01 0.00 -0.00 -0.03 -0.00 -0.00 -0.00 0.02 0.00

10 6 0.01 0.00 0.00 -0.03 -0.00 -0.00 0.00 0.01 0.00

11 6 0.01 -0.00 0.00 -0.03 0.00 -0.00 -0.00 0.01 -0.00

12 6 -0.00 0.00 -0.00 -0.02 -0.00 0.00 0.00 0.02 -0.00

13 6 -0.01 -0.00 -0.00 -0.03 -0.00 0.00 -0.00 0.02 -0.00

14 6 -0.01 -0.00 0.00 -0.03 -0.00 0.00 0.00 0.01 -0.00

15 6 -0.01 0.00 0.00 -0.03 0.00 0.00 -0.00 0.01 0.00

16 6 -0.01 0.00 -0.00 -0.03 0.00 0.00 0.00 0.02 0.00

17 7 -0.01 0.00 -0.00 -0.04 -0.00 0.00 -0.00 0.02 -0.00

18 6 -0.00 -0.00 -0.00 -0.02 0.00 0.00 -0.00 0.02 0.00

19 6 0.00 -0.01 0.00 -0.02 -0.00 0.00 -0.00 0.04 0.00

20 6 0.00 -0.01 -0.00 -0.01 0.00 -0.00 -0.00 0.04 -0.00

21 6 -0.00 -0.01 -0.00 -0.01 -0.00 0.00 0.00 0.04 -0.00

22 6 -0.00 -0.01 0.00 -0.02 0.00 -0.00 0.00 0.04 0.00

23 7 -0.00 -0.01 0.00 -0.02 -0.00 -0.00 -0.00 0.04 0.00

24 1 0.00 0.01 -0.00 -0.01 -0.00 -0.00 0.00 0.04 0.00

25 1 -0.00 0.01 -0.00 -0.01 0.00 0.00 -0.00 0.04 0.00

26 1 0.01 0.00 0.00 -0.04 -0.00 0.00 0.00 0.01 0.00

27 1 0.01 -0.00 0.00 -0.04 0.00 0.00 -0.00 0.01 -0.00

28 1 -0.01 -0.00 0.00 -0.04 -0.00 -0.00 0.00 0.01 -0.00

29 1 -0.01 0.00 0.00 -0.04 0.00 -0.00 -0.00 0.01 0.00

30 1 0.00 -0.01 -0.00 -0.01 0.00 -0.00 -0.00 0.04 -0.00

31 1 -0.00 -0.01 -0.00 -0.01 -0.00 0.00 0.00 0.04 -0.00

32 30 0.00 0.00 0.00 -0.04 -0.00 0.00 -0.00 0.04 -0.00

33 6 0.00 -0.00 -0.00 -0.02 -0.00 -0.00 0.00 0.02 0.00

34 6 -0.04 0.04 -0.00 0.02 -0.05 0.00 0.05 -0.02 0.00

35 6 0.04 -0.04 -0.00 0.02 -0.05 -0.00 0.05 -0.02 -0.00

36 6 -0.18 0.19 -0.00 0.17 -0.20 0.00 0.19 -0.17 0.00

37 6 0.18 -0.19 -0.00 0.17 -0.20 -0.00 0.19 -0.17 -0.00

38 6 -0.04 -0.04 -0.00 0.02 0.05 0.00 -0.05 -0.02 -0.00

39 6 -0.18 -0.19 -0.00 0.17 0.20 0.00 -0.19 -0.17 -0.00

40 6 0.04 0.04 -0.00 0.02 0.05 -0.00 -0.05 -0.02 0.00

41 6 0.18 0.19 -0.00 0.17 0.20 -0.00 -0.19 -0.17 0.00

42 1 0.29 0.30 -0.00 0.28 0.31 -0.00 -0.30 -0.29 0.00

43 1 -0.29 0.30 -0.00 0.28 -0.31 0.00 0.30 -0.29 0.00

44 1 -0.29 -0.30 -0.00 0.28 0.31 0.00 -0.30 -0.29 -0.00

45 1 0.29 -0.30 -0.00 0.28 -0.31 -0.00 0.30 -0.29 -0.00

10 11 12

A2 A2 B1

Frequencies -- 140.4827 143.6947 144.0914

Red. masses -- 5.4682 4.2030 5.5015

Frc consts -- 0.0636 0.0511 0.0673

IR Inten -- 0.0000 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.00 -0.08 -0.08 0.01 0.00 -0.00 0.00 -0.07

2 6 -0.00 0.00 -0.11 -0.05 0.02 0.00 -0.00 0.00 -0.10

3 7 -0.00 0.00 0.00 -0.04 -0.00 0.00 -0.00 -0.00 0.00

4 6 -0.00 -0.00 0.11 -0.05 -0.02 -0.00 -0.00 -0.00 0.10

5 6 -0.00 -0.00 0.08 -0.08 -0.01 -0.00 -0.00 -0.00 0.07

6 6 -0.00 -0.00 0.18 -0.05 -0.04 -0.00 -0.00 -0.00 0.14

7 6 -0.00 -0.00 0.12 -0.03 -0.05 -0.00 -0.00 -0.00 0.09

8 7 0.00 -0.00 -0.00 -0.00 -0.03 -0.00 -0.00 0.00 0.22

9 6 0.00 -0.00 -0.12 0.03 -0.05 0.00 -0.00 0.00 0.09

10 6 0.00 -0.00 -0.09 0.02 -0.08 0.00 -0.00 0.00 -0.14

11 6 -0.00 -0.00 0.09 -0.02 -0.08 -0.00 -0.00 -0.00 -0.14

12 6 -0.00 0.00 -0.18 -0.05 0.04 0.00 -0.00 0.00 -0.14

13 6 -0.00 0.00 -0.12 -0.03 0.05 0.00 -0.00 0.00 -0.09

14 6 -0.00 0.00 -0.09 -0.02 0.08 0.00 -0.00 0.00 0.14

15 6 0.00 0.00 0.09 0.02 0.08 -0.00 -0.00 -0.00 0.14

16 6 0.00 0.00 0.12 0.03 0.05 -0.00 -0.00 -0.00 -0.09

17 7 -0.00 0.00 -0.00 0.00 0.03 -0.00 -0.00 0.00 -0.22

18 6 0.00 0.00 0.18 0.05 0.04 -0.00 -0.00 -0.00 -0.14

19 6 0.00 0.00 0.11 0.05 0.02 -0.00 -0.00 -0.00 -0.10

20 6 0.00 0.00 0.08 0.08 0.01 -0.00 -0.00 -0.00 -0.07

21 6 0.00 -0.00 -0.08 0.08 -0.01 0.00 -0.00 0.00 0.07

22 6 0.00 -0.00 -0.11 0.05 -0.02 0.00 -0.00 0.00 0.10

23 7 0.00 -0.00 0.00 0.04 0.00 0.00 -0.00 -0.00 -0.00

24 1 -0.00 0.00 -0.15 -0.10 0.03 0.00 -0.00 0.00 -0.14

25 1 -0.00 -0.00 0.15 -0.10 -0.03 -0.00 -0.00 -0.00 0.14

26 1 0.00 -0.00 -0.16 0.03 -0.10 0.00 -0.00 -0.00 -0.29

27 1 -0.00 -0.00 0.16 -0.03 -0.10 -0.00 -0.00 0.00 -0.29

28 1 -0.00 0.00 -0.16 -0.03 0.10 0.00 -0.00 -0.00 0.29

29 1 0.00 0.00 0.16 0.03 0.10 -0.00 -0.00 0.00 0.29

30 1 0.00 0.00 0.15 0.10 0.03 -0.00 -0.00 -0.00 -0.14

31 1 0.00 -0.00 -0.15 0.10 -0.03 0.00 -0.00 0.00 0.14

32 30 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00

33 6 0.00 -0.00 -0.18 0.05 -0.04 0.00 -0.00 0.00 0.14

34 6 0.00 0.00 -0.08 0.02 -0.01 0.00 -0.00 0.00 0.06

35 6 -0.00 -0.00 -0.08 -0.02 0.01 0.00 -0.00 0.00 -0.06

36 6 -0.00 0.00 0.15 -0.15 0.16 -0.00 0.00 -0.00 -0.10

37 6 0.00 -0.00 0.15 0.15 -0.16 -0.00 0.00 -0.00 0.10

38 6 -0.00 0.00 0.08 -0.02 -0.01 -0.00 -0.00 -0.00 0.06

39 6 0.00 0.00 -0.15 0.15 0.16 0.00 0.00 0.00 -0.10

40 6 0.00 -0.00 0.08 0.02 0.01 -0.00 -0.00 -0.00 -0.06

41 6 -0.00 -0.00 -0.15 -0.15 -0.16 0.00 0.00 0.00 0.10

42 1 -0.00 -0.00 -0.31 -0.27 -0.29 0.00 0.00 0.00 0.22

43 1 -0.00 0.00 0.31 -0.27 0.29 -0.00 0.00 -0.00 -0.22

44 1 0.00 0.00 -0.31 0.27 0.29 0.00 0.00 0.00 -0.22

45 1 0.00 -0.00 0.31 0.27 -0.29 -0.00 0.00 -0.00 0.22

13 14 15

B2 A2 A1

Frequencies -- 144.3783 164.0827 201.7316

Red. masses -- 5.4104 9.7055 10.6810

Frc consts -- 0.0664 0.1540 0.2561

IR Inten -- 0.0000 0.0000 84.0387

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.00 -0.16 -0.03 -0.04 0.00 -0.00 -0.00 0.10

2 6 -0.00 0.00 0.08 -0.12 -0.08 0.00 -0.00 -0.00 -0.09

3 7 -0.00 0.00 0.20 -0.16 -0.00 0.00 0.00 -0.00 -0.16

4 6 0.00 0.00 0.08 -0.12 0.08 -0.00 0.00 -0.00 -0.09

5 6 0.00 0.00 -0.16 -0.03 0.04 -0.00 0.00 -0.00 0.10

6 6 0.00 0.00 0.13 -0.14 0.14 -0.00 0.00 -0.00 -0.15

7 6 0.00 0.00 0.12 -0.07 0.12 -0.00 0.00 -0.00 -0.11

8 7 0.00 0.00 -0.00 -0.00 0.16 -0.00 0.00 -0.00 -0.20

9 6 -0.00 0.00 -0.12 0.07 0.12 0.00 0.00 0.00 -0.11

10 6 -0.00 0.00 -0.09 0.04 0.04 0.00 0.00 0.00 0.10

11 6 0.00 0.00 0.09 -0.04 0.04 -0.00 0.00 -0.00 0.10

12 6 -0.00 0.00 0.13 -0.14 -0.14 0.00 -0.00 -0.00 -0.15

13 6 -0.00 0.00 0.12 -0.07 -0.12 0.00 -0.00 -0.00 -0.11

14 6 -0.00 0.00 0.09 -0.04 -0.04 0.00 -0.00 -0.00 0.10

15 6 0.00 0.00 -0.09 0.04 -0.04 -0.00 -0.00 0.00 0.10

16 6 0.00 0.00 -0.12 0.07 -0.12 -0.00 -0.00 0.00 -0.11

17 7 0.00 0.00 0.00 0.00 -0.16 -0.00 -0.00 0.00 -0.20

18 6 0.00 0.00 -0.13 0.14 -0.14 -0.00 -0.00 0.00 -0.15

19 6 0.00 0.00 -0.08 0.12 -0.08 -0.00 -0.00 0.00 -0.09

20 6 0.00 0.00 0.16 0.03 -0.04 -0.00 -0.00 0.00 0.10

21 6 -0.00 0.00 0.16 0.03 0.04 0.00 0.00 0.00 0.10

22 6 -0.00 0.00 -0.08 0.12 0.08 0.00 0.00 0.00 -0.09

23 7 -0.00 0.00 -0.20 0.16 0.00 0.00 -0.00 0.00 -0.16

24 1 0.00 0.00 -0.32 0.02 -0.09 0.00 0.00 -0.00 0.24

25 1 -0.00 0.00 -0.32 0.02 0.09 -0.00 -0.00 -0.00 0.24

26 1 -0.00 0.00 -0.15 0.08 -0.01 0.00 0.00 -0.00 0.24

27 1 0.00 0.00 0.15 -0.08 -0.01 -0.00 0.00 0.00 0.24

28 1 -0.00 0.00 0.15 -0.08 0.01 0.00 -0.00 0.00 0.24

29 1 0.00 0.00 -0.15 0.08 0.01 -0.00 -0.00 -0.00 0.24

30 1 -0.00 0.00 0.32 -0.02 -0.09 -0.00 0.00 0.00 0.24

31 1 0.00 0.00 0.32 -0.02 0.09 0.00 -0.00 0.00 0.24

32 30 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.28

33 6 -0.00 0.00 -0.13 0.14 0.14 0.00 0.00 0.00 -0.15

34 6 0.00 0.00 -0.05 0.14 0.14 0.00 0.00 0.00 -0.08

35 6 0.00 0.00 0.05 -0.14 -0.14 0.00 -0.00 -0.00 -0.08

36 6 0.00 -0.00 0.07 0.15 0.14 -0.00 0.00 0.00 0.03

37 6 0.00 -0.00 -0.07 -0.15 -0.14 -0.00 -0.00 -0.00 0.03

38 6 -0.00 0.00 0.05 -0.14 0.14 -0.00 0.00 -0.00 -0.08

39 6 -0.00 -0.00 -0.07 -0.15 0.14 0.00 0.00 -0.00 0.03

40 6 -0.00 0.00 -0.05 0.14 -0.14 -0.00 -0.00 0.00 -0.08

41 6 -0.00 -0.00 0.07 0.15 -0.14 0.00 -0.00 0.00 0.03

42 1 -0.00 -0.00 0.16 0.16 -0.13 0.00 -0.00 0.00 0.12

43 1 0.00 -0.00 0.16 0.16 0.13 -0.00 0.00 0.00 0.12

44 1 -0.00 -0.00 -0.16 -0.16 0.13 0.00 0.00 -0.00 0.12

45 1 0.00 -0.00 -0.16 -0.16 -0.13 -0.00 -0.00 -0.00 0.12

16 17 18

A1 A1 B2

Frequencies -- 221.1432 223.2524 241.0286

Red. masses -- 8.2857 8.9423 7.0962

Frc consts -- 0.2387 0.2626 0.2429

IR Inten -- 0.3508 0.0001 0.0001

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 -0.06 0.00 0.20 0.00 -0.00 0.00 -0.03

2 6 -0.00 0.00 0.16 -0.02 0.17 -0.00 -0.00 -0.00 0.13

3 7 0.00 0.00 0.34 -0.00 0.17 -0.00 0.00 -0.00 0.31

4 6 0.00 0.00 0.16 0.02 0.17 -0.00 0.00 -0.00 0.13

5 6 -0.00 0.00 -0.06 -0.00 0.20 0.00 0.00 0.00 -0.03

6 6 0.00 0.00 -0.01 0.06 0.07 0.00 0.00 0.00 -0.09

7 6 0.00 0.00 -0.14 0.17 0.02 0.00 0.00 0.00 -0.15

8 7 0.00 -0.00 -0.28 0.17 0.00 0.00 -0.00 0.00 0.00

9 6 0.00 -0.00 -0.14 0.17 -0.02 0.00 -0.00 0.00 0.15

10 6 0.00 0.00 0.04 0.19 0.00 -0.00 -0.00 0.00 0.14

11 6 0.00 -0.00 0.04 0.19 -0.00 -0.00 0.00 0.00 -0.14

12 6 -0.00 0.00 -0.01 -0.06 0.07 0.00 -0.00 0.00 -0.09

13 6 -0.00 0.00 -0.14 -0.17 0.02 0.00 -0.00 0.00 -0.15

14 6 -0.00 -0.00 0.04 -0.19 -0.00 -0.00 -0.00 0.00 -0.14

15 6 -0.00 0.00 0.04 -0.19 0.00 -0.00 0.00 0.00 0.14

16 6 -0.00 -0.00 -0.14 -0.17 -0.02 0.00 0.00 0.00 0.15

17 7 -0.00 0.00 -0.28 -0.17 -0.00 0.00 -0.00 0.00 -0.00

18 6 -0.00 -0.00 -0.01 -0.06 -0.07 0.00 0.00 0.00 0.09

19 6 -0.00 -0.00 0.16 -0.02 -0.17 -0.00 0.00 -0.00 -0.13

20 6 0.00 -0.00 -0.06 0.00 -0.20 0.00 0.00 0.00 0.03

21 6 -0.00 -0.00 -0.06 -0.00 -0.20 0.00 -0.00 0.00 0.03

22 6 0.00 -0.00 0.16 0.02 -0.17 -0.00 -0.00 -0.00 -0.13

23 7 -0.00 -0.00 0.34 0.00 -0.17 -0.00 0.00 -0.00 -0.31

24 1 0.00 0.00 -0.25 0.01 0.19 0.00 0.00 -0.00 -0.19

25 1 -0.00 0.00 -0.25 -0.01 0.19 0.00 -0.00 -0.00 -0.19

26 1 0.00 0.00 0.19 0.19 0.01 -0.00 -0.00 0.00 0.23

27 1 0.00 -0.00 0.19 0.19 -0.01 -0.00 0.00 0.00 -0.23

28 1 -0.00 -0.00 0.19 -0.19 -0.01 -0.00 -0.00 0.00 -0.23

29 1 -0.00 0.00 0.19 -0.19 0.01 -0.00 0.00 0.00 0.23

30 1 0.00 -0.00 -0.25 0.01 -0.19 0.00 -0.00 -0.00 0.19

31 1 -0.00 -0.00 -0.25 -0.01 -0.19 0.00 0.00 -0.00 0.19

32 30 -0.00 -0.00 -0.01 0.00 0.00 0.00 -0.00 -0.00 0.00

33 6 0.00 -0.00 -0.01 0.06 -0.07 0.00 -0.00 0.00 0.09

34 6 0.00 -0.00 -0.02 0.00 -0.01 0.00 -0.00 0.00 0.11

35 6 -0.00 0.00 -0.02 -0.00 0.01 0.00 -0.00 0.00 -0.11

36 6 0.00 -0.00 0.02 0.02 -0.03 -0.00 0.00 0.00 -0.06

37 6 -0.00 0.00 0.02 -0.02 0.03 -0.00 0.00 0.00 0.06

38 6 0.00 0.00 -0.02 0.00 0.01 0.00 0.00 0.00 -0.11

39 6 0.00 0.00 0.02 0.02 0.03 -0.00 -0.00 0.00 0.06

40 6 -0.00 -0.00 -0.02 -0.00 -0.01 0.00 0.00 0.00 0.11

41 6 -0.00 -0.00 0.02 -0.02 -0.03 -0.00 -0.00 0.00 -0.06

42 1 -0.00 -0.00 0.05 -0.03 -0.04 -0.00 -0.00 -0.00 -0.17

43 1 0.00 -0.00 0.05 0.03 -0.04 -0.00 0.00 -0.00 -0.17

44 1 0.00 0.00 0.05 0.03 0.04 -0.00 -0.00 -0.00 0.17

45 1 -0.00 0.00 0.05 -0.03 0.04 -0.00 0.00 -0.00 0.17

19 20 21

B1 B1 B2

Frequencies -- 245.4933 246.2852 250.6997

Red. masses -- 6.6440 17.2937 18.0465

Frc consts -- 0.2359 0.6180 0.6683

IR Inten -- 0.0008 2.1426 15.2890

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.00 0.15 -0.17 0.00 -0.00 0.01 0.03 -0.00

2 6 -0.00 -0.00 0.15 -0.14 -0.00 -0.00 0.03 0.03 0.00

3 7 -0.00 -0.00 -0.00 -0.14 -0.00 0.00 -0.00 0.11 0.00

4 6 -0.00 0.00 -0.15 -0.14 0.00 0.00 -0.03 0.03 0.00

5 6 -0.00 -0.00 -0.15 -0.17 -0.00 0.00 -0.01 0.03 -0.00

6 6 -0.00 -0.00 -0.08 -0.12 -0.01 0.00 -0.00 -0.12 -0.00

7 6 0.00 -0.00 0.13 0.04 -0.03 -0.00 0.00 -0.15 -0.00

8 7 0.00 0.00 0.28 0.11 0.00 -0.01 0.00 -0.14 0.00

9 6 0.00 0.00 0.13 0.04 0.03 -0.00 -0.00 -0.15 0.00

10 6 0.00 0.00 -0.02 0.04 0.01 0.00 0.00 -0.16 0.00

11 6 0.00 -0.00 -0.02 0.04 -0.01 0.00 -0.00 -0.16 -0.00

12 6 -0.00 0.00 0.08 -0.12 0.01 -0.00 0.00 -0.12 -0.00

13 6 0.00 0.00 -0.13 0.04 0.03 0.00 -0.00 -0.15 -0.00

14 6 0.00 0.00 0.02 0.04 0.01 -0.00 0.00 -0.16 -0.00

15 6 0.00 -0.00 0.02 0.04 -0.01 -0.00 -0.00 -0.16 0.00

16 6 0.00 -0.00 -0.13 0.04 -0.03 0.00 0.00 -0.15 0.00

17 7 0.00 0.00 -0.28 0.11 0.00 0.01 0.00 -0.14 -0.00

18 6 -0.00 -0.00 0.08 -0.12 -0.01 -0.00 -0.00 -0.12 0.00

19 6 -0.00 0.00 0.15 -0.14 0.00 -0.00 -0.03 0.03 -0.00

20 6 -0.00 -0.00 0.15 -0.17 -0.00 -0.00 -0.01 0.03 0.00

21 6 -0.00 0.00 -0.15 -0.17 0.00 0.00 0.01 0.03 0.00

22 6 -0.00 -0.00 -0.15 -0.14 -0.00 0.00 0.03 0.03 -0.00

23 7 -0.00 -0.00 0.00 -0.14 -0.00 -0.00 -0.00 0.11 -0.00

24 1 -0.00 0.00 0.27 -0.18 0.01 -0.01 -0.01 0.05 -0.00

25 1 -0.00 -0.00 -0.27 -0.18 -0.01 0.01 0.01 0.05 -0.00

26 1 0.00 -0.00 -0.17 0.05 -0.01 0.01 0.01 -0.17 0.00

27 1 0.00 0.00 -0.17 0.05 0.01 0.01 -0.01 -0.17 -0.00

28 1 0.00 -0.00 0.17 0.05 -0.01 -0.01 0.01 -0.17 -0.00

29 1 0.00 0.00 0.17 0.05 0.01 -0.01 -0.01 -0.17 0.00

30 1 -0.00 -0.00 0.27 -0.18 -0.01 -0.01 0.01 0.05 0.00

31 1 -0.00 0.00 -0.27 -0.18 0.01 0.01 -0.01 0.05 0.00

32 30 0.01 -0.00 -0.00 0.41 -0.00 0.00 0.00 0.43 0.00

33 6 -0.00 0.00 -0.08 -0.12 0.01 0.00 0.00 -0.12 0.00

34 6 -0.00 0.00 -0.10 -0.16 0.03 0.00 0.02 -0.16 0.00

35 6 -0.00 0.00 0.10 -0.16 0.03 -0.00 0.02 -0.16 -0.00

36 6 -0.00 -0.00 0.06 -0.02 -0.11 -0.00 -0.11 -0.02 -0.00

37 6 -0.00 -0.00 -0.06 -0.02 -0.11 0.00 -0.11 -0.02 0.00

38 6 -0.00 -0.00 -0.10 -0.16 -0.03 0.00 -0.02 -0.16 -0.00

39 6 -0.00 0.00 0.06 -0.02 0.11 -0.00 0.11 -0.02 0.00

40 6 -0.00 -0.00 0.10 -0.16 -0.03 -0.00 -0.02 -0.16 0.00

41 6 -0.00 0.00 -0.06 -0.02 0.11 0.00 0.11 -0.02 -0.00

42 1 0.00 0.00 -0.15 0.07 0.21 0.00 0.21 0.08 -0.00

43 1 0.00 -0.00 0.15 0.07 -0.21 -0.00 -0.21 0.08 -0.00

44 1 0.00 0.00 0.15 0.07 0.21 -0.00 0.21 0.08 0.00

45 1 0.00 -0.00 -0.15 0.07 -0.21 0.00 -0.21 0.08 0.00

22 23 24

A2 B1 A1

Frequencies -- 285.3955 319.0225 325.2885

Red. masses -- 5.1662 6.1942 7.4725

Frc consts -- 0.2479 0.3714 0.4659

IR Inten -- 0.0000 74.7295 0.9345

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.16 0.16 -0.09 0.00 -0.00 -0.00 -0.04

2 6 0.00 0.00 0.14 -0.02 -0.13 0.00 -0.00 -0.00 -0.03

3 7 0.00 0.00 0.00 -0.10 0.00 0.00 -0.00 -0.00 -0.13

4 6 0.00 -0.00 -0.14 -0.02 0.13 -0.00 0.00 -0.00 -0.03

5 6 0.00 -0.00 -0.16 0.16 0.09 -0.00 0.00 -0.00 -0.04

6 6 -0.00 -0.00 -0.00 -0.03 0.12 0.00 0.00 -0.00 0.15

7 6 -0.00 0.00 0.16 0.05 0.04 0.00 0.00 -0.00 -0.06

8 7 -0.00 0.00 -0.00 0.04 -0.00 0.00 0.00 0.00 -0.17

9 6 0.00 0.00 -0.16 0.05 -0.04 0.00 0.00 0.00 -0.06

10 6 0.00 0.00 -0.16 0.07 -0.00 -0.00 0.00 0.00 -0.03

11 6 -0.00 0.00 0.16 0.07 0.00 -0.00 0.00 -0.00 -0.03

12 6 -0.00 0.00 0.00 -0.03 -0.12 -0.00 -0.00 -0.00 0.15

13 6 -0.00 -0.00 -0.16 0.05 -0.04 -0.00 -0.00 -0.00 -0.06

14 6 -0.00 -0.00 -0.16 0.07 -0.00 0.00 -0.00 -0.00 -0.03

15 6 0.00 -0.00 0.16 0.07 0.00 0.00 -0.00 0.00 -0.03

16 6 0.00 -0.00 0.16 0.05 0.04 -0.00 -0.00 0.00 -0.06

17 7 0.00 -0.00 -0.00 0.04 -0.00 -0.00 -0.00 -0.00 -0.17

18 6 0.00 0.00 -0.00 -0.03 0.12 -0.00 -0.00 0.00 0.15

19 6 -0.00 0.00 -0.14 -0.02 0.13 0.00 -0.00 0.00 -0.03

20 6 -0.00 0.00 -0.16 0.16 0.09 0.00 -0.00 0.00 -0.04

21 6 -0.00 -0.00 0.16 0.16 -0.09 -0.00 0.00 0.00 -0.04

22 6 -0.00 -0.00 0.14 -0.02 -0.13 -0.00 0.00 0.00 -0.03

23 7 -0.00 0.00 0.00 -0.10 0.00 -0.00 0.00 0.00 -0.13

24 1 0.00 0.00 0.29 0.28 -0.18 0.00 0.00 -0.00 -0.05

25 1 0.00 -0.00 -0.29 0.28 0.18 -0.00 -0.00 -0.00 -0.05

26 1 0.00 0.00 -0.26 0.06 0.01 -0.00 0.00 -0.00 0.03

27 1 -0.00 0.00 0.26 0.06 -0.01 -0.00 0.00 0.00 0.03

28 1 -0.00 -0.00 -0.26 0.06 0.01 0.00 -0.00 0.00 0.03

29 1 0.00 -0.00 0.26 0.06 -0.01 0.00 -0.00 -0.00 0.03

30 1 -0.00 0.00 -0.29 0.28 0.18 0.00 0.00 0.00 -0.05

31 1 -0.00 -0.00 0.29 0.28 -0.18 -0.00 -0.00 0.00 -0.05

32 30 0.00 0.00 0.00 -0.02 -0.00 0.00 0.00 0.00 0.04

33 6 0.00 -0.00 0.00 -0.03 -0.12 0.00 0.00 0.00 0.15

34 6 -0.00 0.00 0.02 -0.08 -0.10 -0.00 0.00 0.00 0.27

35 6 0.00 -0.00 0.02 -0.08 -0.10 0.00 -0.00 -0.00 0.27

36 6 0.00 -0.00 -0.01 -0.10 -0.09 -0.00 0.00 0.00 -0.12

37 6 -0.00 0.00 -0.01 -0.10 -0.09 0.00 -0.00 -0.00 -0.12

38 6 0.00 0.00 -0.02 -0.08 0.10 -0.00 0.00 -0.00 0.27

39 6 -0.00 -0.00 0.01 -0.10 0.09 -0.00 0.00 -0.00 -0.12

40 6 -0.00 -0.00 -0.02 -0.08 0.10 0.00 -0.00 0.00 0.27

41 6 0.00 0.00 0.01 -0.10 0.09 0.00 -0.00 0.00 -0.12

42 1 0.00 0.00 0.03 -0.12 0.07 0.00 -0.00 0.00 -0.33

43 1 0.00 -0.00 -0.03 -0.12 -0.07 -0.00 0.00 0.00 -0.33

44 1 -0.00 -0.00 0.03 -0.12 0.07 -0.00 0.00 -0.00 -0.33

45 1 -0.00 0.00 -0.03 -0.12 -0.07 0.00 -0.00 -0.00 -0.33

25 26 27

B2 A1 B2

Frequencies -- 328.1895 330.7135 363.2355

Red. masses -- 6.1697 8.5417 6.0340

Frc consts -- 0.3915 0.5504 0.4691

IR Inten -- 20.4735 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.08 0.00 -0.00 -0.13 0.00 0.00 0.00 0.04

2 6 -0.04 0.06 -0.00 -0.04 -0.12 0.00 0.00 0.00 -0.00

3 7 0.00 0.05 -0.00 -0.00 -0.12 0.00 -0.00 0.00 0.05

4 6 0.04 0.06 -0.00 0.04 -0.12 0.00 -0.00 0.00 -0.00

5 6 0.00 0.08 0.00 0.00 -0.13 0.00 -0.00 0.00 0.04

6 6 0.11 -0.03 -0.00 0.09 -0.10 -0.00 -0.00 -0.00 -0.08

7 6 0.13 -0.02 0.00 0.13 -0.04 0.00 -0.00 -0.00 0.13

8 7 0.00 -0.11 0.00 0.13 0.00 0.00 0.00 -0.00 -0.00

9 6 -0.13 -0.02 -0.00 0.13 0.04 0.00 0.00 -0.00 -0.13

10 6 -0.09 0.16 -0.00 0.14 0.01 0.00 0.00 -0.00 -0.17

11 6 0.09 0.16 0.00 0.14 -0.01 0.00 -0.00 -0.00 0.17

12 6 -0.11 -0.03 -0.00 -0.09 -0.10 -0.00 0.00 -0.00 -0.08

13 6 -0.13 -0.02 0.00 -0.13 -0.04 0.00 0.00 -0.00 0.13

14 6 -0.09 0.16 0.00 -0.14 -0.01 0.00 0.00 -0.00 0.17

15 6 0.09 0.16 -0.00 -0.14 0.01 0.00 -0.00 -0.00 -0.17

16 6 0.13 -0.02 -0.00 -0.13 0.04 0.00 -0.00 -0.00 -0.13

17 7 0.00 -0.11 -0.00 -0.13 -0.00 0.00 0.00 -0.00 0.00

18 6 0.11 -0.03 0.00 -0.09 0.10 -0.00 -0.00 -0.00 0.08

19 6 0.04 0.06 0.00 -0.04 0.12 0.00 -0.00 0.00 0.00

20 6 0.00 0.08 -0.00 -0.00 0.13 0.00 -0.00 0.00 -0.04

21 6 -0.00 0.08 -0.00 0.00 0.13 0.00 0.00 0.00 -0.04

22 6 -0.04 0.06 0.00 0.04 0.12 0.00 0.00 0.00 0.00

23 7 0.00 0.05 0.00 -0.00 0.12 0.00 -0.00 0.00 -0.05

24 1 0.02 0.06 0.00 0.01 -0.15 0.00 -0.00 0.00 0.08

25 1 -0.02 0.06 0.00 -0.01 -0.15 0.00 0.00 0.00 0.08

26 1 -0.19 0.28 -0.00 0.16 -0.01 -0.00 0.00 -0.00 -0.28

27 1 0.19 0.28 0.00 0.16 0.01 -0.00 -0.00 -0.00 0.28

28 1 -0.19 0.28 0.00 -0.16 0.01 -0.00 0.00 -0.00 0.28

29 1 0.19 0.28 -0.00 -0.16 -0.01 -0.00 -0.00 -0.00 -0.28

30 1 -0.02 0.06 -0.00 0.01 0.15 0.00 0.00 0.00 -0.08

31 1 0.02 0.06 -0.00 -0.01 0.15 0.00 -0.00 0.00 -0.08

32 30 0.00 -0.03 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

33 6 -0.11 -0.03 0.00 0.09 0.10 -0.00 0.00 -0.00 0.08

34 6 -0.09 -0.08 -0.00 0.12 0.13 -0.00 0.00 -0.00 0.23

35 6 -0.09 -0.08 0.00 -0.12 -0.13 -0.00 0.00 -0.00 -0.23

36 6 -0.09 -0.09 -0.00 0.13 0.13 0.00 0.00 0.00 -0.09

37 6 -0.09 -0.09 0.00 -0.13 -0.13 0.00 0.00 0.00 0.09

38 6 0.09 -0.08 0.00 0.12 -0.13 -0.00 -0.00 -0.00 -0.23

39 6 0.09 -0.09 0.00 0.13 -0.13 0.00 -0.00 0.00 0.09

40 6 0.09 -0.08 -0.00 -0.12 0.13 -0.00 -0.00 -0.00 0.23

41 6 0.09 -0.09 -0.00 -0.13 0.13 0.00 -0.00 0.00 -0.09

42 1 0.08 -0.11 -0.00 -0.14 0.13 0.00 0.00 0.00 -0.23

43 1 -0.08 -0.11 -0.00 0.14 0.13 0.00 -0.00 0.00 -0.23

44 1 0.08 -0.11 0.00 0.14 -0.13 0.00 0.00 0.00 0.23

45 1 -0.08 -0.11 0.00 -0.14 -0.13 0.00 -0.00 0.00 0.23

28 29 30

B1 B1 B2

Frequencies -- 377.7145 391.3704 395.3106

Red. masses -- 5.8005 8.8602 8.5363

Frc consts -- 0.4876 0.7996 0.7860

IR Inten -- 0.0000 130.5996 12.8229

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.00 0.17 0.11 -0.00 0.00 -0.01 -0.20 -0.00

2 6 -0.00 0.00 0.12 0.06 0.01 0.00 -0.03 -0.16 0.00

3 7 -0.00 0.00 -0.00 0.06 -0.00 -0.00 -0.00 -0.16 0.00

4 6 -0.00 -0.00 -0.12 0.06 -0.01 -0.00 0.03 -0.16 0.00

5 6 -0.00 -0.00 -0.17 0.11 0.00 -0.00 0.01 -0.20 -0.00

6 6 -0.00 -0.00 0.08 0.01 0.04 0.00 0.04 0.00 -0.00

7 6 0.00 -0.00 -0.02 -0.17 0.03 -0.00 -0.00 0.06 0.00

8 7 0.00 -0.00 -0.08 -0.16 0.00 -0.00 0.00 0.07 -0.00

9 6 0.00 0.00 -0.02 -0.17 -0.03 -0.00 0.00 0.06 -0.00

10 6 0.00 0.00 -0.02 -0.20 -0.01 0.00 -0.00 0.12 -0.00

11 6 0.00 -0.00 -0.02 -0.20 0.01 0.00 0.00 0.12 0.00

12 6 -0.00 0.00 -0.08 0.01 -0.04 -0.00 -0.04 0.00 -0.00

13 6 0.00 0.00 0.02 -0.17 -0.03 0.00 0.00 0.06 0.00

14 6 0.00 0.00 0.02 -0.20 -0.01 -0.00 -0.00 0.12 0.00

15 6 0.00 -0.00 0.02 -0.20 0.01 -0.00 0.00 0.12 -0.00

16 6 0.00 -0.00 0.02 -0.17 0.03 0.00 -0.00 0.06 -0.00

17 7 0.00 -0.00 0.08 -0.16 0.00 0.00 0.00 0.07 0.00

18 6 -0.00 -0.00 -0.08 0.01 0.04 -0.00 0.04 0.00 0.00

19 6 -0.00 -0.00 0.12 0.06 -0.01 0.00 0.03 -0.16 -0.00

20 6 -0.00 -0.00 0.17 0.11 0.00 0.00 0.01 -0.20 0.00

21 6 -0.00 0.00 -0.17 0.11 -0.00 -0.00 -0.01 -0.20 0.00

22 6 -0.00 0.00 -0.12 0.06 0.01 -0.00 -0.03 -0.16 -0.00

23 7 -0.00 0.00 0.00 0.06 -0.00 0.00 -0.00 -0.16 -0.00

24 1 -0.00 0.00 0.31 0.14 -0.02 0.00 0.01 -0.21 -0.00

25 1 -0.00 -0.00 -0.31 0.14 0.02 -0.00 -0.01 -0.21 -0.00

26 1 0.00 -0.00 -0.02 -0.22 0.01 0.00 -0.02 0.15 -0.00

27 1 0.00 0.00 -0.02 -0.22 -0.01 0.00 0.02 0.15 0.00

28 1 0.00 -0.00 0.02 -0.22 0.01 -0.00 -0.02 0.15 0.00

29 1 0.00 0.00 0.02 -0.22 -0.01 -0.00 0.02 0.15 -0.00

30 1 -0.00 -0.00 0.31 0.14 0.02 0.00 -0.01 -0.21 0.00

31 1 -0.00 0.00 -0.31 0.14 -0.02 -0.00 0.01 -0.21 0.00

32 30 -0.00 -0.00 0.00 0.16 0.00 0.00 -0.00 0.14 0.00

33 6 -0.00 0.00 0.08 0.01 -0.04 0.00 -0.04 0.00 0.00

34 6 -0.00 0.00 0.23 0.11 -0.15 0.00 -0.16 0.10 0.00

35 6 -0.00 0.00 -0.23 0.11 -0.15 -0.00 -0.16 0.10 -0.00

36 6 0.00 0.00 -0.08 -0.05 0.00 -0.00 -0.01 -0.06 -0.00

37 6 0.00 0.00 0.08 -0.05 0.00 0.00 -0.01 -0.06 0.00

38 6 -0.00 -0.00 0.23 0.11 0.15 0.00 0.16 0.10 -0.00

39 6 0.00 -0.00 -0.08 -0.05 -0.00 -0.00 0.01 -0.06 0.00

40 6 -0.00 -0.00 -0.23 0.11 0.15 -0.00 0.16 0.10 0.00

41 6 0.00 -0.00 0.08 -0.05 -0.00 0.00 0.01 -0.06 -0.00

42 1 0.00 0.00 0.21 -0.15 -0.11 0.00 -0.10 -0.17 -0.00

43 1 0.00 -0.00 -0.21 -0.15 0.11 -0.00 0.10 -0.17 -0.00

44 1 0.00 0.00 -0.21 -0.15 -0.11 -0.00 -0.10 -0.17 0.00

45 1 0.00 -0.00 0.21 -0.15 0.11 0.00 0.10 -0.17 0.00

31 32 33

A2 A2 A2

Frequencies -- 395.4691 406.4436 408.1889

Red. masses -- 5.9615 5.6024 4.6369

Frc consts -- 0.5493 0.5453 0.4552

IR Inten -- 0.0000 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.00 -0.13 -0.05 0.07 0.00 0.20 -0.06 -0.00

2 6 -0.00 0.00 -0.09 0.06 0.10 -0.00 0.04 -0.05 -0.00

3 7 0.00 0.00 -0.00 0.11 0.00 -0.00 -0.03 0.00 -0.00

4 6 -0.00 -0.00 0.09 0.06 -0.10 0.00 0.04 0.05 0.00

5 6 -0.00 -0.00 0.13 -0.05 -0.07 -0.00 0.20 0.06 0.00

6 6 0.00 -0.00 -0.05 0.00 0.01 0.00 -0.02 0.01 -0.00

7 6 0.00 0.00 0.08 -0.11 0.04 -0.00 -0.03 -0.06 0.00

8 7 0.00 0.00 -0.00 -0.00 0.13 -0.00 -0.00 -0.01 0.00

9 6 -0.00 0.00 -0.08 0.11 0.04 0.00 0.03 -0.06 -0.00

10 6 -0.00 0.00 -0.11 0.09 -0.11 0.00 0.03 -0.17 -0.00

11 6 0.00 0.00 0.11 -0.09 -0.11 -0.00 -0.03 -0.17 0.00

12 6 0.00 0.00 0.05 0.00 -0.01 -0.00 -0.02 -0.01 0.00

13 6 0.00 -0.00 -0.08 -0.11 -0.04 0.00 -0.03 0.06 -0.00

14 6 0.00 -0.00 -0.11 -0.09 0.11 0.00 -0.03 0.17 -0.00

15 6 -0.00 -0.00 0.11 0.09 0.11 -0.00 0.03 0.17 0.00

16 6 -0.00 -0.00 0.08 0.11 -0.04 -0.00 0.03 0.06 0.00

17 7 0.00 -0.00 -0.00 0.00 -0.13 -0.00 -0.00 0.01 0.00

18 6 -0.00 0.00 -0.05 -0.00 -0.01 0.00 0.02 -0.01 -0.00

19 6 0.00 0.00 0.09 -0.06 0.10 0.00 -0.04 -0.05 0.00

20 6 0.00 0.00 0.13 0.05 0.07 -0.00 -0.20 -0.06 0.00

21 6 0.00 -0.00 -0.13 0.05 -0.07 0.00 -0.20 0.06 -0.00

22 6 0.00 -0.00 -0.09 -0.06 -0.10 -0.00 -0.04 0.05 -0.00

23 7 -0.00 0.00 -0.00 -0.11 0.00 -0.00 0.03 -0.00 -0.00

24 1 -0.00 0.00 -0.25 -0.14 0.14 -0.00 0.29 -0.13 -0.00

25 1 -0.00 -0.00 0.25 -0.14 -0.14 0.00 0.29 0.13 0.00

26 1 -0.00 0.00 -0.19 0.18 -0.23 0.00 0.09 -0.24 -0.00

27 1 0.00 0.00 0.19 -0.18 -0.23 -0.00 -0.09 -0.24 0.00

28 1 0.00 -0.00 -0.19 -0.18 0.23 0.00 -0.09 0.24 -0.00

29 1 -0.00 -0.00 0.19 0.18 0.23 -0.00 0.09 0.24 0.00

30 1 0.00 0.00 0.25 0.14 0.14 0.00 -0.29 -0.13 0.00

31 1 0.00 -0.00 -0.25 0.14 -0.14 -0.00 -0.29 0.13 -0.00

32 30 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

33 6 -0.00 -0.00 0.05 -0.00 0.01 -0.00 0.02 0.01 0.00

34 6 -0.00 0.00 0.24 -0.12 0.12 -0.00 0.02 -0.01 0.00

35 6 0.00 -0.00 0.24 0.12 -0.12 -0.00 -0.02 0.01 0.00

36 6 -0.00 -0.00 -0.08 0.02 -0.02 0.00 0.01 0.01 -0.00

37 6 0.00 0.00 -0.08 -0.02 0.02 0.00 -0.01 -0.01 -0.00

38 6 0.00 0.00 -0.24 0.12 0.12 0.00 -0.02 -0.01 -0.00

39 6 0.00 -0.00 0.08 -0.02 -0.02 -0.00 -0.01 0.01 0.00

40 6 -0.00 -0.00 -0.24 -0.12 -0.12 0.00 0.02 0.01 -0.00

41 6 -0.00 0.00 0.08 0.02 0.02 -0.00 0.01 -0.01 0.00

42 1 0.00 0.00 0.20 0.11 0.11 -0.00 -0.00 -0.03 0.00

43 1 0.00 -0.00 -0.20 0.11 -0.11 0.00 -0.00 0.03 -0.00

44 1 -0.00 -0.00 0.20 -0.11 -0.11 -0.00 0.00 0.03 0.00

45 1 -0.00 0.00 -0.20 -0.11 0.11 0.00 0.00 -0.03 -0.00

34 35 36

A1 A1 B2

Frequencies -- 456.9307 459.8236 479.9417

Red. masses -- 7.1246 8.1749 6.0495

Frc consts -- 0.8764 1.0184 0.8210

IR Inten -- 0.0000 0.0000 32.4959

Atom AN X Y Z X Y Z X Y Z

1 6 -0.01 0.04 0.00 0.01 0.15 0.00 0.00 -0.09 -0.00

2 6 -0.05 0.01 -0.00 -0.00 0.10 -0.00 0.03 -0.05 0.00

3 7 -0.00 0.01 -0.00 -0.00 0.13 -0.00 -0.00 -0.06 0.00

4 6 0.05 0.01 -0.00 0.00 0.10 -0.00 -0.03 -0.05 0.00

5 6 0.01 0.04 0.00 -0.01 0.15 0.00 -0.00 -0.09 -0.00

6 6 0.08 0.04 -0.00 0.05 -0.09 -0.00 -0.06 0.00 0.00

7 6 -0.03 0.03 -0.00 -0.09 -0.03 -0.00 0.07 0.00 -0.00

8 7 -0.05 0.00 -0.00 -0.11 0.00 -0.00 -0.00 -0.04 0.00

9 6 -0.03 -0.03 -0.00 -0.09 0.03 -0.00 -0.07 0.00 0.00

10 6 -0.03 -0.01 0.00 -0.14 -0.00 0.00 -0.06 0.14 0.00

11 6 -0.03 0.01 0.00 -0.14 0.00 0.00 0.06 0.14 -0.00

12 6 -0.08 0.04 -0.00 -0.05 -0.09 -0.00 0.06 0.00 0.00

13 6 0.03 0.03 -0.00 0.09 -0.03 -0.00 -0.07 0.00 -0.00

14 6 0.03 0.01 0.00 0.14 0.00 0.00 -0.06 0.14 -0.00

15 6 0.03 -0.01 0.00 0.14 -0.00 0.00 0.06 0.14 0.00

16 6 0.03 -0.03 -0.00 0.09 0.03 -0.00 0.07 0.00 0.00

17 7 0.05 -0.00 -0.00 0.11 -0.00 -0.00 -0.00 -0.04 -0.00

18 6 -0.08 -0.04 -0.00 -0.05 0.09 -0.00 -0.06 0.00 -0.00

19 6 -0.05 -0.01 -0.00 -0.00 -0.10 -0.00 -0.03 -0.05 -0.00

20 6 -0.01 -0.04 0.00 0.01 -0.15 0.00 -0.00 -0.09 0.00

21 6 0.01 -0.04 0.00 -0.01 -0.15 0.00 0.00 -0.09 0.00

22 6 0.05 -0.01 -0.00 0.00 -0.10 -0.00 0.03 -0.05 -0.00

23 7 0.00 -0.01 -0.00 0.00 -0.13 -0.00 -0.00 -0.06 -0.00

24 1 0.01 0.02 0.00 0.00 0.15 0.00 -0.00 -0.09 -0.00

25 1 -0.01 0.02 0.00 -0.00 0.15 0.00 0.00 -0.09 -0.00

26 1 -0.05 0.01 0.00 -0.14 -0.01 0.00 -0.14 0.24 0.00

27 1 -0.05 -0.01 0.00 -0.14 0.01 0.00 0.14 0.24 -0.00

28 1 0.05 -0.01 0.00 0.14 0.01 0.00 -0.14 0.24 -0.00

29 1 0.05 0.01 0.00 0.14 -0.01 0.00 0.14 0.24 0.00

30 1 0.01 -0.02 0.00 0.00 -0.15 0.00 0.00 -0.09 0.00

31 1 -0.01 -0.02 0.00 -0.00 -0.15 0.00 -0.00 -0.09 0.00

32 30 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.03 -0.00

33 6 0.08 -0.04 -0.00 0.05 0.09 -0.00 0.06 0.00 -0.00

34 6 0.27 -0.21 0.00 0.05 0.19 0.00 0.22 -0.10 0.00

35 6 -0.27 0.21 0.00 -0.05 -0.19 0.00 0.22 -0.10 -0.00

36 6 0.01 0.06 -0.00 0.14 0.12 -0.00 0.05 0.08 -0.00

37 6 -0.01 -0.06 -0.00 -0.14 -0.12 -0.00 0.05 0.08 0.00

38 6 0.27 0.21 0.00 0.05 -0.19 0.00 -0.22 -0.10 -0.00

39 6 0.01 -0.06 -0.00 0.14 -0.12 -0.00 -0.05 0.08 0.00

40 6 -0.27 -0.21 0.00 -0.05 0.19 0.00 -0.22 -0.10 0.00

41 6 -0.01 0.06 -0.00 -0.14 0.12 -0.00 -0.05 0.08 -0.00

42 1 0.19 0.27 0.00 -0.21 0.06 0.00 0.07 0.21 0.00

43 1 -0.19 0.27 0.00 0.21 0.06 0.00 -0.07 0.21 0.00

44 1 -0.19 -0.27 0.00 0.21 -0.06 0.00 0.07 0.21 -0.00

45 1 0.19 -0.27 0.00 -0.21 -0.06 0.00 -0.07 0.21 -0.00

37 38 39

B1 B1 A2

Frequencies -- 482.6239 501.5115 501.6000

Red. masses -- 5.8833 1.4511 1.4490

Frc consts -- 0.8074 0.2150 0.2148

IR Inten -- 16.1053 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.14 -0.06 -0.00 0.00 -0.00 0.02 0.00 -0.00 -0.02

2 6 -0.00 -0.07 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00

3 7 -0.04 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00

4 6 -0.00 0.07 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00

5 6 0.14 0.06 0.00 0.00 0.00 -0.02 0.00 0.00 0.02

6 6 0.00 -0.06 -0.00 -0.00 -0.00 0.04 0.00 -0.00 -0.04

7 6 -0.04 -0.03 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00

8 7 -0.06 0.00 -0.00 -0.00 -0.00 -0.02 0.00 -0.00 0.00

9 6 -0.04 0.03 -0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00

10 6 -0.08 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.02

11 6 -0.08 -0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.02

12 6 0.00 0.06 0.00 -0.00 0.00 -0.04 0.00 0.00 0.04

13 6 -0.04 0.03 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00

14 6 -0.08 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.02

15 6 -0.08 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 0.02

16 6 -0.04 -0.03 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00

17 7 -0.06 0.00 0.00 -0.00 -0.00 0.02 -0.00 0.00 0.00

18 6 0.00 -0.06 0.00 -0.00 -0.00 -0.04 -0.00 0.00 -0.04

19 6 -0.00 0.07 0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00

20 6 0.14 0.06 -0.00 0.00 0.00 0.02 -0.00 -0.00 0.02

21 6 0.14 -0.06 0.00 0.00 -0.00 -0.02 -0.00 0.00 -0.02

22 6 -0.00 -0.07 -0.00 0.00 -0.00 0.00 0.00 0.00 0.00

23 7 -0.04 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00

24 1 0.25 -0.15 -0.00 0.00 -0.00 0.03 0.00 -0.00 -0.03

25 1 0.25 0.15 0.00 0.00 0.00 -0.03 0.00 0.00 0.03

26 1 -0.08 -0.00 0.00 -0.00 -0.00 0.01 0.00 -0.00 -0.03

27 1 -0.08 0.00 0.00 -0.00 0.00 0.01 -0.00 -0.00 0.03

28 1 -0.08 -0.00 -0.00 -0.00 -0.00 -0.01 -0.00 0.00 -0.03

29 1 -0.08 0.00 -0.00 -0.00 0.00 -0.01 0.00 0.00 0.03

30 1 0.25 0.15 -0.00 0.00 0.00 0.03 -0.00 -0.00 0.03

31 1 0.25 -0.15 0.00 0.00 -0.00 -0.03 -0.00 0.00 -0.03

32 30 0.03 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00

33 6 0.00 0.06 -0.00 -0.00 0.00 0.04 -0.00 -0.00 0.04

34 6 -0.10 0.22 0.00 -0.00 0.00 -0.05 0.00 -0.00 -0.04

35 6 -0.10 0.22 -0.00 -0.00 0.00 0.05 -0.00 0.00 -0.04

36 6 0.08 0.05 -0.00 0.00 0.00 0.08 -0.00 0.00 0.08

37 6 0.08 0.05 0.00 0.00 0.00 -0.08 0.00 -0.00 0.08

38 6 -0.10 -0.22 0.00 -0.00 -0.00 -0.05 -0.00 -0.00 0.04

39 6 0.08 -0.05 -0.00 0.00 -0.00 0.08 0.00 0.00 -0.08

40 6 -0.10 -0.22 -0.00 -0.00 -0.00 0.05 0.00 0.00 0.04

41 6 0.08 -0.05 0.00 0.00 -0.00 -0.08 -0.00 -0.00 -0.08

42 1 0.21 0.09 -0.00 0.00 0.00 0.49 0.00 0.00 0.49

43 1 0.21 -0.09 0.00 0.00 -0.00 -0.49 0.00 -0.00 -0.49

44 1 0.21 0.09 0.00 0.00 0.00 -0.49 -0.00 -0.00 0.49

45 1 0.21 -0.09 -0.00 0.00 -0.00 0.49 -0.00 0.00 -0.49

40 41 42

A1 B2 A2

Frequencies -- 501.8550 501.9201 553.8665

Red. masses -- 1.4532 1.4524 3.6561

Frc consts -- 0.2156 0.2156 0.6608

IR Inten -- 284.0779 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 0.09

2 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.04

3 7 0.00 -0.00 0.02 0.00 0.00 -0.02 -0.00 0.00 0.00

4 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 0.04

5 6 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.09

6 6 -0.00 0.00 -0.04 0.00 0.00 0.04 -0.00 0.00 0.17

7 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.03

8 7 0.00 -0.00 0.02 -0.00 0.00 0.00 -0.00 -0.00 0.00

9 6 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.03

10 6 0.00 0.00 0.00 0.00 -0.00 0.02 -0.00 -0.00 0.10

11 6 0.00 -0.00 0.00 -0.00 -0.00 -0.02 0.00 -0.00 -0.10

12 6 0.00 0.00 -0.04 -0.00 0.00 0.04 -0.00 -0.00 -0.17

13 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.03

14 6 -0.00 -0.00 0.00 0.00 -0.00 -0.02 0.00 0.00 0.10

15 6 -0.00 0.00 0.00 -0.00 -0.00 0.02 -0.00 0.00 -0.10

16 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.03

17 7 -0.00 0.00 0.02 -0.00 0.00 -0.00 0.00 0.00 0.00

18 6 0.00 -0.00 -0.04 0.00 0.00 -0.04 0.00 -0.00 0.17

19 6 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00 0.04

20 6 -0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 -0.09

21 6 0.00 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 0.09

22 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.04

23 7 -0.00 0.00 0.02 0.00 0.00 0.02 0.00 -0.00 0.00

24 1 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.16

25 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.16

26 1 0.00 0.00 -0.01 0.00 -0.00 0.03 -0.00 0.00 0.16

27 1 0.00 -0.00 -0.01 -0.00 -0.00 -0.03 0.00 0.00 -0.16

28 1 -0.00 -0.00 -0.01 0.00 -0.00 -0.03 0.00 -0.00 0.16

29 1 -0.00 0.00 -0.01 -0.00 -0.00 0.03 -0.00 -0.00 -0.16

30 1 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 -0.16

31 1 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.16

32 30 -0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

33 6 -0.00 -0.00 -0.04 -0.00 0.00 -0.04 0.00 0.00 -0.17

34 6 -0.00 -0.00 0.05 -0.00 0.00 0.05 -0.00 0.00 0.11

35 6 0.00 0.00 0.05 -0.00 0.00 -0.05 0.00 -0.00 0.11

36 6 -0.00 -0.00 -0.08 -0.00 -0.00 -0.08 0.00 0.00 0.01

37 6 0.00 0.00 -0.08 -0.00 -0.00 0.08 -0.00 -0.00 0.01

38 6 -0.00 0.00 0.05 0.00 0.00 -0.05 0.00 0.00 -0.11

39 6 -0.00 0.00 -0.08 0.00 -0.00 0.08 -0.00 0.00 -0.01

40 6 0.00 -0.00 0.05 0.00 0.00 0.05 -0.00 -0.00 -0.11

41 6 0.00 -0.00 -0.08 0.00 -0.00 -0.08 0.00 -0.00 -0.01

42 1 0.00 -0.00 0.49 0.00 -0.00 0.49 0.00 0.00 0.37

43 1 -0.00 -0.00 0.49 -0.00 -0.00 0.49 0.00 -0.00 -0.37

44 1 -0.00 0.00 0.49 0.00 -0.00 -0.49 -0.00 -0.00 0.37

45 1 0.00 0.00 0.49 -0.00 -0.00 -0.49 -0.00 0.00 -0.37

43 44 45

B2 B1 A1

Frequencies -- 559.0810 559.3352 564.6678

Red. masses -- 4.1279 4.0713 4.6749

Frc consts -- 0.7602 0.7505 0.8782

IR Inten -- 0.0000 0.0000 88.2257

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.00 -0.02 0.00 -0.00 0.10 0.00 0.00 -0.02

2 6 -0.00 0.00 0.04 -0.00 -0.00 -0.05 -0.00 0.00 0.05

3 7 -0.00 0.00 -0.11 -0.00 0.00 0.00 -0.00 0.00 -0.12

4 6 0.00 0.00 0.04 -0.00 0.00 0.05 0.00 0.00 0.05

5 6 0.00 0.00 -0.02 0.00 0.00 -0.10 -0.00 0.00 -0.02

6 6 0.00 0.00 0.19 -0.00 -0.00 0.19 0.00 -0.00 0.21

7 6 -0.00 -0.00 0.03 -0.00 -0.00 0.02 -0.00 -0.00 0.03

8 7 -0.00 0.00 -0.00 -0.00 0.00 -0.10 -0.00 0.00 -0.11

9 6 0.00 -0.00 -0.03 -0.00 0.00 0.02 -0.00 0.00 0.03

10 6 0.00 -0.00 0.10 -0.00 -0.00 -0.02 -0.00 -0.00 -0.02

11 6 -0.00 -0.00 -0.10 -0.00 0.00 -0.02 -0.00 0.00 -0.02

12 6 -0.00 0.00 0.19 -0.00 0.00 -0.19 -0.00 -0.00 0.21

13 6 0.00 -0.00 0.03 -0.00 0.00 -0.02 0.00 -0.00 0.03

14 6 0.00 -0.00 -0.10 -0.00 -0.00 0.02 0.00 0.00 -0.02

15 6 -0.00 -0.00 0.10 -0.00 0.00 0.02 0.00 -0.00 -0.02

16 6 -0.00 -0.00 -0.03 -0.00 -0.00 -0.02 0.00 0.00 0.03

17 7 -0.00 0.00 0.00 -0.00 0.00 0.10 0.00 -0.00 -0.11

18 6 0.00 0.00 -0.19 -0.00 -0.00 -0.19 -0.00 0.00 0.21

19 6 0.00 0.00 -0.04 -0.00 0.00 -0.05 -0.00 -0.00 0.05

20 6 0.00 0.00 0.02 0.00 0.00 0.10 0.00 -0.00 -0.02

21 6 -0.00 0.00 0.02 0.00 -0.00 -0.10 -0.00 -0.00 -0.02

22 6 -0.00 0.00 -0.04 -0.00 -0.00 0.05 0.00 -0.00 0.05

23 7 -0.00 0.00 0.11 -0.00 0.00 -0.00 0.00 -0.00 -0.12

24 1 0.00 0.00 -0.04 0.00 -0.00 0.17 0.00 0.00 -0.05

25 1 -0.00 0.00 -0.04 0.00 0.00 -0.17 -0.00 0.00 -0.05

26 1 0.00 -0.00 0.17 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

27 1 -0.00 -0.00 -0.17 -0.00 0.00 -0.00 -0.00 0.00 -0.00

28 1 0.00 -0.00 -0.17 -0.00 -0.00 0.00 0.00 0.00 -0.00

29 1 -0.00 -0.00 0.17 -0.00 0.00 0.00 0.00 -0.00 -0.00

30 1 -0.00 0.00 0.04 0.00 0.00 0.17 0.00 -0.00 -0.05

31 1 0.00 0.00 0.04 0.00 -0.00 -0.17 -0.00 -0.00 -0.05

32 30 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.01

33 6 -0.00 0.00 -0.19 -0.00 0.00 0.19 0.00 0.00 0.21

34 6 -0.00 -0.00 0.13 0.00 0.00 -0.12 0.00 0.00 -0.14

35 6 -0.00 -0.00 -0.13 0.00 0.00 0.12 -0.00 -0.00 -0.14

36 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

37 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

38 6 0.00 -0.00 -0.13 0.00 -0.00 -0.12 0.00 -0.00 -0.14

39 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

40 6 0.00 -0.00 0.13 0.00 -0.00 0.12 -0.00 0.00 -0.14

41 6 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

42 1 -0.00 -0.00 -0.39 -0.00 -0.00 -0.39 -0.00 0.00 0.41

43 1 0.00 -0.00 -0.39 -0.00 0.00 0.39 0.00 0.00 0.41

44 1 -0.00 -0.00 0.39 -0.00 -0.00 0.39 0.00 -0.00 0.41

45 1 0.00 -0.00 0.39 -0.00 0.00 -0.39 -0.00 -0.00 0.41

46 47 48

A2 B2 B1

Frequencies -- 579.9816 591.2741 601.5008

Red. masses -- 6.9133 7.2059 7.2539

Frc consts -- 1.3701 1.4843 1.5463

IR Inten -- 0.0000 1.9938 0.1472

Atom AN X Y Z X Y Z X Y Z

1 6 -0.05 -0.05 -0.00 0.00 0.00 -0.00 0.07 0.12 0.00

2 6 -0.07 -0.06 0.00 -0.01 0.00 0.00 0.12 0.12 -0.00

3 7 -0.13 -0.00 -0.00 -0.00 0.01 0.00 0.23 0.00 -0.00

4 6 -0.07 0.06 -0.00 0.01 0.00 0.00 0.12 -0.12 0.00

5 6 -0.05 0.05 0.00 -0.00 0.00 -0.00 0.07 -0.12 -0.00

6 6 -0.01 0.00 -0.00 0.02 -0.02 -0.00 -0.01 0.02 0.00

7 6 0.08 -0.09 -0.00 -0.12 0.12 -0.00 -0.00 0.01 -0.00

8 7 -0.00 -0.17 -0.00 -0.00 0.23 0.00 -0.00 0.00 -0.00

9 6 -0.08 -0.09 0.00 0.12 0.12 0.00 -0.00 -0.01 -0.00

10 6 -0.08 -0.05 -0.00 0.11 0.07 -0.00 -0.00 0.00 0.00

11 6 0.08 -0.05 0.00 -0.11 0.07 0.00 -0.00 -0.00 0.00

12 6 -0.01 -0.00 0.00 -0.02 -0.02 -0.00 -0.01 -0.02 -0.00

13 6 0.08 0.09 0.00 0.12 0.12 -0.00 -0.00 -0.01 0.00

14 6 0.08 0.05 -0.00 0.11 0.07 0.00 -0.00 0.00 -0.00

15 6 -0.08 0.05 0.00 -0.11 0.07 -0.00 -0.00 -0.00 -0.00

16 6 -0.08 0.09 -0.00 -0.12 0.12 0.00 -0.00 0.01 0.00

17 7 0.00 0.17 -0.00 -0.00 0.23 -0.00 -0.00 0.00 0.00

18 6 0.01 -0.00 -0.00 0.02 -0.02 0.00 -0.01 0.02 -0.00

19 6 0.07 -0.06 -0.00 0.01 0.00 -0.00 0.12 -0.12 -0.00

20 6 0.05 -0.05 0.00 -0.00 0.00 0.00 0.07 -0.12 0.00

21 6 0.05 0.05 -0.00 0.00 0.00 0.00 0.07 0.12 -0.00

22 6 0.07 0.06 0.00 -0.01 0.00 -0.00 0.12 0.12 0.00

23 7 0.13 0.00 -0.00 -0.00 0.01 -0.00 0.23 0.00 0.00

24 1 0.00 -0.10 0.00 0.01 -0.00 -0.00 -0.06 0.22 0.00

25 1 0.00 0.10 -0.00 -0.01 -0.00 -0.00 -0.06 -0.22 -0.00

26 1 -0.14 0.03 -0.00 0.21 -0.06 -0.00 -0.01 0.01 0.00

27 1 0.14 0.03 0.00 -0.21 -0.06 0.00 -0.01 -0.01 0.00

28 1 0.14 -0.03 -0.00 0.21 -0.06 0.00 -0.01 0.01 -0.00

29 1 -0.14 -0.03 0.00 -0.21 -0.06 -0.00 -0.01 -0.01 -0.00

30 1 -0.00 -0.10 -0.00 -0.01 -0.00 0.00 -0.06 -0.22 0.00

31 1 -0.00 0.10 0.00 0.01 -0.00 0.00 -0.06 0.22 -0.00

32 30 0.00 0.00 0.00 -0.00 -0.01 -0.00 -0.01 -0.00 0.00

33 6 0.01 0.00 0.00 -0.02 -0.02 0.00 -0.01 -0.02 0.00

34 6 -0.17 0.20 -0.00 0.03 -0.20 -0.00 -0.20 0.03 -0.00

35 6 0.17 -0.20 -0.00 0.03 -0.20 0.00 -0.20 0.03 0.00

36 6 0.02 0.01 0.00 -0.10 -0.10 -0.00 -0.10 -0.10 -0.00

37 6 -0.02 -0.01 0.00 -0.10 -0.10 0.00 -0.10 -0.10 0.00

38 6 0.17 0.20 0.00 -0.03 -0.20 0.00 -0.20 -0.03 -0.00

39 6 -0.02 0.01 -0.00 0.10 -0.10 0.00 -0.10 0.10 -0.00

40 6 -0.17 -0.20 0.00 -0.03 -0.20 -0.00 -0.20 -0.03 0.00

41 6 0.02 -0.01 -0.00 0.10 -0.10 -0.00 -0.10 0.10 0.00

42 1 0.22 0.20 -0.00 0.25 0.05 0.00 0.03 0.25 -0.00

43 1 0.22 -0.20 0.00 -0.25 0.05 0.00 0.03 -0.25 0.00

44 1 -0.22 -0.20 -0.00 0.25 0.05 -0.00 0.03 0.25 0.00

45 1 -0.22 0.20 0.00 -0.25 0.05 -0.00 0.03 -0.25 -0.00

49 50 51

A2 A1 B1

Frequencies -- 611.4121 655.3153 655.3931

Red. masses -- 7.1417 1.2869 1.3017

Frc consts -- 1.5730 0.3256 0.3294

IR Inten -- 0.0000 0.0000 182.0171

Atom AN X Y Z X Y Z X Y Z

1 6 0.04 0.11 -0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00

2 6 0.10 0.11 0.00 0.00 0.00 0.00 -0.00 -0.00 0.00

3 7 0.16 -0.00 0.00 -0.00 -0.00 -0.00 -0.01 0.00 0.00

4 6 0.10 -0.11 -0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00

5 6 0.04 -0.11 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00

6 6 -0.02 0.03 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00

7 6 0.09 -0.07 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

8 7 -0.00 -0.12 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00

9 6 -0.09 -0.07 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

10 6 -0.08 -0.03 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00

11 6 0.08 -0.03 0.00 -0.00 0.00 0.00 0.00 0.00 -0.00

12 6 -0.02 -0.03 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00

13 6 0.09 0.07 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

14 6 0.08 0.03 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00

15 6 -0.08 0.03 0.00 0.00 -0.00 0.00 0.00 0.00 0.00

16 6 -0.09 0.07 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

17 7 0.00 0.12 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00

18 6 0.02 -0.03 0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00

19 6 -0.10 0.11 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00

20 6 -0.04 0.11 0.00 0.00 0.00 0.00 -0.00 0.00 -0.00

21 6 -0.04 -0.11 -0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00

22 6 -0.10 -0.11 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00

23 7 -0.16 0.00 0.00 0.00 0.00 -0.00 -0.01 0.00 -0.00

24 1 -0.09 0.20 -0.00 0.00 -0.00 -0.00 0.00 -0.01 -0.00

25 1 -0.09 -0.20 0.00 -0.00 -0.00 -0.00 0.00 0.01 0.00

26 1 -0.16 0.07 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

27 1 0.16 0.07 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

28 1 0.16 -0.07 -0.00 0.00 0.00 0.00 0.00 0.00 0.00

29 1 -0.16 -0.07 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

30 1 0.09 0.20 0.00 0.00 0.00 -0.00 0.00 0.01 -0.00

31 1 0.09 -0.20 -0.00 -0.00 0.00 -0.00 0.00 -0.01 0.00

32 30 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 -0.00

33 6 0.02 0.03 -0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00

34 6 0.13 0.08 0.00 -0.02 0.02 -0.00 0.03 -0.02 0.00

35 6 -0.13 -0.08 0.00 0.02 -0.02 -0.00 0.03 -0.02 -0.00

36 6 0.13 0.13 0.00 0.05 -0.05 0.00 -0.05 0.05 -0.00

37 6 -0.13 -0.13 0.00 -0.05 0.05 0.00 -0.05 0.05 0.00

38 6 -0.13 0.08 -0.00 -0.02 -0.02 -0.00 0.03 0.02 0.00

39 6 -0.13 0.13 -0.00 0.05 0.05 0.00 -0.05 -0.05 -0.00

40 6 0.13 -0.08 -0.00 0.02 0.02 -0.00 0.03 0.02 -0.00

41 6 0.13 -0.13 -0.00 -0.05 -0.05 0.00 -0.05 -0.05 0.00

42 1 0.12 -0.15 -0.00 0.34 0.35 -0.00 0.35 0.35 -0.00

43 1 0.12 0.15 0.00 -0.34 0.35 -0.00 0.35 -0.35 0.00

44 1 -0.12 0.15 -0.00 -0.34 -0.35 -0.00 0.35 0.35 0.00

45 1 -0.12 -0.15 0.00 0.34 -0.35 -0.00 0.35 -0.35 -0.00

52 53 54

A2 B2 B2

Frequencies -- 655.4826 655.4938 667.7482

Red. masses -- 1.3121 1.3037 3.5146

Frc consts -- 0.3322 0.3300 0.9233

IR Inten -- 0.0000 152.4510 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

2 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.14

3 7 0.01 -0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.14

4 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.14

5 6 0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

6 6 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00

7 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.13

8 7 -0.00 0.01 -0.00 -0.00 -0.01 -0.00 -0.00 0.00 0.00

9 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.13

10 6 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.10

11 6 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.10

12 6 0.00 -0.00 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00

13 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 0.13

14 6 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.10

15 6 0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 0.10

16 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.13

17 7 0.00 -0.01 -0.00 -0.00 -0.01 0.00 -0.00 0.00 -0.00

18 6 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00

19 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.14

20 6 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

21 6 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

22 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.14

23 7 -0.01 0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.14

24 1 -0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 0.37

25 1 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 -0.00 0.37

26 1 0.01 -0.00 -0.00 -0.01 0.00 0.00 -0.00 0.00 0.24

27 1 -0.01 -0.00 0.00 0.01 0.00 -0.00 0.00 0.00 -0.24

28 1 -0.01 0.00 -0.00 -0.01 0.00 -0.00 -0.00 0.00 -0.24

29 1 0.01 0.00 0.00 0.01 0.00 0.00 0.00 0.00 0.24

30 1 0.00 0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 -0.37

31 1 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.37

32 30 0.00 0.00 0.00 0.00 0.00 0.00 -0.00 0.00 -0.00

33 6 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 0.00

34 6 0.03 -0.03 0.00 -0.02 0.03 -0.00 -0.00 0.00 -0.01

35 6 -0.03 0.03 0.00 -0.02 0.03 0.00 -0.00 0.00 0.01

36 6 -0.05 0.05 -0.00 0.05 -0.05 0.00 -0.00 0.00 0.00

37 6 0.05 -0.05 -0.00 0.05 -0.05 -0.00 -0.00 0.00 -0.00

38 6 -0.03 -0.03 -0.00 0.02 0.03 0.00 0.00 0.00 0.01

39 6 0.05 0.05 0.00 -0.05 -0.05 -0.00 0.00 0.00 -0.00

40 6 0.03 0.03 -0.00 0.02 0.03 -0.00 0.00 0.00 -0.01

41 6 -0.05 -0.05 0.00 -0.05 -0.05 0.00 0.00 0.00 0.00

42 1 0.34 0.35 -0.00 0.34 0.36 -0.00 -0.00 -0.00 0.01

43 1 0.34 -0.35 0.00 -0.34 0.36 -0.00 0.00 -0.00 0.01

44 1 -0.34 -0.35 -0.00 0.34 0.36 0.00 -0.00 -0.00 -0.01

45 1 -0.34 0.35 0.00 -0.34 0.36 0.00 0.00 -0.00 -0.01

55 56 57

A1 A2 B1

Frequencies -- 673.8686 677.0687 689.9141

Red. masses -- 2.9110 4.6667 3.2644

Frc consts -- 0.7788 1.2605 0.9155

IR Inten -- 0.9115 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.00 -0.01 0.00 -0.00 -0.10 -0.00 -0.00 0.08

2 6 0.00 -0.00 -0.13 -0.00 0.00 0.15 -0.00 -0.00 -0.12

3 7 -0.00 0.00 0.13 -0.00 0.00 0.00 -0.00 0.00 -0.00

4 6 -0.00 -0.00 -0.13 -0.00 -0.00 -0.15 -0.00 0.00 0.12

5 6 -0.00 -0.00 -0.01 0.00 0.00 0.10 -0.00 0.00 -0.08

6 6 -0.00 -0.00 0.03 -0.00 -0.00 -0.02 0.00 0.00 -0.02

7 6 -0.00 -0.00 0.09 -0.00 -0.00 0.19 0.00 0.00 -0.13

8 7 0.00 0.00 -0.11 0.00 -0.00 -0.00 -0.00 -0.00 0.15

9 6 -0.00 0.00 0.09 0.00 -0.00 -0.19 0.00 -0.00 -0.13

10 6 -0.00 0.00 -0.01 -0.00 0.00 0.13 0.00 -0.00 -0.01

11 6 -0.00 -0.00 -0.01 0.00 0.00 -0.13 0.00 0.00 -0.01

12 6 0.00 -0.00 0.03 -0.00 0.00 0.02 0.00 -0.00 0.02

13 6 0.00 -0.00 0.09 -0.00 0.00 -0.19 0.00 -0.00 0.13

14 6 0.00 -0.00 -0.01 0.00 -0.00 0.13 0.00 -0.00 0.01

15 6 0.00 0.00 -0.01 -0.00 -0.00 -0.13 0.00 0.00 0.01

16 6 0.00 0.00 0.09 0.00 0.00 0.19 0.00 0.00 0.13

17 7 -0.00 -0.00 -0.11 -0.00 0.00 -0.00 -0.00 -0.00 -0.15

18 6 0.00 0.00 0.03 0.00 0.00 -0.02 0.00 0.00 0.02

19 6 0.00 0.00 -0.13 0.00 0.00 -0.15 -0.00 0.00 -0.12

20 6 0.00 0.00 -0.01 -0.00 -0.00 0.10 -0.00 0.00 0.08

21 6 -0.00 0.00 -0.01 -0.00 0.00 -0.10 -0.00 -0.00 -0.08

22 6 -0.00 0.00 -0.13 0.00 -0.00 0.15 -0.00 -0.00 0.12

23 7 0.00 -0.00 0.13 0.00 -0.00 0.00 -0.00 0.00 0.00

24 1 -0.00 -0.00 0.38 0.00 -0.00 -0.24 -0.00 0.00 0.19

25 1 0.00 -0.00 0.38 0.00 0.00 0.24 -0.00 -0.00 -0.19

26 1 0.00 -0.00 -0.25 -0.00 0.00 0.33 0.00 0.00 0.41

27 1 0.00 0.00 -0.25 0.00 0.00 -0.33 0.00 -0.00 0.41

28 1 -0.00 0.00 -0.25 0.00 -0.00 0.33 0.00 0.00 -0.41

29 1 -0.00 -0.00 -0.25 -0.00 -0.00 -0.33 0.00 -0.00 -0.41

30 1 -0.00 0.00 0.38 -0.00 -0.00 0.24 -0.00 -0.00 0.19

31 1 0.00 0.00 0.38 -0.00 0.00 -0.24 -0.00 0.00 -0.19

32 30 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00

33 6 -0.00 0.00 0.03 0.00 -0.00 0.02 0.00 -0.00 -0.02

34 6 0.00 -0.00 -0.01 -0.00 0.00 -0.01 -0.00 0.00 0.01

35 6 -0.00 0.00 -0.01 0.00 -0.00 -0.01 -0.00 0.00 -0.01

36 6 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.00

37 6 0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 0.00 0.00

38 6 0.00 0.00 -0.01 0.00 0.00 0.01 -0.00 -0.00 0.01

39 6 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00

40 6 -0.00 -0.00 -0.01 -0.00 -0.00 0.01 -0.00 -0.00 -0.01

41 6 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00

42 1 0.00 0.00 0.02 0.00 0.00 -0.01 0.00 0.00 0.01

43 1 -0.00 0.00 0.02 0.00 -0.00 0.01 0.00 -0.00 -0.01

44 1 -0.00 -0.00 0.02 -0.00 -0.00 -0.01 0.00 0.00 -0.01

45 1 0.00 -0.00 0.02 -0.00 0.00 0.01 0.00 -0.00 0.01

58 59 60

A1 B2 B1

Frequencies -- 710.3662 711.6189 716.5204

Red. masses -- 2.0091 3.3101 2.8661

Frc consts -- 0.5973 0.9876 0.8670

IR Inten -- 79.4118 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.00 -0.01 -0.00 0.00 0.02 -0.00 -0.00 -0.07

2 6 -0.00 -0.00 -0.06 -0.00 0.00 0.09 -0.00 -0.00 0.14

3 7 0.00 0.00 0.06 -0.00 -0.00 -0.09 -0.00 0.00 0.00

4 6 0.00 -0.00 -0.06 0.00 0.00 0.09 -0.00 0.00 -0.14

5 6 0.00 -0.00 -0.01 0.00 0.00 0.02 -0.00 0.00 0.07

6 6 0.00 0.00 0.06 0.00 0.00 -0.11 0.00 0.00 0.09

7 6 0.00 0.00 -0.08 0.00 -0.00 0.15 0.00 0.00 -0.07

8 7 -0.00 0.00 0.09 0.00 -0.00 -0.00 -0.00 -0.00 0.07

9 6 0.00 -0.00 -0.08 -0.00 -0.00 -0.15 0.00 -0.00 -0.07

10 6 0.00 0.00 -0.03 -0.00 -0.00 0.07 0.00 -0.00 -0.03

11 6 0.00 -0.00 -0.03 0.00 -0.00 -0.07 0.00 0.00 -0.03

12 6 -0.00 0.00 0.06 -0.00 0.00 -0.11 0.00 -0.00 -0.09

13 6 -0.00 0.00 -0.08 -0.00 -0.00 0.15 0.00 -0.00 0.07

14 6 -0.00 -0.00 -0.03 -0.00 -0.00 -0.07 0.00 -0.00 0.03

15 6 -0.00 0.00 -0.03 0.00 -0.00 0.07 0.00 0.00 0.03

16 6 -0.00 -0.00 -0.08 0.00 -0.00 -0.15 0.00 0.00 0.07

17 7 0.00 -0.00 0.09 0.00 -0.00 -0.00 -0.00 -0.00 -0.07

18 6 -0.00 -0.00 0.06 0.00 0.00 0.11 0.00 0.00 -0.09

19 6 -0.00 0.00 -0.06 0.00 0.00 -0.09 -0.00 0.00 0.14

20 6 -0.00 0.00 -0.01 0.00 0.00 -0.02 -0.00 0.00 -0.07

21 6 0.00 0.00 -0.01 -0.00 0.00 -0.02 -0.00 -0.00 0.07

22 6 0.00 0.00 -0.06 -0.00 0.00 -0.09 -0.00 -0.00 -0.14

23 7 -0.00 -0.00 0.06 -0.00 -0.00 0.09 -0.00 0.00 -0.00

24 1 -0.00 -0.00 0.22 0.00 0.00 -0.36 -0.00 -0.00 -0.19

25 1 0.00 -0.00 0.22 -0.00 0.00 -0.36 -0.00 0.00 0.19

26 1 0.00 0.00 0.42 -0.00 -0.00 0.25 -0.00 0.00 0.41

27 1 0.00 -0.00 0.42 0.00 -0.00 -0.25 -0.00 -0.00 0.41

28 1 -0.00 -0.00 0.42 -0.00 -0.00 -0.25 -0.00 0.00 -0.41

29 1 -0.00 0.00 0.42 0.00 -0.00 0.25 -0.00 -0.00 -0.41

30 1 -0.00 0.00 0.22 -0.00 0.00 0.36 -0.00 0.00 -0.19

31 1 0.00 0.00 0.22 0.00 0.00 0.36 -0.00 -0.00 0.19

32 30 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

33 6 0.00 -0.00 0.06 -0.00 0.00 0.11 0.00 -0.00 0.09

34 6 -0.00 -0.00 -0.01 0.00 -0.00 -0.03 0.00 0.00 -0.02

35 6 0.00 0.00 -0.01 0.00 -0.00 0.03 0.00 0.00 0.02

36 6 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

37 6 0.00 0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.00

38 6 -0.00 0.00 -0.01 -0.00 -0.00 0.03 0.00 -0.00 -0.02

39 6 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

40 6 0.00 -0.00 -0.01 -0.00 -0.00 -0.03 0.00 -0.00 0.02

41 6 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

42 1 0.00 -0.00 0.03 0.00 0.00 0.06 0.00 0.00 -0.05

43 1 -0.00 -0.00 0.03 -0.00 0.00 0.06 0.00 -0.00 0.05

44 1 -0.00 0.00 0.03 0.00 0.00 -0.06 0.00 0.00 0.05

45 1 0.00 0.00 0.03 -0.00 0.00 -0.06 0.00 -0.00 -0.05

61 62 63

A2 B1 A1

Frequencies -- 723.4767 765.5016 765.5718

Red. masses -- 5.6833 2.2881 2.2157

Frc consts -- 1.7527 0.7900 0.7651

IR Inten -- 0.0000 0.0000 117.4620

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.00 -0.10 0.00 0.00 0.00 0.00 0.00 0.01

2 6 0.00 0.00 0.21 -0.00 0.00 -0.02 0.00 0.00 0.01

3 7 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.01

4 6 0.00 -0.00 -0.21 -0.00 -0.00 0.02 -0.00 0.00 0.01

5 6 -0.00 0.00 0.10 0.00 -0.00 -0.00 -0.00 0.00 0.01

6 6 -0.00 0.00 0.16 -0.00 -0.00 -0.05 -0.00 -0.00 -0.04

7 6 0.00 -0.00 -0.15 -0.00 -0.00 0.12 -0.00 -0.00 0.12

8 7 -0.00 0.00 -0.00 0.00 -0.00 -0.07 0.00 -0.00 -0.07

9 6 -0.00 -0.00 0.15 -0.00 0.00 0.12 -0.00 0.00 0.12

10 6 0.00 0.00 -0.06 -0.00 0.00 -0.09 -0.00 0.00 -0.09

11 6 -0.00 0.00 0.06 -0.00 -0.00 -0.09 -0.00 -0.00 -0.09

12 6 -0.00 -0.00 -0.16 -0.00 0.00 0.05 0.00 -0.00 -0.04

13 6 0.00 0.00 0.15 -0.00 0.00 -0.12 0.00 -0.00 0.12

14 6 -0.00 -0.00 -0.06 -0.00 0.00 0.09 0.00 -0.00 -0.09

15 6 0.00 -0.00 0.06 -0.00 -0.00 0.09 0.00 0.00 -0.09

16 6 -0.00 0.00 -0.15 -0.00 -0.00 -0.12 0.00 0.00 0.12

17 7 0.00 -0.00 -0.00 0.00 -0.00 0.07 -0.00 0.00 -0.07

18 6 0.00 -0.00 0.16 -0.00 -0.00 0.05 0.00 0.00 -0.04

19 6 -0.00 0.00 -0.21 -0.00 -0.00 -0.02 0.00 -0.00 0.01

20 6 0.00 -0.00 0.10 0.00 -0.00 0.00 0.00 -0.00 0.01

21 6 0.00 0.00 -0.10 0.00 0.00 -0.00 -0.00 -0.00 0.01

22 6 -0.00 -0.00 0.21 -0.00 0.00 0.02 -0.00 -0.00 0.01

23 7 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 -0.01

24 1 -0.00 -0.00 -0.27 0.00 0.00 0.03 -0.00 0.00 -0.09

25 1 -0.00 0.00 0.27 0.00 -0.00 -0.03 0.00 0.00 -0.09

26 1 0.00 0.00 -0.26 -0.00 -0.00 0.47 -0.00 -0.00 0.46

27 1 -0.00 0.00 0.26 -0.00 0.00 0.47 -0.00 0.00 0.46

28 1 -0.00 -0.00 -0.26 -0.00 -0.00 -0.47 0.00 0.00 0.46

29 1 0.00 -0.00 0.26 -0.00 0.00 -0.47 0.00 -0.00 0.46

30 1 0.00 -0.00 0.27 0.00 -0.00 0.03 -0.00 -0.00 -0.09

31 1 0.00 0.00 -0.27 0.00 0.00 -0.03 0.00 -0.00 -0.09

32 30 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 0.00

33 6 0.00 0.00 -0.16 -0.00 0.00 -0.05 -0.00 0.00 -0.04

34 6 -0.00 -0.00 0.04 0.00 -0.00 0.01 0.00 -0.00 0.01

35 6 0.00 0.00 0.04 0.00 -0.00 -0.01 -0.00 0.00 0.01

36 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00

37 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00

38 6 0.00 -0.00 -0.04 0.00 0.00 0.01 0.00 0.00 0.01

39 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00

40 6 -0.00 0.00 -0.04 0.00 0.00 -0.01 -0.00 -0.00 0.01

41 6 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00

42 1 -0.00 0.00 0.08 -0.00 -0.00 0.01 0.00 0.00 -0.01

43 1 -0.00 -0.00 -0.08 -0.00 0.00 -0.01 -0.00 0.00 -0.01

44 1 0.00 -0.00 0.08 -0.00 -0.00 -0.01 -0.00 -0.00 -0.01

45 1 0.00 0.00 -0.08 -0.00 0.00 0.01 0.00 -0.00 -0.01

64 65 66

A1 B2 A2

Frequencies -- 795.0722 795.1581 845.8270

Red. masses -- 1.8384 1.8367 7.8896

Frc consts -- 0.6847 0.6842 3.3256

IR Inten -- 178.3370 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.00 -0.09 -0.00 0.00 -0.09 0.17 0.12 -0.00

2 6 -0.00 0.00 0.09 -0.00 0.00 0.09 -0.09 0.13 -0.00

3 7 0.00 -0.00 -0.05 0.00 -0.00 -0.05 -0.11 -0.00 -0.00

4 6 0.00 0.00 0.09 0.00 0.00 0.09 -0.09 -0.13 0.00

5 6 0.00 0.00 -0.09 0.00 0.00 -0.09 0.17 -0.12 0.00

6 6 0.00 0.00 -0.03 0.00 0.00 -0.03 -0.15 -0.12 -0.00

7 6 -0.00 0.00 0.01 0.00 0.00 0.01 -0.08 -0.08 -0.00

8 7 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.03 -0.00

9 6 -0.00 -0.00 0.01 -0.00 0.00 -0.01 0.08 -0.08 0.00

10 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.07 0.15 0.00

11 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.07 0.15 -0.00

12 6 -0.00 0.00 -0.03 -0.00 0.00 -0.03 -0.15 0.12 0.00

13 6 0.00 0.00 0.01 -0.00 0.00 0.01 -0.08 0.08 0.00

14 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.07 -0.15 0.00

15 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.07 -0.15 -0.00

16 6 0.00 -0.00 0.01 0.00 0.00 -0.01 0.08 0.08 -0.00

17 7 0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.03 -0.00

18 6 -0.00 -0.00 -0.03 0.00 0.00 0.03 0.15 0.12 -0.00

19 6 -0.00 -0.00 0.09 0.00 0.00 -0.09 0.09 0.13 0.00

20 6 -0.00 -0.00 -0.09 0.00 0.00 0.09 -0.17 0.12 0.00

21 6 0.00 -0.00 -0.09 -0.00 0.00 0.09 -0.17 -0.12 -0.00

22 6 0.00 -0.00 0.09 -0.00 0.00 -0.09 0.09 -0.13 -0.00

23 7 -0.00 0.00 -0.05 0.00 -0.00 0.05 0.11 0.00 -0.00

24 1 0.00 0.00 0.48 0.00 0.00 0.48 0.18 0.11 -0.00

25 1 -0.00 0.00 0.48 -0.00 0.00 0.48 0.18 -0.11 0.00

26 1 -0.00 0.00 0.02 -0.00 -0.00 0.04 0.02 0.21 -0.00

27 1 -0.00 -0.00 0.02 0.00 -0.00 -0.04 -0.02 0.21 0.00

28 1 0.00 -0.00 0.02 -0.00 -0.00 -0.04 -0.02 -0.21 -0.00

29 1 0.00 0.00 0.02 0.00 -0.00 0.04 0.02 -0.21 0.00

30 1 0.00 -0.00 0.48 -0.00 0.00 -0.48 -0.18 0.11 0.00

31 1 -0.00 -0.00 0.48 0.00 0.00 -0.48 -0.18 -0.11 -0.00

32 30 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 0.00

33 6 0.00 -0.00 -0.03 -0.00 0.00 0.03 0.15 -0.12 0.00

34 6 -0.00 0.00 0.01 0.00 -0.00 -0.01 -0.05 0.03 -0.00

35 6 0.00 -0.00 0.01 0.00 -0.00 0.01 0.05 -0.03 -0.00

36 6 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.01 -0.01 -0.00

37 6 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.01 0.01 -0.00

38 6 -0.00 -0.00 0.01 -0.00 -0.00 0.01 0.05 0.03 0.00

39 6 0.00 0.00 -0.00 -0.00 0.00 -0.00 0.01 -0.01 0.00

40 6 0.00 0.00 0.01 -0.00 -0.00 -0.01 -0.05 -0.03 0.00

41 6 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.01 0.01 0.00

42 1 -0.00 -0.00 -0.01 0.00 0.00 0.01 0.04 0.06 -0.00

43 1 0.00 -0.00 -0.01 -0.00 0.00 0.01 0.04 -0.06 0.00

44 1 0.00 0.00 -0.01 0.00 0.00 -0.01 -0.04 -0.06 -0.00

45 1 -0.00 0.00 -0.01 -0.00 0.00 -0.01 -0.04 0.06 0.00

67 68 69

B1 A2 B2

Frequencies -- 852.5227 855.1701 855.2121

Red. masses -- 8.2171 1.3467 1.3499

Frc consts -- 3.5187 0.5803 0.5817

IR Inten -- 7.8924 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.18 0.13 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00

2 6 -0.10 0.14 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.01

3 7 -0.11 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 0.00

4 6 -0.10 -0.14 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.01

5 6 0.18 -0.13 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00

6 6 -0.16 -0.14 0.00 -0.00 -0.00 0.01 -0.00 -0.00 0.01

7 6 0.00 -0.11 -0.00 -0.00 -0.00 -0.02 -0.00 -0.00 -0.02

8 7 0.13 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00

9 6 0.00 0.11 -0.00 0.00 -0.00 0.02 0.00 -0.00 0.02

10 6 0.00 0.02 0.00 0.00 0.00 -0.08 0.00 0.00 -0.08

11 6 0.00 -0.02 0.00 -0.00 0.00 0.08 -0.00 0.00 0.08

12 6 -0.16 0.14 -0.00 -0.00 0.00 -0.01 0.00 -0.00 0.01

13 6 0.00 0.11 0.00 -0.00 0.00 0.02 0.00 -0.00 -0.02

14 6 0.00 0.02 -0.00 -0.00 -0.00 -0.08 0.00 0.00 0.08

15 6 0.00 -0.02 -0.00 0.00 -0.00 0.08 -0.00 0.00 -0.08

16 6 0.00 -0.11 0.00 0.00 0.00 -0.02 -0.00 -0.00 0.02

17 7 0.13 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00

18 6 -0.16 -0.14 -0.00 0.00 0.00 0.01 -0.00 -0.00 -0.01

19 6 -0.10 -0.14 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.01

20 6 0.18 -0.13 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00

21 6 0.18 0.13 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00

22 6 -0.10 0.14 0.00 0.00 -0.00 0.00 0.00 -0.00 0.01

23 7 -0.11 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00

24 1 0.20 0.12 -0.00 0.00 0.00 -0.02 -0.00 0.00 -0.01

25 1 0.20 -0.12 0.00 0.00 -0.00 0.02 0.00 0.00 -0.01

26 1 0.12 -0.12 -0.00 -0.00 0.00 0.49 -0.00 0.00 0.49

27 1 0.12 0.12 -0.00 0.00 0.00 -0.49 0.00 0.00 -0.49

28 1 0.12 -0.12 0.00 0.00 -0.00 0.49 -0.00 0.00 -0.49

29 1 0.12 0.12 0.00 -0.00 -0.00 -0.49 0.00 0.00 0.49

30 1 0.20 -0.12 -0.00 -0.00 0.00 0.02 0.00 0.00 0.01

31 1 0.20 0.12 0.00 -0.00 -0.00 -0.02 -0.00 0.00 0.01

32 30 -0.02 0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 0.00

33 6 -0.16 0.14 0.00 0.00 -0.00 -0.01 0.00 -0.00 -0.01

34 6 0.06 -0.05 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

35 6 0.06 -0.05 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

36 6 0.00 0.01 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00

37 6 0.00 0.01 0.00 0.00 0.00 -0.00 0.00 -0.00 0.00

38 6 0.06 0.05 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

39 6 0.00 -0.01 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00

40 6 0.06 0.05 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

41 6 0.00 -0.01 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00

42 1 -0.05 -0.06 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

43 1 -0.05 0.06 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

44 1 -0.05 -0.06 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

45 1 -0.05 0.06 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

70 71 72

B2 A1 A2

Frequencies -- 862.7180 878.9016 883.6869

Red. masses -- 7.9902 7.1082 6.2814

Frc consts -- 3.5038 3.2351 2.8900

IR Inten -- 108.6146 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.02 -0.01 -0.00 0.02 -0.03 -0.00 -0.04 -0.11 0.00

2 6 0.13 0.00 0.00 0.15 -0.00 0.00 -0.02 -0.07 0.00

3 7 0.00 0.15 -0.00 -0.00 0.17 -0.00 0.20 0.00 0.00

4 6 -0.13 0.00 0.00 -0.15 -0.00 0.00 -0.02 0.07 -0.00

5 6 -0.02 -0.01 -0.00 -0.02 -0.03 -0.00 -0.04 0.11 -0.00

6 6 -0.15 -0.16 -0.00 -0.16 -0.16 -0.00 0.06 -0.10 0.00

7 6 -0.12 -0.09 0.00 -0.00 -0.14 -0.00 -0.11 -0.02 -0.00

8 7 0.00 -0.10 0.00 0.15 0.00 0.00 0.00 -0.19 0.00

9 6 0.12 -0.09 -0.00 -0.00 0.14 -0.00 0.11 -0.02 0.00

10 6 0.12 0.17 0.00 -0.02 0.02 0.00 0.13 0.09 0.00

11 6 -0.12 0.17 -0.00 -0.02 -0.02 0.00 -0.13 0.09 -0.00

12 6 0.15 -0.16 -0.00 0.16 -0.16 -0.00 0.06 0.10 -0.00

13 6 0.12 -0.09 0.00 0.00 -0.14 -0.00 -0.11 0.02 0.00

14 6 0.12 0.17 -0.00 0.02 -0.02 0.00 -0.13 -0.09 0.00

15 6 -0.12 0.17 0.00 0.02 0.02 0.00 0.13 -0.09 -0.00

16 6 -0.12 -0.09 -0.00 0.00 0.14 -0.00 0.11 0.02 -0.00

17 7 0.00 -0.10 -0.00 -0.15 -0.00 0.00 -0.00 0.19 0.00

18 6 -0.15 -0.16 0.00 0.16 0.16 -0.00 -0.06 0.10 0.00

19 6 -0.13 0.00 -0.00 0.15 0.00 0.00 0.02 -0.07 -0.00

20 6 -0.02 -0.01 0.00 0.02 0.03 -0.00 0.04 -0.11 -0.00

21 6 0.02 -0.01 0.00 -0.02 0.03 -0.00 0.04 0.11 0.00

22 6 0.13 0.00 -0.00 -0.15 0.00 0.00 0.02 0.07 0.00

23 7 0.00 0.15 0.00 0.00 -0.17 -0.00 -0.20 -0.00 0.00

24 1 -0.15 0.12 0.00 -0.20 0.14 0.00 0.13 -0.24 0.00

25 1 0.15 0.12 0.00 0.20 0.14 0.00 0.13 0.24 -0.00

26 1 0.10 0.20 -0.00 0.14 -0.18 -0.00 0.23 -0.04 0.00

27 1 -0.10 0.20 0.00 0.14 0.18 -0.00 -0.23 -0.04 -0.00

28 1 0.10 0.20 0.00 -0.14 0.18 -0.00 -0.23 0.04 0.00

29 1 -0.10 0.20 -0.00 -0.14 -0.18 -0.00 0.23 0.04 -0.00

30 1 0.15 0.12 -0.00 -0.20 -0.14 0.00 -0.13 -0.24 -0.00

31 1 -0.15 0.12 -0.00 0.20 -0.14 0.00 -0.13 0.24 0.00

32 30 0.00 -0.02 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00

33 6 0.15 -0.16 0.00 -0.16 0.16 -0.00 -0.06 -0.10 -0.00

34 6 -0.06 0.06 -0.00 0.07 -0.07 0.00 0.04 0.05 0.00

35 6 -0.06 0.06 0.00 -0.07 0.07 0.00 -0.04 -0.05 0.00

36 6 0.01 -0.00 -0.00 -0.00 0.01 -0.00 0.05 0.05 0.00

37 6 0.01 -0.00 0.00 0.00 -0.01 -0.00 -0.05 -0.05 0.00

38 6 0.06 0.06 0.00 0.07 0.07 0.00 -0.04 0.05 -0.00

39 6 -0.01 -0.00 0.00 -0.00 -0.01 -0.00 -0.05 0.05 -0.00

40 6 0.06 0.06 -0.00 -0.07 -0.07 0.00 0.04 -0.05 -0.00

41 6 -0.01 -0.00 -0.00 0.00 0.01 -0.00 0.05 -0.05 -0.00

42 1 -0.06 -0.05 -0.00 0.06 0.06 -0.00 0.06 -0.05 -0.00

43 1 0.06 -0.05 -0.00 -0.06 0.06 -0.00 0.06 0.05 0.00

44 1 -0.06 -0.05 0.00 -0.06 -0.06 -0.00 -0.06 0.05 -0.00

45 1 0.06 -0.05 0.00 0.06 -0.06 -0.00 -0.06 -0.05 0.00

73 74 75

B1 A2 B1

Frequencies -- 917.5180 917.5356 959.8367

Red. masses -- 1.3188 1.3187 4.3705

Frc consts -- 0.6541 0.6541 2.3723

IR Inten -- 0.0000 0.0000 358.9468

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.00 -0.08 0.00 -0.00 -0.08 -0.06 -0.14 0.00

2 6 -0.00 0.00 0.01 0.00 0.00 0.01 0.02 -0.00 -0.00

3 7 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.14 -0.00 0.00

4 6 -0.00 -0.00 -0.01 0.00 -0.00 -0.01 0.02 0.00 0.00

5 6 0.00 0.00 0.08 0.00 0.00 0.08 -0.06 0.14 -0.00

6 6 -0.00 -0.00 0.01 -0.00 0.00 0.01 0.01 -0.11 0.00

7 6 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.02 -0.10 -0.00

8 7 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.12 -0.00 0.00

9 6 0.00 0.00 -0.00 -0.00 0.00 0.00 0.02 0.10 -0.00

10 6 0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.08 0.01 -0.00

11 6 0.00 0.00 0.00 0.00 -0.00 0.00 -0.08 -0.01 -0.00

12 6 -0.00 0.00 -0.01 -0.00 -0.00 -0.01 0.01 0.11 -0.00

13 6 0.00 0.00 0.00 0.00 -0.00 0.00 0.02 0.10 0.00

14 6 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.08 0.01 0.00

15 6 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.08 -0.01 0.00

16 6 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.02 -0.10 0.00

17 7 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.12 -0.00 -0.00

18 6 -0.00 -0.00 -0.01 0.00 -0.00 0.01 0.01 -0.11 -0.00

19 6 -0.00 -0.00 0.01 -0.00 0.00 -0.01 0.02 0.00 -0.00

20 6 0.00 0.00 -0.08 -0.00 -0.00 0.08 -0.06 0.14 0.00

21 6 0.00 -0.00 0.08 -0.00 0.00 -0.08 -0.06 -0.14 -0.00

22 6 -0.00 0.00 -0.01 -0.00 -0.00 0.01 0.02 -0.00 0.00

23 7 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.14 -0.00 -0.00

24 1 0.00 0.00 0.49 0.00 0.00 0.49 0.17 -0.32 0.00

25 1 0.00 -0.00 -0.49 0.00 -0.00 -0.49 0.17 0.32 -0.00

26 1 0.00 0.00 -0.00 -0.00 0.00 0.02 0.07 -0.19 -0.00

27 1 0.00 -0.00 -0.00 0.00 0.00 -0.02 0.07 0.19 -0.00

28 1 0.00 0.00 0.00 0.00 -0.00 0.02 0.07 -0.19 0.00

29 1 0.00 -0.00 0.00 -0.00 -0.00 -0.02 0.07 0.19 0.00

30 1 0.00 -0.00 0.49 -0.00 0.00 -0.49 0.17 0.32 0.00

31 1 0.00 0.00 -0.49 -0.00 -0.00 0.49 0.17 -0.32 -0.00

32 30 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.01 0.00 -0.00

33 6 -0.00 0.00 0.01 0.00 0.00 -0.01 0.01 0.11 0.00

34 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.01 -0.04 -0.00

35 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.01 -0.04 0.00

36 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.04 -0.04 -0.00

37 6 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.04 -0.04 0.00

38 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.01 0.04 -0.00

39 6 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.04 0.04 -0.00

40 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.01 0.04 0.00

41 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.04 0.04 0.00

42 1 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.06 0.03 0.00

43 1 -0.00 0.00 0.00 -0.00 -0.00 0.00 -0.06 -0.03 -0.00

44 1 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.06 0.03 -0.00

45 1 -0.00 0.00 -0.00 0.00 0.00 0.00 -0.06 -0.03 0.00

76 77 78

B2 A1 A2

Frequencies -- 960.9205 990.2484 1022.8078

Red. masses -- 5.6749 5.9809 2.6405

Frc consts -- 3.0873 3.4555 1.6275

IR Inten -- 108.4363 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 -0.14 0.00 -0.00 -0.19 -0.00 -0.02 -0.08 0.00

2 6 0.10 0.05 0.00 0.07 0.07 0.00 -0.02 0.06 -0.00

3 7 0.00 0.18 -0.00 0.00 0.21 -0.00 0.10 0.00 -0.00

4 6 -0.10 0.05 0.00 -0.07 0.07 0.00 -0.02 -0.06 0.00

5 6 -0.01 -0.14 0.00 0.00 -0.19 -0.00 -0.02 0.08 -0.00

6 6 -0.09 0.02 -0.00 -0.04 0.09 -0.00 -0.05 -0.05 -0.00

7 6 0.03 0.05 0.00 -0.02 0.10 0.00 -0.02 -0.01 -0.00

8 7 0.00 0.12 -0.00 -0.13 -0.00 -0.00 0.00 0.11 -0.00

9 6 -0.03 0.05 -0.00 -0.02 -0.10 0.00 0.02 -0.01 0.00

10 6 -0.14 -0.08 -0.00 0.09 0.01 -0.00 -0.08 -0.03 -0.00

11 6 0.14 -0.08 0.00 0.09 -0.01 -0.00 0.08 -0.03 0.00

12 6 0.09 0.02 -0.00 0.04 0.09 -0.00 -0.05 0.05 0.00

13 6 -0.03 0.05 0.00 0.02 0.10 0.00 -0.02 0.01 0.00

14 6 -0.14 -0.08 0.00 -0.09 -0.01 -0.00 0.08 0.03 -0.00

15 6 0.14 -0.08 -0.00 -0.09 0.01 -0.00 -0.08 0.03 0.00

16 6 0.03 0.05 -0.00 0.02 -0.10 0.00 0.02 0.01 -0.00

17 7 0.00 0.12 0.00 0.13 0.00 -0.00 -0.00 -0.11 -0.00

18 6 -0.09 0.02 0.00 0.04 -0.09 -0.00 0.05 0.05 -0.00

19 6 -0.10 0.05 -0.00 0.07 -0.07 0.00 0.02 0.06 0.00

20 6 -0.01 -0.14 -0.00 -0.00 0.19 -0.00 0.02 -0.08 -0.00

21 6 0.01 -0.14 -0.00 0.00 0.19 -0.00 0.02 0.08 0.00

22 6 0.10 0.05 -0.00 -0.07 -0.07 0.00 0.02 -0.06 -0.00

23 7 0.00 0.18 0.00 -0.00 -0.21 -0.00 -0.10 -0.00 -0.00

24 1 -0.22 0.03 0.00 -0.23 -0.03 0.00 0.21 -0.26 0.00

25 1 0.22 0.03 0.00 0.23 -0.03 0.00 0.21 0.26 -0.00

26 1 -0.29 0.11 -0.00 -0.10 0.27 -0.00 -0.25 0.19 -0.00

27 1 0.29 0.11 0.00 -0.10 -0.27 -0.00 0.25 0.19 0.00

28 1 -0.29 0.11 0.00 0.10 -0.27 -0.00 0.25 -0.19 -0.00

29 1 0.29 0.11 -0.00 0.10 0.27 -0.00 -0.25 -0.19 0.00

30 1 0.22 0.03 -0.00 -0.23 0.03 0.00 -0.21 -0.26 -0.00

31 1 -0.22 0.03 -0.00 0.23 0.03 0.00 -0.21 0.26 0.00

32 30 -0.00 -0.02 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

33 6 0.09 0.02 0.00 -0.04 -0.09 -0.00 0.05 -0.05 0.00

34 6 -0.04 -0.01 -0.00 0.02 0.03 -0.00 -0.01 0.01 -0.00

35 6 -0.04 -0.01 0.00 -0.02 -0.03 -0.00 0.01 -0.01 -0.00

36 6 -0.04 -0.05 -0.00 0.05 0.04 0.00 0.00 0.00 0.00

37 6 -0.04 -0.05 0.00 -0.05 -0.04 0.00 -0.00 -0.00 0.00

38 6 0.04 -0.01 0.00 0.02 -0.03 -0.00 0.01 0.01 0.00

39 6 0.04 -0.05 0.00 0.05 -0.04 0.00 -0.00 0.00 -0.00

40 6 0.04 -0.01 -0.00 -0.02 0.03 -0.00 -0.01 -0.01 0.00

41 6 0.04 -0.05 -0.00 -0.05 0.04 0.00 0.00 -0.00 -0.00

42 1 0.04 -0.06 -0.00 -0.05 0.04 0.00 0.01 0.01 -0.00

43 1 -0.04 -0.06 -0.00 0.05 0.04 0.00 0.01 -0.01 0.00

44 1 0.04 -0.06 0.00 0.05 -0.04 0.00 -0.01 -0.01 -0.00

45 1 -0.04 -0.06 0.00 -0.05 -0.04 0.00 -0.01 0.01 0.00

79 80 81

B2 A1 B1

Frequencies -- 1029.8405 1049.5218 1050.1104

Red. masses -- 4.1112 5.2545 4.6239

Frc consts -- 2.5690 3.4101 3.0042

IR Inten -- 113.1048 0.0000 191.8012

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 -0.15 0.00 0.01 -0.12 0.00 0.01 0.07 -0.00

2 6 -0.03 0.08 0.00 -0.06 0.07 0.00 0.04 -0.08 0.00

3 7 -0.00 0.15 -0.00 0.00 0.13 -0.00 -0.10 -0.00 -0.00

4 6 0.03 0.08 0.00 0.06 0.07 0.00 0.04 0.08 -0.00

5 6 -0.01 -0.15 0.00 -0.01 -0.12 0.00 0.01 -0.07 0.00

6 6 0.07 0.05 0.00 0.09 0.05 0.00 0.06 0.05 0.00

7 6 0.04 0.03 0.00 0.06 -0.02 -0.00 0.07 -0.02 -0.00

8 7 0.00 -0.13 0.00 0.17 -0.00 0.00 0.19 0.00 0.00

9 6 -0.04 0.03 -0.00 0.06 0.02 -0.00 0.07 0.02 -0.00

10 6 0.08 0.02 0.00 -0.17 -0.02 -0.00 -0.18 -0.00 -0.00

11 6 -0.08 0.02 -0.00 -0.17 0.02 -0.00 -0.18 0.00 -0.00

12 6 -0.07 0.05 0.00 -0.09 0.05 0.00 0.06 -0.05 -0.00

13 6 -0.04 0.03 0.00 -0.06 -0.02 -0.00 0.07 0.02 0.00

14 6 0.08 0.02 -0.00 0.17 0.02 -0.00 -0.18 -0.00 0.00

15 6 -0.08 0.02 0.00 0.17 -0.02 -0.00 -0.18 0.00 0.00

16 6 0.04 0.03 -0.00 -0.06 0.02 -0.00 0.07 -0.02 0.00

17 7 0.00 -0.13 -0.00 -0.17 0.00 0.00 0.19 0.00 -0.00

18 6 0.07 0.05 -0.00 -0.09 -0.05 0.00 0.06 0.05 -0.00

19 6 0.03 0.08 -0.00 -0.06 -0.07 0.00 0.04 0.08 0.00

20 6 -0.01 -0.15 -0.00 0.01 0.12 0.00 0.01 -0.07 -0.00

21 6 0.01 -0.15 -0.00 -0.01 0.12 0.00 0.01 0.07 0.00

22 6 -0.03 0.08 -0.00 0.06 -0.07 0.00 0.04 -0.08 -0.00

23 7 -0.00 0.15 0.00 0.00 -0.13 -0.00 -0.10 -0.00 0.00

24 1 0.06 -0.20 0.00 0.20 -0.28 0.00 -0.26 0.28 -0.00

25 1 -0.06 -0.20 0.00 -0.20 -0.28 0.00 -0.26 -0.28 0.00

26 1 0.29 -0.24 0.00 -0.05 -0.20 -0.00 -0.08 -0.16 -0.00

27 1 -0.29 -0.24 -0.00 -0.05 0.20 -0.00 -0.08 0.16 -0.00

28 1 0.29 -0.24 -0.00 0.05 0.20 -0.00 -0.08 -0.16 0.00

29 1 -0.29 -0.24 0.00 0.05 -0.20 -0.00 -0.08 0.16 0.00

30 1 -0.06 -0.20 -0.00 0.20 0.28 0.00 -0.26 -0.28 -0.00

31 1 0.06 -0.20 -0.00 -0.20 0.28 0.00 -0.26 0.28 0.00

32 30 -0.00 -0.01 0.00 0.00 -0.00 -0.00 -0.02 0.00 -0.00

33 6 -0.07 0.05 -0.00 0.09 -0.05 0.00 0.06 -0.05 0.00

34 6 0.01 -0.00 -0.00 -0.02 0.00 -0.00 -0.01 0.00 -0.00

35 6 0.01 -0.00 0.00 0.02 -0.00 -0.00 -0.01 0.00 0.00

36 6 0.01 0.01 -0.00 -0.01 -0.01 -0.00 -0.00 -0.00 -0.00

37 6 0.01 0.01 0.00 0.01 0.01 -0.00 -0.00 -0.00 0.00

38 6 -0.01 -0.00 0.00 -0.02 -0.00 -0.00 -0.01 -0.00 -0.00

39 6 -0.01 0.01 0.00 -0.01 0.01 -0.00 -0.00 0.00 -0.00

40 6 -0.01 -0.00 -0.00 0.02 0.00 -0.00 -0.01 -0.00 0.00

41 6 -0.01 0.01 -0.00 0.01 -0.01 -0.00 -0.00 0.00 0.00

42 1 0.00 0.02 -0.00 0.00 -0.03 -0.00 0.00 0.01 0.00

43 1 -0.00 0.02 -0.00 -0.00 -0.03 -0.00 0.00 -0.01 -0.00

44 1 0.00 0.02 0.00 -0.00 0.03 -0.00 0.00 0.01 -0.00

45 1 -0.00 0.02 0.00 0.00 0.03 -0.00 0.00 -0.01 0.00

82 83 84

B1 A1 B2

Frequencies -- 1066.3377 1080.5898 1089.1492

Red. masses -- 1.2451 1.2736 1.1895

Frc consts -- 0.8342 0.8762 0.8314

IR Inten -- 814.6039 0.0000 113.9040

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.01 0.00 0.00 0.01 -0.00 0.04 0.01 0.00

2 6 0.00 0.01 0.00 0.00 -0.01 -0.00 -0.01 0.00 0.00

3 7 0.00 -0.00 0.00 0.00 -0.01 0.00 -0.00 0.03 -0.00

4 6 0.00 -0.01 -0.00 -0.00 -0.01 -0.00 0.01 0.00 0.00

5 6 -0.00 0.01 -0.00 -0.00 0.01 -0.00 -0.04 0.01 0.00

6 6 -0.01 -0.02 -0.00 -0.01 -0.01 0.00 -0.02 -0.02 0.00

7 6 0.02 0.01 -0.00 0.01 -0.00 -0.00 -0.02 -0.00 -0.00

8 7 0.04 0.00 0.00 0.06 -0.00 0.00 0.00 0.02 -0.00

9 6 0.02 -0.01 -0.00 0.01 0.00 -0.00 0.02 -0.00 0.00

10 6 -0.01 0.06 -0.00 -0.02 0.05 -0.00 -0.02 -0.01 -0.00

11 6 -0.01 -0.06 -0.00 -0.02 -0.05 -0.00 0.02 -0.01 0.00

12 6 -0.01 0.02 0.00 0.01 -0.01 0.00 0.02 -0.02 0.00

13 6 0.02 -0.01 0.00 -0.01 -0.00 -0.00 0.02 -0.00 -0.00

14 6 -0.01 0.06 0.00 0.02 -0.05 -0.00 -0.02 -0.01 0.00

15 6 -0.01 -0.06 0.00 0.02 0.05 -0.00 0.02 -0.01 -0.00

16 6 0.02 0.01 0.00 -0.01 0.00 -0.00 -0.02 -0.00 0.00

17 7 0.04 0.00 -0.00 -0.06 0.00 0.00 0.00 0.02 0.00

18 6 -0.01 -0.02 0.00 0.01 0.01 0.00 -0.02 -0.02 -0.00

19 6 0.00 -0.01 0.00 0.00 0.01 -0.00 0.01 0.00 -0.00

20 6 -0.00 0.01 0.00 0.00 -0.01 -0.00 -0.04 0.01 -0.00

21 6 -0.00 -0.01 -0.00 -0.00 -0.01 -0.00 0.04 0.01 -0.00

22 6 0.00 0.01 -0.00 -0.00 0.01 -0.00 -0.01 0.00 -0.00

23 7 0.00 -0.00 -0.00 -0.00 0.01 0.00 -0.00 0.03 0.00

24 1 0.03 -0.03 0.00 0.03 -0.01 0.00 0.41 -0.27 0.00

25 1 0.03 0.03 -0.00 -0.03 -0.01 0.00 -0.41 -0.27 0.00

26 1 -0.28 0.41 -0.00 -0.28 0.40 -0.00 -0.07 0.07 -0.00

27 1 -0.28 -0.41 -0.00 -0.28 -0.40 -0.00 0.07 0.07 0.00

28 1 -0.28 0.41 0.00 0.28 -0.40 -0.00 -0.07 0.07 0.00

29 1 -0.28 -0.41 0.00 0.28 0.40 -0.00 0.07 0.07 -0.00

30 1 0.03 0.03 0.00 0.03 0.01 0.00 -0.41 -0.27 -0.00

31 1 0.03 -0.03 -0.00 -0.03 0.01 0.00 0.41 -0.27 -0.00

32 30 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

33 6 -0.01 0.02 -0.00 -0.01 0.01 0.00 0.02 -0.02 -0.00

34 6 0.00 -0.01 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

35 6 0.00 -0.01 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

36 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00

37 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 0.00

38 6 0.00 0.01 -0.00 0.00 0.00 0.00 0.00 0.00 0.00

39 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00

40 6 0.00 0.01 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

41 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00

42 1 -0.01 0.00 0.00 0.00 0.00 -0.00 -0.01 -0.00 -0.00

43 1 -0.01 -0.00 -0.00 -0.00 0.00 -0.00 0.01 -0.00 -0.00

44 1 -0.01 0.00 -0.00 -0.00 -0.00 -0.00 -0.01 -0.00 0.00

45 1 -0.01 -0.00 0.00 0.00 -0.00 -0.00 0.01 -0.00 0.00

85 86 87

A2 A1 A1

Frequencies -- 1093.3709 1096.2834 1139.0985

Red. masses -- 7.9980 1.3172 6.9880

Frc consts -- 5.6334 0.9327 5.3423

IR Inten -- 0.0000 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.08 -0.14 0.00 0.04 0.01 -0.00 -0.03 -0.04 -0.00

2 6 0.18 0.11 -0.00 -0.00 -0.00 0.00 -0.08 -0.02 0.00

3 7 -0.16 0.00 0.00 -0.00 0.04 -0.00 0.00 0.14 -0.00

4 6 0.18 -0.11 0.00 0.00 -0.00 0.00 0.08 -0.02 0.00

5 6 -0.08 0.14 -0.00 -0.04 0.01 -0.00 0.03 -0.04 -0.00

6 6 -0.01 0.02 -0.00 -0.02 -0.03 -0.00 0.19 -0.19 0.00

7 6 0.11 -0.16 0.00 -0.01 -0.01 0.00 0.02 -0.07 0.00

8 7 0.00 0.12 -0.00 -0.04 0.00 -0.00 -0.16 -0.00 -0.00

9 6 -0.11 -0.16 -0.00 -0.01 0.01 0.00 0.02 0.07 0.00

10 6 0.14 0.08 0.00 0.04 0.01 0.00 0.04 0.02 -0.00

11 6 -0.14 0.08 -0.00 0.04 -0.01 0.00 0.04 -0.02 -0.00

12 6 -0.01 -0.02 0.00 0.02 -0.03 -0.00 -0.19 -0.19 0.00

13 6 0.11 0.16 -0.00 0.01 -0.01 0.00 -0.02 -0.07 0.00

14 6 -0.14 -0.08 0.00 -0.04 -0.01 0.00 -0.04 -0.02 -0.00

15 6 0.14 -0.08 -0.00 -0.04 0.01 0.00 -0.04 0.02 -0.00

16 6 -0.11 0.16 0.00 0.01 0.01 0.00 -0.02 0.07 0.00

17 7 -0.00 -0.12 -0.00 0.04 -0.00 -0.00 0.16 0.00 -0.00

18 6 0.01 -0.02 -0.00 0.02 0.03 -0.00 -0.19 0.19 0.00

19 6 -0.18 0.11 0.00 -0.00 0.00 0.00 -0.08 0.02 0.00

20 6 0.08 -0.14 -0.00 0.04 -0.01 -0.00 -0.03 0.04 -0.00

21 6 0.08 0.14 0.00 -0.04 -0.01 -0.00 0.03 0.04 -0.00

22 6 -0.18 -0.11 -0.00 0.00 0.00 0.00 0.08 0.02 0.00

23 7 0.16 -0.00 0.00 0.00 -0.04 -0.00 -0.00 -0.14 -0.00

24 1 0.01 -0.21 0.00 0.41 -0.27 0.00 -0.24 0.11 -0.00

25 1 0.01 0.21 -0.00 -0.41 -0.27 0.00 0.24 0.11 -0.00

26 1 0.22 -0.03 0.00 0.03 0.02 0.00 -0.04 0.15 -0.00

27 1 -0.22 -0.03 -0.00 0.03 -0.02 0.00 -0.04 -0.15 -0.00

28 1 -0.22 0.03 0.00 -0.03 -0.02 0.00 0.04 -0.15 -0.00

29 1 0.22 0.03 -0.00 -0.03 0.02 0.00 0.04 0.15 -0.00

30 1 -0.01 -0.21 -0.00 0.41 0.27 0.00 -0.24 -0.11 -0.00

31 1 -0.01 0.21 0.00 -0.41 0.27 0.00 0.24 -0.11 -0.00

32 30 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 0.00

33 6 0.01 0.02 0.00 -0.02 0.03 -0.00 0.19 0.19 0.00

34 6 -0.01 -0.01 -0.00 0.00 -0.01 -0.00 -0.04 -0.04 -0.00

35 6 0.01 0.01 -0.00 -0.00 0.01 -0.00 0.04 0.04 -0.00

36 6 0.03 0.03 0.00 -0.00 -0.00 -0.00 -0.09 -0.09 -0.00

37 6 -0.03 -0.03 0.00 0.00 0.00 -0.00 0.09 0.09 -0.00

38 6 0.01 -0.01 0.00 0.00 0.01 -0.00 -0.04 0.04 -0.00

39 6 -0.03 0.03 -0.00 -0.00 0.00 -0.00 -0.09 0.09 -0.00

40 6 -0.01 0.01 0.00 -0.00 -0.01 -0.00 0.04 -0.04 -0.00

41 6 0.03 -0.03 -0.00 0.00 -0.00 -0.00 0.09 -0.09 -0.00

42 1 0.03 -0.03 -0.00 0.01 0.00 -0.00 0.11 -0.10 -0.00

43 1 0.03 0.03 0.00 -0.01 0.00 -0.00 -0.11 -0.10 -0.00

44 1 -0.03 0.03 -0.00 -0.01 -0.00 -0.00 -0.11 0.10 -0.00

45 1 -0.03 -0.03 0.00 0.01 -0.00 -0.00 0.11 0.10 -0.00

88 89 90

B2 B1 A2

Frequencies -- 1159.7133 1160.1966 1184.3175

Red. masses -- 6.2668 6.6912 2.2186

Frc consts -- 4.9659 5.3066 1.8334

IR Inten -- 7.0325 12.3887 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 -0.04 0.00 -0.03 -0.02 0.00 0.01 -0.00 -0.00

2 6 -0.10 -0.04 0.00 -0.04 0.07 -0.00 0.04 -0.08 0.00

3 7 -0.00 0.15 -0.00 0.13 0.00 0.00 -0.05 0.00 0.00

4 6 0.10 -0.04 0.00 -0.04 -0.07 0.00 0.04 0.08 -0.00

5 6 0.03 -0.04 0.00 -0.03 0.02 -0.00 0.01 0.00 0.00

6 6 0.18 -0.16 0.00 -0.15 0.20 -0.00 0.06 -0.06 0.00

7 6 -0.03 -0.05 -0.00 -0.04 0.09 -0.00 -0.07 -0.05 -0.00

8 7 -0.00 0.16 -0.00 0.20 0.00 0.00 0.00 0.07 -0.00

9 6 0.03 -0.05 0.00 -0.04 -0.09 -0.00 0.07 -0.05 0.00

10 6 -0.01 -0.02 -0.00 -0.05 -0.04 -0.00 0.01 -0.01 0.00

11 6 0.01 -0.02 0.00 -0.05 0.04 -0.00 -0.01 -0.01 -0.00

12 6 -0.18 -0.16 0.00 -0.15 -0.20 0.00 0.06 0.06 -0.00

13 6 0.03 -0.05 -0.00 -0.04 -0.09 0.00 -0.07 0.05 0.00

14 6 -0.01 -0.02 0.00 -0.05 -0.04 0.00 -0.01 0.01 0.00

15 6 0.01 -0.02 -0.00 -0.05 0.04 0.00 0.01 0.01 -0.00

16 6 -0.03 -0.05 0.00 -0.04 0.09 0.00 0.07 0.05 -0.00

17 7 -0.00 0.16 0.00 0.20 0.00 -0.00 -0.00 -0.07 -0.00

18 6 0.18 -0.16 -0.00 -0.15 0.20 0.00 -0.06 0.06 0.00

19 6 0.10 -0.04 -0.00 -0.04 -0.07 -0.00 -0.04 -0.08 -0.00

20 6 0.03 -0.04 -0.00 -0.03 0.02 0.00 -0.01 -0.00 0.00

21 6 -0.03 -0.04 -0.00 -0.03 -0.02 -0.00 -0.01 0.00 -0.00

22 6 -0.10 -0.04 -0.00 -0.04 0.07 0.00 -0.04 0.08 0.00

23 7 -0.00 0.15 0.00 0.13 0.00 -0.00 0.05 -0.00 0.00

24 1 -0.19 0.07 -0.00 0.23 -0.22 0.00 -0.24 0.19 -0.00

25 1 0.19 0.07 -0.00 0.23 0.22 -0.00 -0.24 -0.19 0.00

26 1 -0.18 0.21 -0.00 -0.04 -0.07 -0.00 -0.22 0.28 -0.00

27 1 0.18 0.21 0.00 -0.04 0.07 -0.00 0.22 0.28 0.00

28 1 -0.18 0.21 0.00 -0.04 -0.07 0.00 0.22 -0.28 -0.00

29 1 0.18 0.21 -0.00 -0.04 0.07 0.00 -0.22 -0.28 0.00

30 1 0.19 0.07 0.00 0.23 0.22 0.00 0.24 0.19 0.00

31 1 -0.19 0.07 0.00 0.23 -0.22 -0.00 0.24 -0.19 -0.00

32 30 0.00 -0.01 -0.00 -0.01 -0.00 -0.00 -0.00 -0.00 0.00

33 6 -0.18 -0.16 -0.00 -0.15 -0.20 -0.00 -0.06 -0.06 -0.00

34 6 0.04 0.03 -0.00 0.02 0.04 -0.00 0.01 0.01 0.00

35 6 0.04 0.03 0.00 0.02 0.04 0.00 -0.01 -0.01 0.00

36 6 0.08 0.08 0.00 0.08 0.07 -0.00 0.03 0.02 0.00

37 6 0.08 0.08 -0.00 0.08 0.07 0.00 -0.03 -0.02 0.00

38 6 -0.04 0.03 0.00 0.02 -0.04 -0.00 -0.01 0.01 -0.00

39 6 -0.08 0.08 -0.00 0.08 -0.07 -0.00 -0.03 0.02 -0.00

40 6 -0.04 0.03 -0.00 0.02 -0.04 0.00 0.01 -0.01 -0.00

41 6 -0.08 0.08 0.00 0.08 -0.07 0.00 0.03 -0.02 -0.00

42 1 -0.09 0.09 0.00 0.10 -0.08 -0.00 0.03 -0.03 -0.00

43 1 0.09 0.09 0.00 0.10 0.08 0.00 0.03 0.03 0.00

44 1 -0.09 0.09 -0.00 0.10 -0.08 0.00 -0.03 0.03 -0.00

45 1 0.09 0.09 -0.00 0.10 0.08 -0.00 -0.03 -0.03 0.00

91 92 93

B2 A2 B1

Frequencies -- 1237.5280 1239.4400 1244.2295

Red. masses -- 2.5461 4.5085 4.1906

Frc consts -- 2.2974 4.0807 3.8223

IR Inten -- 21.4893 0.0000 478.0002

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 0.03 -0.00 -0.01 -0.04 0.00 0.03 0.01 -0.00

2 6 0.05 -0.05 0.00 0.06 -0.02 -0.00 -0.07 -0.17 0.00

3 7 -0.00 0.03 -0.00 0.06 -0.00 -0.00 0.19 0.00 0.00

4 6 -0.05 -0.05 0.00 0.06 0.02 0.00 -0.07 0.17 -0.00

5 6 -0.01 0.03 -0.00 -0.01 0.04 -0.00 0.03 -0.01 0.00

6 6 -0.02 -0.06 -0.00 -0.13 0.18 -0.00 -0.07 -0.01 0.00

7 6 0.13 -0.01 0.00 -0.09 -0.05 -0.00 -0.06 -0.07 -0.00

8 7 0.00 0.10 -0.00 -0.00 -0.11 0.00 0.02 0.00 -0.00

9 6 -0.13 -0.01 -0.00 0.09 -0.05 0.00 -0.06 0.07 -0.00

10 6 -0.01 0.03 -0.00 0.04 -0.00 0.00 0.04 0.02 0.00

11 6 0.01 0.03 0.00 -0.04 -0.00 -0.00 0.04 -0.02 0.00

12 6 0.02 -0.06 -0.00 -0.13 -0.18 0.00 -0.07 0.01 -0.00

13 6 -0.13 -0.01 0.00 -0.09 0.05 0.00 -0.06 0.07 0.00

14 6 -0.01 0.03 0.00 -0.04 0.00 0.00 0.04 0.02 -0.00

15 6 0.01 0.03 -0.00 0.04 0.00 -0.00 0.04 -0.02 -0.00

16 6 0.13 -0.01 -0.00 0.09 0.05 -0.00 -0.06 -0.07 0.00

17 7 0.00 0.10 0.00 0.00 0.11 0.00 0.02 0.00 0.00

18 6 -0.02 -0.06 0.00 0.13 -0.18 -0.00 -0.07 -0.01 -0.00

19 6 -0.05 -0.05 -0.00 -0.06 -0.02 0.00 -0.07 0.17 0.00

20 6 -0.01 0.03 0.00 0.01 -0.04 -0.00 0.03 -0.01 -0.00

21 6 0.01 0.03 0.00 0.01 0.04 0.00 0.03 0.01 0.00

22 6 0.05 -0.05 -0.00 -0.06 0.02 -0.00 -0.07 -0.17 -0.00

23 7 -0.00 0.03 0.00 -0.06 0.00 -0.00 0.19 0.00 -0.00

24 1 0.07 -0.01 -0.00 -0.13 0.05 0.00 -0.31 0.28 -0.00

25 1 -0.07 -0.01 -0.00 -0.13 -0.05 -0.00 -0.31 -0.28 0.00

26 1 0.28 -0.36 0.00 -0.20 0.32 -0.00 -0.00 0.09 0.00

27 1 -0.28 -0.36 -0.00 0.20 0.32 0.00 -0.00 -0.09 0.00

28 1 0.28 -0.36 -0.00 0.20 -0.32 -0.00 -0.00 0.09 -0.00

29 1 -0.28 -0.36 0.00 -0.20 -0.32 0.00 -0.00 -0.09 -0.00

30 1 -0.07 -0.01 0.00 0.13 0.05 -0.00 -0.31 -0.28 -0.00

31 1 0.07 -0.01 0.00 0.13 -0.05 0.00 -0.31 0.28 0.00

32 30 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00

33 6 0.02 -0.06 0.00 0.13 0.18 0.00 -0.07 0.01 0.00

34 6 -0.01 0.01 -0.00 -0.02 -0.03 -0.00 0.02 -0.01 0.00

35 6 -0.01 0.01 0.00 0.02 0.03 -0.00 0.02 -0.01 -0.00

36 6 0.01 0.01 0.00 -0.05 -0.05 -0.00 0.01 0.02 0.00

37 6 0.01 0.01 -0.00 0.05 0.05 -0.00 0.01 0.02 -0.00

38 6 0.01 0.01 0.00 0.02 -0.03 0.00 0.02 0.01 0.00

39 6 -0.01 0.01 -0.00 0.05 -0.05 0.00 0.01 -0.02 0.00

40 6 0.01 0.01 -0.00 -0.02 0.03 0.00 0.02 0.01 -0.00

41 6 -0.01 0.01 0.00 -0.05 0.05 0.00 0.01 -0.02 -0.00

42 1 -0.02 0.00 0.00 -0.06 0.05 0.00 0.01 -0.03 -0.00

43 1 0.02 0.00 0.00 -0.06 -0.05 -0.00 0.01 0.03 0.00

44 1 -0.02 0.00 -0.00 0.06 -0.05 0.00 0.01 -0.03 0.00

45 1 0.02 0.00 -0.00 0.06 0.05 -0.00 0.01 0.03 -0.00

94 95 96

A2 A1 B2

Frequencies -- 1275.0652 1311.8602 1311.8820

Red. masses -- 5.5248 12.2078 6.4888

Frc consts -- 5.2921 12.3784 6.5796

IR Inten -- 0.0000 0.0000 21.9844

Atom AN X Y Z X Y Z X Y Z

1 6 0.03 0.01 -0.00 -0.05 0.08 -0.00 0.04 0.03 -0.00

2 6 -0.08 -0.13 0.00 -0.09 -0.28 0.00 -0.04 -0.06 0.00

3 7 0.19 -0.00 -0.00 0.00 0.28 -0.00 -0.00 0.04 -0.00

4 6 -0.08 0.13 -0.00 0.09 -0.28 0.00 0.04 -0.06 0.00

5 6 0.03 -0.01 0.00 0.05 0.08 -0.00 -0.04 0.03 -0.00

6 6 -0.10 -0.01 -0.00 0.03 0.02 -0.00 0.00 -0.13 0.00

7 6 0.13 -0.12 0.00 -0.20 0.14 -0.00 -0.09 0.23 -0.00

8 7 -0.00 0.15 -0.00 0.23 -0.00 0.00 0.00 -0.18 0.00

9 6 -0.13 -0.12 -0.00 -0.20 -0.14 -0.00 0.09 0.23 0.00

10 6 0.03 0.03 0.00 0.06 -0.11 0.00 -0.14 0.00 -0.00

11 6 -0.03 0.03 -0.00 0.06 0.11 0.00 0.14 0.00 0.00

12 6 -0.10 0.01 0.00 -0.03 0.02 -0.00 -0.00 -0.13 0.00

13 6 0.13 0.12 -0.00 0.20 0.14 -0.00 0.09 0.23 -0.00

14 6 -0.03 -0.03 0.00 -0.06 0.11 0.00 -0.14 0.00 0.00

15 6 0.03 -0.03 -0.00 -0.06 -0.11 0.00 0.14 0.00 -0.00

16 6 -0.13 0.12 0.00 0.20 -0.14 -0.00 -0.09 0.23 0.00

17 7 0.00 -0.15 -0.00 -0.23 0.00 0.00 0.00 -0.18 -0.00

18 6 0.10 0.01 -0.00 -0.03 -0.02 -0.00 0.00 -0.13 -0.00

19 6 0.08 -0.13 -0.00 -0.09 0.28 0.00 0.04 -0.06 -0.00

20 6 -0.03 0.01 0.00 -0.05 -0.08 -0.00 -0.04 0.03 0.00

21 6 -0.03 -0.01 -0.00 0.05 -0.08 -0.00 0.04 0.03 0.00

22 6 0.08 0.13 0.00 0.09 0.28 0.00 -0.04 -0.06 -0.00

23 7 -0.19 0.00 -0.00 -0.00 -0.28 -0.00 -0.00 0.04 0.00

24 1 -0.23 0.20 -0.00 -0.03 0.07 -0.00 -0.07 0.12 -0.00

25 1 -0.23 -0.20 0.00 0.03 0.07 -0.00 0.07 0.12 -0.00

26 1 0.18 -0.16 0.00 -0.04 0.01 0.00 0.09 -0.31 0.00

27 1 -0.18 -0.16 -0.00 -0.04 -0.01 0.00 -0.09 -0.31 -0.00

28 1 -0.18 0.16 0.00 0.04 -0.01 0.00 0.09 -0.31 -0.00

29 1 0.18 0.16 -0.00 0.04 0.01 0.00 -0.09 -0.31 0.00

30 1 0.23 0.20 0.00 -0.03 -0.07 -0.00 0.07 0.12 0.00

31 1 0.23 -0.20 -0.00 0.03 -0.07 -0.00 -0.07 0.12 0.00

32 30 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

33 6 0.10 -0.01 0.00 0.03 -0.02 -0.00 -0.00 -0.13 -0.00

34 6 -0.02 0.01 -0.00 -0.03 0.02 -0.00 0.01 0.01 -0.00

35 6 0.02 -0.01 -0.00 0.03 -0.02 -0.00 0.01 0.01 0.00

36 6 -0.01 -0.02 -0.00 0.00 -0.00 0.00 0.02 0.02 -0.00

37 6 0.01 0.02 -0.00 -0.00 0.00 0.00 0.02 0.02 0.00

38 6 0.02 0.01 0.00 -0.03 -0.02 -0.00 -0.01 0.01 0.00

39 6 0.01 -0.02 0.00 0.00 0.00 0.00 -0.02 0.02 0.00

40 6 -0.02 -0.01 0.00 0.03 0.02 -0.00 -0.01 0.01 -0.00

41 6 -0.01 0.02 0.00 -0.00 -0.00 0.00 -0.02 0.02 -0.00

42 1 -0.01 0.03 0.00 -0.01 -0.01 0.00 -0.03 0.02 0.00

43 1 -0.01 -0.03 -0.00 0.01 -0.01 0.00 0.03 0.02 0.00

44 1 0.01 -0.03 0.00 0.01 0.01 0.00 -0.03 0.02 -0.00

45 1 0.01 0.03 -0.00 -0.01 0.01 0.00 0.03 0.02 -0.00

97 98 99

B1 B2 A2

Frequencies -- 1323.9106 1347.9487 1354.1965

Red. masses -- 4.3769 11.9700 2.3205

Frc consts -- 4.5199 12.8142 2.5072

IR Inten -- 1317.9493 56.1533 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 0.12 -0.00 -0.10 0.09 -0.00 -0.04 0.10 -0.00

2 6 -0.12 -0.05 0.00 -0.04 -0.35 0.00 -0.04 -0.03 0.00

3 7 0.11 -0.00 0.00 0.00 0.33 -0.00 0.01 -0.00 0.00

4 6 -0.12 0.05 -0.00 0.04 -0.35 0.00 -0.04 0.03 -0.00

5 6 -0.03 -0.12 0.00 0.10 0.09 -0.00 -0.04 -0.10 0.00

6 6 0.03 0.02 0.00 -0.02 0.20 -0.00 0.06 0.05 0.00

7 6 0.15 -0.01 0.00 -0.03 -0.02 0.00 0.03 -0.05 0.00

8 7 -0.12 -0.00 -0.00 -0.00 -0.08 0.00 -0.00 0.04 -0.00

9 6 0.15 0.01 0.00 0.03 -0.02 -0.00 -0.03 -0.05 -0.00

10 6 -0.07 0.02 -0.00 0.02 0.00 -0.00 0.07 -0.02 0.00

11 6 -0.07 -0.02 -0.00 -0.02 0.00 0.00 -0.07 -0.02 -0.00

12 6 0.03 -0.02 -0.00 0.02 0.20 -0.00 0.06 -0.05 -0.00

13 6 0.15 0.01 -0.00 0.03 -0.02 0.00 0.03 0.05 -0.00

14 6 -0.07 0.02 0.00 0.02 0.00 0.00 -0.07 0.02 0.00

15 6 -0.07 -0.02 0.00 -0.02 0.00 -0.00 0.07 0.02 -0.00

16 6 0.15 -0.01 -0.00 -0.03 -0.02 -0.00 -0.03 0.05 0.00

17 7 -0.12 -0.00 0.00 -0.00 -0.08 -0.00 0.00 -0.04 -0.00

18 6 0.03 0.02 -0.00 -0.02 0.20 0.00 -0.06 -0.05 0.00

19 6 -0.12 0.05 0.00 0.04 -0.35 -0.00 0.04 -0.03 -0.00

20 6 -0.03 -0.12 -0.00 0.10 0.09 0.00 0.04 0.10 0.00

21 6 -0.03 0.12 0.00 -0.10 0.09 0.00 0.04 -0.10 -0.00

22 6 -0.12 -0.05 -0.00 -0.04 -0.35 -0.00 0.04 0.03 0.00

23 7 0.11 -0.00 -0.00 0.00 0.33 0.00 -0.01 0.00 0.00

24 1 0.37 -0.18 0.00 0.05 -0.02 -0.00 0.35 -0.19 0.00

25 1 0.37 0.18 -0.00 -0.05 -0.02 -0.00 0.35 0.19 -0.00

26 1 -0.02 -0.05 -0.00 -0.03 0.07 -0.00 -0.11 0.22 -0.00

27 1 -0.02 0.05 -0.00 0.03 0.07 0.00 0.11 0.22 0.00

28 1 -0.02 -0.05 0.00 -0.03 0.07 0.00 0.11 -0.22 -0.00

29 1 -0.02 0.05 0.00 0.03 0.07 -0.00 -0.11 -0.22 0.00

30 1 0.37 0.18 0.00 -0.05 -0.02 0.00 -0.35 -0.19 -0.00

31 1 0.37 -0.18 -0.00 0.05 -0.02 0.00 -0.35 0.19 0.00

32 30 0.00 0.00 0.00 0.00 -0.01 -0.00 -0.00 -0.00 0.00

33 6 0.03 -0.02 0.00 0.02 0.20 0.00 -0.06 0.05 -0.00

34 6 0.00 -0.01 0.00 0.02 -0.03 -0.00 0.00 -0.00 0.00

35 6 0.00 -0.01 -0.00 0.02 -0.03 0.00 -0.00 0.00 0.00

36 6 0.00 0.00 0.00 -0.03 -0.03 -0.00 0.00 0.00 0.00

37 6 0.00 0.00 -0.00 -0.03 -0.03 0.00 -0.00 -0.00 0.00

38 6 0.00 0.01 0.00 -0.02 -0.03 0.00 -0.00 -0.00 -0.00

39 6 0.00 -0.00 0.00 0.03 -0.03 0.00 -0.00 0.00 -0.00

40 6 0.00 0.01 -0.00 -0.02 -0.03 -0.00 0.00 0.00 -0.00

41 6 0.00 -0.00 -0.00 0.03 -0.03 -0.00 0.00 -0.00 -0.00

42 1 0.00 -0.00 -0.00 0.05 -0.02 -0.00 -0.00 -0.01 -0.00

43 1 0.00 0.00 0.00 -0.05 -0.02 -0.00 -0.00 0.01 0.00

44 1 0.00 -0.00 0.00 0.05 -0.02 0.00 0.00 0.01 -0.00

45 1 0.00 0.00 -0.00 -0.05 -0.02 0.00 0.00 -0.01 0.00

100 101 102

B1 A1 B1

Frequencies -- 1357.6743 1383.6084 1426.5050

Red. masses -- 4.9203 10.8815 4.8140

Frc consts -- 5.3436 12.2734 5.7717

IR Inten -- 164.9824 0.0000 57.9473

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 0.10 -0.00 0.02 0.08 -0.00 -0.06 0.09 -0.00

2 6 -0.07 -0.04 0.00 0.09 -0.23 0.00 0.10 -0.04 0.00

3 7 0.00 -0.00 0.00 0.00 0.14 -0.00 -0.06 -0.00 -0.00

4 6 -0.07 0.04 -0.00 -0.09 -0.23 0.00 0.10 0.04 -0.00

5 6 -0.03 -0.10 0.00 -0.02 0.08 -0.00 -0.06 -0.09 0.00

6 6 0.14 -0.03 0.00 -0.03 0.04 -0.00 -0.01 0.08 -0.00

7 6 -0.14 -0.00 -0.00 0.31 0.07 0.00 -0.09 -0.12 -0.00

8 7 0.13 0.00 0.00 -0.19 -0.00 -0.00 0.01 0.00 0.00

9 6 -0.14 0.00 -0.00 0.31 -0.07 0.00 -0.09 0.12 -0.00

10 6 0.05 -0.13 0.00 -0.13 -0.02 -0.00 0.03 0.18 0.00

11 6 0.05 0.13 0.00 -0.13 0.02 -0.00 0.03 -0.18 0.00

12 6 0.14 0.03 -0.00 0.03 0.04 -0.00 -0.01 -0.08 0.00

13 6 -0.14 0.00 0.00 -0.31 0.07 0.00 -0.09 0.12 0.00

14 6 0.05 -0.13 -0.00 0.13 0.02 -0.00 0.03 0.18 -0.00

15 6 0.05 0.13 -0.00 0.13 -0.02 -0.00 0.03 -0.18 -0.00

16 6 -0.14 -0.00 0.00 -0.31 -0.07 0.00 -0.09 -0.12 0.00

17 7 0.13 0.00 -0.00 0.19 0.00 -0.00 0.01 0.00 -0.00

18 6 0.14 -0.03 -0.00 0.03 -0.04 -0.00 -0.01 0.08 0.00

19 6 -0.07 0.04 0.00 0.09 0.23 0.00 0.10 0.04 0.00

20 6 -0.03 -0.10 -0.00 0.02 -0.08 -0.00 -0.06 -0.09 -0.00

21 6 -0.03 0.10 0.00 -0.02 -0.08 -0.00 -0.06 0.09 0.00

22 6 -0.07 -0.04 -0.00 -0.09 0.23 0.00 0.10 -0.04 -0.00

23 7 0.00 -0.00 0.00 -0.00 -0.14 -0.00 -0.06 -0.00 0.00

24 1 0.31 -0.15 0.00 0.06 0.07 -0.00 0.29 -0.17 0.00

25 1 0.31 0.15 -0.00 -0.06 0.07 -0.00 0.29 0.17 -0.00

26 1 -0.15 0.13 -0.00 -0.13 -0.07 -0.00 0.22 -0.03 0.00

27 1 -0.15 -0.13 -0.00 -0.13 0.07 -0.00 0.22 0.03 0.00

28 1 -0.15 0.13 0.00 0.13 0.07 -0.00 0.22 -0.03 -0.00

29 1 -0.15 -0.13 0.00 0.13 -0.07 -0.00 0.22 0.03 -0.00

30 1 0.31 0.15 0.00 0.06 -0.07 -0.00 0.29 0.17 0.00

31 1 0.31 -0.15 -0.00 -0.06 -0.07 -0.00 0.29 -0.17 -0.00

32 30 -0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

33 6 0.14 0.03 0.00 -0.03 -0.04 -0.00 -0.01 -0.08 -0.00

34 6 -0.01 0.00 -0.00 0.00 -0.00 -0.00 0.00 0.01 -0.00

35 6 -0.01 0.00 0.00 -0.00 0.00 -0.00 0.00 0.01 0.00

36 6 -0.02 -0.02 -0.00 0.01 0.01 0.00 0.01 0.01 0.00

37 6 -0.02 -0.02 0.00 -0.01 -0.01 0.00 0.01 0.01 -0.00

38 6 -0.01 -0.00 -0.00 0.00 0.00 -0.00 0.00 -0.01 -0.00

39 6 -0.02 0.02 -0.00 0.01 -0.01 0.00 0.01 -0.01 0.00

40 6 -0.01 -0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.01 0.00

41 6 -0.02 0.02 0.00 -0.01 0.01 0.00 0.01 -0.01 -0.00

42 1 -0.02 0.04 0.00 -0.01 0.02 0.00 0.01 -0.00 -0.00

43 1 -0.02 -0.04 -0.00 0.01 0.02 0.00 0.01 0.00 0.00

44 1 -0.02 0.04 -0.00 0.01 -0.02 0.00 0.01 -0.00 0.00

45 1 -0.02 -0.04 0.00 -0.01 -0.02 0.00 0.01 0.00 -0.00

103 104 105

A1 A2 B2

Frequencies -- 1429.4927 1459.1555 1461.4204

Red. masses -- 7.6421 3.5999 3.8857

Frc consts -- 9.2008 4.5158 4.8896

IR Inten -- 0.0000 0.0000 14.3007

Atom AN X Y Z X Y Z X Y Z

1 6 -0.08 0.01 -0.00 0.05 -0.08 0.00 0.07 0.01 -0.00

2 6 -0.12 -0.07 0.00 -0.09 0.08 -0.00 0.04 -0.04 0.00

3 7 0.00 0.09 -0.00 0.03 0.00 -0.00 -0.00 0.00 -0.00

4 6 0.12 -0.07 0.00 -0.09 -0.08 0.00 -0.04 -0.04 0.00

5 6 0.08 0.01 -0.00 0.05 0.08 -0.00 -0.07 0.01 -0.00

6 6 -0.05 0.14 -0.00 0.03 -0.00 0.00 0.01 -0.04 0.00

7 6 -0.02 -0.14 0.00 0.10 0.07 0.00 0.11 0.12 0.00

8 7 -0.05 -0.00 -0.00 -0.00 -0.02 0.00 0.00 -0.05 0.00

9 6 -0.02 0.14 0.00 -0.10 0.07 -0.00 -0.11 0.12 -0.00

10 6 -0.00 0.27 0.00 0.12 -0.06 0.00 0.14 -0.08 0.00

11 6 -0.00 -0.27 0.00 -0.12 -0.06 -0.00 -0.14 -0.08 -0.00

12 6 0.05 0.14 -0.00 0.03 0.00 -0.00 -0.01 -0.04 0.00

13 6 0.02 -0.14 0.00 0.10 -0.07 -0.00 -0.11 0.12 0.00

14 6 0.00 -0.27 0.00 -0.12 0.06 0.00 0.14 -0.08 -0.00

15 6 0.00 0.27 0.00 0.12 0.06 -0.00 -0.14 -0.08 0.00

16 6 0.02 0.14 0.00 -0.10 -0.07 0.00 0.11 0.12 -0.00

17 7 0.05 0.00 -0.00 0.00 0.02 0.00 0.00 -0.05 -0.00

18 6 0.05 -0.14 -0.00 -0.03 0.00 0.00 0.01 -0.04 -0.00

19 6 -0.12 0.07 0.00 0.09 0.08 0.00 -0.04 -0.04 -0.00

20 6 -0.08 -0.01 -0.00 -0.05 -0.08 -0.00 -0.07 0.01 0.00

21 6 0.08 -0.01 -0.00 -0.05 0.08 0.00 0.07 0.01 0.00

22 6 0.12 0.07 0.00 0.09 -0.08 -0.00 0.04 -0.04 -0.00

23 7 -0.00 -0.09 -0.00 -0.03 -0.00 -0.00 -0.00 0.00 0.00

24 1 -0.04 -0.03 -0.00 -0.23 0.12 -0.00 -0.00 0.09 -0.00

25 1 0.04 -0.03 -0.00 -0.23 -0.12 0.00 0.00 0.09 -0.00

26 1 0.30 -0.07 0.00 -0.15 0.32 -0.00 -0.19 0.38 -0.00

27 1 0.30 0.07 0.00 0.15 0.32 0.00 0.19 0.38 0.00

28 1 -0.30 0.07 0.00 0.15 -0.32 -0.00 -0.19 0.38 0.00

29 1 -0.30 -0.07 0.00 -0.15 -0.32 0.00 0.19 0.38 -0.00

30 1 -0.04 0.03 -0.00 0.23 0.12 0.00 0.00 0.09 0.00

31 1 0.04 0.03 -0.00 0.23 -0.12 -0.00 -0.00 0.09 0.00

32 30 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00

33 6 -0.05 -0.14 -0.00 -0.03 -0.00 -0.00 -0.01 -0.04 -0.00

34 6 -0.00 0.01 -0.00 0.01 0.00 0.00 0.00 0.01 -0.00

35 6 0.00 -0.01 -0.00 -0.01 -0.00 0.00 0.00 0.01 0.00

36 6 0.02 0.02 0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

37 6 -0.02 -0.02 0.00 0.00 0.00 0.00 0.00 0.00 -0.00

38 6 -0.00 -0.01 -0.00 -0.01 0.00 -0.00 -0.00 0.01 0.00

39 6 0.02 -0.02 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00

40 6 0.00 0.01 -0.00 0.01 -0.00 -0.00 -0.00 0.01 -0.00

41 6 -0.02 0.02 0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00

42 1 -0.03 0.02 0.00 -0.00 -0.00 -0.00 -0.01 0.00 0.00

43 1 0.03 0.02 0.00 -0.00 0.00 0.00 0.01 0.00 0.00

44 1 0.03 -0.02 0.00 0.00 0.00 -0.00 -0.01 0.00 -0.00

45 1 -0.03 -0.02 0.00 0.00 -0.00 0.00 0.01 0.00 -0.00

106 107 108

B1 A1 B1

Frequencies -- 1480.1928 1507.1825 1514.9082

Red. masses -- 6.7592 5.7714 6.7367

Frc consts -- 8.7253 7.7244 9.1090

IR Inten -- 388.3296 0.0000 1338.5825

Atom AN X Y Z X Y Z X Y Z

1 6 -0.02 0.05 -0.00 0.16 -0.01 0.00 -0.06 0.07 -0.00

2 6 0.04 -0.09 0.00 0.03 -0.00 -0.00 0.19 -0.10 0.00

3 7 0.01 0.00 0.00 0.00 -0.02 0.00 -0.05 0.00 -0.00

4 6 0.04 0.09 -0.00 -0.03 -0.00 -0.00 0.19 0.10 -0.00

5 6 -0.02 -0.05 0.00 -0.16 -0.01 0.00 -0.06 -0.07 0.00

6 6 -0.04 -0.16 0.00 0.04 -0.07 0.00 -0.17 -0.06 -0.00

7 6 -0.04 0.27 -0.00 -0.02 0.19 -0.00 0.06 -0.03 0.00

8 7 0.07 0.00 0.00 0.05 0.00 0.00 -0.04 -0.00 -0.00

9 6 -0.04 -0.27 -0.00 -0.02 -0.19 -0.00 0.06 0.03 0.00

10 6 -0.01 0.12 -0.00 -0.03 0.19 -0.00 0.01 -0.18 0.00

11 6 -0.01 -0.12 -0.00 -0.03 -0.19 -0.00 0.01 0.18 0.00

12 6 -0.04 0.16 -0.00 -0.04 -0.07 0.00 -0.17 0.06 0.00

13 6 -0.04 -0.27 0.00 0.02 0.19 -0.00 0.06 0.03 -0.00

14 6 -0.01 0.12 0.00 0.03 -0.19 -0.00 0.01 -0.18 -0.00

15 6 -0.01 -0.12 0.00 0.03 0.19 -0.00 0.01 0.18 -0.00

16 6 -0.04 0.27 0.00 0.02 -0.19 -0.00 0.06 -0.03 -0.00

17 7 0.07 0.00 -0.00 -0.05 -0.00 0.00 -0.04 -0.00 0.00

18 6 -0.04 -0.16 -0.00 -0.04 0.07 0.00 -0.17 -0.06 0.00

19 6 0.04 0.09 0.00 0.03 0.00 -0.00 0.19 0.10 0.00

20 6 -0.02 -0.05 -0.00 0.16 0.01 0.00 -0.06 -0.07 -0.00

21 6 -0.02 0.05 0.00 -0.16 0.01 0.00 -0.06 0.07 0.00

22 6 0.04 -0.09 -0.00 -0.03 0.00 -0.00 0.19 -0.10 -0.00

23 7 0.01 0.00 -0.00 -0.00 0.02 0.00 -0.05 0.00 0.00

24 1 0.12 -0.05 0.00 -0.04 0.18 -0.00 0.20 -0.12 0.00

25 1 0.12 0.05 -0.00 0.04 0.18 -0.00 0.20 0.12 -0.00

26 1 0.24 -0.21 0.00 0.27 -0.19 0.00 -0.23 0.10 -0.00

27 1 0.24 0.21 0.00 0.27 0.19 0.00 -0.23 -0.10 -0.00

28 1 0.24 -0.21 -0.00 -0.27 0.19 0.00 -0.23 0.10 0.00

29 1 0.24 0.21 -0.00 -0.27 -0.19 0.00 -0.23 -0.10 0.00

30 1 0.12 0.05 0.00 -0.04 -0.18 -0.00 0.20 0.12 0.00

31 1 0.12 -0.05 -0.00 0.04 -0.18 -0.00 0.20 -0.12 -0.00

32 30 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00

33 6 -0.04 0.16 0.00 0.04 0.07 0.00 -0.17 0.06 -0.00

34 6 0.00 -0.01 -0.00 -0.00 -0.00 0.00 0.02 -0.00 0.00

35 6 0.00 -0.01 0.00 0.00 0.00 0.00 0.02 -0.00 -0.00

36 6 -0.01 -0.01 -0.00 -0.01 -0.01 -0.00 0.01 0.01 0.00

37 6 -0.01 -0.01 0.00 0.01 0.01 -0.00 0.01 0.01 -0.00

38 6 0.00 0.01 -0.00 -0.00 0.00 0.00 0.02 0.00 0.00

39 6 -0.01 0.01 -0.00 -0.01 0.01 -0.00 0.01 -0.01 0.00

40 6 0.00 0.01 0.00 0.00 -0.00 0.00 0.02 0.00 -0.00

41 6 -0.01 0.01 0.00 0.01 -0.01 -0.00 0.01 -0.01 -0.00

42 1 -0.02 0.00 0.00 0.01 -0.01 -0.00 0.00 -0.02 -0.00

43 1 -0.02 -0.00 -0.00 -0.01 -0.01 -0.00 0.00 0.02 0.00

44 1 -0.02 0.00 -0.00 -0.01 0.01 -0.00 0.00 -0.02 0.00

45 1 -0.02 -0.00 0.00 0.01 0.01 -0.00 0.00 0.02 -0.00

109 110 111

A2 B2 B2

Frequencies -- 1520.5903 1528.5848 1556.4105

Red. masses -- 7.8703 10.8200 5.7760

Frc consts -- 10.7218 14.8956 8.2438

IR Inten -- 0.0000 33.8637 128.8083

Atom AN X Y Z X Y Z X Y Z

1 6 0.05 -0.07 0.00 0.11 0.01 -0.00 0.29 -0.02 0.00

2 6 -0.17 0.12 -0.00 0.34 -0.04 -0.00 -0.10 -0.03 0.00

3 7 0.02 -0.00 0.00 0.00 -0.03 0.00 0.00 0.02 -0.00

4 6 -0.17 -0.12 0.00 -0.34 -0.04 -0.00 0.10 -0.03 0.00

5 6 0.05 0.07 -0.00 -0.11 0.01 -0.00 -0.29 -0.02 0.00

6 6 0.18 0.16 0.00 0.27 0.07 0.00 -0.02 0.06 -0.00

7 6 -0.10 -0.16 -0.00 -0.10 -0.02 -0.00 -0.01 -0.07 -0.00

8 7 0.00 0.06 -0.00 -0.00 -0.02 0.00 0.00 0.03 -0.00

9 6 0.10 -0.16 0.00 0.10 -0.02 0.00 0.01 -0.07 0.00

10 6 -0.08 0.05 -0.00 -0.05 0.01 -0.00 -0.02 0.02 -0.00

11 6 0.08 0.05 0.00 0.05 0.01 0.00 0.02 0.02 0.00

12 6 0.18 -0.16 -0.00 -0.27 0.07 0.00 0.02 0.06 -0.00

13 6 -0.10 0.16 0.00 0.10 -0.02 -0.00 0.01 -0.07 -0.00

14 6 0.08 -0.05 -0.00 -0.05 0.01 0.00 -0.02 0.02 0.00

15 6 -0.08 -0.05 0.00 0.05 0.01 -0.00 0.02 0.02 -0.00

16 6 0.10 0.16 -0.00 -0.10 -0.02 0.00 -0.01 -0.07 0.00

17 7 -0.00 -0.06 -0.00 -0.00 -0.02 -0.00 0.00 0.03 0.00

18 6 -0.18 -0.16 0.00 0.27 0.07 -0.00 -0.02 0.06 0.00

19 6 0.17 0.12 0.00 -0.34 -0.04 0.00 0.10 -0.03 -0.00

20 6 -0.05 -0.07 -0.00 -0.11 0.01 0.00 -0.29 -0.02 -0.00

21 6 -0.05 0.07 0.00 0.11 0.01 0.00 0.29 -0.02 -0.00

22 6 0.17 -0.12 -0.00 0.34 -0.04 0.00 -0.10 -0.03 -0.00

23 7 -0.02 0.00 0.00 0.00 -0.03 -0.00 0.00 0.02 0.00

24 1 -0.18 0.10 -0.00 0.13 0.03 -0.00 -0.13 0.35 -0.00

25 1 -0.18 -0.10 0.00 -0.13 0.03 -0.00 0.13 0.35 -0.00

26 1 0.10 -0.20 0.00 0.02 -0.08 0.00 0.04 -0.06 0.00

27 1 -0.10 -0.20 -0.00 -0.02 -0.08 -0.00 -0.04 -0.06 -0.00

28 1 -0.10 0.20 0.00 0.02 -0.08 -0.00 0.04 -0.06 -0.00

29 1 0.10 0.20 -0.00 -0.02 -0.08 0.00 -0.04 -0.06 0.00

30 1 0.18 0.10 0.00 -0.13 0.03 0.00 0.13 0.35 0.00

31 1 0.18 -0.10 -0.00 0.13 0.03 0.00 -0.13 0.35 0.00

32 30 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00

33 6 -0.18 0.16 -0.00 -0.27 0.07 -0.00 0.02 0.06 0.00

34 6 0.02 -0.01 0.00 0.01 -0.01 0.00 0.00 -0.00 -0.00

35 6 -0.02 0.01 0.00 0.01 -0.01 -0.00 0.00 -0.00 0.00

36 6 -0.00 0.00 0.00 0.02 0.02 0.00 -0.00 -0.00 -0.00

37 6 0.00 -0.00 0.00 0.02 0.02 -0.00 -0.00 -0.00 0.00

38 6 -0.02 -0.01 -0.00 -0.01 -0.01 -0.00 -0.00 -0.00 0.00

39 6 0.00 0.00 -0.00 -0.02 0.02 -0.00 0.00 -0.00 0.00

40 6 0.02 0.01 -0.00 -0.01 -0.01 0.00 -0.00 -0.00 -0.00

41 6 -0.00 -0.00 -0.00 -0.02 0.02 0.00 0.00 -0.00 -0.00

42 1 -0.01 -0.01 0.00 -0.01 0.03 0.00 0.01 -0.00 -0.00

43 1 -0.01 0.01 -0.00 0.01 0.03 0.00 -0.01 -0.00 -0.00

44 1 0.01 0.01 0.00 -0.01 0.03 -0.00 0.01 -0.00 0.00

45 1 0.01 -0.01 -0.00 0.01 0.03 -0.00 -0.01 -0.00 0.00

112 113 114

A1 A1 A2

Frequencies -- 1562.0040 1572.9830 2147.1564

Red. masses -- 7.4611 8.2546 6.1964

Frc consts -- 10.7254 12.0335 16.8314

IR Inten -- 0.0000 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.27 -0.01 -0.00 -0.15 0.03 -0.00 0.00 -0.00 0.00

2 6 0.05 -0.06 0.00 0.29 -0.03 -0.00 0.03 0.01 -0.00

3 7 -0.00 0.02 -0.00 -0.00 -0.02 0.00 -0.02 -0.00 0.00

4 6 -0.05 -0.06 0.00 -0.29 -0.03 -0.00 0.03 -0.01 0.00

5 6 -0.27 -0.01 -0.00 0.15 0.03 -0.00 0.00 0.00 -0.00

6 6 0.10 0.14 0.00 0.20 0.06 0.00 0.02 -0.03 0.00

7 6 -0.05 -0.18 -0.00 -0.06 -0.02 -0.00 0.01 -0.02 0.00

8 7 -0.01 0.00 -0.00 0.04 0.00 0.00 0.00 0.02 -0.00

9 6 -0.05 0.18 -0.00 -0.06 0.02 -0.00 -0.01 -0.02 -0.00

10 6 0.03 -0.05 0.00 0.00 0.07 0.00 0.00 -0.00 0.00

11 6 0.03 0.05 0.00 0.00 -0.07 0.00 -0.00 -0.00 -0.00

12 6 -0.10 0.14 0.00 -0.20 0.06 0.00 0.02 0.03 -0.00

13 6 0.05 -0.18 -0.00 0.06 -0.02 -0.00 0.01 0.02 -0.00

14 6 -0.03 0.05 0.00 -0.00 -0.07 0.00 -0.00 0.00 0.00

15 6 -0.03 -0.05 0.00 -0.00 0.07 0.00 0.00 0.00 -0.00

16 6 0.05 0.18 -0.00 0.06 0.02 -0.00 -0.01 0.02 0.00

17 7 0.01 -0.00 -0.00 -0.04 -0.00 0.00 -0.00 -0.02 -0.00

18 6 -0.10 -0.14 0.00 -0.20 -0.06 0.00 -0.02 0.03 0.00

19 6 0.05 0.06 0.00 0.29 0.03 -0.00 -0.03 0.01 0.00

20 6 0.27 0.01 -0.00 -0.15 -0.03 -0.00 -0.00 -0.00 -0.00

21 6 -0.27 0.01 -0.00 0.15 -0.03 -0.00 -0.00 0.00 0.00

22 6 -0.05 0.06 0.00 -0.29 0.03 -0.00 -0.03 -0.01 -0.00

23 7 0.00 -0.02 -0.00 0.00 0.02 0.00 0.02 0.00 0.00

24 1 -0.05 0.29 -0.00 0.17 -0.22 0.00 -0.00 -0.00 -0.00

25 1 0.05 0.29 -0.00 -0.17 -0.22 0.00 -0.00 0.00 0.00

26 1 -0.08 0.10 -0.00 0.09 -0.02 0.00 0.00 -0.00 -0.00

27 1 -0.08 -0.10 -0.00 0.09 0.02 0.00 -0.00 -0.00 0.00

28 1 0.08 -0.10 -0.00 -0.09 0.02 0.00 -0.00 0.00 -0.00

29 1 0.08 0.10 -0.00 -0.09 -0.02 0.00 0.00 0.00 0.00

30 1 -0.05 -0.29 -0.00 0.17 0.22 0.00 0.00 -0.00 0.00

31 1 0.05 -0.29 -0.00 -0.17 0.22 0.00 0.00 0.00 -0.00

32 30 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00

33 6 0.10 -0.14 0.00 0.20 -0.06 0.00 -0.02 -0.03 -0.00

34 6 -0.01 0.01 -0.00 -0.01 0.00 -0.00 0.20 0.19 0.00

35 6 0.01 -0.01 -0.00 0.01 -0.00 -0.00 -0.20 -0.19 0.00

36 6 0.00 0.00 0.00 -0.01 -0.01 -0.00 -0.14 -0.14 -0.00

37 6 -0.00 -0.00 0.00 0.01 0.01 -0.00 0.14 0.14 -0.00

38 6 -0.01 -0.01 -0.00 -0.01 -0.00 -0.00 -0.20 0.19 -0.00

39 6 0.00 -0.00 0.00 -0.01 0.01 -0.00 0.14 -0.14 0.00

40 6 0.01 0.01 -0.00 0.01 0.00 -0.00 0.20 -0.19 -0.00

41 6 -0.00 0.00 0.00 0.01 -0.01 -0.00 -0.14 0.14 0.00

42 1 -0.01 -0.01 0.00 0.00 -0.02 -0.00 -0.26 0.25 0.00

43 1 0.01 -0.01 0.00 -0.00 -0.02 -0.00 -0.26 -0.25 -0.00

44 1 0.01 0.01 0.00 -0.00 0.02 -0.00 0.26 -0.25 0.00

45 1 -0.01 0.01 0.00 0.00 0.02 -0.00 0.26 0.25 -0.00

115 116 117

B1 B2 A1

Frequencies -- 2161.6197 2168.0384 2170.0774

Red. masses -- 6.1376 6.1161 6.1012

Frc consts -- 16.8970 16.9378 16.9283

IR Inten -- 2036.6843 490.7964 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

2 6 -0.01 -0.00 0.00 -0.01 0.00 0.00 0.01 -0.00 -0.00

3 7 0.01 0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00

4 6 -0.01 0.00 -0.00 0.01 0.00 0.00 -0.01 -0.00 -0.00

5 6 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

6 6 -0.03 0.03 -0.00 0.03 -0.03 0.00 -0.03 0.03 -0.00

7 6 0.00 0.01 0.00 -0.00 -0.01 -0.00 0.00 0.01 0.00

8 7 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00

9 6 0.00 -0.01 0.00 0.00 -0.01 0.00 0.00 -0.01 0.00

10 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00

11 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00

12 6 -0.03 -0.03 0.00 -0.03 -0.03 0.00 0.03 0.03 -0.00

13 6 0.00 -0.01 -0.00 0.00 -0.01 -0.00 -0.00 0.01 0.00

14 6 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 0.00 -0.00

15 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00

16 6 0.00 0.01 -0.00 -0.00 -0.01 0.00 -0.00 -0.01 0.00

17 7 -0.00 0.00 0.00 0.00 0.00 0.00 -0.00 0.00 -0.00

18 6 -0.03 0.03 0.00 0.03 -0.03 -0.00 0.03 -0.03 -0.00

19 6 -0.01 0.00 0.00 0.01 0.00 -0.00 0.01 0.00 -0.00

20 6 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

21 6 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

22 6 -0.01 -0.00 -0.00 -0.01 0.00 -0.00 -0.01 0.00 -0.00

23 7 0.01 0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00

24 1 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

25 1 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

26 1 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00

27 1 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00

28 1 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00

29 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00

30 1 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

31 1 -0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

32 30 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00

33 6 -0.03 -0.03 -0.00 -0.03 -0.03 -0.00 -0.03 -0.03 -0.00

34 6 0.20 0.19 0.00 0.20 0.19 0.00 0.20 0.19 0.00

35 6 0.20 0.19 -0.00 0.20 0.19 -0.00 -0.20 -0.19 0.00

36 6 -0.14 -0.14 -0.00 -0.14 -0.14 -0.00 -0.14 -0.14 -0.00

37 6 -0.14 -0.14 0.00 -0.14 -0.14 0.00 0.14 0.14 -0.00

38 6 0.20 -0.19 0.00 -0.20 0.19 -0.00 0.20 -0.19 0.00

39 6 -0.14 0.14 -0.00 0.14 -0.14 0.00 -0.14 0.14 -0.00

40 6 0.20 -0.19 -0.00 -0.20 0.19 0.00 -0.20 0.19 0.00

41 6 -0.14 0.14 0.00 0.14 -0.14 -0.00 0.14 -0.14 -0.00

42 1 -0.26 0.25 0.00 0.26 -0.25 -0.00 0.26 -0.25 -0.00

43 1 -0.26 -0.25 -0.00 -0.26 -0.25 -0.00 -0.26 -0.25 -0.00

44 1 -0.26 0.25 -0.00 0.26 -0.25 0.00 -0.26 0.25 -0.00

45 1 -0.26 -0.25 0.00 -0.26 -0.25 0.00 0.26 0.25 -0.00

118 119 120

A2 B2 A2

Frequencies -- 3227.6963 3227.7403 3233.5677

Red. masses -- 1.0900 1.0901 1.0897

Frc consts -- 6.6907 6.6911 6.7130

IR Inten -- 0.0000 19.5876 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.03 -0.04 0.00

2 6 0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

3 7 -0.00 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00

4 6 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

5 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.03 0.04 -0.00

6 6 0.00 0.00 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00

7 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00

8 7 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00

9 6 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00

10 6 -0.04 -0.02 -0.00 -0.04 -0.02 -0.00 0.00 0.00 0.00

11 6 0.04 -0.02 0.00 0.04 -0.02 0.00 -0.00 0.00 -0.00

12 6 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00

13 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00

14 6 0.04 0.02 -0.00 -0.04 -0.02 0.00 -0.00 -0.00 0.00

15 6 -0.04 0.02 0.00 0.04 -0.02 -0.00 0.00 -0.00 -0.00

16 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00

17 7 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.00 -0.00

18 6 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00

19 6 -0.00 0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.00

20 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.03 -0.04 -0.00

21 6 0.00 0.00 0.00 0.00 0.00 0.00 0.03 0.04 0.00

22 6 -0.00 -0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

23 7 0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00

24 1 0.01 0.01 -0.00 -0.00 -0.00 0.00 0.30 0.40 -0.00

25 1 0.01 -0.01 0.00 0.00 -0.00 0.00 0.30 -0.40 0.00

26 1 0.40 0.30 0.00 0.40 0.30 0.00 -0.01 -0.01 -0.00

27 1 -0.40 0.30 -0.00 -0.40 0.30 -0.00 0.01 -0.01 0.00

28 1 -0.40 -0.30 0.00 0.40 0.30 -0.00 0.01 0.01 -0.00

29 1 0.40 -0.30 -0.00 -0.40 0.30 0.00 -0.01 0.01 0.00

30 1 -0.01 0.01 0.00 0.00 -0.00 -0.00 -0.30 0.40 0.00

31 1 -0.01 -0.01 -0.00 -0.00 -0.00 -0.00 -0.30 -0.40 -0.00

32 30 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00

33 6 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00

34 6 -0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 0.00 0.00

35 6 0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00

36 6 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00

37 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00

38 6 0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00

39 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00

40 6 -0.00 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00

41 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

42 1 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

43 1 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

44 1 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

45 1 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

121 122 123

B1 B1 A1

Frequencies -- 3233.6361 3243.7311 3243.8058

Red. masses -- 1.0897 1.1017 1.1017

Frc consts -- 6.7136 6.8300 6.8301

IR Inten -- 2.2742 59.4458 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 -0.04 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

2 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00

3 7 0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

4 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00

5 6 -0.03 0.04 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

6 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

7 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

8 7 -0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 0.00 0.00

9 6 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

10 6 0.00 0.00 0.00 -0.04 -0.03 -0.00 -0.04 -0.03 -0.00

11 6 0.00 -0.00 0.00 -0.04 0.03 -0.00 -0.04 0.03 -0.00

12 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

13 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

14 6 0.00 0.00 -0.00 -0.04 -0.03 0.00 0.04 0.03 -0.00

15 6 0.00 -0.00 -0.00 -0.04 0.03 0.00 0.04 -0.03 -0.00

16 6 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

17 7 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00

18 6 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

19 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00

20 6 -0.03 0.04 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

21 6 -0.03 -0.04 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

22 6 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 0.00 -0.00

23 7 0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

24 1 0.30 0.40 -0.00 0.01 0.01 -0.00 0.01 0.01 -0.00

25 1 0.30 -0.40 0.00 0.01 -0.01 0.00 -0.01 0.01 -0.00

26 1 -0.01 -0.01 -0.00 0.40 0.30 0.00 0.39 0.30 0.00

27 1 -0.01 0.01 -0.00 0.40 -0.30 0.00 0.39 -0.30 0.00

28 1 -0.01 -0.01 0.00 0.40 0.30 -0.00 -0.39 -0.30 0.00

29 1 -0.01 0.01 0.00 0.40 -0.30 -0.00 -0.39 0.30 0.00

30 1 0.30 -0.40 -0.00 0.01 -0.01 -0.00 0.01 -0.01 -0.00

31 1 0.30 0.40 0.00 0.01 0.01 0.00 -0.01 -0.01 -0.00

32 30 0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.00 -0.00

33 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

34 6 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

35 6 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

36 6 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

37 6 -0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

38 6 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

39 6 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

40 6 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

41 6 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

42 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

43 1 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

44 1 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

45 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

124 125 126

B2 A1 A2

Frequencies -- 3251.0062 3251.0778 3430.1052

Red. masses -- 1.1041 1.1041 1.1553

Frc consts -- 6.8755 6.8756 8.0087

IR Inten -- 38.1202 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 -0.04 0.00 -0.03 -0.04 0.00 0.00 -0.00 0.00

2 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 0.00

3 7 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00 0.00

4 6 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00

5 6 0.03 -0.04 0.00 0.03 -0.04 0.00 0.00 0.00 -0.00

6 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00

7 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00

8 7 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00

9 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00

10 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00

11 6 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00

12 6 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00

13 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00

14 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00

15 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.00

16 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00

17 7 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00

18 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00

19 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00

20 6 0.03 -0.04 -0.00 -0.03 0.04 0.00 -0.00 -0.00 -0.00

21 6 -0.03 -0.04 -0.00 0.03 0.04 0.00 -0.00 0.00 0.00

22 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00

23 7 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00

24 1 0.30 0.39 -0.00 0.30 0.39 -0.00 0.00 0.00 -0.00

25 1 -0.30 0.39 -0.00 -0.30 0.39 -0.00 0.00 -0.00 0.00

26 1 0.00 0.00 0.00 -0.01 -0.01 -0.00 -0.00 -0.00 -0.00

27 1 -0.00 0.00 -0.00 -0.01 0.01 -0.00 0.00 -0.00 0.00

28 1 0.00 0.00 -0.00 0.01 0.01 -0.00 0.00 0.00 -0.00

29 1 -0.00 0.00 0.00 0.01 -0.01 -0.00 -0.00 0.00 0.00

30 1 -0.30 0.39 0.00 0.30 -0.39 -0.00 -0.00 0.00 0.00

31 1 0.30 0.39 0.00 -0.30 -0.39 -0.00 -0.00 -0.00 -0.00

32 30 -0.00 0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.00

34 6 -0.00 0.00 -0.00 0.00 0.00 0.00 0.01 0.01 0.00

35 6 -0.00 0.00 0.00 -0.00 -0.00 0.00 -0.01 -0.01 0.00

36 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.04 -0.04 -0.00

37 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.04 0.04 -0.00

38 6 0.00 0.00 0.00 0.00 -0.00 0.00 -0.01 0.01 -0.00

39 6 0.00 0.00 -0.00 0.00 0.00 -0.00 0.04 -0.04 0.00

40 6 0.00 0.00 -0.00 -0.00 0.00 0.00 0.01 -0.01 -0.00

41 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.04 0.04 0.00

42 1 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.36 -0.35 -0.00

43 1 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.36 0.35 0.00

44 1 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.36 0.35 -0.00

45 1 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.36 -0.35 0.00

127 128 129

B1 B2 A1

Frequencies -- 3431.8622 3432.5400 3433.0083

Red. masses -- 1.1577 1.1586 1.1592

Frc consts -- 8.0334 8.0433 8.0491

IR Inten -- 1214.8268 644.4244 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00

2 6 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

3 7 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 0.00 0.00

4 6 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

5 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00

6 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

7 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

8 7 -0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

9 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

10 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

11 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

12 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

13 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

14 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

15 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

16 6 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

17 7 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

18 6 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

19 6 -0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

20 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00

21 6 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00

22 6 -0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

23 7 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00

24 1 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

25 1 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

26 1 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

27 1 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

28 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

29 1 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

30 1 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

31 1 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.00

32 30 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00

33 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.00

34 6 0.01 0.01 0.00 -0.01 -0.01 -0.00 -0.01 -0.01 -0.00

35 6 0.01 0.01 -0.00 -0.01 -0.01 0.00 0.01 0.01 -0.00

36 6 -0.04 -0.04 -0.00 0.04 0.04 0.00 0.04 0.04 0.00

37 6 -0.04 -0.04 0.00 0.04 0.04 -0.00 -0.04 -0.04 0.00

38 6 0.01 -0.01 0.00 0.01 -0.01 0.00 -0.01 0.01 -0.00

39 6 -0.04 0.04 -0.00 -0.04 0.04 -0.00 0.04 -0.04 0.00

40 6 0.01 -0.01 -0.00 0.01 -0.01 -0.00 0.01 -0.01 -0.00

41 6 -0.04 0.04 0.00 -0.04 0.04 0.00 -0.04 0.04 0.00

42 1 0.36 -0.35 -0.00 0.36 -0.35 -0.00 0.36 -0.35 -0.00

43 1 0.36 0.35 0.00 -0.36 -0.35 -0.00 -0.36 -0.35 -0.00

44 1 0.36 -0.35 0.00 0.36 -0.35 0.00 -0.36 0.35 -0.00

45 1 0.36 0.35 -0.00 -0.36 -0.35 0.00 0.36 0.35 -0.00

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- Thermochemistry -

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Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Atom 1 has atomic number 6 and mass 12.00000

Atom 2 has atomic number 6 and mass 12.00000

Atom 3 has atomic number 7 and mass 14.00307

Atom 4 has atomic number 6 and mass 12.00000

Atom 5 has atomic number 6 and mass 12.00000

Atom 6 has atomic number 6 and mass 12.00000

Atom 7 has atomic number 6 and mass 12.00000

Atom 8 has atomic number 7 and mass 14.00307

Atom 9 has atomic number 6 and mass 12.00000

Atom 10 has atomic number 6 and mass 12.00000

Atom 11 has atomic number 6 and mass 12.00000

Atom 12 has atomic number 6 and mass 12.00000

Atom 13 has atomic number 6 and mass 12.00000

Atom 14 has atomic number 6 and mass 12.00000

Atom 15 has atomic number 6 and mass 12.00000

Atom 16 has atomic number 6 and mass 12.00000

Atom 17 has atomic number 7 and mass 14.00307

Atom 18 has atomic number 6 and mass 12.00000

Atom 19 has atomic number 6 and mass 12.00000

Atom 20 has atomic number 6 and mass 12.00000

Atom 21 has atomic number 6 and mass 12.00000

Atom 22 has atomic number 6 and mass 12.00000

Atom 23 has atomic number 7 and mass 14.00307

Atom 24 has atomic number 1 and mass 1.00783

Atom 25 has atomic number 1 and mass 1.00783

Atom 26 has atomic number 1 and mass 1.00783

Atom 27 has atomic number 1 and mass 1.00783

Atom 28 has atomic number 1 and mass 1.00783

Atom 29 has atomic number 1 and mass 1.00783

Atom 30 has atomic number 1 and mass 1.00783

Atom 31 has atomic number 1 and mass 1.00783

Atom 32 has atomic number 30 and mass 63.92915

Atom 33 has atomic number 6 and mass 12.00000

Atom 34 has atomic number 6 and mass 12.00000

Atom 35 has atomic number 6 and mass 12.00000

Atom 36 has atomic number 6 and mass 12.00000

Atom 37 has atomic number 6 and mass 12.00000

Atom 38 has atomic number 6 and mass 12.00000

Atom 39 has atomic number 6 and mass 12.00000

Atom 40 has atomic number 6 and mass 12.00000

Atom 41 has atomic number 6 and mass 12.00000

Atom 42 has atomic number 1 and mass 1.00783

Atom 43 has atomic number 1 and mass 1.00783

Atom 44 has atomic number 1 and mass 1.00783

Atom 45 has atomic number 1 and mass 1.00783

Molecular mass: 468.03534 amu.

Principal axes and moments of inertia in atomic units:

1 2 3

Eigenvalues -- \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

X 0.00000 1.00000 0.00000

Y 1.00000 -0.00000 0.00000

Z -0.00000 -0.00000 1.00000

This molecule is an asymmetric top.

Rotational symmetry number 2.

Warning -- assumption of classical behavior for rotation

may cause significant error

Rotational temperatures (Kelvin) 0.00700 0.00697 0.00349

Rotational constants (GHZ): 0.14594 0.14531 0.07281

Zero-point vibrational energy 794718.2 (Joules/Mol)

189.94220 (Kcal/Mol)

Warning -- explicit consideration of 49 degrees of freedom as

vibrations may cause significant error

Vibrational temperatures: 18.69 57.52 71.73 86.97 94.90

(Kelvin) 129.53 159.88 163.62 163.90 202.12

206.74 207.32 207.73 236.08 290.25

318.18 321.21 346.79 353.21 354.35

360.70 410.62 459.00 468.02 472.19

475.82 522.61 543.45 563.09 568.76

568.99 584.78 587.29 657.42 661.58

690.53 694.39 721.56 721.69 722.06

722.15 796.89 804.39 804.76 812.43

834.46 850.71 865.42 879.68 942.85

942.96 943.09 943.11 960.74 969.55

974.15 992.63 1022.06 1023.86 1030.91

1040.92 1101.38 1101.49 1143.93 1144.05

1216.95 1226.59 1230.40 1230.46 1241.26

1264.54 1271.43 1320.10 1320.13 1380.99

1382.55 1424.74 1471.59 1481.71 1510.03

1510.87 1534.22 1554.73 1567.04 1573.11

1577.31 1638.91 1668.57 1669.26 1703.97

1780.52 1783.28 1790.17 1834.53 1887.47

1887.50 1904.81 1939.40 1948.38 1953.39

1990.70 2052.42 2056.72 2099.40 2102.66

2129.66 2168.50 2179.61 2187.79 2199.29

2239.32 2247.37 2263.17 3089.28 3110.08

3119.32 3122.25 4643.93 4643.99 4652.38

4652.48 4667.00 4667.11 4677.47 4677.57

4935.15 4937.68 4938.65 4939.33

Zero-point correction= 0.302692 (Hartree/Particle)

Thermal correction to Energy= 0.329903

Thermal correction to Enthalpy= 0.330848

Thermal correction to Gibbs Free Energy= 0.246251

Sum of electronic and zero-point Energies= -1358.880009

Sum of electronic and thermal Energies= -1358.852797

Sum of electronic and thermal Enthalpies= -1358.851853

Sum of electronic and thermal Free Energies= -1358.936450

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 207.017 108.637 178.049

Electronic 0.000 0.000 1.377

Translational 0.889 2.981 44.319

Rotational 0.889 2.981 35.208

Vibrational 205.240 102.675 97.145

Vibration 1 0.593 1.987 7.492

Vibration 2 0.594 1.981 5.260

Vibration 3 0.595 1.978 4.823

Vibration 4 0.597 1.973 4.442

Vibration 5 0.597 1.971 4.271

Vibration 6 0.602 1.956 3.659

Vibration 7 0.607 1.940 3.249

Vibration 8 0.607 1.938 3.204

Vibration 9 0.607 1.938 3.201

Vibration 10 0.615 1.913 2.797

Vibration 11 0.616 1.909 2.754

Vibration 12 0.616 1.909 2.749

Vibration 13 0.616 1.909 2.745

Vibration 14 0.623 1.887 2.502

Vibration 15 0.639 1.837 2.117

Vibration 16 0.648 1.809 1.950

Vibration 17 0.649 1.806 1.933

Vibration 18 0.658 1.778 1.795

Vibration 19 0.660 1.770 1.763

Vibration 20 0.661 1.769 1.757

Vibration 21 0.663 1.762 1.726

Vibration 22 0.683 1.701 1.501

Vibration 23 0.705 1.637 1.315

Vibration 24 0.709 1.625 1.283

Vibration 25 0.711 1.619 1.269

Vibration 26 0.713 1.614 1.257

Vibration 27 0.737 1.548 1.108

Vibration 28 0.748 1.518 1.048

Vibration 29 0.759 1.489 0.995

Vibration 30 0.762 1.480 0.980

Vibration 31 0.762 1.480 0.979

Vibration 32 0.771 1.456 0.939

Vibration 33 0.773 1.452 0.933

Vibration 34 0.815 1.346 0.775

Vibration 35 0.818 1.339 0.767

Vibration 36 0.836 1.295 0.710

Vibration 37 0.839 1.289 0.703

Vibration 38 0.857 1.247 0.654

Vibration 39 0.857 1.246 0.654

Vibration 40 0.857 1.246 0.654

Vibration 41 0.857 1.246 0.653

Vibration 42 0.909 1.131 0.536

Vibration 43 0.915 1.120 0.526

Vibration 44 0.915 1.119 0.525

Vibration 45 0.920 1.108 0.515

Vibration 46 0.937 1.075 0.485

Vibration 47 0.949 1.050 0.465

Vibration 48 0.960 1.029 0.447

Vibration 49 0.971 1.008 0.430

Q Log10(Q) Ln(Q)

Total Bot 0.540572-113 -113.267147 -260.807244

Total V=0 0.914717D+26 25.961287 59.778072

Vib (Bot) 0.614972-129 -129.211145 -297.519656

Vib (Bot) 1 0.159513D+02 1.202796 2.769539

Vib (Bot) 2 0.517526D+01 0.713932 1.643890

Vib (Bot) 3 0.414633D+01 0.617664 1.422223

Vib (Bot) 4 0.341595D+01 0.533511 1.228455

Vib (Bot) 5 0.312857D+01 0.495345 1.140575

Vib (Bot) 6 0.228381D+01 0.358659 0.825844

Vib (Bot) 7 0.184266D+01 0.265445 0.611209

Vib (Bot) 8 0.179954D+01 0.255161 0.587530

Vib (Bot) 9 0.179636D+01 0.254395 0.585765

Vib (Bot) 10 0.144722D+01 0.160534 0.369644

Vib (Bot) 11 0.141363D+01 0.150335 0.346159

Vib (Bot) 12 0.140958D+01 0.149090 0.343291

Vib (Bot) 13 0.140667D+01 0.148191 0.341223

Vib (Bot) 14 0.123053D+01 0.090092 0.207445

Vib (Bot) 15 0.987762D+00 -0.005348 -0.012313

Vib (Bot) 16 0.894031D+00 -0.048648 -0.112015

Vib (Bot) 17 0.884794D+00 -0.053158 -0.122401

Vib (Bot) 18 0.813135D+00 -0.089837 -0.206858

Vib (Bot) 19 0.796703D+00 -0.098703 -0.227273

Vib (Bot) 20 0.793848D+00 -0.100262 -0.230863

Vib (Bot) 21 0.778250D+00 -0.108881 -0.250708

Vib (Bot) 22 0.671736D+00 -0.172801 -0.397890

Vib (Bot) 23 0.589589D+00 -0.229451 -0.528329

Vib (Bot) 24 0.576057D+00 -0.239534 -0.551548

Vib (Bot) 25 0.569957D+00 -0.244158 -0.562195

Vib (Bot) 26 0.564731D+00 -0.248158 -0.571405

Vib (Bot) 27 0.503515D+00 -0.297987 -0.686141

Vib (Bot) 28 0.479447D+00 -0.319260 -0.735123

Vib (Bot) 29 0.458274D+00 -0.338875 -0.780288

Vib (Bot) 30 0.452419D+00 -0.344459 -0.793147

Vib (Bot) 31 0.452186D+00 -0.344683 -0.793662

Vib (Bot) 32 0.436449D+00 -0.360067 -0.829085

Vib (Bot) 33 0.434019D+00 -0.362491 -0.834668

Vib (Bot) 34 0.373184D+00 -0.428077 -0.985684

Vib (Bot) 35 0.369953D+00 -0.431854 -0.994381

Vib (Bot) 36 0.348490D+00 -0.457809 -1.054145

Vib (Bot) 37 0.345755D+00 -0.461231 -1.062024

Vib (Bot) 38 0.327276D+00 -0.485086 -1.116953

Vib (Bot) 39 0.327192D+00 -0.485197 -1.117208

Vib (Bot) 40 0.326952D+00 -0.485516 -1.117943

Vib (Bot) 41 0.326890D+00 -0.485598 -1.118130

Vib (Bot) 42 0.282287D+00 -0.549308 -1.264830

Vib (Bot) 43 0.278245D+00 -0.555573 -1.279253

Vib (Bot) 44 0.278050D+00 -0.555877 -1.279955

Vib (Bot) 45 0.273993D+00 -0.562260 -1.294652

Vib (Bot) 46 0.262741D+00 -0.580472 -1.336586

Vib (Bot) 47 0.254803D+00 -0.593796 -1.367266

Vib (Bot) 48 0.247862D+00 -0.605790 -1.394883

Vib (Bot) 49 0.241350D+00 -0.617352 -1.421505

Vib (V=0) 0.104061D+11 10.017289 23.065659

Vib (V=0) 1 0.164591D+02 1.216406 2.800879

Vib (V=0) 2 0.569936D+01 0.755826 1.740354

Vib (V=0) 3 0.467637D+01 0.669909 1.542521

Vib (V=0) 4 0.395235D+01 0.596855 1.374310

Vib (V=0) 5 0.366827D+01 0.564461 1.299720

Vib (V=0) 6 0.283790D+01 0.452997 1.043064

Vib (V=0) 7 0.240929D+01 0.381889 0.879332

Vib (V=0) 8 0.236771D+01 0.374328 0.861923

Vib (V=0) 9 0.236465D+01 0.373767 0.860631

Vib (V=0) 10 0.203116D+01 0.307744 0.708606

Vib (V=0) 11 0.199945D+01 0.300910 0.692871

Vib (V=0) 12 0.199563D+01 0.300080 0.690961

Vib (V=0) 13 0.199289D+01 0.299483 0.689584

Vib (V=0) 14 0.182823D+01 0.262032 0.603350

Vib (V=0) 15 0.160710D+01 0.206043 0.474432

Vib (V=0) 16 0.152435D+01 0.183084 0.421567

Vib (V=0) 17 0.151630D+01 0.180784 0.416271

Vib (V=0) 18 0.145456D+01 0.162732 0.374705

Vib (V=0) 19 0.144060D+01 0.158545 0.365062

Vib (V=0) 20 0.143819D+01 0.157815 0.363383

Vib (V=0) 21 0.142503D+01 0.153823 0.354190

Vib (V=0) 22 0.133739D+01 0.126259 0.290723

Vib (V=0) 23 0.127306D+01 0.104847 0.241420

Vib (V=0) 24 0.126279D+01 0.101330 0.233320

Vib (V=0) 25 0.125819D+01 0.099746 0.229674

Vib (V=0) 26 0.125427D+01 0.098391 0.226553

Vib (V=0) 27 0.120960D+01 0.082641 0.190287

Vib (V=0) 28 0.119273D+01 0.076541 0.176241

Vib (V=0) 29 0.117824D+01 0.071235 0.164025

Vib (V=0) 30 0.117430D+01 0.069780 0.160674

Vib (V=0) 31 0.117415D+01 0.069722 0.160540

Vib (V=0) 32 0.116369D+01 0.065838 0.151598

Vib (V=0) 33 0.116210D+01 0.065242 0.150226

Vib (V=0) 34 0.112391D+01 0.050732 0.116815

Vib (V=0) 35 0.112198D+01 0.049987 0.115099

Vib (V=0) 36 0.110946D+01 0.045113 0.103876

Vib (V=0) 37 0.110790D+01 0.044502 0.102470

Vib (V=0) 38 0.109759D+01 0.040439 0.093113

Vib (V=0) 39 0.109754D+01 0.040421 0.093072

Vib (V=0) 40 0.109741D+01 0.040368 0.092952

Vib (V=0) 41 0.109738D+01 0.040355 0.092921

Vib (V=0) 42 0.107418D+01 0.031078 0.071560

Vib (V=0) 43 0.107221D+01 0.030278 0.069719

Vib (V=0) 44 0.107211D+01 0.030240 0.069630

Vib (V=0) 45 0.107015D+01 0.029445 0.067800

Vib (V=0) 46 0.106483D+01 0.027280 0.062815

Vib (V=0) 47 0.106118D+01 0.025790 0.059383

Vib (V=0) 48 0.105806D+01 0.024512 0.056441

Vib (V=0) 49 0.105520D+01 0.023336 0.053733

Electronic 0.200000D+01 0.301030 0.693147

Translational 0.397991D+09 8.599873 19.801940

Rotational 0.110432D+08 7.043095 16.217325

ZnTSPsimanion

IR Spectrum

333333333333 2222111111111111111111111111111111111111

444422222222 111155555554444433333332222111100000000099998888887777777766666666665555555544444433333333322222222111111

333355443322 766476522108652285542117433866399886553296618765549966211197765555109865500088650099976322185444220644111966541

332011444488 082732691570199748484225498400963916000301084935365566372007485555121059422230078655183185951651312440441060003

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X X X X

X X X X

X X X X

X X X X

X X X

X

X

X

X

X

X

X

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000000063 -0.000002223 0.000000002

2 6 0.000000504 -0.000000985 -0.000000040

3 7 -0.000007341 -0.000000000 0.000001959

4 6 0.000000504 0.000000985 -0.000000040

5 6 -0.000000063 0.000002223 0.000000002

6 6 0.000000577 0.000000585 -0.000000005

7 6 -0.000000924 0.000000285 -0.000000047

8 7 0.000000000 -0.000004908 0.000002340

9 6 0.000000924 0.000000285 -0.000000047

10 6 -0.000001883 -0.000000442 0.000000000

11 6 0.000001883 -0.000000442 0.000000000

12 6 0.000000577 -0.000000585 -0.000000005

13 6 -0.000000924 -0.000000285 -0.000000047

14 6 0.000001883 0.000000442 0.000000000

15 6 -0.000001883 0.000000442 0.000000000

16 6 0.000000924 -0.000000285 -0.000000047

17 7 0.000000000 0.000004908 0.000002340

18 6 -0.000000577 -0.000000585 -0.000000005

19 6 -0.000000504 -0.000000985 -0.000000040

20 6 0.000000063 -0.000002223 0.000000002

21 6 0.000000063 0.000002223 0.000000002

22 6 -0.000000504 0.000000985 -0.000000040

23 7 0.000007341 0.000000000 0.000001959

24 1 -0.000000114 -0.000000113 -0.000000006

25 1 -0.000000114 0.000000113 -0.000000006

26 1 -0.000000048 -0.000000061 -0.000000006

27 1 0.000000048 -0.000000061 -0.000000006

28 1 0.000000048 0.000000061 -0.000000006

29 1 -0.000000048 0.000000061 -0.000000006

30 1 0.000000114 -0.000000113 -0.000000006

31 1 0.000000114 0.000000113 -0.000000006

32 30 -0.000000000 -0.000000000 -0.000008213

33 6 -0.000000577 0.000000585 -0.000000005

34 6 -0.000000172 -0.000000177 0.000000003

35 6 0.000000172 0.000000177 0.000000003

36 6 -0.000000149 -0.000000079 0.000000003

37 6 0.000000149 0.000000079 0.000000003

38 6 0.000000172 -0.000000177 0.000000003

39 6 0.000000149 -0.000000079 0.000000003

40 6 -0.000000172 0.000000177 0.000000003

41 6 -0.000000149 0.000000079 0.000000003

42 1 0.000000232 0.000000090 -0.000000000

43 1 0.000000232 -0.000000090 -0.000000000

44 1 -0.000000232 -0.000000090 -0.000000000

45 1 -0.000000232 0.000000090 -0.000000000

-------------------------------------------------------------------

Cartesian Forces: Max 0.000008213 RMS 0.000001463

Red2BG is reusing G-inverse.

Leave Link 716 at Wed Jul 31 05:38:58 2019, MaxMem= 4294967296 cpu: 1.3

(Enter /home/kira/g09/l9999.exe)

1\1\ WCSS.PL-BEM-LOCALHOST\Freq\UB3LYP\GenECP\C28H12N4Zn1(1-,2)\KIRA\3

1-Jul-2019\0\\#p opt=calcall b3lyp/genecp scrf=(solvent=dmso,smd) empi

ricaldispersion=gd3bj\\ZnTSPsimanion\\-1,2\C,-4.2916029867,0.679463229

6,-0.024405114\C,-2.9029144048,1.1095426569,-0.024396559\N,-2.09656335

36,0.,-0.0243912249\C,-2.9029144048,-1.1095426569,-0.024396559\C,-4.29

16029867,-0.6794632296,-0.024405114\C,-2.4693076492,-2.4457789056,-0.0

243988245\C,-1.1070534684,-2.9105405592,-0.0243995013\N,0.,-2.10119374

88,-0.0243936467\C,1.1070534684,-2.9105405592,-0.0243995013\C,0.691944

3496,-4.2758814207,-0.0244106905\C,-0.6919443496,-4.2758814207,-0.0244

106905\C,-2.4693076492,2.4457789056,-0.0243988245\C,-1.1070534684,2.91

05405592,-0.0243995013\C,-0.6919443496,4.2758814207,-0.0244106905\C,0.

6919443496,4.2758814207,-0.0244106905\C,1.1070534684,2.9105405592,-0.0

243995013\N,0.,2.1011937488,-0.0243936467\C,2.4693076492,2.4457789056,

-0.0243988245\C,2.9029144048,1.1095426569,-0.024396559\C,4.2916029867,

0.6794632296,-0.024405114\C,4.2916029867,-0.6794632296,-0.024405114\C,

2.9029144048,-1.1095426569,-0.024396559\N,2.0965633536,0.,-0.024391224

9\H,-5.1491235842,1.3365428427,-0.0244121738\H,-5.1491235842,-1.336542

8427,-0.0244121738\H,1.3458616209,-5.1359809533,-0.0244191385\H,-1.345

8616209,-5.1359809533,-0.0244191385\H,-1.3458616209,5.1359809533,-0.02

44191385\H,1.3458616209,5.1359809533,-0.0244191385\H,5.1491235842,1.33

65428427,-0.0244121738\H,5.1491235842,-1.3365428427,-0.0244121738\Zn,0

.,0.,-0.0243129378\C,2.4693076492,-2.4457789056,-0.0243988245\C,3.4764

97716,-3.4528287863,-0.0244048716\C,-3.476497716,3.4528287863,-0.02440

48716\C,4.3160508964,-4.3219725925,-0.0244108448\C,-4.3160508964,4.321

9725925,-0.0244108448\C,-3.476497716,-3.4528287863,-0.0244048716\C,-4.

3160508964,-4.3219725925,-0.0244108448\C,3.476497716,3.4528287863,-0.0

244048716\C,4.3160508964,4.3219725925,-0.0244108448\H,5.0614612568,5.0

851551012,-0.0244162246\H,5.0614612568,-5.0851551012,-0.0244162246\H,-

5.0614612568,-5.0851551012,-0.0244162246\H,-5.0614612568,5.0851551012,

-0.0244162246\\Version=ES64L-G09RevE.01\State=2-B2\HF=-1359.1827007\S2

=0.763087\S2-1=0.\S2A=0.750117\RMSD=7.730e-09\RMSF=1.463e-06\ZeroPoint

=0.3026922\Thermal=0.3299034\Dipole=0.,0.,0.0001926\DipoleDeriv=0.5195

883,0.0847322,0.,0.7986427,0.2171149,-0.0000017,0.0000068,0.0000012,-0

.227252,-0.4772059,-0.4716875,0.0000031,0.3070492,1.7122594,-0.0000076

,-0.0000039,0.0000013,0.1161948,-1.0463666,0.0000094,0.000022,-0.00000

01,-2.3950874,0.,-0.0000127,0.,-0.4710957,-0.4772061,0.4716851,0.00000

31,-0.3070491,1.7122587,0.0000076,-0.0000039,-0.0000014,0.1161948,0.51

95883,-0.0847333,0.,-0.7986429,0.2171098,0.0000017,0.0000068,-0.000001

1,-0.227252,0.1836527,-1.1032705,-0.0000014,-0.2275509,-0.7964009,-0.0

000016,-0.0000018,0.0000089,-0.1052843,-0.0421959,0.2501295,0.0000059,

-0.3745413,-1.4518194,0.000003,0.0000015,-0.0000145,0.0610761,-0.34269

31,0.0000034,0.,-0.0000005,-1.0182278,0.000022,0.,-0.0000152,-0.431350

6,-0.0421957,-0.2501343,-0.0000059,0.374541,-1.4518169,0.000003,-0.000

0015,-0.0000145,0.0610761,-0.0281506,2.118035,0.0000002,-0.1672118,1.0

98425,0.000001,-0.0000038,0.0000127,-0.2827211,-0.028151,-2.118033,-0.

0000002,0.1672121,1.0984299,0.000001,0.0000038,0.0000127,-0.2827211,0.

1836528,1.1032719,-0.0000014,0.2275513,-0.7963994,0.0000016,-0.0000018

,-0.0000087,-0.1052843,-0.042196,-0.2501344,0.0000059,0.374541,-1.4518

171,-0.000003,0.0000015,0.0000145,0.0610761,-0.0281505,2.1180342,-0.00

00002,-0.1672123,1.0984299,-0.000001,0.0000038,-0.0000126,-0.2827211,-

0.028151,-2.1180338,0.0000002,0.1672121,1.0984283,-0.000001,-0.0000038

,-0.0000126,-0.2827211,-0.0421968,0.2501365,-0.0000059,-0.3745411,-1.4

518185,-0.000003,-0.0000015,0.0000145,0.0610761,-0.3426921,-0.0000003,

0.,0.,-1.0182261,-0.000022,0.,0.0000151,-0.4313506,0.1836532,-1.103276

4,0.0000014,-0.2275516,-0.7963947,0.0000016,0.0000017,-0.0000088,-0.10

52843,-0.477206,0.4716861,-0.0000031,-0.3070483,1.7122531,-0.0000076,0

.0000039,0.0000014,0.1161948,0.5195879,-0.0847318,0.,-0.7986432,0.2171

107,-0.0000017,-0.0000068,0.0000012,-0.227252,0.5195885,0.0847321,0.,0

.7986434,0.2171109,0.0000017,-0.0000068,-0.0000011,-0.227252,-0.477206

7,-0.4716864,-0.0000031,0.307049,1.7122588,0.0000076,0.0000039,-0.0000

013,0.1161948,-1.0463658,-0.000001,-0.000022,-0.0000006,-2.3950849,0.,

0.0000127,0.,-0.4710957,-0.0465219,0.0905965,-0.0000015,0.1277622,0.08

42738,0.0000006,-0.0000019,0.000001,0.2016167,-0.0465219,-0.0905963,-0

.0000015,-0.1277621,0.0842733,-0.0000006,-0.0000019,-0.000001,0.201616

7,0.0605185,0.2011405,0.000001,0.1248795,-0.0613256,-0.0000023,0.00000

18,-0.0000031,0.211075,0.0605181,-0.201142,-0.000001,-0.1248796,-0.061

3269,-0.0000023,-0.0000018,-0.0000031,0.211075,0.060518,0.201143,-0.00

0001,0.1248798,-0.0613279,0.0000023,-0.0000018,0.0000031,0.211075,0.06

05184,-0.2011432,0.000001,-0.1248795,-0.061327,0.0000023,0.0000018,0.0

000031,0.211075,-0.0465219,-0.0905956,0.0000015,-0.1277622,0.0842747,0

.0000006,0.0000019,0.000001,0.2016167,-0.0465219,0.0905966,0.0000015,0

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-0.0000043,0.,0.0000009,1.2289675,0.,0.,0.,1.3311538,0.1836525,1.10327

31,0.0000014,0.2275504,-0.7963936,-0.0000016,0.0000017,0.0000088,-0.10

52843,0.6238644,-1.4923125,-0.000003,-0.8577388,1.6263327,0.0000031,-0

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506,0.00015575,0.,-0.00012752,-0.00007068,0.,0.00005093,-0.00010750,0.

,-0.00152594,0.00052015,-0.00000001,0.00012864,-0.00048924,0.,-0.00008

969,0.00008314,0.,-0.00004694,-0.00002560,0.,-0.00010821,0.00001233,0.

,0.00014028,0.00009680,0.,0.00003805,-0.00009765,0.,-0.00004427,0.0000

7629,0.,0.00004373,-0.00005792,0.,0.00005981,0.00007135,0.,-0.00010984

,0.00006836,0.,0.00000279,-0.00007531,0.,0.00078319,0.00098191,0.00000

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,0.00000003,0.00775362,-0.00000008,-0.00000005,0.00387273,-0.00000005,

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.,0.,-0.00000285,0.,0.,-0.00001563,0.,0.00000001,0.00081675,0.,0.,-0.0

0093774,0.,0.,-0.00014931,0.,0.,0.00001987,0.,0.,-0.00012892,0.,0.0000

0002,0.00019320,0.,0.,0.00002381,0.,0.,-0.00000508,0.,0.,-0.00000621,0

.,0.,0.00000019,0.,0.,0.00000629,0.,0.,-0.00002042,0.00000003,-0.00000

001,-0.00419478,0.00000185,0.00000131,0.02231317,-0.00003808,0.0000511

5,0.,0.00005198,-0.00009178,0.,0.00011164,0.00009154,0.,-0.00065286,-0

.00031287,0.,0.00013057,0.00003745,0.,0.00059998,0.00156355,0.00000001

,-0.00566065,-0.00035765,0.,0.00019193,-0.00351542,-0.00000003,0.00975

959,-0.00732726,-0.00000007,-0.16383539,0.14103233,0.00000142,-0.00574

386,0.02332515,0.00000024,-0.00020786,0.00009919,0.,0.00015578,0.00014

505,0.,-0.00019528,-0.00011336,0.,0.00022628,-0.00014504,0.,0.00000219

,0.00026074,0.,-0.00009758,-0.00001448,0.,0.00011380,-0.00008197,0.,0.

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49,0.,0.00016828,0.00014963,0.,-0.00002344,-0.00007675,0.,0.00000502,0

.00001914,0.,-0.00000718,-0.00000699,0.,0.16597438,0.00004553,-0.00006

688,0.,0.00000262,0.00035767,0.,0.00028529,-0.00050214,0.00000003,-0.0

0006337,0.00007734,0.,-0.00005439,0.00010244,0.,-0.00018700,0.00047197

,0.,-0.00206994,-0.00092620,-0.00000007,0.00018740,-0.00622427,-0.0000

0010,0.01841062,-0.00936076,-0.00000009,0.13959105,-0.24426157,-0.0000

0209,-0.00429321,0.00790852,0.00000007,0.00008983,-0.00018883,0.,-0.00

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266,0.00017298,0.,-0.00015805,-0.00021042,0.,-0.00001211,-0.00008466,0

.,-0.00000319,0.00001574,0.,-0.00005037,-0.00039031,0.,-0.00014099,0.0

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0.15369389,0.25099367,0.,0.,0.00000792,0.,0.,-0.00007644,-0.00000002,0

.,0.00006117,0.,0.,-0.00044780,0.,0.,-0.00018028,-0.00000001,0.,0.0013

1301,-0.00000004,-0.00000010,0.00540976,0.00000006,-0.00000011,0.00509

231,0.00000018,-0.00000006,-0.00200559,0.00000145,-0.00000211,-0.02581

840,-0.00000008,0.00000009,0.00058927,0.,0.,-0.00000930,0.,0.,0.000008

54,0.,0.,0.00000082,0.,0.,-0.00000130,0.,0.,0.00000327,0.,0.,-0.000027

89,0.,0.,-0.00000499,0.,0.,0.00003882,0.,0.,0.00001395,0.,0.,0.0000148

8,0.,0.,-0.00013486,0.,0.00000001,-0.00003769,0.,0.,0.00005847,0.,0.,-

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.,0.00010258,-0.00015725,0.,-0.00002344,0.00007676,0.,0.00016828,-0.00

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233,-0.00000142,0.00011380,0.00008197,0.,0.00000219,-0.00026074,0.,0.0

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8,0.00001211,-0.00008466,0.,0.00015805,-0.00021042,0.,0.00014099,0.000

27326,0.00000003,0.00005037,-0.00039031,0.,0.00000319,0.00001574,0.,-0

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5,0.,-0.00001912,-0.00000264,0.,0.00012781,0.00006423,0.,-0.00017075,0

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,0.,-0.00004553,-0.00006688,0.,0.00005439,0.00010244,0.,0.00006337,0.0

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.,0.00002999,0.00000676,0.,-0.00083317,-0.00008654,0.00000003,0.153693

89,0.25099367,0.,0.,0.00001395,0.,0.,0.00003882,0.,0.00000001,-0.00003

769,0.,0.,-0.00013486,0.,0.,0.00001488,0.,0.00000001,-0.00167109,-0.00

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0145,-0.00000211,-0.02581840,0.,0.,-0.00000499,0.,0.,0.00000327,0.,0.,

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,-0.00044780,0.00000002,0.,0.00006117,0.,0.,-0.00002365,0.,0.,0.000045

02,-0.00000001,0.00000003,-0.00317626,0.00000154,0.00000224,0.02035892

,-0.00011358,-0.00004249,0.,0.00016828,0.00014963,0.,-0.00002344,-0.00

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504,0.,0.00007391,0.00073655,0.,0.00975959,-0.00732726,0.00000007,-0.1

6383539,0.14103233,-0.00000142,-0.00574386,0.02332515,-0.00000024,-0.0

0566065,-0.00035765,0.,0.00019193,-0.00351542,0.00000003,0.00059998,0.

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61,0.00000213,0.,0.00000881,0.00000395,0.,0.16597438,-0.00000319,0.000

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.00010244,0.,0.00004553,-0.00006688,0.,0.00000262,0.00035767,0.,0.0002

8529,-0.00050214,-0.00000003,-0.00002999,0.00000676,0.,-0.00001079,-0.

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369389,0.25099367,0.,0.,0.00001488,0.,0.,-0.00013486,0.,-0.00000001,-0

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,-0.00000145,0.00000211,-0.02581840,0.00000008,-0.00000009,0.00058927,

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,-0.00002365,0.,0.,0.00000341,0.,0.,-0.00000218,0.00000154,-0.00000224

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4,0.,0.00000881,-0.00000395,0.,-0.00000761,-0.00000213,0.,0.00092338,0

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4,0.,0.00007737,0.00005275,0.,-0.00001912,-0.00000264,0.,0.00018700,0.

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1,-0.00008466,0.,0.00015805,-0.00021042,0.,0.00014099,0.00027326,-0.00

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1,-0.00000003,-0.00317626,-0.00000154,-0.00000224,0.02035892,0.0000528

9,0.00006041,0.,-0.00013922,0.00022614,0.,0.00001150,-0.00024240,-0.00

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,-0.00015286,0.,0.00031241,0.00007693,0.,-0.00051181,-0.00025259,-0.00

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3083,-0.01807926,0.00000009,-0.24486289,-0.14158461,0.00000170,0.00816

712,0.00457455,-0.00000004,-0.00113527,0.00234718,0.00000008,-0.005649

33,-0.00033858,0.00000007,-0.00000671,0.00000273,0.,-0.00000130,-0.000

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18,0.00001170,0.,0.00001218,0.00002999,0.,0.25053019,0.00005981,0.0000

7135,0.,-0.00010984,0.00006836,0.,0.00000279,-0.00007531,0.,-0.0000442

7,0.00007629,0.,0.00004373,-0.00005792,0.,0.00003805,-0.00009765,0.,-0

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4,0.,-0.00008969,0.00008314,0.,-0.00004694,-0.00002560,0.,0.00008404,-

0.00000562,0.,-0.00019506,0.00015575,0.,-0.00012752,-0.00007068,0.,0.0

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4,0.,-0.00065264,0.00026969,0.,0.00761225,0.00986567,-0.00000007,-0.14

199109,-0.16509197,0.00000121,-0.02391275,-0.00677867,0.00000020,0.000

73009,-0.00551887,-0.00000001,0.00375405,0.00020146,-0.00000003,-0.000

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0.,0.00007941,-0.00020820,0.,0.00001150,0.00024241,-0.00000001,-0.0001

3922,-0.00022614,0.,0.00005289,-0.00006041,0.,0.00014898,0.00012663,0.

,-0.00023982,-0.00023102,0.,0.00030456,-0.00010581,-0.00000002,-0.0003

3242,-0.00001778,0.,0.00001955,-0.00001824,0.,-0.00012894,0.00001853,0

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82,0.00025259,-0.00000003,0.00039712,0.00006120,0.,-0.00113527,-0.0023

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461,0.00000170,-0.00883083,0.01807926,0.00000009,-0.00564933,0.0003385

6,0.00000007,-0.00000130,0.00000143,0.,-0.00000671,-0.00000273,0.,0.00

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,0.,0.00000322,0.00001079,0.,-0.00003401,0.00078319,-0.00000003,0.2505

3019,-0.00004373,-0.00005792,0.,0.00004427,0.00007629,0.,-0.00000279,-

0.00007532,0.,0.00010984,0.00006836,0.,-0.00005981,0.00007135,0.,-0.00

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4694,-0.00002560,0.,0.00008969,0.00008314,0.,-0.00012864,-0.00048924,0

.,-0.00014028,0.00009680,0.,0.00152594,0.00052015,-0.00000001,-0.00073

009,-0.00551887,0.00000001,0.02391275,-0.00677867,-0.00000020,0.141991

09,-0.16509197,-0.00000121,-0.00761225,0.00986567,0.00000007,-0.003754

05,0.00020146,0.00000003,0.00000143,-0.00000256,0.,0.00000273,0.000003

06,0.,-0.00001146,0.00000676,0.,0.00000699,0.00000296,0.,0.00001914,0.

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256,0.,0.,0.00004502,0.,0.,-0.00000698,0.,0.,0.00005847,0.,0.,-0.00002

365,-0.00000003,-0.00000001,-0.00419478,-0.00000185,0.00000131,0.02231

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5,-0.02673711,0.00000005,-0.00181606,0.01966517,0.00000003,-0.00123861

,0.00150840,0.00000004,0.00188587,0.00126372,-0.00000004,-0.00513458,0

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,0.,-0.00009374,-0.00003725,0.,0.00003980,0.00003256,0.,-0.00010619,-0

.00009356,0.,-0.00003462,-0.00002176,0.,-0.00059716,-0.00009757,0.,0.0

0084818,0.00042731,0.,-0.00004179,-0.00005825,0.,0.00061963,-0.0001304

5,0.00000019,0.00450038,-0.00651656,0.00000005,-0.00409346,0.00431149,

0.00000004,0.00260577,-0.00268123,0.00000002,0.00298862,-0.00310523,-0

.00000003,-0.00188169,0.00197475,-0.00000002,-0.00214265,-0.00203555,-

0.00000002,0.00127399,0.00129300,0.00000001,-0.50723683,-0.49401748,0.

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,-0.00497330,-0.00516427,0.,0.00647465,0.00028679,-0.00000006,-0.00537

055,0.00229525,-0.00000001,0.00065257,-0.00015313,-0.00000002,-0.00268

671,0.00197902,0.00000004,-0.00387038,0.00379023,0.00000003,0.00617850

,-0.00444147,0.,0.00131228,0.00198281,-0.00000004,0.00107199,-0.000444

76,0.00000003,0.01455007,-0.00304142,0.00000005,-0.00940621,0.00052642

,-0.00000006,-0.02162604,-0.02143477,0.00000005,0.00079628,0.02043639,

0.00000002,-0.00045394,0.00079713,0.00000004,0.00127423,0.00123813,-0.

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85,0.00076316,0.,0.00003913,-0.00045655,0.,-0.00002813,-0.00007157,0.,

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496673,-0.53568324,0.00000347,0.70594314,0.77128070,0.,0.,0.00000659,-

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,-0.00000551,0.00000004,-0.00000004,-0.00010701,-0.00000006,0.00000004

,-0.00004828,-0.00000001,-0.00000002,-0.00015946,0.,0.,0.00019145,-0.0

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0.,0.,-0.00013625,0.,0.,0.00002600,0.,0.,-0.00006683,-0.00000004,0.000

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0003,0.00002155,-0.00000003,0.00000003,0.00001977,0.00000002,-0.000000

02,0.00000746,0.00000002,0.00000002,0.00000362,-0.00000001,-0.00000001

,0.00000023,0.00000323,0.00000353,-0.02340103,-0.00000471,-0.00000513,

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974,-0.00035592,0.,0.00016056,0.00038694,0.,-0.00004954,0.00004133,0.,

-0.00013080,-0.00024672,0.,0.00031057,0.00027497,0.,-0.00036412,-0.000

02947,0.,0.00024489,-0.00014672,0.,-0.00002116,0.00002103,0.,0.0001362

4,-0.00010372,0.,0.00025561,-0.00019156,0.,-0.00032624,0.00029207,0.,-

0.00007063,-0.00004546,0.,0.00002320,0.00005401,0.,-0.00013954,0.00062

274,0.,0.00067905,-0.00011662,0.,0.00421441,-0.00202555,0.00000002,-0.

00096106,-0.00128117,0.,0.00008930,-0.00016104,0.,-0.00002366,-0.00000

157,0.,0.00016964,-0.00066326,0.,0.00017796,0.00066359,0.,-0.00000140,

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,0.,0.00000282,-0.00001160,0.,0.00000411,0.00000956,0.,-0.00000258,-0.

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814,0.00294804,-0.00000003,-0.21102701,-0.19523905,0.00000140,0.203059

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0038342,0.,0.00016670,0.00041057,0.,-0.00005455,0.00004158,0.,-0.00014

169,-0.00025916,0.,0.00032209,0.00027747,0.,-0.00036716,-0.00002423,0.

,0.00024789,-0.00016383,0.,-0.00001067,0.00002635,0.,0.00013300,-0.000

09971,0.,0.00026550,-0.00016522,0.,-0.00042392,0.00015112,0.,-0.000030

10,-0.00004135,0.,-0.00010622,0.00004896,0.,-0.00094173,-0.00082000,0.

,0.00038081,0.00011336,0.,-0.00214081,0.00436455,0.00000002,0.00051395

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0057,0.,0.00000612,0.00000279,0.,-0.00000276,-0.00000136,0.,0.00000684

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017774,0.00017806,0.,-0.00019137,0.00019795,0.,0.00012410,-0.00013159,

0.,0.00012438,0.00011792,0.,-0.00006936,-0.00007024,0.,0.00217394,0.00

330780,-0.00000003,-0.19456197,-0.22013120,0.00000151,0.19452370,0.212

59480,0.,0.,-0.00000224,0.,0.,-0.00000362,0.,0.,-0.00000402,0.,0.,-0.0

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2782,0.,0.,0.00003515,0.,0.,0.00003398,0.,0.,0.00004386,0.,0.,0.000007

53,0.,0.,-0.00001737,0.,0.,-0.00000432,0.,0.,-0.00000011,0.,0.,-0.0000

0062,-0.00000003,-0.00000004,-0.00250419,0.00000140,0.00000151,-0.0111

8312,-0.00000139,-0.00000149,0.00845350,-0.00004954,-0.00004133,0.,0.0

0016056,-0.00038694,0.,-0.00001974,0.00035592,0.,-0.00015984,-0.000254

05,0.,0.00004262,-0.00003205,0.,0.00025561,0.00019156,0.,-0.00032624,-

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002320,-0.00005401,0.,-0.00007063,0.00004546,0.,-0.00013080,0.00024672

,0.,0.00031057,-0.00027497,0.,0.00013624,0.00010372,0.,-0.00002116,-0.

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7919,-0.00046142,0.,0.00016964,0.00066326,0.,-0.00002366,0.00000157,0.

,0.00008930,0.00016104,0.,-0.00096106,0.00128117,0.,0.00017796,-0.0006

6360,0.,0.00000617,-0.00000275,0.,-0.00000140,0.00000064,0.,0.00002758

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0,0.,-0.00000258,0.00000471,-0.00000002,0.00421441,0.00202555,0.000000

02,0.00377814,-0.00294804,-0.00000003,0.00011571,-0.00010954,0.,-0.211

02701,0.19523905,0.00000140,-0.00006466,0.00006490,0.,-0.00015529,-0.0

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86,-0.00019286,0.,0.00001221,0.00001142,0.,0.20305903,0.00005455,0.000

04158,0.,-0.00016670,0.00041057,0.,0.00002595,-0.00038343,0.,0.0001669

7,0.00026426,0.,-0.00004657,0.00003298,0.,-0.00026550,-0.00016522,0.,0

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2,0.,0.19456197,-0.22013120,-0.00000151,0.00006936,-0.00007024,0.,0.00

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2,0.,0.00019137,0.00019795,0.,-0.00001142,-0.00001332,0.,-0.19452370,0

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66,-0.00000157,0.,0.00016964,-0.00066326,0.,0.00017796,0.00066359,0.,-

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0282,-0.00001160,0.,-0.00000351,-0.00000223,0.,0.00002758,0.00002961,0

.,-0.00000288,-0.00000117,0.,0.00000682,0.00000573,0.,0.00000617,0.000

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8,-0.00059848,0.,-0.00006389,0.00097006,0.,0.00051395,-0.00043718,0.,0

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3,-0.00082000,0.,0.00038081,0.00011336,0.,-0.00042392,0.00015112,0.,-0

.00003010,-0.00004135,0.,-0.00010622,0.00004896,0.,-0.00021022,0.00048

169,0.,0.00024789,-0.00016383,0.,-0.00001067,0.00002635,0.,0.00013300,

-0.00009971,0.,0.00032209,0.00027747,0.,-0.00036716,-0.00002423,0.,-0.

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8,0.,0.00004657,0.00003298,0.,-0.00016697,0.00026426,0.,-0.00002595,-0

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62,0.,0.,-0.00000402,0.,0.,-0.00002782,0.,0.,0.00005418,0.,0.,-0.00001

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7,0.,0.,0.00000046,0.,0.,0.00003515,0.,0.,0.00001859,0.,0.,0.00000753,

0.,0.,0.00004386,0.,0.,-0.00000432,0.,0.,-0.00001737,0.00000003,0.0000

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2624,-0.00029207,0.,0.00067906,0.00011662,0.,0.00025561,0.00019156,0.,

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82,0.00001160,0.,0.00000411,-0.00000956,0.,0.00000682,-0.00000573,0.,-

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223,0.,-0.00000140,0.00000064,0.,0.00000617,-0.00000275,0.,-0.00000258

,0.00000471,0.00000002,-0.00013080,0.00024672,0.,0.00011571,-0.0001095

4,0.,0.00377814,-0.00294804,0.00000003,-0.00006466,0.00006490,0.,-0.21

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.,0.20305903,-0.00012727,-0.00002188,0.,-0.00051395,-0.00043718,0.,0.0

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4,0.,0.00021022,0.00048169,0.,-0.00024789,-0.00016383,0.,0.00036716,-0

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8,0.,-0.00016670,0.00041057,0.,0.00002595,-0.00038343,0.,-0.00001979,0

.00002105,0.,0.00000074,-0.00000060,0.,-0.00000684,0.00000631,0.,0.000

00276,-0.00000136,0.,0.00001617,0.00000400,0.,-0.00000776,0.00000314,0

.,0.00000143,-0.00000057,0.,-0.00000612,0.00000279,0.,0.00004370,0.000

03786,-0.00000002,0.00014169,-0.00025916,0.,-0.00012438,0.00011792,0.,

-0.00217394,0.00330780,-0.00000003,0.00006936,-0.00007024,0.,0.1945619

7,-0.22013120,0.00000151,-0.00026661,-0.00026752,0.,0.00019137,0.00019

795,0.,0.00017774,0.00017806,0.,-0.00012410,-0.00013159,0.,0.00000756,

0.00000882,0.,-0.00000298,0.00000337,0.,-0.00001142,-0.00001332,0.,-0.

19452370,0.21259480,0.,0.,0.00014074,0.,0.,0.00019138,0.,0.,-0.0002409

2,0.,0.,-0.00015660,0.,0.,0.00001351,0.,0.,0.00003398,0.,0.,-0.0000136

5,0.,0.,-0.00000263,0.,0.,-0.00000415,0.,0.,-0.00000342,0.,0.,0.000002

00,-0.00000002,0.00000002,0.00517559,0.,0.,0.00012884,0.,0.,-0.0000572

6,0.,0.,0.00004360,0.,0.,-0.00006584,0.,0.,-0.00013778,0.,0.,0.0000185

9,0.,0.,-0.00000362,0.,0.,-0.00000224,0.,0.,-0.00000007,0.,0.,-0.00000

003,0.,0.,-0.00000402,0.,0.,0.00005418,0.,0.,-0.00002782,0.,0.,0.00000

053,0.,0.,0.00000157,0.,0.,0.00008966,0.,0.,-0.00001280,0.,0.,0.000000

46,0.,0.,0.00000067,0.,0.,0.00003515,0.,0.,0.00000193,0.,0.,-0.0000001

1,0.00000003,-0.00000004,-0.00250419,0.,0.,-0.00000062,-0.00000140,0.0

0000151,-0.01118312,0.,0.,0.00004386,0.,0.,-0.00001737,0.,0.,0.0000075

3,0.,0.,-0.00000432,0.,0.,0.00000135,0.,0.,0.00000043,0.,0.,0.00000350

,0.00000139,-0.00000149,0.00845350\\0.00000006,0.00000222,0.,-0.000000

50,0.00000099,0.00000004,0.00000734,0.,-0.00000196,-0.00000050,-0.0000

0099,0.00000004,0.00000006,-0.00000222,0.,-0.00000058,-0.00000059,0.,0

.00000092,-0.00000028,0.00000005,0.,0.00000491,-0.00000234,-0.00000092

,-0.00000028,0.00000005,0.00000188,0.00000044,0.,-0.00000188,0.0000004

4,0.,-0.00000058,0.00000059,0.,0.00000092,0.00000028,0.00000005,-0.000

00188,-0.00000044,0.,0.00000188,-0.00000044,0.,-0.00000092,0.00000028,

0.00000005,0.,-0.00000491,-0.00000234,0.00000058,0.00000059,0.,0.00000

050,0.00000099,0.00000004,-0.00000006,0.00000222,0.,-0.00000006,-0.000

00222,0.,0.00000050,-0.00000099,0.00000004,-0.00000734,0.,-0.00000196,

0.00000011,0.00000011,0.,0.00000011,-0.00000011,0.,0.00000005,0.000000

06,0.,-0.00000005,0.00000006,0.,-0.00000005,-0.00000006,0.,0.00000005,

-0.00000006,0.,-0.00000011,0.00000011,0.,-0.00000011,-0.00000011,0.,0.

,0.,0.00000821,0.00000058,-0.00000059,0.,0.00000017,0.00000018,0.,-0.0

0000017,-0.00000018,0.,0.00000015,0.00000008,0.,-0.00000015,-0.0000000

8,0.,-0.00000017,0.00000018,0.,-0.00000015,0.00000008,0.,0.00000017,-0

.00000018,0.,0.00000015,-0.00000008,0.,-0.00000023,-0.00000009,0.,-0.0

0000023,0.00000009,0.,0.00000023,0.00000009,0.,0.00000023,-0.00000009,

0.\\\@

ERWIN WITH HIS PSI CAN DO

CALCULATIONS QUITE A FEW.

BUT ONE THING HAS NOT BEEN SEEN

JUST WHAT DOES PSI REALLY MEAN.

-- WALTER HUCKEL, TRANS. BY FELIX BLOCH

Job cpu time: 6 days 16 hours 9 minutes 47.1 seconds.

File lengths (MBytes): RWF= 2327 Int= 0 D2E= 0 Chk= 54 Scr= 1

Normal termination of Gaussian 09 at Wed Jul 31 05:38:58 2019.