Entering Gaussian System, Link 0=g09

Input=ZnTPP0.com

Output=ZnTPP0.log

Initial command:

/home/kira/g09/l1.exe "/home/kira/g09/scratch/Gau-5142.inp" -scrdir="/home/kira/g09/scratch/"

Entering Link 1 = /home/kira/g09/l1.exe PID= 5150.

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Cite this work as:

Gaussian 09, Revision E.01,

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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

13-Aug-2019

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

%nprocshared=4

Will use up to 4 processors via shared memory.

%mem=5GB

%chk=ZnTPP0.chk

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

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

d3bj

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

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

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

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

4//1;

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

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

7//1,2,3,16;

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

2/9=110/2;

99//99;

2/9=110/2;

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

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

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

7//1,2,3,16;

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

2/9=110/2;

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

99/9=1/99;

Leave Link 1 at Tue Aug 13 17:57:33 2019, MaxMem= 671088640 cpu: 0.2

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

------

ZnTPP0

------

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C -0.68332 4.282 0.14077

C -1.11148 2.89954 0.03164

N 0. 2.09593 -0.02263

C 1.11148 2.89954 0.03164

C 0.68332 4.282 0.14077

C 2.45929 2.45929 0.

C 2.89954 1.11148 -0.03164

N 2.09593 0. 0.02263

C 2.89954 -1.11148 -0.03164

C 4.282 -0.68332 -0.14077

C 4.282 0.68332 -0.14077

C -2.45929 2.45929 0.

C -2.89954 1.11148 -0.03164

C -4.282 0.68332 -0.14077

C -4.282 -0.68332 -0.14077

C -2.89954 -1.11148 -0.03164

N -2.09593 0. 0.02263

C -2.45929 -2.45929 0.

C -1.11148 -2.89954 0.03164

C -0.68332 -4.282 0.14077

C 0.68332 -4.282 0.14077

C 1.11148 -2.89954 0.03164

N 0. -2.09593 -0.02263

C 2.45929 -2.45929 0.

C 3.52052 3.52052 0.

C 3.6939 4.36294 -1.11182

C 4.68502 5.3494 -1.11387

C 5.51516 5.51516 0.

C 5.3494 4.68502 1.11387

C 4.36294 3.6939 1.11182

C -5.51516 5.51516 0.

C -4.68502 5.3494 -1.11387

C -3.6939 4.36294 -1.11182

C -3.52052 3.52052 0.

C -4.36294 3.6939 1.11182

C -5.3494 4.68502 1.11387

C 3.52052 -3.52052 0.

C 4.36294 -3.6939 1.11182

C 5.3494 -4.68502 1.11387

C 5.51516 -5.51516 0.

C 4.68502 -5.3494 -1.11387

C 3.6939 -4.36294 -1.11182

C -3.52052 -3.52052 0.

C -4.36294 -3.6939 1.11182

C -5.3494 -4.68502 1.11387

C -5.51516 -5.51516 0.

C -4.68502 -5.3494 -1.11387

C -3.6939 -4.36294 -1.11182

H -1.33363 5.14162 0.22169

H 1.33363 5.14162 0.22169

H 5.14162 -1.33363 -0.22169

H 5.14162 1.33363 -0.22169

H -5.14162 1.33363 -0.22169

H -5.14162 -1.33363 -0.22169

H -1.33363 -5.14162 0.22169

H 1.33363 -5.14162 0.22169

H 3.05468 4.23853 -1.98172

H 4.8076 5.98685 -1.98557

H 6.2836 6.2836 0.

H 5.98685 4.8076 1.98557

H 4.23853 3.05468 1.98172

H -6.2836 6.2836 0.

H -4.8076 5.98685 -1.98557

H -3.05468 4.23853 -1.98172

H -4.23853 3.05468 1.98172

H -5.98685 4.8076 1.98557

H 4.23853 -3.05468 1.98172

H 5.98685 -4.8076 1.98557

H 6.2836 -6.2836 0.

H 4.8076 -5.98685 -1.98557

H 3.05468 -4.23853 -1.98172

H -4.23853 -3.05468 1.98172

H -5.98685 -4.8076 1.98557

H -6.2836 -6.2836 0.

H -4.8076 -5.98685 -1.98557

H -3.05468 -4.23853 -1.98172

Zn 0. 0. 0.

NAtoms= 77 NQM= 77 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 12 12 12 12 12 12 12

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

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

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

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

Atom 31 32 33 34 35 36 37 38 39 40

IAtWgt= 12 12 12 12 12 12 12 12 12 12

AtmWgt= 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000

NucSpn= 0 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= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

AtZNuc= 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000

Atom 41 42 43 44 45 46 47 48 49 50

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

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

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

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

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

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

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

Atom 51 52 53 54 55 56 57 58 59 60

IAtWgt= 1 1 1 1 1 1 1 1 1 1

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 1 1 1 1 1 1 1 1 1 1

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

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

NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Atom 61 62 63 64 65 66 67 68 69 70

IAtWgt= 1 1 1 1 1 1 1 1 1 1

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 1 1 1 1 1 1 1 1 1 1

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

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

NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Atom 71 72 73 74 75 76 77

IAtWgt= 1 1 1 1 1 1 64

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 63.9291454

NucSpn= 1 1 1 1 1 1 0

AtZEff= 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

NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 0.0000000

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 30.0000000

Leave Link 101 at Tue Aug 13 17:57:33 2019, MaxMem= 671088640 cpu: 0.9

(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) 1.4514 estimate D2E/DX2 !

! R2 R(1,5) 1.3666 estimate D2E/DX2 !

! R3 R(1,49) 1.0809 estimate D2E/DX2 !

! R4 R(2,3) 1.3726 estimate D2E/DX2 !

! R5 R(2,12) 1.4182 estimate D2E/DX2 !

! R6 R(3,4) 1.3726 estimate D2E/DX2 !

! R7 R(3,77) 2.0961 estimate D2E/DX2 !

! R8 R(4,5) 1.4514 estimate D2E/DX2 !

! R9 R(4,6) 1.4182 estimate D2E/DX2 !

! R10 R(5,50) 1.0809 estimate D2E/DX2 !

! R11 R(6,7) 1.4182 estimate D2E/DX2 !

! R12 R(6,25) 1.5008 estimate D2E/DX2 !

! R13 R(7,8) 1.3726 estimate D2E/DX2 !

! R14 R(7,11) 1.4514 estimate D2E/DX2 !

! R15 R(8,9) 1.3726 estimate D2E/DX2 !

! R16 R(8,77) 2.0961 estimate D2E/DX2 !

! R17 R(9,10) 1.4514 estimate D2E/DX2 !

! R18 R(9,24) 1.4182 estimate D2E/DX2 !

! R19 R(10,11) 1.3666 estimate D2E/DX2 !

! R20 R(10,51) 1.0809 estimate D2E/DX2 !

! R21 R(11,52) 1.0809 estimate D2E/DX2 !

! R22 R(12,13) 1.4182 estimate D2E/DX2 !

! R23 R(12,34) 1.5008 estimate D2E/DX2 !

! R24 R(13,14) 1.4514 estimate D2E/DX2 !

! R25 R(13,17) 1.3726 estimate D2E/DX2 !

! R26 R(14,15) 1.3666 estimate D2E/DX2 !

! R27 R(14,53) 1.0809 estimate D2E/DX2 !

! R28 R(15,16) 1.4514 estimate D2E/DX2 !

! R29 R(15,54) 1.0809 estimate D2E/DX2 !

! R30 R(16,17) 1.3726 estimate D2E/DX2 !

! R31 R(16,18) 1.4182 estimate D2E/DX2 !

! R32 R(17,77) 2.0961 estimate D2E/DX2 !

! R33 R(18,19) 1.4182 estimate D2E/DX2 !

! R34 R(18,43) 1.5008 estimate D2E/DX2 !

! R35 R(19,20) 1.4514 estimate D2E/DX2 !

! R36 R(19,23) 1.3726 estimate D2E/DX2 !

! R37 R(20,21) 1.3666 estimate D2E/DX2 !

! R38 R(20,55) 1.0809 estimate D2E/DX2 !

! R39 R(21,22) 1.4514 estimate D2E/DX2 !

! R40 R(21,56) 1.0809 estimate D2E/DX2 !

! R41 R(22,23) 1.3726 estimate D2E/DX2 !

! R42 R(22,24) 1.4182 estimate D2E/DX2 !

! R43 R(23,77) 2.0961 estimate D2E/DX2 !

! R44 R(24,37) 1.5008 estimate D2E/DX2 !

! R45 R(25,26) 1.4057 estimate D2E/DX2 !

! R46 R(25,30) 1.4057 estimate D2E/DX2 !

! R47 R(26,27) 1.3984 estimate D2E/DX2 !

! R48 R(26,57) 1.0867 estimate D2E/DX2 !

! R49 R(27,28) 1.399 estimate D2E/DX2 !

! R50 R(27,58) 1.0868 estimate D2E/DX2 !

! R51 R(28,29) 1.399 estimate D2E/DX2 !

! R52 R(28,59) 1.0867 estimate D2E/DX2 !

! R53 R(29,30) 1.3984 estimate D2E/DX2 !

! R54 R(29,60) 1.0868 estimate D2E/DX2 !

! R55 R(30,61) 1.0867 estimate D2E/DX2 !

! R56 R(31,32) 1.399 estimate D2E/DX2 !

! R57 R(31,36) 1.399 estimate D2E/DX2 !

! R58 R(31,62) 1.0867 estimate D2E/DX2 !

! R59 R(32,33) 1.3984 estimate D2E/DX2 !

! R60 R(32,63) 1.0868 estimate D2E/DX2 !

! R61 R(33,34) 1.4057 estimate D2E/DX2 !

! R62 R(33,64) 1.0867 estimate D2E/DX2 !

! R63 R(34,35) 1.4057 estimate D2E/DX2 !

! R64 R(35,36) 1.3984 estimate D2E/DX2 !

! R65 R(35,65) 1.0867 estimate D2E/DX2 !

! R66 R(36,66) 1.0868 estimate D2E/DX2 !

! R67 R(37,38) 1.4057 estimate D2E/DX2 !

! R68 R(37,42) 1.4057 estimate D2E/DX2 !

! R69 R(38,39) 1.3984 estimate D2E/DX2 !

! R70 R(38,67) 1.0867 estimate D2E/DX2 !

! R71 R(39,40) 1.399 estimate D2E/DX2 !

! R72 R(39,68) 1.0868 estimate D2E/DX2 !

! R73 R(40,41) 1.399 estimate D2E/DX2 !

! R74 R(40,69) 1.0867 estimate D2E/DX2 !

! R75 R(41,42) 1.3984 estimate D2E/DX2 !

! R76 R(41,70) 1.0868 estimate D2E/DX2 !

! R77 R(42,71) 1.0867 estimate D2E/DX2 !

! R78 R(43,44) 1.4057 estimate D2E/DX2 !

! R79 R(43,48) 1.4057 estimate D2E/DX2 !

! R80 R(44,45) 1.3984 estimate D2E/DX2 !

! R81 R(44,72) 1.0867 estimate D2E/DX2 !

! R82 R(45,46) 1.399 estimate D2E/DX2 !

! R83 R(45,73) 1.0868 estimate D2E/DX2 !

! R84 R(46,47) 1.399 estimate D2E/DX2 !

! R85 R(46,74) 1.0867 estimate D2E/DX2 !

! R86 R(47,48) 1.3984 estimate D2E/DX2 !

! R87 R(47,75) 1.0868 estimate D2E/DX2 !

! R88 R(48,76) 1.0867 estimate D2E/DX2 !

! A1 A(2,1,5) 107.1579 estimate D2E/DX2 !

! A2 A(2,1,49) 125.8494 estimate D2E/DX2 !

! A3 A(5,1,49) 126.9865 estimate D2E/DX2 !

! A4 A(1,2,3) 108.7689 estimate D2E/DX2 !

! A5 A(1,2,12) 125.2901 estimate D2E/DX2 !

! A6 A(3,2,12) 125.9384 estimate D2E/DX2 !

! A7 A(2,3,4) 108.1419 estimate D2E/DX2 !

! A8 A(2,3,77) 125.8022 estimate D2E/DX2 !

! A9 A(4,3,77) 125.8022 estimate D2E/DX2 !

! A10 A(3,4,5) 108.7689 estimate D2E/DX2 !

! A11 A(3,4,6) 125.9384 estimate D2E/DX2 !

! A12 A(5,4,6) 125.2901 estimate D2E/DX2 !

! A13 A(1,5,4) 107.1579 estimate D2E/DX2 !

! A14 A(1,5,50) 126.9865 estimate D2E/DX2 !

! A15 A(4,5,50) 125.8494 estimate D2E/DX2 !

! A16 A(4,6,7) 126.1926 estimate D2E/DX2 !

! A17 A(4,6,25) 116.9037 estimate D2E/DX2 !

! A18 A(7,6,25) 116.9037 estimate D2E/DX2 !

! A19 A(6,7,8) 125.9384 estimate D2E/DX2 !

! A20 A(6,7,11) 125.2901 estimate D2E/DX2 !

! A21 A(8,7,11) 108.7689 estimate D2E/DX2 !

! A22 A(7,8,9) 108.1419 estimate D2E/DX2 !

! A23 A(7,8,77) 125.8022 estimate D2E/DX2 !

! A24 A(9,8,77) 125.8022 estimate D2E/DX2 !

! A25 A(8,9,10) 108.7689 estimate D2E/DX2 !

! A26 A(8,9,24) 125.9384 estimate D2E/DX2 !

! A27 A(10,9,24) 125.2901 estimate D2E/DX2 !

! A28 A(9,10,11) 107.1579 estimate D2E/DX2 !

! A29 A(9,10,51) 125.8494 estimate D2E/DX2 !

! A30 A(11,10,51) 126.9865 estimate D2E/DX2 !

! A31 A(7,11,10) 107.1579 estimate D2E/DX2 !

! A32 A(7,11,52) 125.8494 estimate D2E/DX2 !

! A33 A(10,11,52) 126.9865 estimate D2E/DX2 !

! A34 A(2,12,13) 126.1926 estimate D2E/DX2 !

! A35 A(2,12,34) 116.9037 estimate D2E/DX2 !

! A36 A(13,12,34) 116.9037 estimate D2E/DX2 !

! A37 A(12,13,14) 125.2901 estimate D2E/DX2 !

! A38 A(12,13,17) 125.9384 estimate D2E/DX2 !

! A39 A(14,13,17) 108.7689 estimate D2E/DX2 !

! A40 A(13,14,15) 107.1579 estimate D2E/DX2 !

! A41 A(13,14,53) 125.8494 estimate D2E/DX2 !

! A42 A(15,14,53) 126.9865 estimate D2E/DX2 !

! A43 A(14,15,16) 107.1579 estimate D2E/DX2 !

! A44 A(14,15,54) 126.9865 estimate D2E/DX2 !

! A45 A(16,15,54) 125.8494 estimate D2E/DX2 !

! A46 A(15,16,17) 108.7689 estimate D2E/DX2 !

! A47 A(15,16,18) 125.2901 estimate D2E/DX2 !

! A48 A(17,16,18) 125.9384 estimate D2E/DX2 !

! A49 A(13,17,16) 108.1419 estimate D2E/DX2 !

! A50 A(13,17,77) 125.8022 estimate D2E/DX2 !

! A51 A(16,17,77) 125.8022 estimate D2E/DX2 !

! A52 A(16,18,19) 126.1926 estimate D2E/DX2 !

! A53 A(16,18,43) 116.9037 estimate D2E/DX2 !

! A54 A(19,18,43) 116.9037 estimate D2E/DX2 !

! A55 A(18,19,20) 125.2901 estimate D2E/DX2 !

! A56 A(18,19,23) 125.9384 estimate D2E/DX2 !

! A57 A(20,19,23) 108.7689 estimate D2E/DX2 !

! A58 A(19,20,21) 107.1579 estimate D2E/DX2 !

! A59 A(19,20,55) 125.8494 estimate D2E/DX2 !

! A60 A(21,20,55) 126.9865 estimate D2E/DX2 !

! A61 A(20,21,22) 107.1579 estimate D2E/DX2 !

! A62 A(20,21,56) 126.9865 estimate D2E/DX2 !

! A63 A(22,21,56) 125.8494 estimate D2E/DX2 !

! A64 A(21,22,23) 108.7689 estimate D2E/DX2 !

! A65 A(21,22,24) 125.2901 estimate D2E/DX2 !

! A66 A(23,22,24) 125.9384 estimate D2E/DX2 !

! A67 A(19,23,22) 108.1419 estimate D2E/DX2 !

! A68 A(19,23,77) 125.8022 estimate D2E/DX2 !

! A69 A(22,23,77) 125.8022 estimate D2E/DX2 !

! A70 A(9,24,22) 126.1926 estimate D2E/DX2 !

! A71 A(9,24,37) 116.9037 estimate D2E/DX2 !

! A72 A(22,24,37) 116.9037 estimate D2E/DX2 !

! A73 A(6,25,26) 120.7303 estimate D2E/DX2 !

! A74 A(6,25,30) 120.7303 estimate D2E/DX2 !

! A75 A(26,25,30) 118.5394 estimate D2E/DX2 !

! A76 A(25,26,27) 120.7548 estimate D2E/DX2 !

! A77 A(25,26,57) 119.4727 estimate D2E/DX2 !

! A78 A(27,26,57) 119.7705 estimate D2E/DX2 !

! A79 A(26,27,28) 120.1966 estimate D2E/DX2 !

! A80 A(26,27,58) 119.661 estimate D2E/DX2 !

! A81 A(28,27,58) 120.1424 estimate D2E/DX2 !

! A82 A(27,28,29) 119.5563 estimate D2E/DX2 !

! A83 A(27,28,59) 120.2218 estimate D2E/DX2 !

! A84 A(29,28,59) 120.2218 estimate D2E/DX2 !

! A85 A(28,29,30) 120.1966 estimate D2E/DX2 !

! A86 A(28,29,60) 120.1424 estimate D2E/DX2 !

! A87 A(30,29,60) 119.661 estimate D2E/DX2 !

! A88 A(25,30,29) 120.7548 estimate D2E/DX2 !

! A89 A(25,30,61) 119.4727 estimate D2E/DX2 !

! A90 A(29,30,61) 119.7705 estimate D2E/DX2 !

! A91 A(32,31,36) 119.5563 estimate D2E/DX2 !

! A92 A(32,31,62) 120.2218 estimate D2E/DX2 !

! A93 A(36,31,62) 120.2218 estimate D2E/DX2 !

! A94 A(31,32,33) 120.1966 estimate D2E/DX2 !

! A95 A(31,32,63) 120.1424 estimate D2E/DX2 !

! A96 A(33,32,63) 119.661 estimate D2E/DX2 !

! A97 A(32,33,34) 120.7548 estimate D2E/DX2 !

! A98 A(32,33,64) 119.7705 estimate D2E/DX2 !

! A99 A(34,33,64) 119.4727 estimate D2E/DX2 !

! A100 A(12,34,33) 120.7303 estimate D2E/DX2 !

! A101 A(12,34,35) 120.7303 estimate D2E/DX2 !

! A102 A(33,34,35) 118.5394 estimate D2E/DX2 !

! A103 A(34,35,36) 120.7548 estimate D2E/DX2 !

! A104 A(34,35,65) 119.4727 estimate D2E/DX2 !

! A105 A(36,35,65) 119.7705 estimate D2E/DX2 !

! A106 A(31,36,35) 120.1966 estimate D2E/DX2 !

! A107 A(31,36,66) 120.1424 estimate D2E/DX2 !

! A108 A(35,36,66) 119.661 estimate D2E/DX2 !

! A109 A(24,37,38) 120.7303 estimate D2E/DX2 !

! A110 A(24,37,42) 120.7303 estimate D2E/DX2 !

! A111 A(38,37,42) 118.5394 estimate D2E/DX2 !

! A112 A(37,38,39) 120.7548 estimate D2E/DX2 !

! A113 A(37,38,67) 119.4727 estimate D2E/DX2 !

! A114 A(39,38,67) 119.7705 estimate D2E/DX2 !

! A115 A(38,39,40) 120.1966 estimate D2E/DX2 !

! A116 A(38,39,68) 119.661 estimate D2E/DX2 !

! A117 A(40,39,68) 120.1424 estimate D2E/DX2 !

! A118 A(39,40,41) 119.5563 estimate D2E/DX2 !

! A119 A(39,40,69) 120.2218 estimate D2E/DX2 !

! A120 A(41,40,69) 120.2218 estimate D2E/DX2 !

! A121 A(40,41,42) 120.1966 estimate D2E/DX2 !

! A122 A(40,41,70) 120.1424 estimate D2E/DX2 !

! A123 A(42,41,70) 119.661 estimate D2E/DX2 !

! A124 A(37,42,41) 120.7548 estimate D2E/DX2 !

! A125 A(37,42,71) 119.4727 estimate D2E/DX2 !

! A126 A(41,42,71) 119.7705 estimate D2E/DX2 !

! A127 A(18,43,44) 120.7303 estimate D2E/DX2 !

! A128 A(18,43,48) 120.7303 estimate D2E/DX2 !

! A129 A(44,43,48) 118.5394 estimate D2E/DX2 !

! A130 A(43,44,45) 120.7548 estimate D2E/DX2 !

! A131 A(43,44,72) 119.4727 estimate D2E/DX2 !

! A132 A(45,44,72) 119.7705 estimate D2E/DX2 !

! A133 A(44,45,46) 120.1966 estimate D2E/DX2 !

! A134 A(44,45,73) 119.661 estimate D2E/DX2 !

! A135 A(46,45,73) 120.1424 estimate D2E/DX2 !

! A136 A(45,46,47) 119.5563 estimate D2E/DX2 !

! A137 A(45,46,74) 120.2218 estimate D2E/DX2 !

! A138 A(47,46,74) 120.2218 estimate D2E/DX2 !

! A139 A(46,47,48) 120.1966 estimate D2E/DX2 !

! A140 A(46,47,75) 120.1424 estimate D2E/DX2 !

! A141 A(48,47,75) 119.661 estimate D2E/DX2 !

! A142 A(43,48,47) 120.7548 estimate D2E/DX2 !

! A143 A(43,48,76) 119.4727 estimate D2E/DX2 !

! A144 A(47,48,76) 119.7705 estimate D2E/DX2 !

! A145 A(3,77,8) 90.0067 estimate D2E/DX2 !

! A146 A(3,77,17) 90.0067 estimate D2E/DX2 !

! A147 A(8,77,23) 90.0067 estimate D2E/DX2 !

! A148 A(17,77,23) 90.0067 estimate D2E/DX2 !

! A149 L(3,77,23,17,-1) 180.0134 estimate D2E/DX2 !

! A150 L(8,77,17,23,-1) 180.0134 estimate D2E/DX2 !

! A151 L(3,77,23,17,-2) 178.7631 estimate D2E/DX2 !

! A152 L(8,77,17,23,-2) 178.7631 estimate D2E/DX2 !

! D1 D(5,1,2,3) 0.4033 estimate D2E/DX2 !

! D2 D(5,1,2,12) 179.8462 estimate D2E/DX2 !

! D3 D(49,1,2,3) -178.7453 estimate D2E/DX2 !

! D4 D(49,1,2,12) 0.6976 estimate D2E/DX2 !

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

! D6 D(2,1,5,50) -179.136 estimate D2E/DX2 !

! D7 D(49,1,5,4) 179.136 estimate D2E/DX2 !

! D8 D(49,1,5,50) 0.0 estimate D2E/DX2 !

! D9 D(1,2,3,4) -0.6567 estimate D2E/DX2 !

! D10 D(1,2,3,77) 173.8148 estimate D2E/DX2 !

! D11 D(12,2,3,4) 179.905 estimate D2E/DX2 !

! D12 D(12,2,3,77) -5.6235 estimate D2E/DX2 !

! D13 D(1,2,12,13) -176.2696 estimate D2E/DX2 !

! D14 D(1,2,12,34) 3.7304 estimate D2E/DX2 !

! D15 D(3,2,12,13) 3.0788 estimate D2E/DX2 !

! D16 D(3,2,12,34) -176.9212 estimate D2E/DX2 !

! D17 D(2,3,4,5) 0.6567 estimate D2E/DX2 !

! D18 D(2,3,4,6) -179.905 estimate D2E/DX2 !

! D19 D(77,3,4,5) -173.8148 estimate D2E/DX2 !

! D20 D(77,3,4,6) 5.6235 estimate D2E/DX2 !

! D21 D(2,3,77,8) -176.1408 estimate D2E/DX2 !

! D22 D(2,3,77,17) 2.6223 estimate D2E/DX2 !

! D23 D(4,3,77,8) -2.6223 estimate D2E/DX2 !

! D24 D(4,3,77,17) 176.1408 estimate D2E/DX2 !

! D25 D(3,4,5,1) -0.4033 estimate D2E/DX2 !

! D26 D(3,4,5,50) 178.7453 estimate D2E/DX2 !

! D27 D(6,4,5,1) -179.8462 estimate D2E/DX2 !

! D28 D(6,4,5,50) -0.6976 estimate D2E/DX2 !

! D29 D(3,4,6,7) -3.0788 estimate D2E/DX2 !

! D30 D(3,4,6,25) 176.9212 estimate D2E/DX2 !

! D31 D(5,4,6,7) 176.2696 estimate D2E/DX2 !

! D32 D(5,4,6,25) -3.7304 estimate D2E/DX2 !

! D33 D(4,6,7,8) -3.0788 estimate D2E/DX2 !

! D34 D(4,6,7,11) 176.2696 estimate D2E/DX2 !

! D35 D(25,6,7,8) 176.9212 estimate D2E/DX2 !

! D36 D(25,6,7,11) -3.7304 estimate D2E/DX2 !

! D37 D(4,6,25,26) -68.3833 estimate D2E/DX2 !

! D38 D(4,6,25,30) 111.6167 estimate D2E/DX2 !

! D39 D(7,6,25,26) 111.6167 estimate D2E/DX2 !

! D40 D(7,6,25,30) -68.3833 estimate D2E/DX2 !

! D41 D(6,7,8,9) -179.905 estimate D2E/DX2 !

! D42 D(6,7,8,77) 5.6235 estimate D2E/DX2 !

! D43 D(11,7,8,9) 0.6567 estimate D2E/DX2 !

! D44 D(11,7,8,77) -173.8148 estimate D2E/DX2 !

! D45 D(6,7,11,10) -179.8462 estimate D2E/DX2 !

! D46 D(6,7,11,52) -0.6976 estimate D2E/DX2 !

! D47 D(8,7,11,10) -0.4033 estimate D2E/DX2 !

! D48 D(8,7,11,52) 178.7453 estimate D2E/DX2 !

! D49 D(7,8,9,10) -0.6567 estimate D2E/DX2 !

! D50 D(7,8,9,24) 179.905 estimate D2E/DX2 !

! D51 D(77,8,9,10) 173.8148 estimate D2E/DX2 !

! D52 D(77,8,9,24) -5.6235 estimate D2E/DX2 !

! D53 D(7,8,77,3) -2.6223 estimate D2E/DX2 !

! D54 D(7,8,77,23) 176.1408 estimate D2E/DX2 !

! D55 D(9,8,77,3) -176.1408 estimate D2E/DX2 !

! D56 D(9,8,77,23) 2.6223 estimate D2E/DX2 !

! D57 D(8,9,10,11) 0.4033 estimate D2E/DX2 !

! D58 D(8,9,10,51) -178.7453 estimate D2E/DX2 !

! D59 D(24,9,10,11) 179.8462 estimate D2E/DX2 !

! D60 D(24,9,10,51) 0.6976 estimate D2E/DX2 !

! D61 D(8,9,24,22) 3.0788 estimate D2E/DX2 !

! D62 D(8,9,24,37) -176.9212 estimate D2E/DX2 !

! D63 D(10,9,24,22) -176.2696 estimate D2E/DX2 !

! D64 D(10,9,24,37) 3.7304 estimate D2E/DX2 !

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

! D66 D(9,10,11,52) -179.136 estimate D2E/DX2 !

! D67 D(51,10,11,7) 179.136 estimate D2E/DX2 !

! D68 D(51,10,11,52) 0.0 estimate D2E/DX2 !

! D69 D(2,12,13,14) -176.2696 estimate D2E/DX2 !

! D70 D(2,12,13,17) 3.0788 estimate D2E/DX2 !

! D71 D(34,12,13,14) 3.7304 estimate D2E/DX2 !

! D72 D(34,12,13,17) -176.9212 estimate D2E/DX2 !

! D73 D(2,12,34,33) 68.3833 estimate D2E/DX2 !

! D74 D(2,12,34,35) -111.6167 estimate D2E/DX2 !

! D75 D(13,12,34,33) -111.6167 estimate D2E/DX2 !

! D76 D(13,12,34,35) 68.3833 estimate D2E/DX2 !

! D77 D(12,13,14,15) 179.8462 estimate D2E/DX2 !

! D78 D(12,13,14,53) 0.6976 estimate D2E/DX2 !

! D79 D(17,13,14,15) 0.4033 estimate D2E/DX2 !

! D80 D(17,13,14,53) -178.7453 estimate D2E/DX2 !

! D81 D(12,13,17,16) 179.905 estimate D2E/DX2 !

! D82 D(12,13,17,77) -5.6235 estimate D2E/DX2 !

! D83 D(14,13,17,16) -0.6567 estimate D2E/DX2 !

! D84 D(14,13,17,77) 173.8148 estimate D2E/DX2 !

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

! D86 D(13,14,15,54) -179.136 estimate D2E/DX2 !

! D87 D(53,14,15,16) 179.136 estimate D2E/DX2 !

! D88 D(53,14,15,54) 0.0 estimate D2E/DX2 !

! D89 D(14,15,16,17) -0.4033 estimate D2E/DX2 !

! D90 D(14,15,16,18) -179.8462 estimate D2E/DX2 !

! D91 D(54,15,16,17) 178.7453 estimate D2E/DX2 !

! D92 D(54,15,16,18) -0.6976 estimate D2E/DX2 !

! D93 D(15,16,17,13) 0.6567 estimate D2E/DX2 !

! D94 D(15,16,17,77) -173.8148 estimate D2E/DX2 !

! D95 D(18,16,17,13) -179.905 estimate D2E/DX2 !

! D96 D(18,16,17,77) 5.6235 estimate D2E/DX2 !

! D97 D(15,16,18,19) 176.2696 estimate D2E/DX2 !

! D98 D(15,16,18,43) -3.7304 estimate D2E/DX2 !

! D99 D(17,16,18,19) -3.0788 estimate D2E/DX2 !

! D100 D(17,16,18,43) 176.9212 estimate D2E/DX2 !

! D101 D(13,17,77,3) 2.6223 estimate D2E/DX2 !

! D102 D(13,17,77,23) -176.1408 estimate D2E/DX2 !

! D103 D(16,17,77,3) 176.1408 estimate D2E/DX2 !

! D104 D(16,17,77,23) -2.6223 estimate D2E/DX2 !

! D105 D(16,18,19,20) 176.2696 estimate D2E/DX2 !

! D106 D(16,18,19,23) -3.0788 estimate D2E/DX2 !

! D107 D(43,18,19,20) -3.7304 estimate D2E/DX2 !

! D108 D(43,18,19,23) 176.9212 estimate D2E/DX2 !

! D109 D(16,18,43,44) -68.3833 estimate D2E/DX2 !

! D110 D(16,18,43,48) 111.6167 estimate D2E/DX2 !

! D111 D(19,18,43,44) 111.6167 estimate D2E/DX2 !

! D112 D(19,18,43,48) -68.3833 estimate D2E/DX2 !

! D113 D(18,19,20,21) -179.8462 estimate D2E/DX2 !

! D114 D(18,19,20,55) -0.6976 estimate D2E/DX2 !

! D115 D(23,19,20,21) -0.4033 estimate D2E/DX2 !

! D116 D(23,19,20,55) 178.7453 estimate D2E/DX2 !

! D117 D(18,19,23,22) -179.905 estimate D2E/DX2 !

! D118 D(18,19,23,77) 5.6235 estimate D2E/DX2 !

! D119 D(20,19,23,22) 0.6567 estimate D2E/DX2 !

! D120 D(20,19,23,77) -173.8148 estimate D2E/DX2 !

! D121 D(19,20,21,22) 0.0 estimate D2E/DX2 !

! D122 D(19,20,21,56) 179.136 estimate D2E/DX2 !

! D123 D(55,20,21,22) -179.136 estimate D2E/DX2 !

! D124 D(55,20,21,56) 0.0 estimate D2E/DX2 !

! D125 D(20,21,22,23) 0.4033 estimate D2E/DX2 !

! D126 D(20,21,22,24) 179.8462 estimate D2E/DX2 !

! D127 D(56,21,22,23) -178.7453 estimate D2E/DX2 !

! D128 D(56,21,22,24) 0.6976 estimate D2E/DX2 !

! D129 D(21,22,23,19) -0.6567 estimate D2E/DX2 !

! D130 D(21,22,23,77) 173.8148 estimate D2E/DX2 !

! D131 D(24,22,23,19) 179.905 estimate D2E/DX2 !

! D132 D(24,22,23,77) -5.6235 estimate D2E/DX2 !

! D133 D(21,22,24,9) -176.2696 estimate D2E/DX2 !

! D134 D(21,22,24,37) 3.7304 estimate D2E/DX2 !

! D135 D(23,22,24,9) 3.0788 estimate D2E/DX2 !

! D136 D(23,22,24,37) -176.9212 estimate D2E/DX2 !

! D137 D(19,23,77,8) 176.1408 estimate D2E/DX2 !

! D138 D(19,23,77,17) -2.6223 estimate D2E/DX2 !

! D139 D(22,23,77,8) 2.6223 estimate D2E/DX2 !

! D140 D(22,23,77,17) -176.1408 estimate D2E/DX2 !

! D141 D(9,24,37,38) 68.3833 estimate D2E/DX2 !

! D142 D(9,24,37,42) -111.6167 estimate D2E/DX2 !

! D143 D(22,24,37,38) -111.6167 estimate D2E/DX2 !

! D144 D(22,24,37,42) 68.3833 estimate D2E/DX2 !

! D145 D(6,25,26,27) -179.8173 estimate D2E/DX2 !

! D146 D(6,25,26,57) -0.341 estimate D2E/DX2 !

! D147 D(30,25,26,27) 0.1827 estimate D2E/DX2 !

! D148 D(30,25,26,57) 179.659 estimate D2E/DX2 !

! D149 D(6,25,30,29) -179.8173 estimate D2E/DX2 !

! D150 D(6,25,30,61) -0.341 estimate D2E/DX2 !

! D151 D(26,25,30,29) 0.1827 estimate D2E/DX2 !

! D152 D(26,25,30,61) 179.659 estimate D2E/DX2 !

! D153 D(25,26,27,28) -0.3664 estimate D2E/DX2 !

! D154 D(25,26,27,58) 179.6136 estimate D2E/DX2 !

! D155 D(57,26,27,28) -179.8411 estimate D2E/DX2 !

! D156 D(57,26,27,58) 0.1388 estimate D2E/DX2 !

! D157 D(26,27,28,29) 0.1816 estimate D2E/DX2 !

! D158 D(26,27,28,59) -179.8184 estimate D2E/DX2 !

! D159 D(58,27,28,29) -179.7983 estimate D2E/DX2 !

! D160 D(58,27,28,59) 0.2017 estimate D2E/DX2 !

! D161 D(27,28,29,30) 0.1816 estimate D2E/DX2 !

! D162 D(27,28,29,60) -179.7983 estimate D2E/DX2 !

! D163 D(59,28,29,30) -179.8184 estimate D2E/DX2 !

! D164 D(59,28,29,60) 0.2017 estimate D2E/DX2 !

! D165 D(28,29,30,25) -0.3664 estimate D2E/DX2 !

! D166 D(28,29,30,61) -179.8411 estimate D2E/DX2 !

! D167 D(60,29,30,25) 179.6136 estimate D2E/DX2 !

! D168 D(60,29,30,61) 0.1388 estimate D2E/DX2 !

! D169 D(36,31,32,33) -0.1816 estimate D2E/DX2 !

! D170 D(36,31,32,63) 179.7983 estimate D2E/DX2 !

! D171 D(62,31,32,33) 179.8184 estimate D2E/DX2 !

! D172 D(62,31,32,63) -0.2017 estimate D2E/DX2 !

! D173 D(32,31,36,35) -0.1816 estimate D2E/DX2 !

! D174 D(32,31,36,66) 179.7983 estimate D2E/DX2 !

! D175 D(62,31,36,35) 179.8184 estimate D2E/DX2 !

! D176 D(62,31,36,66) -0.2017 estimate D2E/DX2 !

! D177 D(31,32,33,34) 0.3664 estimate D2E/DX2 !

! D178 D(31,32,33,64) 179.8411 estimate D2E/DX2 !

! D179 D(63,32,33,34) -179.6136 estimate D2E/DX2 !

! D180 D(63,32,33,64) -0.1388 estimate D2E/DX2 !

! D181 D(32,33,34,12) 179.8173 estimate D2E/DX2 !

! D182 D(32,33,34,35) -0.1827 estimate D2E/DX2 !

! D183 D(64,33,34,12) 0.341 estimate D2E/DX2 !

! D184 D(64,33,34,35) -179.659 estimate D2E/DX2 !

! D185 D(12,34,35,36) 179.8173 estimate D2E/DX2 !

! D186 D(12,34,35,65) 0.341 estimate D2E/DX2 !

! D187 D(33,34,35,36) -0.1827 estimate D2E/DX2 !

! D188 D(33,34,35,65) -179.659 estimate D2E/DX2 !

! D189 D(34,35,36,31) 0.3664 estimate D2E/DX2 !

! D190 D(34,35,36,66) -179.6136 estimate D2E/DX2 !

! D191 D(65,35,36,31) 179.8411 estimate D2E/DX2 !

! D192 D(65,35,36,66) -0.1388 estimate D2E/DX2 !

! D193 D(24,37,38,39) 179.8173 estimate D2E/DX2 !

! D194 D(24,37,38,67) 0.341 estimate D2E/DX2 !

! D195 D(42,37,38,39) -0.1827 estimate D2E/DX2 !

! D196 D(42,37,38,67) -179.659 estimate D2E/DX2 !

! D197 D(24,37,42,41) 179.8173 estimate D2E/DX2 !

! D198 D(24,37,42,71) 0.341 estimate D2E/DX2 !

! D199 D(38,37,42,41) -0.1827 estimate D2E/DX2 !

! D200 D(38,37,42,71) -179.659 estimate D2E/DX2 !

! D201 D(37,38,39,40) 0.3664 estimate D2E/DX2 !

! D202 D(37,38,39,68) -179.6136 estimate D2E/DX2 !

! D203 D(67,38,39,40) 179.8411 estimate D2E/DX2 !

! D204 D(67,38,39,68) -0.1388 estimate D2E/DX2 !

! D205 D(38,39,40,41) -0.1816 estimate D2E/DX2 !

! D206 D(38,39,40,69) 179.8184 estimate D2E/DX2 !

! D207 D(68,39,40,41) 179.7983 estimate D2E/DX2 !

! D208 D(68,39,40,69) -0.2017 estimate D2E/DX2 !

! D209 D(39,40,41,42) -0.1816 estimate D2E/DX2 !

! D210 D(39,40,41,70) 179.7983 estimate D2E/DX2 !

! D211 D(69,40,41,42) 179.8184 estimate D2E/DX2 !

! D212 D(69,40,41,70) -0.2017 estimate D2E/DX2 !

! D213 D(40,41,42,37) 0.3664 estimate D2E/DX2 !

! D214 D(40,41,42,71) 179.8411 estimate D2E/DX2 !

! D215 D(70,41,42,37) -179.6136 estimate D2E/DX2 !

! D216 D(70,41,42,71) -0.1388 estimate D2E/DX2 !

! D217 D(18,43,44,45) -179.8173 estimate D2E/DX2 !

! D218 D(18,43,44,72) -0.341 estimate D2E/DX2 !

! D219 D(48,43,44,45) 0.1827 estimate D2E/DX2 !

! D220 D(48,43,44,72) 179.659 estimate D2E/DX2 !

! D221 D(18,43,48,47) -179.8173 estimate D2E/DX2 !

! D222 D(18,43,48,76) -0.341 estimate D2E/DX2 !

! D223 D(44,43,48,47) 0.1827 estimate D2E/DX2 !

! D224 D(44,43,48,76) 179.659 estimate D2E/DX2 !

! D225 D(43,44,45,46) -0.3664 estimate D2E/DX2 !

! D226 D(43,44,45,73) 179.6136 estimate D2E/DX2 !

! D227 D(72,44,45,46) -179.8411 estimate D2E/DX2 !

! D228 D(72,44,45,73) 0.1388 estimate D2E/DX2 !

! D229 D(44,45,46,47) 0.1816 estimate D2E/DX2 !

! D230 D(44,45,46,74) -179.8184 estimate D2E/DX2 !

! D231 D(73,45,46,47) -179.7983 estimate D2E/DX2 !

! D232 D(73,45,46,74) 0.2017 estimate D2E/DX2 !

! D233 D(45,46,47,48) 0.1816 estimate D2E/DX2 !

! D234 D(45,46,47,75) -179.7983 estimate D2E/DX2 !

! D235 D(74,46,47,48) -179.8184 estimate D2E/DX2 !

! D236 D(74,46,47,75) 0.2017 estimate D2E/DX2 !

! D237 D(46,47,48,43) -0.3664 estimate D2E/DX2 !

! D238 D(46,47,48,76) -179.8411 estimate D2E/DX2 !

! D239 D(75,47,48,43) 179.6136 estimate D2E/DX2 !

! D240 D(75,47,48,76) 0.1388 estimate D2E/DX2 !

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

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

Number of steps in this run= 462 maximum allowed number of steps= 462.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Aug 13 17:57:33 2019, MaxMem= 671088640 cpu: 0.1

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

Stoichiometry C44H28N4Zn

Framework group D2D[O(Zn),2SGD(N2),X(C44H28)]

Deg. of freedom 29

Full point group D2D NOp 8

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.683316 4.282000 0.140770

2 6 0 -1.111476 2.899536 0.031636

3 7 0 0.000000 2.095932 -0.022626

4 6 0 1.111476 2.899536 0.031636

5 6 0 0.683316 4.282000 0.140770

6 6 0 2.459288 2.459288 -0.000000

7 6 0 2.899536 1.111476 -0.031636

8 7 0 2.095932 -0.000000 0.022626

9 6 0 2.899536 -1.111476 -0.031636

10 6 0 4.282000 -0.683316 -0.140770

11 6 0 4.282000 0.683316 -0.140770

12 6 0 -2.459288 2.459288 -0.000000

13 6 0 -2.899536 1.111476 -0.031636

14 6 0 -4.282000 0.683316 -0.140770

15 6 0 -4.282000 -0.683316 -0.140770

16 6 0 -2.899536 -1.111476 -0.031636

17 7 0 -2.095932 0.000000 0.022626

18 6 0 -2.459288 -2.459288 -0.000000

19 6 0 -1.111476 -2.899536 0.031636

20 6 0 -0.683316 -4.282000 0.140770

21 6 0 0.683316 -4.282000 0.140770

22 6 0 1.111476 -2.899536 0.031636

23 7 0 -0.000000 -2.095932 -0.022626

24 6 0 2.459288 -2.459288 -0.000000

25 6 0 3.520517 3.520517 -0.000000

26 6 0 3.693904 4.362945 -1.111817

27 6 0 4.685017 5.349404 -1.113870

28 6 0 5.515160 5.515160 -0.000000

29 6 0 5.349404 4.685017 1.113870

30 6 0 4.362945 3.693904 1.111817

31 6 0 -5.515160 5.515160 -0.000000

32 6 0 -4.685017 5.349404 -1.113870

33 6 0 -3.693904 4.362945 -1.111817

34 6 0 -3.520517 3.520517 -0.000000

35 6 0 -4.362945 3.693904 1.111817

36 6 0 -5.349404 4.685017 1.113870

37 6 0 3.520517 -3.520517 -0.000000

38 6 0 4.362945 -3.693904 1.111817

39 6 0 5.349404 -4.685017 1.113870

40 6 0 5.515160 -5.515160 -0.000000

41 6 0 4.685017 -5.349404 -1.113870

42 6 0 3.693904 -4.362945 -1.111817

43 6 0 -3.520517 -3.520517 -0.000000

44 6 0 -4.362945 -3.693904 1.111817

45 6 0 -5.349404 -4.685017 1.113870

46 6 0 -5.515160 -5.515160 -0.000000

47 6 0 -4.685017 -5.349404 -1.113870

48 6 0 -3.693904 -4.362945 -1.111817

49 1 0 -1.333630 5.141618 0.221690

50 1 0 1.333630 5.141618 0.221690

51 1 0 5.141618 -1.333630 -0.221690

52 1 0 5.141618 1.333630 -0.221690

53 1 0 -5.141618 1.333630 -0.221690

54 1 0 -5.141618 -1.333630 -0.221690

55 1 0 -1.333630 -5.141618 0.221690

56 1 0 1.333630 -5.141618 0.221690

57 1 0 3.054676 4.238531 -1.981719

58 1 0 4.807600 5.986847 -1.985568

59 1 0 6.283598 6.283598 -0.000000

60 1 0 5.986847 4.807600 1.985568

61 1 0 4.238531 3.054676 1.981719

62 1 0 -6.283598 6.283598 -0.000000

63 1 0 -4.807600 5.986847 -1.985568

64 1 0 -3.054676 4.238531 -1.981719

65 1 0 -4.238531 3.054676 1.981719

66 1 0 -5.986847 4.807600 1.985568

67 1 0 4.238531 -3.054676 1.981719

68 1 0 5.986847 -4.807600 1.985568

69 1 0 6.283598 -6.283598 -0.000000

70 1 0 4.807600 -5.986847 -1.985568

71 1 0 3.054676 -4.238531 -1.981719

72 1 0 -4.238531 -3.054676 1.981719

73 1 0 -5.986847 -4.807600 1.985568

74 1 0 -6.283598 -6.283598 -0.000000

75 1 0 -4.807600 -5.986847 -1.985568

76 1 0 -3.054676 -4.238531 -1.981719

77 30 0 0.000000 0.000000 0.000000

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

Rotational constants (GHZ): 0.0577332 0.0577332 0.0299039

Leave Link 202 at Tue Aug 13 17:57:34 2019, MaxMem= 671088640 cpu: 0.0

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

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

Centers: 77

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: 49 50 51 52 53 54 55 56 57 58

Centers: 59 60 61 62 63 64 65 66 67 68

Centers: 69 70 71 72 73 74 75 76 1 2

Centers: 4 5 6 7 9 10 11 12 13 14

Centers: 15 16 18 19 20 21 22 24 25 26

Centers: 27 28 29 30 31 32 33 34 35 36

Centers: 37 38 39 40 41 42 43 44 45 46

Centers: 47 48 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

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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

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21 6

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22 6

No pseudopotential on this center.

23 7

No pseudopotential on this center.

24 6

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25 6

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48 6

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49 1

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71 1

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72 1

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73 1

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74 1

No pseudopotential on this center.

75 1

No pseudopotential on this center.

76 1

No pseudopotential on this center.

77 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

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

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

There are 272 symmetry adapted cartesian basis functions of A1 symmetry.

There are 243 symmetry adapted cartesian basis functions of A2 symmetry.

There are 254 symmetry adapted cartesian basis functions of B1 symmetry.

There are 254 symmetry adapted cartesian basis functions of B2 symmetry.

There are 256 symmetry adapted basis functions of A1 symmetry.

There are 232 symmetry adapted basis functions of A2 symmetry.

There are 242 symmetry adapted basis functions of B1 symmetry.

There are 242 symmetry adapted basis functions of B2 symmetry.

972 basis functions, 1715 primitive gaussians, 1023 cartesian basis functions

166 alpha electrons 166 beta electrons

nuclear repulsion energy 5717.0343999240 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= 77 NActive= 77 NUniq= 13 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T 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= -0.2209966080 Hartrees.

Nuclear repulsion after empirical dispersion term = 5716.8134033160 Hartrees.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 77.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 77

GePol: Total number of spheres = 77

GePol: Number of exposed spheres = 77 (100.00%)

GePol: Number of points = 5786

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.21D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 312

GePol: Fraction of low-weight points (<1% of avg) = 5.39%

GePol: Cavity surface area = 621.386 Ang\*\*2

GePol: Cavity volume = 635.046 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0018876932 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5716.8115156229 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

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36641 LenP2D= 94862.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 972 RedAO= T EigKep= 6.58D-05 NBF= 256 232 242 242

NBsUse= 972 1.00D-06 EigRej= -1.00D+00 NBFU= 256 232 242 242

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= 952 952 976 976 976 MxSgAt= 77 MxSgA2= 77.

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

DipDrv: MaxL=1.

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(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= 2000

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= -1979.23370499641

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Leave Link 401 at Tue Aug 13 17:57:44 2019, MaxMem= 671088640 cpu: 30.3

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3177123 IEndB= 3177123 NGot= 671088640 MDV= 668975710

LenX= 668975710 LenY= 667928158

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= 520000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 100433388.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.24D-14 for 5784.

Iteration 1 A\*A^-1 deviation from orthogonality is 7.33D-15 for 5505 1335.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.22D-14 for 5784.

Iteration 1 A^-1\*A deviation from orthogonality is 1.37D-12 for 3133 3131.

E= -1977.88704097701

DIIS: error= 9.81D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1977.88704097701 IErMin= 1 ErrMin= 9.81D-02

ErrMax= 9.81D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.24D+00 BMatP= 1.24D+00

IDIUse=3 WtCom= 1.88D-02 WtEn= 9.81D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.107 Goal= None Shift= 0.000

GapD= 0.107 DampG=1.000 DampE=0.250 DampFc=0.2500 IDamp=-1.

Damping current iteration by 2.50D-01

RMSDP=1.81D-03 MaxDP=9.52D-02 OVMax= 1.52D-01

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.48D-04 CP: 9.89D-01

E= -1978.24484758964 Delta-E= -0.357806612633 Rises=F Damp=T

DIIS: error= 4.19D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1978.24484758964 IErMin= 2 ErrMin= 4.19D-02

ErrMax= 4.19D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.65D-01 BMatP= 1.24D+00

IDIUse=3 WtCom= 5.81D-01 WtEn= 4.19D-01

Coeff-Com: -0.102D+01 0.202D+01

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

Coeff: -0.592D+00 0.159D+01

Gap= 0.102 Goal= None Shift= 0.000

RMSDP=7.04D-04 MaxDP=3.80D-02 DE=-3.58D-01 OVMax= 6.24D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.01D-04 CP: 9.72D-01 2.27D+00

E= -1978.86934884958 Delta-E= -0.624501259940 Rises=F Damp=F

DIIS: error= 7.09D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1978.86934884958 IErMin= 3 ErrMin= 7.09D-03

ErrMax= 7.09D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.15D-02 BMatP= 3.65D-01

IDIUse=3 WtCom= 9.29D-01 WtEn= 7.09D-02

Coeff-Com: -0.878D-01 0.350D+00 0.738D+00

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

Coeff: -0.815D-01 0.325D+00 0.757D+00

Gap= 0.100 Goal= None Shift= 0.000

RMSDP=2.66D-04 MaxDP=1.67D-02 DE=-6.25D-01 OVMax= 3.70D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.80D-04 CP: 9.77D-01 1.93D+00 7.08D-01

E= -1978.89465723123 Delta-E= -0.025308381653 Rises=F Damp=F

DIIS: error= 3.41D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1978.89465723123 IErMin= 4 ErrMin= 3.41D-03

ErrMax= 3.41D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.88D-03 BMatP= 3.15D-02

IDIUse=3 WtCom= 9.66D-01 WtEn= 3.41D-02

Coeff-Com: 0.636D-01-0.333D-01 0.421D+00 0.549D+00

Coeff-En: 0.000D+00 0.000D+00 0.109D+00 0.891D+00

Coeff: 0.614D-01-0.322D-01 0.410D+00 0.561D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.12D-04 MaxDP=6.18D-03 DE=-2.53D-02 OVMax= 1.96D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 5.83D-05 CP: 9.76D-01 1.97D+00 8.02D-01 5.24D-01

E= -1978.90172754413 Delta-E= -0.007070312892 Rises=F Damp=F

DIIS: error= 2.09D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1978.90172754413 IErMin= 5 ErrMin= 2.09D-03

ErrMax= 2.09D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.12D-03 BMatP= 7.88D-03

IDIUse=3 WtCom= 9.79D-01 WtEn= 2.09D-02

Coeff-Com: 0.424D-01-0.488D-01 0.173D+00 0.339D+00 0.494D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.634D-01 0.937D+00

Coeff: 0.415D-01-0.478D-01 0.169D+00 0.333D+00 0.503D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=3.20D-05 MaxDP=2.21D-03 DE=-7.07D-03 OVMax= 5.32D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.67D-05 CP: 9.76D-01 1.98D+00 8.13D-01 5.88D-01 5.84D-01

E= -1978.90267205423 Delta-E= -0.000944510105 Rises=F Damp=F

DIIS: error= 6.59D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1978.90267205423 IErMin= 6 ErrMin= 6.59D-04

ErrMax= 6.59D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.78D-05 BMatP= 1.12D-03

IDIUse=3 WtCom= 9.93D-01 WtEn= 6.59D-03

Coeff-Com: 0.148D-01-0.197D-01 0.490D-01 0.117D+00 0.247D+00 0.592D+00

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

Coeff: 0.147D-01-0.196D-01 0.487D-01 0.116D+00 0.246D+00 0.595D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=6.40D-06 MaxDP=3.88D-04 DE=-9.45D-04 OVMax= 1.46D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.57D-06 CP: 9.76D-01 1.97D+00 8.15D-01 5.92D-01 6.11D-01

CP: 7.13D-01

E= -1978.90270771330 Delta-E= -0.000035659067 Rises=F Damp=F

DIIS: error= 8.07D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1978.90270771330 IErMin= 7 ErrMin= 8.07D-05

ErrMax= 8.07D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.93D-06 BMatP= 4.78D-05

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

Coeff-Com: 0.640D-02-0.882D-02 0.196D-01 0.501D-01 0.112D+00 0.313D+00

Coeff-Com: 0.508D+00

Coeff: 0.640D-02-0.882D-02 0.196D-01 0.501D-01 0.112D+00 0.313D+00

Coeff: 0.508D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.71D-06 MaxDP=8.22D-05 DE=-3.57D-05 OVMax= 4.62D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.18D-06 CP: 9.76D-01 1.97D+00 8.15D-01 5.93D-01 6.15D-01

CP: 7.22D-01 6.74D-01

E= -1978.90271016728 Delta-E= -0.000002453982 Rises=F Damp=F

DIIS: error= 2.30D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1978.90271016728 IErMin= 8 ErrMin= 2.30D-05

ErrMax= 2.30D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.41D-07 BMatP= 2.93D-06

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

Coeff-Com: 0.666D-03-0.981D-03 0.134D-02 0.499D-02 0.124D-01 0.513D-01

Coeff-Com: 0.240D+00 0.690D+00

Coeff: 0.666D-03-0.981D-03 0.134D-02 0.499D-02 0.124D-01 0.513D-01

Coeff: 0.240D+00 0.690D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=6.20D-07 MaxDP=2.45D-05 DE=-2.45D-06 OVMax= 1.19D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.00D-07 CP: 9.76D-01 1.97D+00 8.15D-01 5.94D-01 6.17D-01

CP: 7.24D-01 7.27D-01 6.63D-01

E= -1978.90271036254 Delta-E= -0.000000195261 Rises=F Damp=F

DIIS: error= 1.32D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1978.90271036254 IErMin= 9 ErrMin= 1.32D-05

ErrMax= 1.32D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.34D-08 BMatP= 2.41D-07

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

Coeff-Com: 0.437D-04-0.100D-03-0.288D-03 0.381D-04 0.599D-03 0.105D-01

Coeff-Com: 0.101D+00 0.393D+00 0.496D+00

Coeff: 0.437D-04-0.100D-03-0.288D-03 0.381D-04 0.599D-03 0.105D-01

Coeff: 0.101D+00 0.393D+00 0.496D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.94D-07 MaxDP=9.69D-06 DE=-1.95D-07 OVMax= 3.13D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 8.94D-08 CP: 9.76D-01 1.97D+00 8.15D-01 5.94D-01 6.16D-01

CP: 7.27D-01 7.37D-01 7.19D-01 6.83D-01

E= -1978.90271039525 Delta-E= -0.000000032705 Rises=F Damp=F

DIIS: error= 1.24D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1978.90271039525 IErMin=10 ErrMin= 1.24D-06

ErrMax= 1.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.45D-10 BMatP= 3.34D-08

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

Coeff-Com: -0.499D-04 0.603D-04-0.234D-03-0.482D-03-0.921D-03-0.446D-03

Coeff-Com: 0.168D-01 0.964D-01 0.166D+00 0.723D+00

Coeff: -0.499D-04 0.603D-04-0.234D-03-0.482D-03-0.921D-03-0.446D-03

Coeff: 0.168D-01 0.964D-01 0.166D+00 0.723D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=3.69D-08 MaxDP=1.90D-06 DE=-3.27D-08 OVMax= 6.64D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.83D-08 CP: 9.76D-01 1.97D+00 8.15D-01 5.94D-01 6.16D-01

CP: 7.27D-01 7.39D-01 7.30D-01 6.99D-01 8.67D-01

E= -1978.90271039585 Delta-E= -0.000000000606 Rises=F Damp=F

DIIS: error= 1.01D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1978.90271039585 IErMin=11 ErrMin= 1.01D-06

ErrMax= 1.01D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.82D-10 BMatP= 7.45D-10

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

Coeff-Com: -0.307D-04 0.410D-04-0.983D-04-0.273D-03-0.547D-03-0.121D-02

Coeff-Com: -0.560D-03 0.175D-01 0.456D-01 0.426D+00 0.514D+00

Coeff: -0.307D-04 0.410D-04-0.983D-04-0.273D-03-0.547D-03-0.121D-02

Coeff: -0.560D-03 0.175D-01 0.456D-01 0.426D+00 0.514D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.56D-08 MaxDP=8.83D-07 DE=-6.06D-10 OVMax= 3.38D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 7.04D-09 CP: 9.76D-01 1.97D+00 8.15D-01 5.94D-01 6.16D-01

CP: 7.27D-01 7.39D-01 7.33D-01 7.01D-01 9.21D-01

CP: 6.47D-01

E= -1978.90271039630 Delta-E= -0.000000000448 Rises=F Damp=F

DIIS: error= 1.59D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1978.90271039630 IErMin=12 ErrMin= 1.59D-07

ErrMax= 1.59D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.98D-12 BMatP= 2.82D-10

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

Coeff-Com: -0.479D-05 0.662D-05-0.114D-04-0.489D-04-0.879D-04-0.309D-03

Coeff-Com: -0.128D-02-0.137D-02 0.210D-02 0.643D-01 0.135D+00 0.802D+00

Coeff: -0.479D-05 0.662D-05-0.114D-04-0.489D-04-0.879D-04-0.309D-03

Coeff: -0.128D-02-0.137D-02 0.210D-02 0.643D-01 0.135D+00 0.802D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=2.73D-09 MaxDP=1.29D-07 DE=-4.48D-10 OVMax= 3.94D-07

Error on total polarization charges = 0.08566

SCF Done: E(RB3LYP) = -1978.90271040 A.U. after 12 cycles

NFock= 12 Conv=0.27D-08 -V/T= 1.9796

KE= 2.020018907872D+03 PE=-1.611523604103D+04 EE= 6.399502907140D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.18

(included in total energy above)

Leave Link 502 at Tue Aug 13 18:05:21 2019, MaxMem= 671088640 cpu: 1823.7

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

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

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Population analysis using the SCF density.

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

Orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The electronic state is 1-A1.

Alpha occ. eigenvalues -- -14.30367 -14.30367 -14.30367 -14.30367 -10.21016

Alpha occ. eigenvalues -- -10.21016 -10.21016 -10.21015 -10.21015 -10.21015

Alpha occ. eigenvalues -- -10.21015 -10.21015 -10.19773 -10.19772 -10.19772

Alpha occ. eigenvalues -- -10.19772 -10.18871 -10.18870 -10.18870 -10.18870

Alpha occ. eigenvalues -- -10.17500 -10.17500 -10.17500 -10.17500 -10.17499

Alpha occ. eigenvalues -- -10.17499 -10.17499 -10.17498 -10.17448 -10.17448

Alpha occ. eigenvalues -- -10.17448 -10.17448 -10.17420 -10.17420 -10.17420

Alpha occ. eigenvalues -- -10.17420 -10.17380 -10.17380 -10.17380 -10.17380

Alpha occ. eigenvalues -- -10.16974 -10.16974 -10.16974 -10.16974 -10.16910

Alpha occ. eigenvalues -- -10.16910 -10.16910 -10.16909 -0.96157 -0.95328

Alpha occ. eigenvalues -- -0.95328 -0.94463 -0.86638 -0.86286 -0.86286

Alpha occ. eigenvalues -- -0.86114 -0.82069 -0.80419 -0.80419 -0.78659

Alpha occ. eigenvalues -- -0.76565 -0.76519 -0.76519 -0.76084 -0.74773

Alpha occ. eigenvalues -- -0.74722 -0.74722 -0.74702 -0.74008 -0.73326

Alpha occ. eigenvalues -- -0.73326 -0.71773 -0.70753 -0.66028 -0.66028

Alpha occ. eigenvalues -- -0.62025 -0.60861 -0.60692 -0.60692 -0.60589

Alpha occ. eigenvalues -- -0.59871 -0.59871 -0.59415 -0.59389 -0.58566

Alpha occ. eigenvalues -- -0.56987 -0.56539 -0.56182 -0.56182 -0.56024

Alpha occ. eigenvalues -- -0.55366 -0.55366 -0.54807 -0.54270 -0.52605

Alpha occ. eigenvalues -- -0.52605 -0.52593 -0.51773 -0.51361 -0.51361

Alpha occ. eigenvalues -- -0.49841 -0.49798 -0.49042 -0.49042 -0.46173

Alpha occ. eigenvalues -- -0.45844 -0.45757 -0.45626 -0.45626 -0.45010

Alpha occ. eigenvalues -- -0.45010 -0.44867 -0.44328 -0.42465 -0.42411

Alpha occ. eigenvalues -- -0.42191 -0.42191 -0.42130 -0.42114 -0.42087

Alpha occ. eigenvalues -- -0.42087 -0.41736 -0.41196 -0.40750 -0.40750

Alpha occ. eigenvalues -- -0.40119 -0.40119 -0.39241 -0.39070 -0.38333

Alpha occ. eigenvalues -- -0.38212 -0.37793 -0.37793 -0.36797 -0.36723

Alpha occ. eigenvalues -- -0.36583 -0.36583 -0.35756 -0.35155 -0.34802

Alpha occ. eigenvalues -- -0.34694 -0.34694 -0.34613 -0.34612 -0.34612

Alpha occ. eigenvalues -- -0.33892 -0.31693 -0.31349 -0.31349 -0.28426

Alpha occ. eigenvalues -- -0.28426 -0.26290 -0.26029 -0.25941 -0.25897

Alpha occ. eigenvalues -- -0.25864 -0.25864 -0.25730 -0.25257 -0.25257

Alpha occ. eigenvalues -- -0.25250 -0.24765 -0.24765 -0.24653 -0.20224

Alpha occ. eigenvalues -- -0.19040

Alpha virt. eigenvalues -- -0.09150 -0.09150 -0.03633 -0.01514 -0.01443

Alpha virt. eigenvalues -- -0.01443 -0.01224 -0.01193 -0.01187 -0.01059

Alpha virt. eigenvalues -- -0.01059 0.03325 0.03761 0.04456 0.04623

Alpha virt. eigenvalues -- 0.04623 0.05489 0.05489 0.05771 0.06072

Alpha virt. eigenvalues -- 0.06992 0.06992 0.07089 0.08527 0.08966

Alpha virt. eigenvalues -- 0.08966 0.09072 0.09107 0.09446 0.09446

Alpha virt. eigenvalues -- 0.09837 0.10157 0.10195 0.10253 0.11250

Alpha virt. eigenvalues -- 0.11250 0.11722 0.11722 0.11940 0.12435

Alpha virt. eigenvalues -- 0.12873 0.12873 0.13167 0.13426 0.13626

Alpha virt. eigenvalues -- 0.13626 0.13739 0.13932 0.14034 0.14354

Alpha virt. eigenvalues -- 0.14974 0.14974 0.15355 0.15355 0.15745

Alpha virt. eigenvalues -- 0.16236 0.18232 0.18232 0.20588 0.21262

Alpha virt. eigenvalues -- 0.22454 0.23433 0.23433 0.23572 0.23740

Alpha virt. eigenvalues -- 0.24070 0.24912 0.25352 0.25352 0.26546

Alpha virt. eigenvalues -- 0.26588 0.26588 0.26878 0.27392 0.27850

Alpha virt. eigenvalues -- 0.27851 0.27851 0.28085 0.28274 0.28274

Alpha virt. eigenvalues -- 0.28659 0.28708 0.28936 0.28936 0.29714

Alpha virt. eigenvalues -- 0.29811 0.29811 0.29844 0.30371 0.31148

Alpha virt. eigenvalues -- 0.31148 0.31276 0.32057 0.34190 0.35059

Alpha virt. eigenvalues -- 0.35216 0.35216 0.35255 0.35671 0.35671

Alpha virt. eigenvalues -- 0.36199 0.36337 0.36348 0.36348 0.36607

Alpha virt. eigenvalues -- 0.36607 0.37278 0.37348 0.37860 0.38639

Alpha virt. eigenvalues -- 0.38786 0.39540 0.39638 0.39638 0.39682

Alpha virt. eigenvalues -- 0.39806 0.39806 0.40474 0.40522 0.40843

Alpha virt. eigenvalues -- 0.40843 0.41140 0.41188 0.41508 0.41508

Alpha virt. eigenvalues -- 0.41630 0.41632 0.41788 0.41788 0.42014

Alpha virt. eigenvalues -- 0.42536 0.42536 0.42920 0.42992 0.42992

Alpha virt. eigenvalues -- 0.43118 0.43659 0.44137 0.44331 0.44331

Alpha virt. eigenvalues -- 0.44365 0.44850 0.44919 0.44919 0.45193

Alpha virt. eigenvalues -- 0.45216 0.46261 0.46261 0.46500 0.46500

Alpha virt. eigenvalues -- 0.46670 0.46747 0.47450 0.48075 0.48075

Alpha virt. eigenvalues -- 0.48617 0.48617 0.49401 0.49463 0.49583

Alpha virt. eigenvalues -- 0.49583 0.50068 0.51147 0.51223 0.51373

Alpha virt. eigenvalues -- 0.51706 0.52447 0.52447 0.53449 0.53449

Alpha virt. eigenvalues -- 0.53497 0.53893 0.53939 0.53939 0.54656

Alpha virt. eigenvalues -- 0.56161 0.56335 0.56707 0.57148 0.57356

Alpha virt. eigenvalues -- 0.57580 0.57580 0.58347 0.58347 0.59413

Alpha virt. eigenvalues -- 0.59413 0.60345 0.60471 0.60665 0.60833

Alpha virt. eigenvalues -- 0.60833 0.60900 0.61261 0.61261 0.61395

Alpha virt. eigenvalues -- 0.61435 0.61481 0.61501 0.61501 0.61781

Alpha virt. eigenvalues -- 0.62263 0.62263 0.62302 0.62857 0.63486

Alpha virt. eigenvalues -- 0.63797 0.63797 0.64294 0.64574 0.64574

Alpha virt. eigenvalues -- 0.64576 0.64860 0.65232 0.65373 0.65450

Alpha virt. eigenvalues -- 0.65458 0.65458 0.66787 0.66801 0.66801

Alpha virt. eigenvalues -- 0.66904 0.67924 0.67924 0.67985 0.69319

Alpha virt. eigenvalues -- 0.69319 0.70021 0.70578 0.71678 0.71859

Alpha virt. eigenvalues -- 0.71859 0.72574 0.72574 0.72731 0.72871

Alpha virt. eigenvalues -- 0.73477 0.73477 0.73857 0.74300 0.74493

Alpha virt. eigenvalues -- 0.75047 0.75047 0.75309 0.75513 0.75590

Alpha virt. eigenvalues -- 0.75590 0.76084 0.76084 0.76781 0.77780

Alpha virt. eigenvalues -- 0.78224 0.78886 0.78886 0.79335 0.79578

Alpha virt. eigenvalues -- 0.79604 0.80216 0.80216 0.80663 0.80663

Alpha virt. eigenvalues -- 0.81278 0.81342 0.82215 0.82215 0.82362

Alpha virt. eigenvalues -- 0.83987 0.84078 0.84967 0.85002 0.85002

Alpha virt. eigenvalues -- 0.85434 0.86639 0.86639 0.86717 0.86746

Alpha virt. eigenvalues -- 0.89059 0.89059 0.89294 0.89402 0.89490

Alpha virt. eigenvalues -- 0.90128 0.90128 0.91264 0.91870 0.91870

Alpha virt. eigenvalues -- 0.92288 0.93180 0.93466 0.94282 0.94282

Alpha virt. eigenvalues -- 0.95308 0.95965 0.96717 0.96717 0.97154

Alpha virt. eigenvalues -- 0.97332 0.98853 0.98853 0.99823 1.00060

Alpha virt. eigenvalues -- 1.01146 1.01146 1.02175 1.02203 1.02211

Alpha virt. eigenvalues -- 1.04106 1.04106 1.04845 1.05047 1.05047

Alpha virt. eigenvalues -- 1.05427 1.05654 1.06672 1.08171 1.08487

Alpha virt. eigenvalues -- 1.08487 1.08578 1.10945 1.10945 1.11574

Alpha virt. eigenvalues -- 1.11856 1.12699 1.12699 1.14767 1.14837

Alpha virt. eigenvalues -- 1.14846 1.14846 1.15065 1.16451 1.16990

Alpha virt. eigenvalues -- 1.17331 1.17331 1.17668 1.17668 1.18264

Alpha virt. eigenvalues -- 1.19152 1.20193 1.20193 1.20530 1.20997

Alpha virt. eigenvalues -- 1.21120 1.21120 1.21120 1.21527 1.21527

Alpha virt. eigenvalues -- 1.22178 1.22225 1.22786 1.23066 1.23955

Alpha virt. eigenvalues -- 1.23955 1.24430 1.24462 1.24462 1.24959

Alpha virt. eigenvalues -- 1.25369 1.26169 1.26289 1.26289 1.27548

Alpha virt. eigenvalues -- 1.27958 1.27958 1.28173 1.30066 1.30696

Alpha virt. eigenvalues -- 1.30843 1.32361 1.32361 1.37432 1.38019

Alpha virt. eigenvalues -- 1.38023 1.38023 1.39971 1.39971 1.40352

Alpha virt. eigenvalues -- 1.41460 1.41625 1.43940 1.43940 1.44180

Alpha virt. eigenvalues -- 1.45645 1.46726 1.46726 1.47152 1.47292

Alpha virt. eigenvalues -- 1.47562 1.48383 1.48383 1.48434 1.49014

Alpha virt. eigenvalues -- 1.49788 1.49788 1.50110 1.50305 1.52394

Alpha virt. eigenvalues -- 1.52394 1.53691 1.54244 1.54302 1.54302

Alpha virt. eigenvalues -- 1.55568 1.55568 1.55935 1.56778 1.56778

Alpha virt. eigenvalues -- 1.56975 1.58208 1.59511 1.60878 1.60878

Alpha virt. eigenvalues -- 1.61256 1.61372 1.62042 1.62042 1.64509

Alpha virt. eigenvalues -- 1.64509 1.65037 1.66804 1.68220 1.68442

Alpha virt. eigenvalues -- 1.68442 1.68444 1.69824 1.69824 1.69936

Alpha virt. eigenvalues -- 1.70823 1.70823 1.71470 1.72762 1.73469

Alpha virt. eigenvalues -- 1.74060 1.74996 1.74996 1.75931 1.76008

Alpha virt. eigenvalues -- 1.76051 1.76051 1.77165 1.77204 1.77204

Alpha virt. eigenvalues -- 1.78658 1.78887 1.79660 1.80039 1.80039

Alpha virt. eigenvalues -- 1.80732 1.80833 1.81224 1.81576 1.81576

Alpha virt. eigenvalues -- 1.83296 1.83296 1.83570 1.83936 1.84100

Alpha virt. eigenvalues -- 1.84230 1.84911 1.84911 1.85072 1.85856

Alpha virt. eigenvalues -- 1.87017 1.87017 1.87809 1.87809 1.88074

Alpha virt. eigenvalues -- 1.88383 1.88737 1.89159 1.91390 1.91678

Alpha virt. eigenvalues -- 1.91679 1.91679 1.91941 1.92018 1.92018

Alpha virt. eigenvalues -- 1.92147 1.92540 1.92554 1.92554 1.93709

Alpha virt. eigenvalues -- 1.93820 1.94017 1.94017 1.94085 1.95458

Alpha virt. eigenvalues -- 1.95958 1.95958 1.96100 1.96646 1.96646

Alpha virt. eigenvalues -- 1.98507 1.98957 1.98957 1.98970 1.99218

Alpha virt. eigenvalues -- 1.99751 1.99878 1.99878 2.00912 2.06349

Alpha virt. eigenvalues -- 2.06689 2.07816 2.07816 2.08712 2.08712

Alpha virt. eigenvalues -- 2.08741 2.11323 2.12606 2.13037 2.13736

Alpha virt. eigenvalues -- 2.13736 2.18769 2.21032 2.22676 2.23046

Alpha virt. eigenvalues -- 2.23046 2.25131 2.25425 2.25425 2.25859

Alpha virt. eigenvalues -- 2.26254 2.26309 2.26834 2.26834 2.27515

Alpha virt. eigenvalues -- 2.27561 2.28114 2.28114 2.28319 2.29024

Alpha virt. eigenvalues -- 2.29127 2.29127 2.29184 2.30170 2.30170

Alpha virt. eigenvalues -- 2.31907 2.31927 2.32031 2.32514 2.32514

Alpha virt. eigenvalues -- 2.33603 2.33603 2.35018 2.35048 2.35170

Alpha virt. eigenvalues -- 2.35679 2.35679 2.36436 2.37887 2.38264

Alpha virt. eigenvalues -- 2.39237 2.39237 2.40058 2.40058 2.40154

Alpha virt. eigenvalues -- 2.43591 2.44406 2.44406 2.44549 2.46756

Alpha virt. eigenvalues -- 2.47704 2.49585 2.49585 2.53119 2.53657

Alpha virt. eigenvalues -- 2.53657 2.54218 2.54941 2.56213 2.57238

Alpha virt. eigenvalues -- 2.57238 2.57548 2.58815 2.59406 2.59406

Alpha virt. eigenvalues -- 2.60375 2.60671 2.60671 2.60897 2.61678

Alpha virt. eigenvalues -- 2.62007 2.62030 2.63632 2.63632 2.64270

Alpha virt. eigenvalues -- 2.64270 2.64576 2.64665 2.66249 2.68949

Alpha virt. eigenvalues -- 2.69465 2.69465 2.69886 2.71795 2.71795

Alpha virt. eigenvalues -- 2.72526 2.74212 2.74246 2.74246 2.74285

Alpha virt. eigenvalues -- 2.75976 2.75976 2.77602 2.78407 2.79088

Alpha virt. eigenvalues -- 2.79290 2.79290 2.79823 2.80272 2.81958

Alpha virt. eigenvalues -- 2.81958 2.83430 2.84314 2.84638 2.84638

Alpha virt. eigenvalues -- 2.85526 2.86520 2.89105 2.89105 2.89460

Alpha virt. eigenvalues -- 2.89460 2.90223 2.92616 2.93634 2.95413

Alpha virt. eigenvalues -- 2.95413 2.96209 2.98147 2.98304 2.98304

Alpha virt. eigenvalues -- 2.98998 3.00249 3.02283 3.03388 3.04399

Alpha virt. eigenvalues -- 3.04399 3.06122 3.06619 3.06619 3.06981

Alpha virt. eigenvalues -- 3.07430 3.07430 3.07681 3.10232 3.10453

Alpha virt. eigenvalues -- 3.10750 3.10761 3.10761 3.13059 3.15861

Alpha virt. eigenvalues -- 3.15861 3.15937 3.18804 3.18982 3.19005

Alpha virt. eigenvalues -- 3.19005 3.22094 3.24998 3.25036 3.25036

Alpha virt. eigenvalues -- 3.25497 3.25881 3.25881 3.28090 3.28186

Alpha virt. eigenvalues -- 3.28545 3.28545 3.28948 3.29045 3.29045

Alpha virt. eigenvalues -- 3.29110 3.29377 3.30059 3.30059 3.30085

Alpha virt. eigenvalues -- 3.30200 3.30301 3.30948 3.33226 3.33226

Alpha virt. eigenvalues -- 3.34442 3.35273 3.35434 3.35434 3.37476

Alpha virt. eigenvalues -- 3.37476 3.39392 3.39899 3.40705 3.41786

Alpha virt. eigenvalues -- 3.41786 3.43914 3.49939 3.51578 3.51578

Alpha virt. eigenvalues -- 3.51581 3.55668 3.56739 3.56739 3.58095

Alpha virt. eigenvalues -- 3.58472 3.58472 3.59304 3.61425 3.61817

Alpha virt. eigenvalues -- 3.65643 3.65935 3.65935 3.71922 3.72825

Alpha virt. eigenvalues -- 3.75298 3.75298 3.82128 3.82128 3.82207

Alpha virt. eigenvalues -- 3.84243 3.86900 3.86900 3.88420 3.91328

Alpha virt. eigenvalues -- 3.93958 3.93958 3.94902 3.95419 3.95489

Alpha virt. eigenvalues -- 3.95489 3.95525 3.95573 3.98751 4.00460

Alpha virt. eigenvalues -- 4.00460 4.11459 4.32773 4.34239 4.38989

Alpha virt. eigenvalues -- 4.38989 4.45210 4.49171 4.53355 4.53355

Alpha virt. eigenvalues -- 4.61289 4.66494 4.66494 4.67199 4.77851

Alpha virt. eigenvalues -- 4.77859 4.77859 4.77867 5.10680 5.17950

Alpha virt. eigenvalues -- 5.17950 5.31496 7.77437 7.77437 7.87875

Alpha virt. eigenvalues -- 7.92463 8.13477 11.11370 23.25256 23.28813

Alpha virt. eigenvalues -- 23.28813 23.30389 23.45737 23.52522 23.52522

Alpha virt. eigenvalues -- 23.57200 23.74177 23.75336 23.75336 23.77189

Alpha virt. eigenvalues -- 23.79656 23.79780 23.79780 23.79979 23.83578

Alpha virt. eigenvalues -- 23.84575 23.84575 23.85334 23.90908 23.93044

Alpha virt. eigenvalues -- 23.93044 23.95471 23.95879 23.96966 23.96979

Alpha virt. eigenvalues -- 23.96979 24.02674 24.02801 24.02801 24.02949

Alpha virt. eigenvalues -- 24.06956 24.07394 24.07394 24.07784 24.11820

Alpha virt. eigenvalues -- 24.12215 24.12215 24.12951 24.14296 24.14312

Alpha virt. eigenvalues -- 24.14333 24.14333 35.62728 35.63900 35.65597

Alpha virt. eigenvalues -- 35.65597

Condensed to atoms (all electrons):

Mulliken charges:

1

1 C -0.259781

2 C 0.310423

3 N -0.704084

4 C 0.310423

5 C -0.259781

6 C -0.154256

7 C 0.310423

8 N -0.704084

9 C 0.310423

10 C -0.259781

11 C -0.259781

12 C -0.154256

13 C 0.310423

14 C -0.259781

15 C -0.259781

16 C 0.310423

17 N -0.704084

18 C -0.154256

19 C 0.310423

20 C -0.259781

21 C -0.259781

22 C 0.310423

23 N -0.704084

24 C -0.154256

25 C -0.112930

26 C -0.207149

27 C -0.219068

28 C -0.221901

29 C -0.219068

30 C -0.207149

31 C -0.221901

32 C -0.219068

33 C -0.207149

34 C -0.112930

35 C -0.207149

36 C -0.219068

37 C -0.112930

38 C -0.207149

39 C -0.219068

40 C -0.221901

41 C -0.219068

42 C -0.207149

43 C -0.112930

44 C -0.207149

45 C -0.219068

46 C -0.221901

47 C -0.219068

48 C -0.207149

49 H 0.238124

50 H 0.238124

51 H 0.238124

52 H 0.238124

53 H 0.238124

54 H 0.238124

55 H 0.238124

56 H 0.238124

57 H 0.222683

58 H 0.226545

59 H 0.226444

60 H 0.226545

61 H 0.222683

62 H 0.226444

63 H 0.226545

64 H 0.222683

65 H 0.222683

66 H 0.226545

67 H 0.222683

68 H 0.226545

69 H 0.226444

70 H 0.226545

71 H 0.222683

72 H 0.222683

73 H 0.226545

74 H 0.226444

75 H 0.226545

76 H 0.222683

77 Zn 1.372692

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 C -0.021656

2 C 0.310423

3 N -0.704084

4 C 0.310423

5 C -0.021656

6 C -0.154256

7 C 0.310423

8 N -0.704084

9 C 0.310423

10 C -0.021656

11 C -0.021656

12 C -0.154256

13 C 0.310423

14 C -0.021656

15 C -0.021656

16 C 0.310423

17 N -0.704084

18 C -0.154256

19 C 0.310423

20 C -0.021656

21 C -0.021656

22 C 0.310423

23 N -0.704084

24 C -0.154256

25 C -0.112930

26 C 0.015534

27 C 0.007477

28 C 0.004542

29 C 0.007477

30 C 0.015534

31 C 0.004542

32 C 0.007477

33 C 0.015534

34 C -0.112930

35 C 0.015534

36 C 0.007477

37 C -0.112930

38 C 0.015534

39 C 0.007477

40 C 0.004542

41 C 0.007477

42 C 0.015534

43 C -0.112930

44 C 0.015534

45 C 0.007477

46 C 0.004542

47 C 0.007477

48 C 0.015534

77 Zn 1.372692

Electronic spatial extent (au): <R\*\*2>= 33586.7438

Charge= -0.0000 electrons

Dipole moment (field-independent basis, Debye):

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

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

XX= -249.3089 YY= -249.3089 ZZ= -274.6620

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XX= 8.4510 YY= 8.4510 ZZ= -16.9021

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

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

XXY= -0.0000 XXZ= 80.6530 XZZ= 0.0000 YZZ= 0.0000

YYZ= -80.6530 XYZ= -0.0000

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

XXXX= -21779.9389 YYYY= -21779.9389 ZZZZ= -1122.5110 XXXY= 0.0000

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

ZZZY= -0.0000 XXYY= -5732.9357 XXZZ= -3824.2007 YYZZ= -3824.2007

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

N-N= 5.716811515623D+03 E-N=-1.611523602343D+04 KE= 2.020018907872D+03

Symmetry A1 KE= 5.776625547584D+02

Symmetry A2 KE= 4.452193542407D+02

Symmetry B1 KE= 4.985684994364D+02

Symmetry B2 KE= 4.985684994364D+02

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Tue Aug 13 18:05:28 2019, MaxMem= 671088640 cpu: 26.8

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36641 LenP2D= 94862.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 187

Leave Link 701 at Tue Aug 13 18:06:14 2019, MaxMem= 671088640 cpu: 184.8

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

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

Leave Link 702 at Tue Aug 13 18:06:14 2019, MaxMem= 671088640 cpu: 0.1

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 0 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Tue Aug 13 18:07:02 2019, MaxMem= 671088640 cpu: 190.8

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

Dipole = 8.61533067D-13 2.20268248D-13-3.90798505D-14

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.002268134 -0.000674533 -0.000120063

2 6 -0.003415705 -0.001939225 -0.000379710

3 7 0.000000000 0.002571020 0.000410099

4 6 0.003415705 -0.001939225 -0.000379710

5 6 -0.002268134 -0.000674533 -0.000120063

6 6 -0.001078066 -0.001078066 -0.000000000

7 6 -0.001939225 0.003415705 0.000379710

8 7 0.002571020 0.000000000 -0.000410099

9 6 -0.001939225 -0.003415705 0.000379710

10 6 -0.000674533 0.002268134 0.000120063

11 6 -0.000674533 -0.002268134 0.000120063

12 6 0.001078066 -0.001078066 0.000000000

13 6 0.001939225 0.003415705 0.000379710

14 6 0.000674533 -0.002268134 0.000120063

15 6 0.000674533 0.002268134 0.000120063

16 6 0.001939225 -0.003415705 0.000379710

17 7 -0.002571020 -0.000000000 -0.000410099

18 6 0.001078066 0.001078066 -0.000000000

19 6 -0.003415705 0.001939225 -0.000379710

20 6 0.002268134 0.000674533 -0.000120063

21 6 -0.002268134 0.000674533 -0.000120063

22 6 0.003415705 0.001939225 -0.000379710

23 7 0.000000000 -0.002571020 0.000410099

24 6 -0.001078066 0.001078066 -0.000000000

25 6 0.001714866 0.001714866 -0.000000000

26 6 0.001393476 0.000087552 0.002529780

27 6 -0.000638937 -0.002037782 0.002857707

28 6 -0.002657837 -0.002657837 -0.000000000

29 6 -0.002037782 -0.000638937 -0.002857707

30 6 0.000087552 0.001393476 -0.002529780

31 6 0.002657837 -0.002657837 0.000000000

32 6 0.000638937 -0.002037782 0.002857707

33 6 -0.001393476 0.000087552 0.002529780

34 6 -0.001714866 0.001714866 0.000000000

35 6 -0.000087552 0.001393476 -0.002529780

36 6 0.002037782 -0.000638937 -0.002857707

37 6 0.001714866 -0.001714866 0.000000000

38 6 0.000087552 -0.001393476 -0.002529780

39 6 -0.002037782 0.000638937 -0.002857707

40 6 -0.002657837 0.002657837 -0.000000000

41 6 -0.000638937 0.002037782 0.002857707

42 6 0.001393476 -0.000087552 0.002529780

43 6 -0.001714866 -0.001714866 0.000000000

44 6 -0.000087552 -0.001393476 -0.002529780

45 6 0.002037782 0.000638937 -0.002857707

46 6 0.002657837 0.002657837 0.000000000

47 6 0.000638937 0.002037782 0.002857707

48 6 -0.001393476 -0.000087552 0.002529780

49 1 0.000474944 -0.001067965 -0.000143566

50 1 -0.000474944 -0.001067965 -0.000143566

51 1 -0.001067965 0.000474944 0.000143566

52 1 -0.001067965 -0.000474944 0.000143566

53 1 0.001067965 -0.000474944 0.000143566

54 1 0.001067965 0.000474944 0.000143566

55 1 0.000474944 0.001067965 -0.000143566

56 1 -0.000474944 0.001067965 -0.000143566

57 1 0.000623926 -0.000032689 0.001281385

58 1 -0.000149879 -0.000779311 0.001043576

59 1 -0.000921051 -0.000921051 -0.000000000

60 1 -0.000779311 -0.000149879 -0.001043576

61 1 -0.000032689 0.000623926 -0.001281385

62 1 0.000921051 -0.000921051 -0.000000000

63 1 0.000149879 -0.000779311 0.001043576

64 1 -0.000623926 -0.000032689 0.001281385

65 1 0.000032689 0.000623926 -0.001281385

66 1 0.000779311 -0.000149879 -0.001043576

67 1 -0.000032689 -0.000623926 -0.001281385

68 1 -0.000779311 0.000149879 -0.001043576

69 1 -0.000921051 0.000921051 -0.000000000

70 1 -0.000149879 0.000779311 0.001043576

71 1 0.000623926 0.000032689 0.001281385

72 1 0.000032689 -0.000623926 -0.001281385

73 1 0.000779311 0.000149879 -0.001043576

74 1 0.000921051 0.000921051 -0.000000000

75 1 0.000149879 0.000779311 0.001043576

76 1 -0.000623926 0.000032689 0.001281385

77 30 0.000000000 -0.000000000 -0.000000000

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

Cartesian Forces: Max 0.003415705 RMS 0.001474806

Leave Link 716 at Tue Aug 13 18:07:02 2019, MaxMem= 671088640 cpu: 0.1

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

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

Internal Forces: Max 0.005604429 RMS 0.001590103

Search for a local minimum.

Step number 1 out of a maximum of 462

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

RMS Force = .15901D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Second derivative matrix not updated -- first step.

ITU= 0

Eigenvalues --- 0.00755 0.00755 0.00755 0.00755 0.01174

Eigenvalues --- 0.01317 0.01444 0.01469 0.01469 0.01548

Eigenvalues --- 0.01582 0.01582 0.01582 0.01595 0.01622

Eigenvalues --- 0.01622 0.01622 0.01622 0.01678 0.01701

Eigenvalues --- 0.01701 0.01743 0.01782 0.01782 0.01784

Eigenvalues --- 0.01808 0.01812 0.01813 0.01813 0.01821

Eigenvalues --- 0.01878 0.01879 0.01879 0.01885 0.01899

Eigenvalues --- 0.01899 0.01916 0.01943 0.02025 0.02025

Eigenvalues --- 0.02025 0.02025 0.02058 0.02058 0.02058

Eigenvalues --- 0.02058 0.02066 0.02066 0.02066 0.02066

Eigenvalues --- 0.02089 0.02089 0.02089 0.02089 0.02101

Eigenvalues --- 0.02101 0.02101 0.02101 0.02104 0.02104

Eigenvalues --- 0.02104 0.02104 0.02106 0.02106 0.02106

Eigenvalues --- 0.02106 0.02107 0.02107 0.02107 0.02107

Eigenvalues --- 0.02122 0.02128 0.02128 0.02131 0.12208

Eigenvalues --- 0.12208 0.14155 0.15996 0.15996 0.15996

Eigenvalues --- 0.15996 0.15998 0.15998 0.15998 0.15998

Eigenvalues --- 0.15999 0.15999 0.15999 0.15999 0.15999

Eigenvalues --- 0.15999 0.15999 0.15999 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16527 0.21805 0.21805 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22000 0.22827 0.22859 0.22891 0.22891

Eigenvalues --- 0.23473 0.23473 0.23473 0.23473 0.24755

Eigenvalues --- 0.24781 0.24781 0.24819 0.24825 0.24925

Eigenvalues --- 0.24936 0.24936 0.24986 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.32293 0.32293 0.32293 0.32293

Eigenvalues --- 0.35015 0.35015 0.35139 0.35158 0.35181

Eigenvalues --- 0.35181 0.35181 0.35181 0.35181 0.35181

Eigenvalues --- 0.35181 0.35181 0.35193 0.35193 0.35193

Eigenvalues --- 0.35193 0.35202 0.35202 0.35202 0.35202

Eigenvalues --- 0.35202 0.35202 0.35202 0.35202 0.35740

Eigenvalues --- 0.35883 0.35883 0.35883 0.35883 0.35883

Eigenvalues --- 0.35883 0.35883 0.35883 0.36273 0.37162

Eigenvalues --- 0.37162 0.38243 0.39011 0.40031 0.40031

Eigenvalues --- 0.41233 0.41233 0.41330 0.41330 0.41330

Eigenvalues --- 0.41330 0.41389 0.41389 0.41389 0.41389

Eigenvalues --- 0.41586 0.42296 0.43129 0.43334 0.43334

Eigenvalues --- 0.44302 0.44943 0.44943 0.44943 0.44943

Eigenvalues --- 0.45297 0.45297 0.45297 0.45297 0.45804

Eigenvalues --- 0.45804 0.45804 0.45804 0.45893 0.45893

Eigenvalues --- 0.45893 0.45893 0.46895 0.47953 0.47953

Eigenvalues --- 0.48887 0.50576 0.50967 0.50967 0.51069

RFO step: Lambda=-3.39154589D-03 EMin= 7.55306179D-03

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.04570743 RMS(Int)= 0.00061161

Iteration 2 RMS(Cart)= 0.00101169 RMS(Int)= 0.00000213

Iteration 3 RMS(Cart)= 0.00000048 RMS(Int)= 0.00000211

ITry= 1 IFail=0 DXMaxC= 1.71D-01 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.12D-07 for atom 77.

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

(Linear) (Quad) (Total)

R1 2.74267 -0.00162 0.00000 -0.00453 -0.00453 2.73813

R2 2.58256 -0.00254 0.00000 -0.00568 -0.00568 2.57688

R3 2.04265 -0.00115 0.00000 -0.00316 -0.00316 2.03949

R4 2.59389 -0.00334 0.00000 -0.00629 -0.00629 2.58760

R5 2.68009 -0.00515 0.00000 -0.01440 -0.01440 2.66569

R6 2.59389 -0.00334 0.00000 -0.00629 -0.00629 2.58760

R7 3.96097 -0.00339 0.00000 -0.01483 -0.01483 3.94613

R8 2.74267 -0.00162 0.00000 -0.00453 -0.00453 2.73813

R9 2.68009 -0.00515 0.00000 -0.01440 -0.01440 2.66569

R10 2.04265 -0.00115 0.00000 -0.00316 -0.00316 2.03949

R11 2.68009 -0.00515 0.00000 -0.01440 -0.01440 2.66569

R12 2.83611 -0.00481 0.00000 -0.01472 -0.01472 2.82138

R13 2.59389 -0.00334 0.00000 -0.00629 -0.00629 2.58760

R14 2.74267 -0.00162 0.00000 -0.00453 -0.00453 2.73813

R15 2.59389 -0.00334 0.00000 -0.00629 -0.00629 2.58760

R16 3.96097 -0.00339 0.00000 -0.01483 -0.01483 3.94613

R17 2.74267 -0.00162 0.00000 -0.00453 -0.00453 2.73813

R18 2.68009 -0.00515 0.00000 -0.01440 -0.01440 2.66569

R19 2.58256 -0.00254 0.00000 -0.00568 -0.00568 2.57688

R20 2.04265 -0.00115 0.00000 -0.00316 -0.00316 2.03949

R21 2.04265 -0.00115 0.00000 -0.00316 -0.00316 2.03949

R22 2.68009 -0.00515 0.00000 -0.01440 -0.01440 2.66569

R23 2.83611 -0.00481 0.00000 -0.01472 -0.01472 2.82138

R24 2.74267 -0.00162 0.00000 -0.00453 -0.00453 2.73813

R25 2.59389 -0.00334 0.00000 -0.00629 -0.00629 2.58760

R26 2.58256 -0.00254 0.00000 -0.00568 -0.00568 2.57688

R27 2.04265 -0.00115 0.00000 -0.00316 -0.00316 2.03949

R28 2.74267 -0.00162 0.00000 -0.00453 -0.00453 2.73813

R29 2.04265 -0.00115 0.00000 -0.00316 -0.00316 2.03949

R30 2.59389 -0.00334 0.00000 -0.00629 -0.00629 2.58760

R31 2.68009 -0.00515 0.00000 -0.01440 -0.01440 2.66569

R32 3.96097 -0.00339 0.00000 -0.01483 -0.01483 3.94613

R33 2.68009 -0.00515 0.00000 -0.01440 -0.01440 2.66569

R34 2.83611 -0.00481 0.00000 -0.01472 -0.01472 2.82138

R35 2.74267 -0.00162 0.00000 -0.00453 -0.00453 2.73813

R36 2.59389 -0.00334 0.00000 -0.00629 -0.00629 2.58760

R37 2.58256 -0.00254 0.00000 -0.00568 -0.00568 2.57688

R38 2.04265 -0.00115 0.00000 -0.00316 -0.00316 2.03949

R39 2.74267 -0.00162 0.00000 -0.00453 -0.00453 2.73813

R40 2.04265 -0.00115 0.00000 -0.00316 -0.00316 2.03949

R41 2.59389 -0.00334 0.00000 -0.00629 -0.00629 2.58760

R42 2.68009 -0.00515 0.00000 -0.01440 -0.01440 2.66569

R43 3.96097 -0.00339 0.00000 -0.01483 -0.01483 3.94613

R44 2.83611 -0.00481 0.00000 -0.01472 -0.01472 2.82138

R45 2.65632 -0.00560 0.00000 -0.01249 -0.01249 2.64382

R46 2.65632 -0.00560 0.00000 -0.01249 -0.01249 2.64382

R47 2.64252 -0.00508 0.00000 -0.01099 -0.01099 2.63153

R48 2.05348 -0.00139 0.00000 -0.00391 -0.00391 2.04957

R49 2.64381 -0.00458 0.00000 -0.00989 -0.00989 2.63391

R50 2.05383 -0.00131 0.00000 -0.00369 -0.00369 2.05014

R51 2.64381 -0.00458 0.00000 -0.00989 -0.00989 2.63391

R52 2.05363 -0.00130 0.00000 -0.00367 -0.00367 2.04997

R53 2.64252 -0.00508 0.00000 -0.01099 -0.01099 2.63153

R54 2.05383 -0.00131 0.00000 -0.00369 -0.00369 2.05014

R55 2.05348 -0.00139 0.00000 -0.00391 -0.00391 2.04957

R56 2.64381 -0.00458 0.00000 -0.00989 -0.00989 2.63391

R57 2.64381 -0.00458 0.00000 -0.00989 -0.00989 2.63391

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D97 3.07649 0.00004 0.00000 0.00380 0.00380 3.08029

D98 -0.06511 0.00004 0.00000 0.00380 0.00380 -0.06130

D99 -0.05374 -0.00002 0.00000 0.00093 0.00093 -0.05281

D100 3.08786 -0.00002 0.00000 0.00093 0.00093 3.08878

D101 0.04577 -0.00004 0.00000 -0.00086 -0.00086 0.04491

D102 -3.07424 -0.00008 0.00000 -0.00155 -0.00155 -3.07578

D103 3.07424 0.00008 0.00000 0.00155 0.00155 3.07578

D104 -0.04577 0.00004 0.00000 0.00086 0.00086 -0.04491

D105 3.07649 0.00004 0.00000 0.00380 0.00380 3.08029

D106 -0.05374 -0.00002 0.00000 0.00093 0.00093 -0.05281

D107 -0.06511 0.00004 0.00000 0.00380 0.00380 -0.06130

D108 3.08786 -0.00002 0.00000 0.00093 0.00093 3.08878

D109 -1.19351 0.00052 0.00000 0.04747 0.04747 -1.14604

D110 1.94808 0.00052 0.00000 0.04747 0.04747 1.99555

D111 1.94808 0.00052 0.00000 0.04747 0.04747 1.99555

D112 -1.19351 0.00052 0.00000 0.04747 0.04747 -1.14604

D113 -3.13891 0.00001 0.00000 -0.00106 -0.00106 -3.13997

D114 -0.01218 0.00001 0.00000 0.00003 0.00003 -0.01215

D115 -0.00704 0.00007 0.00000 0.00140 0.00140 -0.00564

D116 3.11969 0.00007 0.00000 0.00249 0.00249 3.12218

D117 -3.13993 -0.00004 0.00000 0.00022 0.00022 -3.13971

D118 0.09815 -0.00004 0.00000 -0.00172 -0.00172 0.09643

D119 0.01146 -0.00011 0.00000 -0.00227 -0.00227 0.00919

D120 -3.03364 -0.00011 0.00000 -0.00421 -0.00421 -3.03785

D121 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D122 3.12651 -0.00001 0.00000 0.00107 0.00107 3.12758

D123 -3.12651 0.00001 0.00000 -0.00107 -0.00107 -3.12758

D124 0.00000 -0.00000 0.00000 0.00000 -0.00000 0.00000

D125 0.00704 -0.00007 0.00000 -0.00140 -0.00140 0.00564

D126 3.13891 -0.00001 0.00000 0.00106 0.00106 3.13997

D127 -3.11969 -0.00007 0.00000 -0.00249 -0.00249 -3.12218

D128 0.01218 -0.00001 0.00000 -0.00003 -0.00003 0.01215

D129 -0.01146 0.00011 0.00000 0.00227 0.00227 -0.00919

D130 3.03364 0.00011 0.00000 0.00421 0.00421 3.03785

D131 3.13993 0.00004 0.00000 -0.00022 -0.00022 3.13971

D132 -0.09815 0.00004 0.00000 0.00172 0.00172 -0.09643

D133 -3.07649 -0.00004 0.00000 -0.00380 -0.00380 -3.08029

D134 0.06511 -0.00004 0.00000 -0.00380 -0.00380 0.06130

D135 0.05374 0.00002 0.00000 -0.00093 -0.00093 0.05281

D136 -3.08786 0.00002 0.00000 -0.00093 -0.00093 -3.08878

D137 3.07424 0.00008 0.00000 0.00155 0.00155 3.07578

D138 -0.04577 0.00004 0.00000 0.00086 0.00086 -0.04491

D139 0.04577 -0.00004 0.00000 -0.00086 -0.00086 0.04491

D140 -3.07424 -0.00008 0.00000 -0.00155 -0.00155 -3.07578

D141 1.19351 -0.00052 0.00000 -0.04747 -0.04747 1.14604

D142 -1.94808 -0.00052 0.00000 -0.04747 -0.04747 -1.99555

D143 -1.94808 -0.00052 0.00000 -0.04747 -0.04747 -1.99555

D144 1.19351 -0.00052 0.00000 -0.04747 -0.04747 1.14604

D145 -3.13840 -0.00004 0.00000 -0.00182 -0.00182 -3.14022

D146 -0.00595 0.00004 0.00000 0.00165 0.00165 -0.00430

D147 0.00319 -0.00004 0.00000 -0.00182 -0.00182 0.00137

D148 3.13564 0.00004 0.00000 0.00165 0.00165 3.13729

D149 -3.13840 -0.00004 0.00000 -0.00182 -0.00182 -3.14022

D150 -0.00595 0.00004 0.00000 0.00165 0.00165 -0.00430

D151 0.00319 -0.00004 0.00000 -0.00182 -0.00182 0.00137

D152 3.13564 0.00004 0.00000 0.00165 0.00165 3.13729

D153 -0.00639 0.00009 0.00000 0.00365 0.00365 -0.00275

D154 3.13485 0.00004 0.00000 0.00164 0.00163 3.13648

D155 -3.13882 0.00001 0.00000 0.00019 0.00018 -3.13864

D156 0.00242 -0.00004 0.00000 -0.00182 -0.00183 0.00060

D157 0.00317 -0.00004 0.00000 -0.00180 -0.00180 0.00136

D158 -3.13842 -0.00004 0.00000 -0.00180 -0.00180 -3.14023

D159 -3.13807 0.00001 0.00000 0.00022 0.00022 -3.13786

D160 0.00352 0.00001 0.00000 0.00022 0.00022 0.00374

D161 0.00317 -0.00004 0.00000 -0.00180 -0.00180 0.00136

D162 -3.13807 0.00001 0.00000 0.00022 0.00022 -3.13786

D163 -3.13842 -0.00004 0.00000 -0.00180 -0.00180 -3.14023

D164 0.00352 0.00001 0.00000 0.00022 0.00022 0.00374

D165 -0.00639 0.00009 0.00000 0.00365 0.00365 -0.00275

D166 -3.13882 0.00001 0.00000 0.00019 0.00018 -3.13864

D167 3.13485 0.00004 0.00000 0.00164 0.00163 3.13648

D168 0.00242 -0.00004 0.00000 -0.00182 -0.00183 0.00060

D169 -0.00317 0.00004 0.00000 0.00180 0.00180 -0.00136

D170 3.13807 -0.00001 0.00000 -0.00022 -0.00022 3.13786

D171 3.13842 0.00004 0.00000 0.00180 0.00180 3.14023

D172 -0.00352 -0.00001 0.00000 -0.00022 -0.00022 -0.00374

D173 -0.00317 0.00004 0.00000 0.00180 0.00180 -0.00136

D174 3.13807 -0.00001 0.00000 -0.00022 -0.00022 3.13786

D175 3.13842 0.00004 0.00000 0.00180 0.00180 3.14023

D176 -0.00352 -0.00001 0.00000 -0.00022 -0.00022 -0.00374

D177 0.00639 -0.00009 0.00000 -0.00365 -0.00365 0.00275

D178 3.13882 -0.00001 0.00000 -0.00019 -0.00018 3.13864

D179 -3.13485 -0.00004 0.00000 -0.00164 -0.00163 -3.13648

D180 -0.00242 0.00004 0.00000 0.00182 0.00183 -0.00060

D181 3.13840 0.00004 0.00000 0.00182 0.00182 3.14022

D182 -0.00319 0.00004 0.00000 0.00182 0.00182 -0.00137

D183 0.00595 -0.00004 0.00000 -0.00165 -0.00165 0.00430

D184 -3.13564 -0.00004 0.00000 -0.00165 -0.00165 -3.13729

D185 3.13840 0.00004 0.00000 0.00182 0.00182 3.14022

D186 0.00595 -0.00004 0.00000 -0.00165 -0.00165 0.00430

D187 -0.00319 0.00004 0.00000 0.00182 0.00182 -0.00137

D188 -3.13564 -0.00004 0.00000 -0.00165 -0.00165 -3.13729

D189 0.00639 -0.00009 0.00000 -0.00365 -0.00365 0.00275

D190 -3.13485 -0.00004 0.00000 -0.00164 -0.00163 -3.13648

D191 3.13882 -0.00001 0.00000 -0.00019 -0.00018 3.13864

D192 -0.00242 0.00004 0.00000 0.00182 0.00183 -0.00060

D193 3.13840 0.00004 0.00000 0.00182 0.00182 3.14022

D194 0.00595 -0.00004 0.00000 -0.00165 -0.00165 0.00430

D195 -0.00319 0.00004 0.00000 0.00182 0.00182 -0.00137

D196 -3.13564 -0.00004 0.00000 -0.00165 -0.00165 -3.13729

D197 3.13840 0.00004 0.00000 0.00182 0.00182 3.14022

D198 0.00595 -0.00004 0.00000 -0.00165 -0.00165 0.00430

D199 -0.00319 0.00004 0.00000 0.00182 0.00182 -0.00137

D200 -3.13564 -0.00004 0.00000 -0.00165 -0.00165 -3.13729

D201 0.00639 -0.00009 0.00000 -0.00365 -0.00365 0.00275

D202 -3.13485 -0.00004 0.00000 -0.00164 -0.00163 -3.13648

D203 3.13882 -0.00001 0.00000 -0.00019 -0.00018 3.13864

D204 -0.00242 0.00004 0.00000 0.00182 0.00183 -0.00060

D205 -0.00317 0.00004 0.00000 0.00180 0.00180 -0.00136

D206 3.13842 0.00004 0.00000 0.00180 0.00180 3.14023

D207 3.13807 -0.00001 0.00000 -0.00022 -0.00022 3.13786

D208 -0.00352 -0.00001 0.00000 -0.00022 -0.00022 -0.00374

D209 -0.00317 0.00004 0.00000 0.00180 0.00180 -0.00136

D210 3.13807 -0.00001 0.00000 -0.00022 -0.00022 3.13786

D211 3.13842 0.00004 0.00000 0.00180 0.00180 3.14023

D212 -0.00352 -0.00001 0.00000 -0.00022 -0.00022 -0.00374

D213 0.00639 -0.00009 0.00000 -0.00365 -0.00365 0.00275

D214 3.13882 -0.00001 0.00000 -0.00019 -0.00018 3.13864

D215 -3.13485 -0.00004 0.00000 -0.00164 -0.00163 -3.13648

D216 -0.00242 0.00004 0.00000 0.00182 0.00183 -0.00060

D217 -3.13840 -0.00004 0.00000 -0.00182 -0.00182 -3.14022

D218 -0.00595 0.00004 0.00000 0.00165 0.00165 -0.00430

D219 0.00319 -0.00004 0.00000 -0.00182 -0.00182 0.00137

D220 3.13564 0.00004 0.00000 0.00165 0.00165 3.13729

D221 -3.13840 -0.00004 0.00000 -0.00182 -0.00182 -3.14022

D222 -0.00595 0.00004 0.00000 0.00165 0.00165 -0.00430

D223 0.00319 -0.00004 0.00000 -0.00182 -0.00182 0.00137

D224 3.13564 0.00004 0.00000 0.00165 0.00165 3.13729

D225 -0.00639 0.00009 0.00000 0.00365 0.00365 -0.00275

D226 3.13485 0.00004 0.00000 0.00164 0.00163 3.13648

D227 -3.13882 0.00001 0.00000 0.00019 0.00018 -3.13864

D228 0.00242 -0.00004 0.00000 -0.00182 -0.00183 0.00060

D229 0.00317 -0.00004 0.00000 -0.00180 -0.00180 0.00136

D230 -3.13842 -0.00004 0.00000 -0.00180 -0.00180 -3.14023

D231 -3.13807 0.00001 0.00000 0.00022 0.00022 -3.13786

D232 0.00352 0.00001 0.00000 0.00022 0.00022 0.00374

D233 0.00317 -0.00004 0.00000 -0.00180 -0.00180 0.00136

D234 -3.13807 0.00001 0.00000 0.00022 0.00022 -3.13786

D235 -3.13842 -0.00004 0.00000 -0.00180 -0.00180 -3.14023

D236 0.00352 0.00001 0.00000 0.00022 0.00022 0.00374

D237 -0.00639 0.00009 0.00000 0.00365 0.00365 -0.00275

D238 -3.13882 0.00001 0.00000 0.00019 0.00018 -3.13864

D239 3.13485 0.00004 0.00000 0.00164 0.00163 3.13648

D240 0.00242 -0.00004 0.00000 -0.00182 -0.00183 0.00060

Item Value Threshold Converged?

Maximum Force 0.005604 0.000450 NO

RMS Force 0.001590 0.000300 NO

Maximum Displacement 0.170979 0.001800 NO

RMS Displacement 0.045642 0.001200 NO

Predicted change in Energy=-1.771666D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Aug 13 18:07:02 2019, MaxMem= 671088640 cpu: 1.0

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

Stoichiometry C44H28N4Zn

Framework group D2D[O(Zn),2SGD(N2),X(C44H28)]

Deg. of freedom 29

Full point group D2D NOp 8

RotChk: IX=0 Diff= 0.00D+00

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681813 4.269322 0.135498

2 6 0 -1.109482 2.888844 0.031286

3 7 0 0.000000 2.088090 -0.021827

4 6 0 1.109482 2.888844 0.031286

5 6 0 0.681813 4.269322 0.135498

6 6 0 2.449616 2.449616 -0.000000

7 6 0 2.888844 1.109482 -0.031286

8 7 0 2.088090 -0.000000 0.021827

9 6 0 2.888844 -1.109482 -0.031286

10 6 0 4.269322 -0.681813 -0.135498

11 6 0 4.269322 0.681813 -0.135498

12 6 0 -2.449616 2.449616 -0.000000

13 6 0 -2.888844 1.109482 -0.031286

14 6 0 -4.269322 0.681813 -0.135498

15 6 0 -4.269322 -0.681813 -0.135498

16 6 0 -2.888844 -1.109482 -0.031286

17 7 0 -2.088090 0.000000 0.021827

18 6 0 -2.449616 -2.449616 -0.000000

19 6 0 -1.109482 -2.888844 0.031286

20 6 0 -0.681813 -4.269322 0.135498

21 6 0 0.681813 -4.269322 0.135498

22 6 0 1.109482 -2.888844 0.031286

23 7 0 -0.000000 -2.088090 -0.021827

24 6 0 2.449616 -2.449616 -0.000000

25 6 0 3.505336 3.505336 -0.000000

26 6 0 3.638727 4.378940 -1.084604

27 6 0 4.624276 5.362745 -1.085831

28 6 0 5.488990 5.488990 -0.000000

29 6 0 5.362745 4.624276 1.085831

30 6 0 4.378940 3.638727 1.084604

31 6 0 -5.488990 5.488990 -0.000000

32 6 0 -4.624276 5.362745 -1.085831

33 6 0 -3.638727 4.378940 -1.084604

34 6 0 -3.505336 3.505336 -0.000000

35 6 0 -4.378940 3.638727 1.084604

36 6 0 -5.362745 4.624276 1.085831

37 6 0 3.505336 -3.505336 -0.000000

38 6 0 4.378940 -3.638727 1.084604

39 6 0 5.362745 -4.624276 1.085831

40 6 0 5.488990 -5.488990 -0.000000

41 6 0 4.624276 -5.362745 -1.085831

42 6 0 3.638727 -4.378940 -1.084604

43 6 0 -3.505336 -3.505336 -0.000000

44 6 0 -4.378940 -3.638727 1.084604

45 6 0 -5.362745 -4.624276 1.085831

46 6 0 -5.488990 -5.488990 -0.000000

47 6 0 -4.624276 -5.362745 -1.085831

48 6 0 -3.638727 -4.378940 -1.084604

49 1 0 -1.332502 5.126925 0.212336

50 1 0 1.332502 5.126925 0.212336

51 1 0 5.126925 -1.332502 -0.212336

52 1 0 5.126925 1.332502 -0.212336

53 1 0 -5.126925 1.332502 -0.212336

54 1 0 -5.126925 -1.332502 -0.212336

55 1 0 -1.332502 -5.126925 0.212336

56 1 0 1.332502 -5.126925 0.212336

57 1 0 2.969404 4.281894 -1.932495

58 1 0 4.717122 6.028970 -1.937006

59 1 0 6.256056 6.256056 -0.000000

60 1 0 6.028970 4.717122 1.937006

61 1 0 4.281894 2.969404 1.932495

62 1 0 -6.256056 6.256056 -0.000000

63 1 0 -4.717122 6.028970 -1.937006

64 1 0 -2.969404 4.281894 -1.932495

65 1 0 -4.281894 2.969404 1.932495

66 1 0 -6.028970 4.717122 1.937006

67 1 0 4.281894 -2.969404 1.932495

68 1 0 6.028970 -4.717122 1.937006

69 1 0 6.256056 -6.256056 -0.000000

70 1 0 4.717122 -6.028970 -1.937006

71 1 0 2.969404 -4.281894 -1.932495

72 1 0 -4.281894 -2.969404 1.932495

73 1 0 -6.028970 -4.717122 1.937006

74 1 0 -6.256056 -6.256056 -0.000000

75 1 0 -4.717122 -6.028970 -1.937006

76 1 0 -2.969404 -4.281894 -1.932495

77 30 0 0.000000 0.000000 0.000000

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

Rotational constants (GHZ): 0.0582830 0.0582830 0.0301452

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

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

Pseudo-potential data read from rwf file.

There are 272 symmetry adapted cartesian basis functions of A1 symmetry.

There are 243 symmetry adapted cartesian basis functions of A2 symmetry.

There are 254 symmetry adapted cartesian basis functions of B1 symmetry.

There are 254 symmetry adapted cartesian basis functions of B2 symmetry.

There are 256 symmetry adapted basis functions of A1 symmetry.

There are 232 symmetry adapted basis functions of A2 symmetry.

There are 242 symmetry adapted basis functions of B1 symmetry.

There are 242 symmetry adapted basis functions of B2 symmetry.

972 basis functions, 1715 primitive gaussians, 1023 cartesian basis functions

166 alpha electrons 166 beta electrons

nuclear repulsion energy 5742.0081753727 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= 77 NActive= 77 NUniq= 13 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T 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= -0.2224696032 Hartrees.

Nuclear repulsion after empirical dispersion term = 5741.7857057695 Hartrees.

No density basis found on file 724.

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Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 77.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 77

GePol: Total number of spheres = 77

GePol: Number of exposed spheres = 77 (100.00%)

GePol: Number of points = 5754

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.14D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 376

GePol: Fraction of low-weight points (<1% of avg) = 6.53%

GePol: Cavity surface area = 614.051 Ang\*\*2

GePol: Cavity volume = 630.325 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021400157 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5741.7835657538 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

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36781 LenP2D= 95334.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 972 RedAO= T EigKep= 6.26D-05 NBF= 256 232 242 242

NBsUse= 972 1.00D-06 EigRej= -1.00D+00 NBFU= 256 232 242 242

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= 952 960 976 976 976 MxSgAt= 77 MxSgA2= 77.

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Aug 13 18:07:05 2019, MaxMem= 671088640 cpu: 0.9

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

Initial guess from the checkpoint file: "ZnTPP0.chk"

B after Tr= 0.000000 -0.000000 0.000000

Rot= 1.000000 0.000000 -0.000000 -0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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= -1979.25737182729

Leave Link 401 at Tue Aug 13 18:07:14 2019, MaxMem= 671088640 cpu: 33.8

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3177123 IEndB= 3177123 NGot= 671088640 MDV= 668975710

LenX= 668975710 LenY= 667928158

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= 530000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 99325548.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.88D-15 for 5739.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.77D-15 for 5238 2643.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.11D-15 for 5739.

Iteration 1 A^-1\*A deviation from orthogonality is 2.32D-13 for 4912 4893.

E= -1978.88802053462

DIIS: error= 5.75D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1978.88802053462 IErMin= 1 ErrMin= 5.75D-03

ErrMax= 5.75D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.52D-03 BMatP= 7.52D-03

IDIUse=3 WtCom= 9.42D-01 WtEn= 5.75D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.444 Goal= None Shift= 0.000

GapD= 0.444 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.36D-04 MaxDP=3.16D-03 OVMax= 2.40D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.36D-04 CP: 1.00D+00

E= -1978.90389475825 Delta-E= -0.015874223633 Rises=F Damp=F

DIIS: error= 8.06D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1978.90389475825 IErMin= 2 ErrMin= 8.06D-04

ErrMax= 8.06D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.53D-04 BMatP= 7.52D-03

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.06D-03

Coeff-Com: -0.517D-01 0.105D+01

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

Coeff: -0.513D-01 0.105D+01

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=2.85D-05 MaxDP=1.16D-03 DE=-1.59D-02 OVMax= 4.06D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.81D-05 CP: 1.00D+00 1.03D+00

E= -1978.90412037772 Delta-E= -0.000225619463 Rises=F Damp=F

DIIS: error= 5.27D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1978.90412037772 IErMin= 3 ErrMin= 5.27D-04

ErrMax= 5.27D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-04 BMatP= 1.53D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.27D-03

Coeff-Com: -0.386D-01 0.493D+00 0.545D+00

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

Coeff: -0.384D-01 0.491D+00 0.548D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.42D-05 MaxDP=8.09D-04 DE=-2.26D-04 OVMax= 2.36D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 9.43D-06 CP: 1.00D+00 1.06D+00 6.53D-01

E= -1978.90421453780 Delta-E= -0.000094160080 Rises=F Damp=F

DIIS: error= 1.60D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1978.90421453780 IErMin= 4 ErrMin= 1.60D-04

ErrMax= 1.60D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.61D-05 BMatP= 1.04D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.60D-03

Coeff-Com: -0.144D-01 0.149D+00 0.304D+00 0.562D+00

Coeff-En: 0.000D+00 0.000D+00 0.776D-01 0.922D+00

Coeff: -0.144D-01 0.148D+00 0.303D+00 0.563D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=4.26D-06 MaxDP=2.36D-04 DE=-9.42D-05 OVMax= 8.10D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.04D-06 CP: 1.00D+00 1.06D+00 7.08D-01 7.28D-01

E= -1978.90422977193 Delta-E= -0.000015234133 Rises=F Damp=F

DIIS: error= 4.57D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1978.90422977193 IErMin= 5 ErrMin= 4.57D-05

ErrMax= 4.57D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.48D-06 BMatP= 1.61D-05

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

Coeff-Com: -0.192D-02 0.585D-02 0.780D-01 0.278D+00 0.640D+00

Coeff: -0.192D-02 0.585D-02 0.780D-01 0.278D+00 0.640D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.36D-06 MaxDP=8.51D-05 DE=-1.52D-05 OVMax= 2.14D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.67D-07 CP: 1.00D+00 1.07D+00 7.18D-01 7.80D-01 7.49D-01

E= -1978.90423116873 Delta-E= -0.000001396805 Rises=F Damp=F

DIIS: error= 3.74D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1978.90423116873 IErMin= 6 ErrMin= 3.74D-05

ErrMax= 3.74D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.75D-07 BMatP= 1.48D-06

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

Coeff-Com: 0.432D-03-0.125D-01 0.778D-02 0.837D-01 0.325D+00 0.596D+00

Coeff: 0.432D-03-0.125D-01 0.778D-02 0.837D-01 0.325D+00 0.596D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=4.68D-07 MaxDP=2.28D-05 DE=-1.40D-06 OVMax= 8.48D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.88D-07 CP: 1.00D+00 1.06D+00 7.25D-01 7.83D-01 7.84D-01

CP: 6.90D-01

E= -1978.90423130069 Delta-E= -0.000000131956 Rises=F Damp=F

DIIS: error= 7.47D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1978.90423130069 IErMin= 7 ErrMin= 7.47D-06

ErrMax= 7.47D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.63D-08 BMatP= 1.75D-07

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

Coeff-Com: 0.386D-03-0.773D-02-0.187D-02 0.271D-01 0.138D+00 0.353D+00

Coeff-Com: 0.491D+00

Coeff: 0.386D-03-0.773D-02-0.187D-02 0.271D-01 0.138D+00 0.353D+00

Coeff: 0.491D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.73D-07 MaxDP=9.40D-06 DE=-1.32D-07 OVMax= 3.66D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.52D-08 CP: 1.00D+00 1.06D+00 7.24D-01 7.89D-01 7.86D-01

CP: 6.83D-01 5.14D-01

E= -1978.90423132355 Delta-E= -0.000000022855 Rises=F Damp=F

DIIS: error= 2.76D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1978.90423132355 IErMin= 8 ErrMin= 2.76D-06

ErrMax= 2.76D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.41D-09 BMatP= 2.63D-08

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

Coeff-Com: 0.178D-03-0.327D-02-0.170D-02 0.867D-02 0.517D-01 0.149D+00

Coeff-Com: 0.263D+00 0.532D+00

Coeff: 0.178D-03-0.327D-02-0.170D-02 0.867D-02 0.517D-01 0.149D+00

Coeff: 0.263D+00 0.532D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=3.86D-08 MaxDP=3.14D-06 DE=-2.29D-08 OVMax= 7.58D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.90D-08 CP: 1.00D+00 1.06D+00 7.24D-01 7.89D-01 7.85D-01

CP: 6.88D-01 5.76D-01 8.14D-01

E= -1978.90423132473 Delta-E= -0.000000001185 Rises=F Damp=F

DIIS: error= 8.91D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1978.90423132473 IErMin= 9 ErrMin= 8.91D-07

ErrMax= 8.91D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-10 BMatP= 1.41D-09

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

Coeff-Com: 0.136D-04-0.107D-03-0.493D-03-0.958D-03-0.877D-03 0.711D-02

Coeff-Com: 0.375D-01 0.236D+00 0.722D+00

Coeff: 0.136D-04-0.107D-03-0.493D-03-0.958D-03-0.877D-03 0.711D-02

Coeff: 0.375D-01 0.236D+00 0.722D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.11D-08 MaxDP=5.95D-07 DE=-1.19D-09 OVMax= 1.96D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 8.78D-09 CP: 1.00D+00 1.06D+00 7.24D-01 7.89D-01 7.85D-01

CP: 6.91D-01 5.76D-01 8.59D-01 8.39D-01

E= -1978.90423132482 Delta-E= -0.000000000090 Rises=F Damp=F

DIIS: error= 1.69D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1978.90423132482 IErMin=10 ErrMin= 1.69D-07

ErrMax= 1.69D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.63D-11 BMatP= 1.02D-10

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

Coeff-Com: -0.183D-05 0.121D-03-0.197D-03-0.107D-02-0.342D-02-0.410D-02

Coeff-Com: 0.742D-02 0.106D+00 0.421D+00 0.474D+00

Coeff: -0.183D-05 0.121D-03-0.197D-03-0.107D-02-0.342D-02-0.410D-02

Coeff: 0.742D-02 0.106D+00 0.421D+00 0.474D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=3.81D-09 MaxDP=2.91D-07 DE=-9.00D-11 OVMax= 5.83D-07

Error on total polarization charges = 0.08507

SCF Done: E(RB3LYP) = -1978.90423132 A.U. after 10 cycles

NFock= 10 Conv=0.38D-08 -V/T= 1.9793

KE= 2.020800233511D+03 PE=-1.616577664049D+04 EE= 6.424288609905D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.34

(included in total energy above)

Leave Link 502 at Tue Aug 13 18:13:38 2019, MaxMem= 671088640 cpu: 1536.0

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36781 LenP2D= 95334.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 189

Leave Link 701 at Tue Aug 13 18:14:25 2019, MaxMem= 671088640 cpu: 186.1

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

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

Leave Link 702 at Tue Aug 13 18:14:25 2019, MaxMem= 671088640 cpu: 0.1

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 0 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Tue Aug 13 18:15:13 2019, MaxMem= 671088640 cpu: 193.2

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

Dipole = 5.25801624D-13 1.73550063D-12-3.81916720D-14

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000623629 0.000516528 0.000216044

2 6 -0.000417475 -0.000491117 -0.000751214

3 7 -0.000000000 0.000476004 0.000236316

4 6 0.000417475 -0.000491117 -0.000751214

5 6 -0.000623629 0.000516528 0.000216044

6 6 0.000317225 0.000317225 0.000000000

7 6 -0.000491117 0.000417475 0.000751214

8 7 0.000476004 0.000000000 -0.000236316

9 6 -0.000491117 -0.000417475 0.000751214

10 6 0.000516528 0.000623629 -0.000216044

11 6 0.000516528 -0.000623629 -0.000216044

12 6 -0.000317225 0.000317225 -0.000000000

13 6 0.000491117 0.000417475 0.000751214

14 6 -0.000516528 -0.000623629 -0.000216044

15 6 -0.000516528 0.000623629 -0.000216044

16 6 0.000491117 -0.000417475 0.000751214

17 7 -0.000476004 -0.000000000 -0.000236316

18 6 -0.000317225 -0.000317225 0.000000000

19 6 -0.000417475 0.000491117 -0.000751214

20 6 0.000623629 -0.000516528 0.000216044

21 6 -0.000623629 -0.000516528 0.000216044

22 6 0.000417475 0.000491117 -0.000751214

23 7 0.000000000 -0.000476004 0.000236316

24 6 0.000317225 -0.000317225 0.000000000

25 6 -0.000481452 -0.000481452 -0.000000000

26 6 -0.000080158 0.000566150 -0.000444534

27 6 0.000012310 0.000242589 -0.000327947

28 6 0.000241822 0.000241822 0.000000000

29 6 0.000242589 0.000012310 0.000327947

30 6 0.000566150 -0.000080158 0.000444534

31 6 -0.000241822 0.000241822 0.000000000

32 6 -0.000012310 0.000242589 -0.000327947

33 6 0.000080158 0.000566150 -0.000444534

34 6 0.000481452 -0.000481452 -0.000000000

35 6 -0.000566150 -0.000080158 0.000444534

36 6 -0.000242589 0.000012310 0.000327947

37 6 -0.000481452 0.000481452 -0.000000000

38 6 0.000566150 0.000080158 0.000444534

39 6 0.000242589 -0.000012310 0.000327947

40 6 0.000241822 -0.000241822 -0.000000000

41 6 0.000012310 -0.000242589 -0.000327947

42 6 -0.000080158 -0.000566150 -0.000444534

43 6 0.000481452 0.000481452 -0.000000000

44 6 -0.000566150 0.000080158 0.000444534

45 6 -0.000242589 -0.000012310 0.000327947

46 6 -0.000241822 -0.000241822 0.000000000

47 6 -0.000012310 -0.000242589 -0.000327947

48 6 0.000080158 -0.000566150 -0.000444534

49 1 0.000143908 -0.000044677 0.000107913

50 1 -0.000143908 -0.000044677 0.000107913

51 1 -0.000044677 0.000143908 -0.000107913

52 1 -0.000044677 -0.000143908 -0.000107913

53 1 0.000044677 -0.000143908 -0.000107913

54 1 0.000044677 0.000143908 -0.000107913

55 1 0.000143908 0.000044677 0.000107913

56 1 -0.000143908 0.000044677 0.000107913

57 1 0.000029595 -0.000093848 -0.000005993

58 1 0.000078079 0.000109282 -0.000067851

59 1 0.000091523 0.000091523 0.000000000

60 1 0.000109282 0.000078079 0.000067851

61 1 -0.000093848 0.000029595 0.000005993

62 1 -0.000091523 0.000091523 -0.000000000

63 1 -0.000078079 0.000109282 -0.000067851

64 1 -0.000029595 -0.000093848 -0.000005993

65 1 0.000093848 0.000029595 0.000005993

66 1 -0.000109282 0.000078079 0.000067851

67 1 -0.000093848 -0.000029595 0.000005993

68 1 0.000109282 -0.000078079 0.000067851

69 1 0.000091523 -0.000091523 0.000000000

70 1 0.000078079 -0.000109282 -0.000067851

71 1 0.000029595 0.000093848 -0.000005993

72 1 0.000093848 -0.000029595 0.000005993

73 1 -0.000109282 -0.000078079 0.000067851

74 1 -0.000091523 -0.000091523 -0.000000000

75 1 -0.000078079 -0.000109282 -0.000067851

76 1 -0.000029595 0.000093848 -0.000005993

77 30 0.000000000 -0.000000000 0.000000000

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

Cartesian Forces: Max 0.000751214 RMS 0.000321281

Leave Link 716 at Tue Aug 13 18:15:13 2019, MaxMem= 671088640 cpu: 0.1

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.001012425 RMS 0.000288337

Search for a local minimum.

Step number 2 out of a maximum of 462

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

RMS Force = .28834D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 2

DE= -1.52D-03 DEPred=-1.77D-03 R= 8.58D-01

TightC=F SS= 1.41D+00 RLast= 2.11D-01 DXNew= 5.0454D-01 6.3422D-01

Trust test= 8.58D-01 RLast= 2.11D-01 DXMaxT set to 5.05D-01

ITU= 1 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.00755 0.00755 0.00755 0.00771 0.01174

Eigenvalues --- 0.01318 0.01443 0.01469 0.01469 0.01547

Eigenvalues --- 0.01583 0.01583 0.01583 0.01595 0.01624

Eigenvalues --- 0.01624 0.01624 0.01624 0.01678 0.01700

Eigenvalues --- 0.01700 0.01743 0.01782 0.01782 0.01784

Eigenvalues --- 0.01812 0.01814 0.01814 0.01821 0.01827

Eigenvalues --- 0.01878 0.01880 0.01880 0.01886 0.01899

Eigenvalues --- 0.01899 0.01916 0.01952 0.02025 0.02025

Eigenvalues --- 0.02025 0.02025 0.02058 0.02058 0.02058

Eigenvalues --- 0.02061 0.02066 0.02066 0.02066 0.02066

Eigenvalues --- 0.02089 0.02089 0.02089 0.02090 0.02101

Eigenvalues --- 0.02101 0.02101 0.02101 0.02104 0.02104

Eigenvalues --- 0.02104 0.02104 0.02106 0.02106 0.02106

Eigenvalues --- 0.02106 0.02107 0.02107 0.02107 0.02107

Eigenvalues --- 0.02123 0.02129 0.02129 0.02132 0.12214

Eigenvalues --- 0.12214 0.14174 0.15972 0.15997 0.15997

Eigenvalues --- 0.15997 0.15997 0.15998 0.15998 0.15998

Eigenvalues --- 0.15999 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16011

Eigenvalues --- 0.16859 0.21814 0.21814 0.21996 0.22000

Eigenvalues --- 0.22000 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22000 0.22827 0.22859 0.22891 0.22891

Eigenvalues --- 0.23475 0.23475 0.23475 0.23603 0.24758

Eigenvalues --- 0.24786 0.24786 0.24828 0.24839 0.24881

Eigenvalues --- 0.24940 0.24940 0.24987 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.32293 0.32293 0.32293 0.32785

Eigenvalues --- 0.35006 0.35006 0.35104 0.35131 0.35149

Eigenvalues --- 0.35181 0.35181 0.35181 0.35181 0.35181

Eigenvalues --- 0.35181 0.35181 0.35187 0.35193 0.35193

Eigenvalues --- 0.35193 0.35202 0.35202 0.35202 0.35202

Eigenvalues --- 0.35202 0.35202 0.35202 0.35206 0.35709

Eigenvalues --- 0.35883 0.35883 0.35883 0.35883 0.35883

Eigenvalues --- 0.35883 0.35883 0.36128 0.36248 0.37152

Eigenvalues --- 0.37152 0.38061 0.38999 0.40015 0.40015

Eigenvalues --- 0.41220 0.41220 0.41292 0.41292 0.41292

Eigenvalues --- 0.41374 0.41374 0.41374 0.41374 0.41473

Eigenvalues --- 0.41577 0.42294 0.43125 0.43325 0.43325

Eigenvalues --- 0.44285 0.44941 0.44941 0.44941 0.44941

Eigenvalues --- 0.45296 0.45296 0.45296 0.45705 0.45804

Eigenvalues --- 0.45804 0.45804 0.45804 0.45893 0.45893

Eigenvalues --- 0.45893 0.46884 0.47948 0.47948 0.48886

Eigenvalues --- 0.49277 0.50572 0.50965 0.50965 0.51399

RFO step: Lambda=-1.29512779D-04 EMin= 7.55306179D-03

Quartic linear search produced a step of -0.10560.

Iteration 1 RMS(Cart)= 0.01310533 RMS(Int)= 0.00004968

Iteration 2 RMS(Cart)= 0.00008203 RMS(Int)= 0.00000270

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000270

ITry= 1 IFail=0 DXMaxC= 4.43D-02 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.13D-08 for atom 53.

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

(Linear) (Quad) (Total)

R1 2.73813 0.00059 0.00048 0.00080 0.00128 2.73941

R2 2.57688 -0.00036 0.00060 -0.00135 -0.00075 2.57613

R3 2.03949 -0.00011 0.00033 -0.00070 -0.00037 2.03912

R4 2.58760 0.00078 0.00066 0.00061 0.00127 2.58887

R5 2.66569 0.00072 0.00152 0.00002 0.00154 2.66723

R6 2.58760 0.00078 0.00066 0.00061 0.00127 2.58887

R7 3.94613 0.00084 0.00157 0.00224 0.00380 3.94994

R8 2.73813 0.00059 0.00048 0.00080 0.00128 2.73941

R9 2.66569 0.00072 0.00152 0.00002 0.00154 2.66723

R10 2.03949 -0.00011 0.00033 -0.00070 -0.00037 2.03912

R11 2.66569 0.00072 0.00152 0.00002 0.00154 2.66723

R12 2.82138 0.00101 0.00156 0.00086 0.00241 2.82380

R13 2.58760 0.00078 0.00066 0.00061 0.00127 2.58887

R14 2.73813 0.00059 0.00048 0.00080 0.00128 2.73941

R15 2.58760 0.00078 0.00066 0.00061 0.00127 2.58887

R16 3.94613 0.00084 0.00157 0.00224 0.00380 3.94994

R17 2.73813 0.00059 0.00048 0.00080 0.00128 2.73941

R18 2.66569 0.00072 0.00152 0.00002 0.00154 2.66723

R19 2.57688 -0.00036 0.00060 -0.00135 -0.00075 2.57613

R20 2.03949 -0.00011 0.00033 -0.00070 -0.00037 2.03912

R21 2.03949 -0.00011 0.00033 -0.00070 -0.00037 2.03912

R22 2.66569 0.00072 0.00152 0.00002 0.00154 2.66723

R23 2.82138 0.00101 0.00156 0.00086 0.00241 2.82380

R24 2.73813 0.00059 0.00048 0.00080 0.00128 2.73941

R25 2.58760 0.00078 0.00066 0.00061 0.00127 2.58887

R26 2.57688 -0.00036 0.00060 -0.00135 -0.00075 2.57613

R27 2.03949 -0.00011 0.00033 -0.00070 -0.00037 2.03912

R28 2.73813 0.00059 0.00048 0.00080 0.00128 2.73941

R29 2.03949 -0.00011 0.00033 -0.00070 -0.00037 2.03912

R30 2.58760 0.00078 0.00066 0.00061 0.00127 2.58887

R31 2.66569 0.00072 0.00152 0.00002 0.00154 2.66723

R32 3.94613 0.00084 0.00157 0.00224 0.00380 3.94994

R33 2.66569 0.00072 0.00152 0.00002 0.00154 2.66723

R34 2.82138 0.00101 0.00156 0.00086 0.00241 2.82380

R35 2.73813 0.00059 0.00048 0.00080 0.00128 2.73941

R36 2.58760 0.00078 0.00066 0.00061 0.00127 2.58887

R37 2.57688 -0.00036 0.00060 -0.00135 -0.00075 2.57613

R38 2.03949 -0.00011 0.00033 -0.00070 -0.00037 2.03912

R39 2.73813 0.00059 0.00048 0.00080 0.00128 2.73941

R40 2.03949 -0.00011 0.00033 -0.00070 -0.00037 2.03912

R41 2.58760 0.00078 0.00066 0.00061 0.00127 2.58887

R42 2.66569 0.00072 0.00152 0.00002 0.00154 2.66723

R43 3.94613 0.00084 0.00157 0.00224 0.00380 3.94994

R44 2.82138 0.00101 0.00156 0.00086 0.00241 2.82380

R45 2.64382 0.00100 0.00132 0.00039 0.00171 2.64554

R46 2.64382 0.00100 0.00132 0.00039 0.00171 2.64554

R47 2.63153 0.00055 0.00116 -0.00037 0.00079 2.63231

R48 2.04957 -0.00001 0.00041 -0.00053 -0.00012 2.04946

R49 2.63391 0.00042 0.00104 -0.00052 0.00052 2.63443

R50 2.05014 0.00013 0.00039 -0.00016 0.00023 2.05036

R51 2.63391 0.00042 0.00104 -0.00052 0.00052 2.63443

R52 2.04997 0.00013 0.00039 -0.00015 0.00023 2.05020

R53 2.63153 0.00055 0.00116 -0.00037 0.00079 2.63231

R54 2.05014 0.00013 0.00039 -0.00016 0.00023 2.05036

R55 2.04957 -0.00001 0.00041 -0.00053 -0.00012 2.04946

R56 2.63391 0.00042 0.00104 -0.00052 0.00052 2.63443

R57 2.63391 0.00042 0.00104 -0.00052 0.00052 2.63443

R58 2.04997 0.00013 0.00039 -0.00015 0.00023 2.05020

R59 2.63153 0.00055 0.00116 -0.00037 0.00079 2.63231

R60 2.05014 0.00013 0.00039 -0.00016 0.00023 2.05036

R61 2.64382 0.00100 0.00132 0.00039 0.00171 2.64554

R62 2.04957 -0.00001 0.00041 -0.00053 -0.00012 2.04946

R63 2.64382 0.00100 0.00132 0.00039 0.00171 2.64554

R64 2.63153 0.00055 0.00116 -0.00037 0.00079 2.63231

R65 2.04957 -0.00001 0.00041 -0.00053 -0.00012 2.04946

R66 2.05014 0.00013 0.00039 -0.00016 0.00023 2.05036

R67 2.64382 0.00100 0.00132 0.00039 0.00171 2.64554

R68 2.64382 0.00100 0.00132 0.00039 0.00171 2.64554

R69 2.63153 0.00055 0.00116 -0.00037 0.00079 2.63231

R70 2.04957 -0.00001 0.00041 -0.00053 -0.00012 2.04946

R71 2.63391 0.00042 0.00104 -0.00052 0.00052 2.63443

R72 2.05014 0.00013 0.00039 -0.00016 0.00023 2.05036

R73 2.63391 0.00042 0.00104 -0.00052 0.00052 2.63443

R74 2.04997 0.00013 0.00039 -0.00015 0.00023 2.05020

R75 2.63153 0.00055 0.00116 -0.00037 0.00079 2.63231

R76 2.05014 0.00013 0.00039 -0.00016 0.00023 2.05036

R77 2.04957 -0.00001 0.00041 -0.00053 -0.00012 2.04946

R78 2.64382 0.00100 0.00132 0.00039 0.00171 2.64554

R79 2.64382 0.00100 0.00132 0.00039 0.00171 2.64554

R80 2.63153 0.00055 0.00116 -0.00037 0.00079 2.63231

R81 2.04957 -0.00001 0.00041 -0.00053 -0.00012 2.04946

R82 2.63391 0.00042 0.00104 -0.00052 0.00052 2.63443

R83 2.05014 0.00013 0.00039 -0.00016 0.00023 2.05036

R84 2.63391 0.00042 0.00104 -0.00052 0.00052 2.63443

R85 2.04997 0.00013 0.00039 -0.00015 0.00023 2.05020

R86 2.63153 0.00055 0.00116 -0.00037 0.00079 2.63231

R87 2.05014 0.00013 0.00039 -0.00016 0.00023 2.05036

R88 2.04957 -0.00001 0.00041 -0.00053 -0.00012 2.04946

A1 1.87042 0.00028 -0.00002 0.00085 0.00083 1.87125

A2 2.19474 -0.00005 0.00018 -0.00014 0.00004 2.19479

A3 2.21794 -0.00024 -0.00017 -0.00074 -0.00091 2.21702

A4 1.89736 -0.00035 0.00011 -0.00174 -0.00165 1.89571

A5 2.18788 -0.00001 -0.00012 0.00025 0.00012 2.18800

A6 2.19792 0.00036 0.00001 0.00144 0.00145 2.19937

A7 1.88918 0.00014 -0.00018 0.00170 0.00151 1.89069

A8 2.19488 -0.00007 0.00008 -0.00082 -0.00074 2.19414

A9 2.19488 -0.00007 0.00008 -0.00082 -0.00074 2.19414

A10 1.89736 -0.00035 0.00011 -0.00174 -0.00165 1.89571

A11 2.19792 0.00036 0.00001 0.00144 0.00145 2.19937

A12 2.18788 -0.00001 -0.00012 0.00025 0.00012 2.18800

A13 1.87042 0.00028 -0.00002 0.00085 0.00083 1.87125

A14 2.21794 -0.00024 -0.00017 -0.00074 -0.00091 2.21702

A15 2.19474 -0.00005 0.00018 -0.00014 0.00004 2.19479

A16 2.20448 -0.00058 -0.00021 -0.00115 -0.00135 2.20313

A17 2.03935 0.00029 0.00011 0.00057 0.00068 2.04003

A18 2.03935 0.00029 0.00011 0.00057 0.00068 2.04003

A19 2.19792 0.00036 0.00001 0.00144 0.00145 2.19937

A20 2.18788 -0.00001 -0.00012 0.00025 0.00012 2.18800

A21 1.89736 -0.00035 0.00011 -0.00174 -0.00165 1.89571

A22 1.88918 0.00014 -0.00018 0.00170 0.00151 1.89069

A23 2.19488 -0.00007 0.00008 -0.00082 -0.00074 2.19414

A24 2.19488 -0.00007 0.00008 -0.00082 -0.00074 2.19414

A25 1.89736 -0.00035 0.00011 -0.00174 -0.00165 1.89571

A26 2.19792 0.00036 0.00001 0.00144 0.00145 2.19937

A27 2.18788 -0.00001 -0.00012 0.00025 0.00012 2.18800

A28 1.87042 0.00028 -0.00002 0.00085 0.00083 1.87125

A29 2.19474 -0.00005 0.00018 -0.00014 0.00004 2.19479

A30 2.21794 -0.00024 -0.00017 -0.00074 -0.00091 2.21702

A31 1.87042 0.00028 -0.00002 0.00085 0.00083 1.87125

A32 2.19474 -0.00005 0.00018 -0.00014 0.00004 2.19479

A33 2.21794 -0.00024 -0.00017 -0.00074 -0.00091 2.21702

A34 2.20448 -0.00058 -0.00021 -0.00115 -0.00135 2.20313

A35 2.03935 0.00029 0.00011 0.00057 0.00068 2.04003

A36 2.03935 0.00029 0.00011 0.00057 0.00068 2.04003

A37 2.18788 -0.00001 -0.00012 0.00025 0.00012 2.18800

A38 2.19792 0.00036 0.00001 0.00144 0.00145 2.19937

A39 1.89736 -0.00035 0.00011 -0.00174 -0.00165 1.89571

A40 1.87042 0.00028 -0.00002 0.00085 0.00083 1.87125

A41 2.19474 -0.00005 0.00018 -0.00014 0.00004 2.19479

A42 2.21794 -0.00024 -0.00017 -0.00074 -0.00091 2.21702

A43 1.87042 0.00028 -0.00002 0.00085 0.00083 1.87125

A44 2.21794 -0.00024 -0.00017 -0.00074 -0.00091 2.21702

A45 2.19474 -0.00005 0.00018 -0.00014 0.00004 2.19479

A46 1.89736 -0.00035 0.00011 -0.00174 -0.00165 1.89571

A47 2.18788 -0.00001 -0.00012 0.00025 0.00012 2.18800

A48 2.19792 0.00036 0.00001 0.00144 0.00145 2.19937

A49 1.88918 0.00014 -0.00018 0.00170 0.00151 1.89069

A50 2.19488 -0.00007 0.00008 -0.00082 -0.00074 2.19414

A51 2.19488 -0.00007 0.00008 -0.00082 -0.00074 2.19414

A52 2.20448 -0.00058 -0.00021 -0.00115 -0.00135 2.20313

A53 2.03935 0.00029 0.00011 0.00057 0.00068 2.04003

A54 2.03935 0.00029 0.00011 0.00057 0.00068 2.04003

A55 2.18788 -0.00001 -0.00012 0.00025 0.00012 2.18800

A56 2.19792 0.00036 0.00001 0.00144 0.00145 2.19937

A57 1.89736 -0.00035 0.00011 -0.00174 -0.00165 1.89571

A58 1.87042 0.00028 -0.00002 0.00085 0.00083 1.87125

A59 2.19474 -0.00005 0.00018 -0.00014 0.00004 2.19479

A60 2.21794 -0.00024 -0.00017 -0.00074 -0.00091 2.21702

A61 1.87042 0.00028 -0.00002 0.00085 0.00083 1.87125

A62 2.21794 -0.00024 -0.00017 -0.00074 -0.00091 2.21702

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A66 2.19792 0.00036 0.00001 0.00144 0.00145 2.19937

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A74 2.10477 0.00024 0.00025 0.00048 0.00073 2.10549

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A77 2.08443 -0.00015 0.00008 -0.00082 -0.00074 2.08369

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A80 2.08875 0.00006 -0.00003 0.00048 0.00045 2.08920

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A84 2.09755 -0.00002 0.00008 -0.00007 0.00000 2.09756

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A89 2.08443 -0.00015 0.00008 -0.00082 -0.00074 2.08369

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A94 2.09714 0.00004 0.00007 -0.00006 0.00002 2.09716

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A96 2.08875 0.00006 -0.00003 0.00048 0.00045 2.08920

A97 2.10517 0.00018 0.00025 0.00046 0.00071 2.10589

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A107 2.09728 -0.00010 -0.00004 -0.00042 -0.00047 2.09682

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A110 2.10477 0.00024 0.00025 0.00048 0.00073 2.10549

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A128 2.10477 0.00024 0.00025 0.00048 0.00073 2.10549

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D1 0.00564 0.00010 0.00015 0.00448 0.00463 0.01027

D2 3.13997 -0.00006 -0.00011 -0.00290 -0.00301 3.13696

D3 -3.12218 0.00015 0.00026 0.00689 0.00715 -3.11503

D4 0.01215 -0.00001 0.00000 -0.00049 -0.00049 0.01166

D5 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D6 -3.12758 0.00005 0.00011 0.00244 0.00255 -3.12503

D7 3.12758 -0.00005 -0.00011 -0.00244 -0.00255 3.12503

D8 0.00000 -0.00000 -0.00000 0.00000 -0.00000 0.00000

D9 -0.00919 -0.00016 -0.00024 -0.00732 -0.00756 -0.01675

D10 3.03785 -0.00016 -0.00044 -0.00672 -0.00717 3.03069

D11 3.13971 -0.00000 0.00002 0.00012 0.00015 3.13986

D12 -0.09643 -0.00000 -0.00018 0.00072 0.00054 -0.09589

D13 -3.08029 0.00019 0.00040 0.00831 0.00871 -3.07158

D14 0.06130 0.00019 0.00040 0.00831 0.00871 0.07001

D15 0.05281 0.00000 0.00010 -0.00034 -0.00024 0.05256

D16 -3.08878 0.00000 0.00010 -0.00034 -0.00024 -3.08903

D17 0.00919 0.00016 0.00024 0.00732 0.00756 0.01675

D18 -3.13971 0.00000 -0.00002 -0.00012 -0.00015 -3.13986

D19 -3.03785 0.00016 0.00044 0.00672 0.00717 -3.03069

D20 0.09643 0.00000 0.00018 -0.00072 -0.00054 0.09589

D21 -3.07578 0.00000 0.00016 -0.00042 -0.00026 -3.07604

D22 0.04491 -0.00002 0.00009 -0.00040 -0.00031 0.04459

D23 -0.04491 0.00002 -0.00009 0.00040 0.00031 -0.04459

D24 3.07578 -0.00000 -0.00016 0.00042 0.00026 3.07604

D25 -0.00564 -0.00010 -0.00015 -0.00448 -0.00463 -0.01027

D26 3.12218 -0.00015 -0.00026 -0.00689 -0.00715 3.11503

D27 -3.13997 0.00006 0.00011 0.00290 0.00301 -3.13696

D28 -0.01215 0.00001 -0.00000 0.00049 0.00049 -0.01166

D29 -0.05281 -0.00000 -0.00010 0.00034 0.00024 -0.05256

D30 3.08878 -0.00000 -0.00010 0.00034 0.00024 3.08903

D31 3.08029 -0.00019 -0.00040 -0.00831 -0.00871 3.07158

D32 -0.06130 -0.00019 -0.00040 -0.00831 -0.00871 -0.07001

D33 -0.05281 -0.00000 -0.00010 0.00034 0.00024 -0.05256

D34 3.08029 -0.00019 -0.00040 -0.00831 -0.00871 3.07158

D35 3.08878 -0.00000 -0.00010 0.00034 0.00024 3.08903

D36 -0.06130 -0.00019 -0.00040 -0.00831 -0.00871 -0.07001

D37 -1.14604 0.00007 -0.00501 0.01936 0.01435 -1.13169

D38 1.99555 0.00007 -0.00501 0.01936 0.01435 2.00990

D39 1.99555 0.00007 -0.00501 0.01936 0.01435 2.00990

D40 -1.14604 0.00007 -0.00501 0.01936 0.01435 -1.13169

D41 -3.13971 0.00000 -0.00002 -0.00012 -0.00015 -3.13986

D42 0.09643 0.00000 0.00018 -0.00072 -0.00054 0.09589

D43 0.00919 0.00016 0.00024 0.00732 0.00756 0.01675

D44 -3.03785 0.00016 0.00044 0.00672 0.00717 -3.03069

D45 -3.13997 0.00006 0.00011 0.00290 0.00301 -3.13696

D46 -0.01215 0.00001 -0.00000 0.00049 0.00049 -0.01166

D47 -0.00564 -0.00010 -0.00015 -0.00448 -0.00463 -0.01027

D48 3.12218 -0.00015 -0.00026 -0.00689 -0.00715 3.11503

D49 -0.00919 -0.00016 -0.00024 -0.00732 -0.00756 -0.01675

D50 3.13971 -0.00000 0.00002 0.00012 0.00015 3.13986

D51 3.03785 -0.00016 -0.00044 -0.00672 -0.00717 3.03069

D52 -0.09643 -0.00000 -0.00018 0.00072 0.00054 -0.09589

D53 -0.04491 0.00002 -0.00009 0.00040 0.00031 -0.04459

D54 3.07578 -0.00000 -0.00016 0.00042 0.00026 3.07604

D55 -3.07578 0.00000 0.00016 -0.00042 -0.00026 -3.07604

D56 0.04491 -0.00002 0.00009 -0.00040 -0.00031 0.04459

D57 0.00564 0.00010 0.00015 0.00448 0.00463 0.01027

D58 -3.12218 0.00015 0.00026 0.00689 0.00715 -3.11503

D59 3.13997 -0.00006 -0.00011 -0.00290 -0.00301 3.13696

D60 0.01215 -0.00001 0.00000 -0.00049 -0.00049 0.01166

D61 0.05281 0.00000 0.00010 -0.00034 -0.00024 0.05256

D62 -3.08878 0.00000 0.00010 -0.00034 -0.00024 -3.08903

D63 -3.08029 0.00019 0.00040 0.00831 0.00871 -3.07158

D64 0.06130 0.00019 0.00040 0.00831 0.00871 0.07001

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D66 -3.12758 0.00005 0.00011 0.00244 0.00255 -3.12503

D67 3.12758 -0.00005 -0.00011 -0.00244 -0.00255 3.12503

D68 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D69 -3.08029 0.00019 0.00040 0.00831 0.00871 -3.07158

D70 0.05281 0.00000 0.00010 -0.00034 -0.00024 0.05256

D71 0.06130 0.00019 0.00040 0.00831 0.00871 0.07001

D72 -3.08878 0.00000 0.00010 -0.00034 -0.00024 -3.08903

D73 1.14604 -0.00007 0.00501 -0.01936 -0.01435 1.13169

D74 -1.99555 -0.00007 0.00501 -0.01936 -0.01435 -2.00990

D75 -1.99555 -0.00007 0.00501 -0.01936 -0.01435 -2.00990

D76 1.14604 -0.00007 0.00501 -0.01936 -0.01435 1.13169

D77 3.13997 -0.00006 -0.00011 -0.00290 -0.00301 3.13696

D78 0.01215 -0.00001 0.00000 -0.00049 -0.00049 0.01166

D79 0.00564 0.00010 0.00015 0.00448 0.00463 0.01027

D80 -3.12218 0.00015 0.00026 0.00689 0.00715 -3.11503

D81 3.13971 -0.00000 0.00002 0.00012 0.00015 3.13986

D82 -0.09643 -0.00000 -0.00018 0.00072 0.00054 -0.09589

D83 -0.00919 -0.00016 -0.00024 -0.00732 -0.00756 -0.01675

D84 3.03785 -0.00016 -0.00044 -0.00672 -0.00717 3.03069

D85 -0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D86 -3.12758 0.00005 0.00011 0.00244 0.00255 -3.12503

D87 3.12758 -0.00005 -0.00011 -0.00244 -0.00255 3.12503

D88 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D89 -0.00564 -0.00010 -0.00015 -0.00448 -0.00463 -0.01027

D90 -3.13997 0.00006 0.00011 0.00290 0.00301 -3.13696

D91 3.12218 -0.00015 -0.00026 -0.00689 -0.00715 3.11503

D92 -0.01215 0.00001 -0.00000 0.00049 0.00049 -0.01166

D93 0.00919 0.00016 0.00024 0.00732 0.00756 0.01675

D94 -3.03785 0.00016 0.00044 0.00672 0.00717 -3.03069

D95 -3.13971 0.00000 -0.00002 -0.00012 -0.00015 -3.13986

D96 0.09643 0.00000 0.00018 -0.00072 -0.00054 0.09589

D97 3.08029 -0.00019 -0.00040 -0.00831 -0.00871 3.07158

D98 -0.06130 -0.00019 -0.00040 -0.00831 -0.00871 -0.07001

D99 -0.05281 -0.00000 -0.00010 0.00034 0.00024 -0.05256

D100 3.08878 -0.00000 -0.00010 0.00034 0.00024 3.08903

D101 0.04491 -0.00002 0.00009 -0.00040 -0.00031 0.04459

D102 -3.07578 0.00000 0.00016 -0.00042 -0.00026 -3.07604

D103 3.07578 -0.00000 -0.00016 0.00042 0.00026 3.07604

D104 -0.04491 0.00002 -0.00009 0.00040 0.00031 -0.04459

D105 3.08029 -0.00019 -0.00040 -0.00831 -0.00871 3.07158

D106 -0.05281 -0.00000 -0.00010 0.00034 0.00024 -0.05256

D107 -0.06130 -0.00019 -0.00040 -0.00831 -0.00871 -0.07001

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D109 -1.14604 0.00007 -0.00501 0.01936 0.01435 -1.13169

D110 1.99555 0.00007 -0.00501 0.01936 0.01435 2.00990

D111 1.99555 0.00007 -0.00501 0.01936 0.01435 2.00990

D112 -1.14604 0.00007 -0.00501 0.01936 0.01435 -1.13169

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D114 -0.01215 0.00001 -0.00000 0.00049 0.00049 -0.01166

D115 -0.00564 -0.00010 -0.00015 -0.00448 -0.00463 -0.01027

D116 3.12218 -0.00015 -0.00026 -0.00689 -0.00715 3.11503

D117 -3.13971 0.00000 -0.00002 -0.00012 -0.00015 -3.13986

D118 0.09643 0.00000 0.00018 -0.00072 -0.00054 0.09589

D119 0.00919 0.00016 0.00024 0.00732 0.00756 0.01675

D120 -3.03785 0.00016 0.00044 0.00672 0.00717 -3.03069

D121 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D122 3.12758 -0.00005 -0.00011 -0.00244 -0.00255 3.12503

D123 -3.12758 0.00005 0.00011 0.00244 0.00255 -3.12503

D124 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D125 0.00564 0.00010 0.00015 0.00448 0.00463 0.01027

D126 3.13997 -0.00006 -0.00011 -0.00290 -0.00301 3.13696

D127 -3.12218 0.00015 0.00026 0.00689 0.00715 -3.11503

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D131 3.13971 -0.00000 0.00002 0.00012 0.00015 3.13986

D132 -0.09643 -0.00000 -0.00018 0.00072 0.00054 -0.09589

D133 -3.08029 0.00019 0.00040 0.00831 0.00871 -3.07158

D134 0.06130 0.00019 0.00040 0.00831 0.00871 0.07001

D135 0.05281 0.00000 0.00010 -0.00034 -0.00024 0.05256

D136 -3.08878 0.00000 0.00010 -0.00034 -0.00024 -3.08903

D137 3.07578 -0.00000 -0.00016 0.00042 0.00026 3.07604

D138 -0.04491 0.00002 -0.00009 0.00040 0.00031 -0.04459

D139 0.04491 -0.00002 0.00009 -0.00040 -0.00031 0.04459

D140 -3.07578 0.00000 0.00016 -0.00042 -0.00026 -3.07604

D141 1.14604 -0.00007 0.00501 -0.01936 -0.01435 1.13169

D142 -1.99555 -0.00007 0.00501 -0.01936 -0.01435 -2.00990

D143 -1.99555 -0.00007 0.00501 -0.01936 -0.01435 -2.00990

D144 1.14604 -0.00007 0.00501 -0.01936 -0.01435 1.13169

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D146 -0.00430 -0.00004 -0.00017 -0.00147 -0.00165 -0.00595

D147 0.00137 0.00001 0.00019 -0.00007 0.00012 0.00149

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D149 -3.14022 0.00001 0.00019 -0.00007 0.00012 -3.14010

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D155 -3.13864 0.00004 -0.00002 0.00156 0.00154 -3.13710

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D157 0.00136 0.00001 0.00019 -0.00007 0.00012 0.00148

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D159 -3.13786 0.00001 -0.00002 0.00059 0.00056 -3.13729

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D164 0.00374 0.00001 -0.00002 0.00059 0.00056 0.00430

D165 -0.00275 -0.00001 -0.00038 0.00015 -0.00024 -0.00299

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D173 -0.00136 -0.00001 -0.00019 0.00007 -0.00012 -0.00148

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D180 -0.00060 -0.00003 -0.00019 -0.00090 -0.00109 -0.00169

D181 3.14022 -0.00001 -0.00019 0.00007 -0.00012 3.14010

D182 -0.00137 -0.00001 -0.00019 0.00007 -0.00012 -0.00149

D183 0.00430 0.00004 0.00017 0.00147 0.00165 0.00595

D184 -3.13729 0.00004 0.00017 0.00147 0.00165 -3.13564

D185 3.14022 -0.00001 -0.00019 0.00007 -0.00012 3.14010

D186 0.00430 0.00004 0.00017 0.00147 0.00165 0.00595

D187 -0.00137 -0.00001 -0.00019 0.00007 -0.00012 -0.00149

D188 -3.13729 0.00004 0.00017 0.00147 0.00165 -3.13564

D189 0.00275 0.00001 0.00038 -0.00015 0.00024 0.00299

D190 -3.13648 0.00002 0.00017 0.00051 0.00068 -3.13580

D191 3.13864 -0.00004 0.00002 -0.00156 -0.00154 3.13710

D192 -0.00060 -0.00003 -0.00019 -0.00090 -0.00109 -0.00169

D193 3.14022 -0.00001 -0.00019 0.00007 -0.00012 3.14010

D194 0.00430 0.00004 0.00017 0.00147 0.00165 0.00595

D195 -0.00137 -0.00001 -0.00019 0.00007 -0.00012 -0.00149

D196 -3.13729 0.00004 0.00017 0.00147 0.00165 -3.13564

D197 3.14022 -0.00001 -0.00019 0.00007 -0.00012 3.14010

D198 0.00430 0.00004 0.00017 0.00147 0.00165 0.00595

D199 -0.00137 -0.00001 -0.00019 0.00007 -0.00012 -0.00149

D200 -3.13729 0.00004 0.00017 0.00147 0.00165 -3.13564

D201 0.00275 0.00001 0.00038 -0.00015 0.00024 0.00299

D202 -3.13648 0.00002 0.00017 0.00051 0.00068 -3.13580

D203 3.13864 -0.00004 0.00002 -0.00156 -0.00154 3.13710

D204 -0.00060 -0.00003 -0.00019 -0.00090 -0.00109 -0.00169

D205 -0.00136 -0.00001 -0.00019 0.00007 -0.00012 -0.00148

D206 3.14023 -0.00001 -0.00019 0.00007 -0.00012 3.14011

D207 3.13786 -0.00001 0.00002 -0.00059 -0.00056 3.13729

D208 -0.00374 -0.00001 0.00002 -0.00059 -0.00056 -0.00430

D209 -0.00136 -0.00001 -0.00019 0.00007 -0.00012 -0.00148

D210 3.13786 -0.00001 0.00002 -0.00059 -0.00056 3.13729

D211 3.14023 -0.00001 -0.00019 0.00007 -0.00012 3.14011

D212 -0.00374 -0.00001 0.00002 -0.00059 -0.00056 -0.00430

D213 0.00275 0.00001 0.00038 -0.00015 0.00024 0.00299

D214 3.13864 -0.00004 0.00002 -0.00156 -0.00154 3.13710

D215 -3.13648 0.00002 0.00017 0.00051 0.00068 -3.13580

D216 -0.00060 -0.00003 -0.00019 -0.00090 -0.00109 -0.00169

D217 -3.14022 0.00001 0.00019 -0.00007 0.00012 -3.14010

D218 -0.00430 -0.00004 -0.00017 -0.00147 -0.00165 -0.00595

D219 0.00137 0.00001 0.00019 -0.00007 0.00012 0.00149

D220 3.13729 -0.00004 -0.00017 -0.00147 -0.00165 3.13564

D221 -3.14022 0.00001 0.00019 -0.00007 0.00012 -3.14010

D222 -0.00430 -0.00004 -0.00017 -0.00147 -0.00165 -0.00595

D223 0.00137 0.00001 0.00019 -0.00007 0.00012 0.00149

D224 3.13729 -0.00004 -0.00017 -0.00147 -0.00165 3.13564

D225 -0.00275 -0.00001 -0.00038 0.00015 -0.00024 -0.00299

D226 3.13648 -0.00002 -0.00017 -0.00051 -0.00068 3.13580

D227 -3.13864 0.00004 -0.00002 0.00156 0.00154 -3.13710

D228 0.00060 0.00003 0.00019 0.00090 0.00109 0.00169

D229 0.00136 0.00001 0.00019 -0.00007 0.00012 0.00148

D230 -3.14023 0.00001 0.00019 -0.00007 0.00012 -3.14011

D231 -3.13786 0.00001 -0.00002 0.00059 0.00056 -3.13729

D232 0.00374 0.00001 -0.00002 0.00059 0.00056 0.00430

D233 0.00136 0.00001 0.00019 -0.00007 0.00012 0.00148

D234 -3.13786 0.00001 -0.00002 0.00059 0.00056 -3.13729

D235 -3.14023 0.00001 0.00019 -0.00007 0.00012 -3.14011

D236 0.00374 0.00001 -0.00002 0.00059 0.00056 0.00430

D237 -0.00275 -0.00001 -0.00038 0.00015 -0.00024 -0.00299

D238 -3.13864 0.00004 -0.00002 0.00156 0.00154 -3.13710

D239 3.13648 -0.00002 -0.00017 -0.00051 -0.00068 3.13580

D240 0.00060 0.00003 0.00019 0.00090 0.00109 0.00169

Item Value Threshold Converged?

Maximum Force 0.001012 0.000450 NO

RMS Force 0.000288 0.000300 YES

Maximum Displacement 0.044331 0.001800 NO

RMS Displacement 0.013106 0.001200 NO

Predicted change in Energy=-8.244415D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Aug 13 18:15:14 2019, MaxMem= 671088640 cpu: 1.0

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

Stoichiometry C44H28N4Zn

Framework group D2D[O(Zn),2SGD(N2),X(C44H28)]

Deg. of freedom 29

Full point group D2D NOp 8

RotChk: IX=0 Diff= 0.00D+00

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681614 4.270408 0.145119

2 6 0 -1.110635 2.890427 0.030942

3 7 0 0.000000 2.090102 -0.021901

4 6 0 1.110635 2.890427 0.030942

5 6 0 0.681614 4.270408 0.145119

6 6 0 2.451846 2.451846 0.000000

7 6 0 2.890427 1.110635 -0.030942

8 7 0 2.090102 -0.000000 0.021901

9 6 0 2.890427 -1.110635 -0.030942

10 6 0 4.270408 -0.681614 -0.145119

11 6 0 4.270408 0.681614 -0.145119

12 6 0 -2.451846 2.451846 0.000000

13 6 0 -2.890427 1.110635 -0.030942

14 6 0 -4.270408 0.681614 -0.145119

15 6 0 -4.270408 -0.681614 -0.145119

16 6 0 -2.890427 -1.110635 -0.030942

17 7 0 -2.090102 0.000000 0.021901

18 6 0 -2.451846 -2.451846 0.000000

19 6 0 -1.110635 -2.890427 0.030942

20 6 0 -0.681614 -4.270408 0.145119

21 6 0 0.681614 -4.270408 0.145119

22 6 0 1.110635 -2.890427 0.030942

23 7 0 -0.000000 -2.090102 -0.021901

24 6 0 2.451846 -2.451846 0.000000

25 6 0 3.508468 3.508468 -0.000000

26 6 0 3.631971 4.393853 -1.077367

27 6 0 4.617899 5.377867 -1.078654

28 6 0 5.493460 5.493460 -0.000000

29 6 0 5.377867 4.617899 1.078654

30 6 0 4.393853 3.631971 1.077367

31 6 0 -5.493460 5.493460 -0.000000

32 6 0 -4.617899 5.377867 -1.078654

33 6 0 -3.631971 4.393853 -1.077367

34 6 0 -3.508468 3.508468 -0.000000

35 6 0 -4.393853 3.631971 1.077367

36 6 0 -5.377867 4.617899 1.078654

37 6 0 3.508468 -3.508468 -0.000000

38 6 0 4.393853 -3.631971 1.077367

39 6 0 5.377867 -4.617899 1.078654

40 6 0 5.493460 -5.493460 -0.000000

41 6 0 4.617899 -5.377867 -1.078654

42 6 0 3.631971 -4.393853 -1.077367

43 6 0 -3.508468 -3.508468 -0.000000

44 6 0 -4.393853 -3.631971 1.077367

45 6 0 -5.377867 -4.617899 1.078654

46 6 0 -5.493460 -5.493460 -0.000000

47 6 0 -4.617899 -5.377867 -1.078654

48 6 0 -3.631971 -4.393853 -1.077367

49 1 0 -1.331399 5.127658 0.230361

50 1 0 1.331399 5.127658 0.230361

51 1 0 5.127658 -1.331399 -0.230361

52 1 0 5.127658 1.331399 -0.230361

53 1 0 -5.127658 1.331399 -0.230361

54 1 0 -5.127658 -1.331399 -0.230361

55 1 0 -1.331399 -5.127658 0.230361

56 1 0 1.331399 -5.127658 0.230361

57 1 0 2.955267 4.304230 -1.920123

58 1 0 4.703109 6.052429 -1.924196

59 1 0 6.260614 6.260614 -0.000000

60 1 0 6.052429 4.703109 1.924196

61 1 0 4.304230 2.955267 1.920123

62 1 0 -6.260614 6.260614 -0.000000

63 1 0 -4.703109 6.052429 -1.924196

64 1 0 -2.955267 4.304230 -1.920123

65 1 0 -4.304230 2.955267 1.920123

66 1 0 -6.052429 4.703109 1.924196

67 1 0 4.304230 -2.955267 1.920123

68 1 0 6.052429 -4.703109 1.924196

69 1 0 6.260614 -6.260614 -0.000000

70 1 0 4.703109 -6.052429 -1.924196

71 1 0 2.955267 -4.304230 -1.920123

72 1 0 -4.304230 -2.955267 1.920123

73 1 0 -6.052429 -4.703109 1.924196

74 1 0 -6.260614 -6.260614 -0.000000

75 1 0 -4.703109 -6.052429 -1.924196

76 1 0 -2.955267 -4.304230 -1.920123

77 30 0 0.000000 0.000000 0.000000

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

Rotational constants (GHZ): 0.0582031 0.0582031 0.0300901

Leave Link 202 at Tue Aug 13 18:15:14 2019, MaxMem= 671088640 cpu: 0.0

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

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

Pseudo-potential data read from rwf file.

There are 272 symmetry adapted cartesian basis functions of A1 symmetry.

There are 243 symmetry adapted cartesian basis functions of A2 symmetry.

There are 254 symmetry adapted cartesian basis functions of B1 symmetry.

There are 254 symmetry adapted cartesian basis functions of B2 symmetry.

There are 256 symmetry adapted basis functions of A1 symmetry.

There are 232 symmetry adapted basis functions of A2 symmetry.

There are 242 symmetry adapted basis functions of B1 symmetry.

There are 242 symmetry adapted basis functions of B2 symmetry.

972 basis functions, 1715 primitive gaussians, 1023 cartesian basis functions

166 alpha electrons 166 beta electrons

nuclear repulsion energy 5738.4869611517 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= 77 NActive= 77 NUniq= 13 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T 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= -0.2223931397 Hartrees.

Nuclear repulsion after empirical dispersion term = 5738.2645680120 Hartrees.

No density basis found on file 724.

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Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 77.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 77

GePol: Total number of spheres = 77

GePol: Number of exposed spheres = 77 (100.00%)

GePol: Number of points = 5690

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.14D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 288

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

GePol: Cavity surface area = 614.414 Ang\*\*2

GePol: Cavity volume = 630.510 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0021369114 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5738.2624311006 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

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36749 LenP2D= 95286.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 972 RedAO= T EigKep= 6.32D-05 NBF= 256 232 242 242

NBsUse= 972 1.00D-06 EigRej= -1.00D+00 NBFU= 256 232 242 242

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= 952 960 976 976 976 MxSgAt= 77 MxSgA2= 77.

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Aug 13 18:15:17 2019, MaxMem= 671088640 cpu: 0.8

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

Initial guess from the checkpoint file: "ZnTPP0.chk"

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 1.000000 -0.000000 0.000000 -0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

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

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

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

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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= -1979.25552399589

Leave Link 401 at Tue Aug 13 18:15:26 2019, MaxMem= 671088640 cpu: 35.6

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3177123 IEndB= 3177123 NGot= 671088640 MDV= 668975710

LenX= 668975710 LenY= 667928158

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= 530000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 97128300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.99D-15 for 5681.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.44D-15 for 5674 1298.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.33D-15 for 5681.

Iteration 1 A^-1\*A deviation from orthogonality is 1.84D-09 for 4955 4953.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.55D-15 for 341.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.05D-15 for 3660 3246.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 5492.

Iteration 2 A^-1\*A deviation from orthogonality is 4.58D-16 for 1768 1546.

E= -1978.90283930300

DIIS: error= 1.61D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1978.90283930300 IErMin= 1 ErrMin= 1.61D-03

ErrMax= 1.61D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.80D-04 BMatP= 6.80D-04

IDIUse=3 WtCom= 9.84D-01 WtEn= 1.61D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.444 Goal= None Shift= 0.000

GapD= 0.444 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=4.12D-05 MaxDP=9.44D-04 OVMax= 6.75D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.12D-05 CP: 1.00D+00

E= -1978.90429675275 Delta-E= -0.001457449758 Rises=F Damp=F

DIIS: error= 2.18D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1978.90429675275 IErMin= 2 ErrMin= 2.18D-04

ErrMax= 2.18D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-05 BMatP= 6.80D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.18D-03

Coeff-Com: -0.661D-01 0.107D+01

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

Coeff: -0.659D-01 0.107D+01

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=7.05D-06 MaxDP=2.39D-04 DE=-1.46D-03 OVMax= 1.06D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 6.35D-06 CP: 1.00D+00 1.07D+00

E= -1978.90431784895 Delta-E= -0.000021096197 Rises=F Damp=F

DIIS: error= 1.22D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1978.90431784895 IErMin= 3 ErrMin= 1.22D-04

ErrMax= 1.22D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.81D-06 BMatP= 1.10D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.22D-03

Coeff-Com: -0.394D-01 0.502D+00 0.537D+00

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

Coeff: -0.394D-01 0.501D+00 0.538D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=3.19D-06 MaxDP=2.32D-04 DE=-2.11D-05 OVMax= 8.26D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.58D-06 CP: 1.00D+00 1.09D+00 7.19D-01

E= -1978.90432278836 Delta-E= -0.000004939411 Rises=F Damp=F

DIIS: error= 6.44D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1978.90432278836 IErMin= 4 ErrMin= 6.44D-05

ErrMax= 6.44D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.61D-06 BMatP= 6.81D-06

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

Coeff-Com: -0.117D-01 0.115D+00 0.330D+00 0.566D+00

Coeff: -0.117D-01 0.115D+00 0.330D+00 0.566D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.24D-06 MaxDP=9.44D-05 DE=-4.94D-06 OVMax= 2.95D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 8.75D-07 CP: 1.00D+00 1.09D+00 7.88D-01 7.07D-01

E= -1978.90432416949 Delta-E= -0.000001381125 Rises=F Damp=F

DIIS: error= 1.55D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1978.90432416949 IErMin= 5 ErrMin= 1.55D-05

ErrMax= 1.55D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.50D-08 BMatP= 1.61D-06

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

Coeff-Com: -0.131D-02 0.540D-04 0.934D-01 0.253D+00 0.655D+00

Coeff: -0.131D-02 0.540D-04 0.934D-01 0.253D+00 0.655D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=3.85D-07 MaxDP=1.76D-05 DE=-1.38D-06 OVMax= 4.95D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.83D-07 CP: 1.00D+00 1.09D+00 8.02D-01 7.42D-01 7.44D-01

E= -1978.90432423590 Delta-E= -0.000000066413 Rises=F Damp=F

DIIS: error= 1.05D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1978.90432423590 IErMin= 6 ErrMin= 1.05D-05

ErrMax= 1.05D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.61D-08 BMatP= 8.50D-08

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

Coeff-Com: 0.635D-03-0.142D-01 0.100D-01 0.682D-01 0.359D+00 0.577D+00

Coeff: 0.635D-03-0.142D-01 0.100D-01 0.682D-01 0.359D+00 0.577D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.44D-07 MaxDP=7.88D-06 DE=-6.64D-08 OVMax= 2.50D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 6.22D-08 CP: 1.00D+00 1.09D+00 8.08D-01 7.54D-01 7.85D-01

CP: 5.90D-01

E= -1978.90432424863 Delta-E= -0.000000012727 Rises=F Damp=F

DIIS: error= 1.69D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1978.90432424863 IErMin= 7 ErrMin= 1.69D-06

ErrMax= 1.69D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.50D-09 BMatP= 1.61D-08

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

Coeff-Com: 0.441D-03-0.839D-02 0.730D-03 0.268D-01 0.179D+00 0.340D+00

Coeff-Com: 0.462D+00

Coeff: 0.441D-03-0.839D-02 0.730D-03 0.268D-01 0.179D+00 0.340D+00

Coeff: 0.462D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=3.85D-08 MaxDP=2.12D-06 DE=-1.27D-08 OVMax= 7.67D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.50D-08 CP: 1.00D+00 1.09D+00 8.08D-01 7.55D-01 7.86D-01

CP: 6.13D-01 5.50D-01

E= -1978.90432425022 Delta-E= -0.000000001596 Rises=F Damp=F

DIIS: error= 5.35D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1978.90432425022 IErMin= 8 ErrMin= 5.35D-07

ErrMax= 5.35D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.74D-11 BMatP= 1.50D-09

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

Coeff-Com: 0.120D-03-0.209D-02-0.833D-03 0.431D-02 0.408D-01 0.877D-01

Coeff-Com: 0.196D+00 0.674D+00

Coeff: 0.120D-03-0.209D-02-0.833D-03 0.431D-02 0.408D-01 0.877D-01

Coeff: 0.196D+00 0.674D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=8.13D-09 MaxDP=5.62D-07 DE=-1.60D-09 OVMax= 1.38D-06

Error on total polarization charges = 0.08501

SCF Done: E(RB3LYP) = -1978.90432425 A.U. after 8 cycles

NFock= 8 Conv=0.81D-08 -V/T= 1.9793

KE= 2.020719894127D+03 PE=-1.615865469740D+04 EE= 6.420768047927D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.34

(included in total energy above)

Leave Link 502 at Tue Aug 13 18:21:24 2019, MaxMem= 671088640 cpu: 1430.7

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36749 LenP2D= 95286.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 180

Leave Link 701 at Tue Aug 13 18:22:13 2019, MaxMem= 671088640 cpu: 192.4

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

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

Leave Link 702 at Tue Aug 13 18:22:13 2019, MaxMem= 671088640 cpu: 0.1

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 0 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Tue Aug 13 18:23:03 2019, MaxMem= 671088640 cpu: 202.3

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

Dipole = 9.11271059D-13 2.00728323D-13 6.57252031D-14

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000232306 0.000162770 -0.000021838

2 6 0.000185755 -0.000218408 0.000222274

3 7 0.000000000 0.000078988 -0.000690365

4 6 -0.000185755 -0.000218408 0.000222274

5 6 -0.000232306 0.000162770 -0.000021838

6 6 0.000300204 0.000300204 0.000000000

7 6 -0.000218408 -0.000185755 -0.000222274

8 7 0.000078988 -0.000000000 0.000690365

9 6 -0.000218408 0.000185755 -0.000222274

10 6 0.000162770 0.000232306 0.000021838

11 6 0.000162770 -0.000232306 0.000021838

12 6 -0.000300204 0.000300204 -0.000000000

13 6 0.000218408 -0.000185755 -0.000222274

14 6 -0.000162770 -0.000232306 0.000021838

15 6 -0.000162770 0.000232306 0.000021838

16 6 0.000218408 0.000185755 -0.000222274

17 7 -0.000078988 -0.000000000 0.000690365

18 6 -0.000300204 -0.000300204 -0.000000000

19 6 0.000185755 0.000218408 0.000222274

20 6 0.000232306 -0.000162770 -0.000021838

21 6 -0.000232306 -0.000162770 -0.000021838

22 6 -0.000185755 0.000218408 0.000222274

23 7 0.000000000 -0.000078988 -0.000690365

24 6 0.000300204 -0.000300204 0.000000000

25 6 -0.000407566 -0.000407566 -0.000000000

26 6 0.000014992 0.000251278 -0.000117258

27 6 -0.000075439 -0.000017073 -0.000100782

28 6 0.000082524 0.000082524 0.000000000

29 6 -0.000017073 -0.000075439 0.000100782

30 6 0.000251278 0.000014992 0.000117258

31 6 -0.000082524 0.000082524 0.000000000

32 6 0.000075439 -0.000017073 -0.000100782

33 6 -0.000014992 0.000251278 -0.000117258

34 6 0.000407566 -0.000407566 0.000000000

35 6 -0.000251278 0.000014992 0.000117258

36 6 0.000017073 -0.000075439 0.000100782

37 6 -0.000407566 0.000407566 -0.000000000

38 6 0.000251278 -0.000014992 0.000117258

39 6 -0.000017073 0.000075439 0.000100782

40 6 0.000082524 -0.000082524 0.000000000

41 6 -0.000075439 0.000017073 -0.000100782

42 6 0.000014992 -0.000251278 -0.000117258

43 6 0.000407566 0.000407566 -0.000000000

44 6 -0.000251278 -0.000014992 0.000117258

45 6 0.000017073 0.000075439 0.000100782

46 6 -0.000082524 -0.000082524 -0.000000000

47 6 0.000075439 0.000017073 -0.000100782

48 6 -0.000014992 -0.000251278 -0.000117258

49 1 0.000020697 0.000055552 0.000022069

50 1 -0.000020697 0.000055552 0.000022069

51 1 0.000055552 0.000020697 -0.000022069

52 1 0.000055552 -0.000020697 -0.000022069

53 1 -0.000055552 -0.000020697 -0.000022069

54 1 -0.000055552 0.000020697 -0.000022069

55 1 0.000020697 -0.000055552 0.000022069

56 1 -0.000020697 -0.000055552 0.000022069

57 1 0.000003113 -0.000025854 -0.000035114

58 1 0.000005288 0.000022680 -0.000025456

59 1 0.000027125 0.000027125 0.000000000

60 1 0.000022680 0.000005288 0.000025456

61 1 -0.000025854 0.000003113 0.000035114

62 1 -0.000027125 0.000027125 -0.000000000

63 1 -0.000005288 0.000022680 -0.000025456

64 1 -0.000003113 -0.000025854 -0.000035114

65 1 0.000025854 0.000003113 0.000035114

66 1 -0.000022680 0.000005288 0.000025456

67 1 -0.000025854 -0.000003113 0.000035114

68 1 0.000022680 -0.000005288 0.000025456

69 1 0.000027125 -0.000027125 0.000000000

70 1 0.000005288 -0.000022680 -0.000025456

71 1 0.000003113 0.000025854 -0.000035114

72 1 0.000025854 -0.000003113 0.000035114

73 1 -0.000022680 -0.000005288 0.000025456

74 1 -0.000027125 -0.000027125 0.000000000

75 1 -0.000005288 -0.000022680 -0.000025456

76 1 -0.000003113 0.000025854 -0.000035114

77 30 0.000000000 0.000000000 0.000000000

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

Cartesian Forces: Max 0.000690365 RMS 0.000168323

Leave Link 716 at Tue Aug 13 18:23:03 2019, MaxMem= 671088640 cpu: 0.1

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.000285063 RMS 0.000069572

Search for a local minimum.

Step number 3 out of a maximum of 462

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

RMS Force = .69572D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3

DE= -9.29D-05 DEPred=-8.24D-05 R= 1.13D+00

TightC=F SS= 1.41D+00 RLast= 8.02D-02 DXNew= 8.4853D-01 2.4053D-01

Trust test= 1.13D+00 RLast= 8.02D-02 DXMaxT set to 5.05D-01

ITU= 1 1 0

Eigenvalues --- 0.00603 0.00755 0.00755 0.00755 0.01174

Eigenvalues --- 0.01318 0.01422 0.01470 0.01470 0.01549

Eigenvalues --- 0.01582 0.01583 0.01583 0.01595 0.01623

Eigenvalues --- 0.01623 0.01623 0.01623 0.01679 0.01701

Eigenvalues --- 0.01701 0.01711 0.01782 0.01782 0.01784

Eigenvalues --- 0.01812 0.01814 0.01814 0.01821 0.01879

Eigenvalues --- 0.01880 0.01880 0.01886 0.01899 0.01899

Eigenvalues --- 0.01915 0.01917 0.02025 0.02025 0.02025

Eigenvalues --- 0.02025 0.02051 0.02058 0.02058 0.02058

Eigenvalues --- 0.02066 0.02066 0.02066 0.02066 0.02089

Eigenvalues --- 0.02089 0.02089 0.02090 0.02101 0.02101

Eigenvalues --- 0.02101 0.02101 0.02104 0.02104 0.02104

Eigenvalues --- 0.02104 0.02106 0.02106 0.02106 0.02106

Eigenvalues --- 0.02107 0.02107 0.02107 0.02107 0.02123

Eigenvalues --- 0.02129 0.02129 0.02132 0.02236 0.12213

Eigenvalues --- 0.12213 0.14171 0.15920 0.15995 0.15995

Eigenvalues --- 0.15995 0.15995 0.15997 0.15997 0.15997

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16009

Eigenvalues --- 0.16941 0.21803 0.21803 0.21996 0.22000

Eigenvalues --- 0.22000 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22000 0.22824 0.22856 0.22888 0.22888

Eigenvalues --- 0.23474 0.23474 0.23474 0.23477 0.24756

Eigenvalues --- 0.24780 0.24780 0.24816 0.24824 0.24905

Eigenvalues --- 0.24934 0.24934 0.24985 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.32293 0.32293 0.32293 0.33934

Eigenvalues --- 0.35010 0.35010 0.35121 0.35135 0.35153

Eigenvalues --- 0.35181 0.35181 0.35181 0.35181 0.35181

Eigenvalues --- 0.35181 0.35181 0.35189 0.35193 0.35193

Eigenvalues --- 0.35193 0.35202 0.35202 0.35202 0.35202

Eigenvalues --- 0.35202 0.35202 0.35202 0.35214 0.35617

Eigenvalues --- 0.35883 0.35883 0.35883 0.35883 0.35883

Eigenvalues --- 0.35883 0.35883 0.35912 0.36240 0.37149

Eigenvalues --- 0.37149 0.37929 0.38999 0.40016 0.40016

Eigenvalues --- 0.41183 0.41221 0.41221 0.41297 0.41297

Eigenvalues --- 0.41297 0.41373 0.41373 0.41373 0.41373

Eigenvalues --- 0.41579 0.42294 0.43125 0.43326 0.43326

Eigenvalues --- 0.44276 0.44942 0.44942 0.44942 0.44942

Eigenvalues --- 0.45182 0.45296 0.45296 0.45296 0.45804

Eigenvalues --- 0.45804 0.45804 0.45804 0.45893 0.45893

Eigenvalues --- 0.45893 0.46792 0.46891 0.47950 0.47950

Eigenvalues --- 0.48890 0.50573 0.50966 0.50966 0.51945

En-DIIS/RFO-DIIS IScMMF= 0 using points: 3 2

RFO step: Lambda=-6.44583173D-06.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 9.29D-05 SmlDif= 1.00D-05

RMS Error= 0.2725046525D-03 NUsed= 2 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.11499 -0.11499

Iteration 1 RMS(Cart)= 0.00560837 RMS(Int)= 0.00001089

Iteration 2 RMS(Cart)= 0.00001869 RMS(Int)= 0.00000279

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000279

ITry= 1 IFail=0 DXMaxC= 1.85D-02 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.10D-05 for atom 62.

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

(Linear) (Quad) (Total)

R1 2.73941 0.00022 0.00015 0.00069 0.00084 2.74025

R2 2.57613 -0.00023 -0.00009 -0.00067 -0.00076 2.57537

R3 2.03912 0.00003 -0.00004 0.00003 -0.00001 2.03911

R4 2.58887 -0.00002 0.00015 0.00007 0.00022 2.58909

R5 2.66723 0.00017 0.00018 0.00047 0.00064 2.66788

R6 2.58887 -0.00002 0.00015 0.00007 0.00022 2.58909

R7 3.94994 0.00008 0.00044 0.00096 0.00140 3.95134

R8 2.73941 0.00022 0.00015 0.00069 0.00084 2.74025

R9 2.66723 0.00017 0.00018 0.00047 0.00064 2.66788

R10 2.03912 0.00003 -0.00004 0.00003 -0.00001 2.03911

R11 2.66723 0.00017 0.00018 0.00047 0.00064 2.66788

R12 2.82380 -0.00017 0.00028 -0.00049 -0.00021 2.82359

R13 2.58887 -0.00002 0.00015 0.00007 0.00022 2.58909

R14 2.73941 0.00022 0.00015 0.00069 0.00084 2.74025

R15 2.58887 -0.00002 0.00015 0.00007 0.00022 2.58909

R16 3.94994 0.00008 0.00044 0.00096 0.00140 3.95134

R17 2.73941 0.00022 0.00015 0.00069 0.00084 2.74025

R18 2.66723 0.00017 0.00018 0.00047 0.00064 2.66788

R19 2.57613 -0.00023 -0.00009 -0.00067 -0.00076 2.57537

R20 2.03912 0.00003 -0.00004 0.00003 -0.00001 2.03911

R21 2.03912 0.00003 -0.00004 0.00003 -0.00001 2.03911

R22 2.66723 0.00017 0.00018 0.00047 0.00064 2.66788

R23 2.82380 -0.00017 0.00028 -0.00049 -0.00021 2.82359

R24 2.73941 0.00022 0.00015 0.00069 0.00084 2.74025

R25 2.58887 -0.00002 0.00015 0.00007 0.00022 2.58909

R26 2.57613 -0.00023 -0.00009 -0.00067 -0.00076 2.57537

R27 2.03912 0.00003 -0.00004 0.00003 -0.00001 2.03911

R28 2.73941 0.00022 0.00015 0.00069 0.00084 2.74025

R29 2.03912 0.00003 -0.00004 0.00003 -0.00001 2.03911

R30 2.58887 -0.00002 0.00015 0.00007 0.00022 2.58909

R31 2.66723 0.00017 0.00018 0.00047 0.00064 2.66788

R32 3.94994 0.00008 0.00044 0.00096 0.00140 3.95134

R33 2.66723 0.00017 0.00018 0.00047 0.00064 2.66788

R34 2.82380 -0.00017 0.00028 -0.00049 -0.00021 2.82359

R35 2.73941 0.00022 0.00015 0.00069 0.00084 2.74025

R36 2.58887 -0.00002 0.00015 0.00007 0.00022 2.58909

R37 2.57613 -0.00023 -0.00009 -0.00067 -0.00076 2.57537

R38 2.03912 0.00003 -0.00004 0.00003 -0.00001 2.03911

R39 2.73941 0.00022 0.00015 0.00069 0.00084 2.74025

R40 2.03912 0.00003 -0.00004 0.00003 -0.00001 2.03911

R41 2.58887 -0.00002 0.00015 0.00007 0.00022 2.58909

R42 2.66723 0.00017 0.00018 0.00047 0.00064 2.66788

R43 3.94994 0.00008 0.00044 0.00096 0.00140 3.95134

R44 2.82380 -0.00017 0.00028 -0.00049 -0.00021 2.82359

R45 2.64554 0.00029 0.00020 0.00077 0.00097 2.64650

R46 2.64554 0.00029 0.00020 0.00077 0.00097 2.64650

R47 2.63231 0.00003 0.00009 0.00005 0.00014 2.63245

R48 2.04946 0.00003 -0.00001 0.00004 0.00002 2.04948

R49 2.63443 0.00015 0.00006 0.00031 0.00037 2.63480

R50 2.05036 0.00003 0.00003 0.00009 0.00012 2.05048

R51 2.63443 0.00015 0.00006 0.00031 0.00037 2.63480

R52 2.05020 0.00004 0.00003 0.00011 0.00013 2.05033

R53 2.63231 0.00003 0.00009 0.00005 0.00014 2.63245

R54 2.05036 0.00003 0.00003 0.00009 0.00012 2.05048

R55 2.04946 0.00003 -0.00001 0.00004 0.00002 2.04948

R56 2.63443 0.00015 0.00006 0.00031 0.00037 2.63480

R57 2.63443 0.00015 0.00006 0.00031 0.00037 2.63480

R58 2.05020 0.00004 0.00003 0.00011 0.00013 2.05033

R59 2.63231 0.00003 0.00009 0.00005 0.00014 2.63245

R60 2.05036 0.00003 0.00003 0.00009 0.00012 2.05048

R61 2.64554 0.00029 0.00020 0.00077 0.00097 2.64650

R62 2.04946 0.00003 -0.00001 0.00004 0.00002 2.04948

R63 2.64554 0.00029 0.00020 0.00077 0.00097 2.64650

R64 2.63231 0.00003 0.00009 0.00005 0.00014 2.63245

R65 2.04946 0.00003 -0.00001 0.00004 0.00002 2.04948

R66 2.05036 0.00003 0.00003 0.00009 0.00012 2.05048

R67 2.64554 0.00029 0.00020 0.00077 0.00097 2.64650

R68 2.64554 0.00029 0.00020 0.00077 0.00097 2.64650

R69 2.63231 0.00003 0.00009 0.00005 0.00014 2.63245

R70 2.04946 0.00003 -0.00001 0.00004 0.00002 2.04948

R71 2.63443 0.00015 0.00006 0.00031 0.00037 2.63480

R72 2.05036 0.00003 0.00003 0.00009 0.00012 2.05048

R73 2.63443 0.00015 0.00006 0.00031 0.00037 2.63480

R74 2.05020 0.00004 0.00003 0.00011 0.00013 2.05033

R75 2.63231 0.00003 0.00009 0.00005 0.00014 2.63245

R76 2.05036 0.00003 0.00003 0.00009 0.00012 2.05048

R77 2.04946 0.00003 -0.00001 0.00004 0.00002 2.04948

R78 2.64554 0.00029 0.00020 0.00077 0.00097 2.64650

R79 2.64554 0.00029 0.00020 0.00077 0.00097 2.64650

R80 2.63231 0.00003 0.00009 0.00005 0.00014 2.63245

R81 2.04946 0.00003 -0.00001 0.00004 0.00002 2.04948

R82 2.63443 0.00015 0.00006 0.00031 0.00037 2.63480

R83 2.05036 0.00003 0.00003 0.00009 0.00012 2.05048

R84 2.63443 0.00015 0.00006 0.00031 0.00037 2.63480

R85 2.05020 0.00004 0.00003 0.00011 0.00013 2.05033

R86 2.63231 0.00003 0.00009 0.00005 0.00014 2.63245

R87 2.05036 0.00003 0.00003 0.00009 0.00012 2.05048

R88 2.04946 0.00003 -0.00001 0.00004 0.00002 2.04948

A1 1.87125 0.00000 0.00010 0.00005 0.00014 1.87139

A2 2.19479 0.00005 0.00001 0.00035 0.00036 2.19514

A3 2.21702 -0.00005 -0.00011 -0.00044 -0.00054 2.21648

A4 1.89571 0.00002 -0.00019 0.00003 -0.00015 1.89556

A5 2.18800 -0.00003 0.00001 -0.00025 -0.00024 2.18776

A6 2.19937 0.00001 0.00017 0.00022 0.00039 2.19976

A7 1.89069 -0.00004 0.00017 -0.00007 0.00009 1.89078

A8 2.19414 0.00002 -0.00008 -0.00038 -0.00047 2.19367

A9 2.19414 0.00002 -0.00008 -0.00038 -0.00047 2.19367

A10 1.89571 0.00002 -0.00019 0.00003 -0.00015 1.89556

A11 2.19937 0.00001 0.00017 0.00022 0.00039 2.19976

A12 2.18800 -0.00003 0.00001 -0.00025 -0.00024 2.18776

A13 1.87125 0.00000 0.00010 0.00005 0.00014 1.87139

A14 2.21702 -0.00005 -0.00011 -0.00044 -0.00054 2.21648

A15 2.19479 0.00005 0.00001 0.00035 0.00036 2.19514

A16 2.20313 -0.00007 -0.00016 -0.00032 -0.00047 2.20266

A17 2.04003 0.00003 0.00008 0.00016 0.00023 2.04026

A18 2.04003 0.00003 0.00008 0.00016 0.00023 2.04026

A19 2.19937 0.00001 0.00017 0.00022 0.00039 2.19976

A20 2.18800 -0.00003 0.00001 -0.00025 -0.00024 2.18776

A21 1.89571 0.00002 -0.00019 0.00003 -0.00015 1.89556

A22 1.89069 -0.00004 0.00017 -0.00007 0.00009 1.89078

A23 2.19414 0.00002 -0.00008 -0.00038 -0.00047 2.19367

A24 2.19414 0.00002 -0.00008 -0.00038 -0.00047 2.19367

A25 1.89571 0.00002 -0.00019 0.00003 -0.00015 1.89556

A26 2.19937 0.00001 0.00017 0.00022 0.00039 2.19976

A27 2.18800 -0.00003 0.00001 -0.00025 -0.00024 2.18776

A28 1.87125 0.00000 0.00010 0.00005 0.00014 1.87139

A29 2.19479 0.00005 0.00001 0.00035 0.00036 2.19514

A30 2.21702 -0.00005 -0.00011 -0.00044 -0.00054 2.21648

A31 1.87125 0.00000 0.00010 0.00005 0.00014 1.87139

A32 2.19479 0.00005 0.00001 0.00035 0.00036 2.19514

A33 2.21702 -0.00005 -0.00011 -0.00044 -0.00054 2.21648

A34 2.20313 -0.00007 -0.00016 -0.00032 -0.00047 2.20266

A35 2.04003 0.00003 0.00008 0.00016 0.00023 2.04026

A36 2.04003 0.00003 0.00008 0.00016 0.00023 2.04026

A37 2.18800 -0.00003 0.00001 -0.00025 -0.00024 2.18776

A38 2.19937 0.00001 0.00017 0.00022 0.00039 2.19976

A39 1.89571 0.00002 -0.00019 0.00003 -0.00015 1.89556

A40 1.87125 0.00000 0.00010 0.00005 0.00014 1.87139

A41 2.19479 0.00005 0.00001 0.00035 0.00036 2.19514

A42 2.21702 -0.00005 -0.00011 -0.00044 -0.00054 2.21648

A43 1.87125 0.00000 0.00010 0.00005 0.00014 1.87139

A44 2.21702 -0.00005 -0.00011 -0.00044 -0.00054 2.21648

A45 2.19479 0.00005 0.00001 0.00035 0.00036 2.19514

A46 1.89571 0.00002 -0.00019 0.00003 -0.00015 1.89556

A47 2.18800 -0.00003 0.00001 -0.00025 -0.00024 2.18776

A48 2.19937 0.00001 0.00017 0.00022 0.00039 2.19976

A49 1.89069 -0.00004 0.00017 -0.00007 0.00009 1.89078

A50 2.19414 0.00002 -0.00008 -0.00038 -0.00047 2.19367

A51 2.19414 0.00002 -0.00008 -0.00038 -0.00047 2.19367

A52 2.20313 -0.00007 -0.00016 -0.00032 -0.00047 2.20266

A53 2.04003 0.00003 0.00008 0.00016 0.00023 2.04026

A54 2.04003 0.00003 0.00008 0.00016 0.00023 2.04026

A55 2.18800 -0.00003 0.00001 -0.00025 -0.00024 2.18776

A56 2.19937 0.00001 0.00017 0.00022 0.00039 2.19976

A57 1.89571 0.00002 -0.00019 0.00003 -0.00015 1.89556

A58 1.87125 0.00000 0.00010 0.00005 0.00014 1.87139

A59 2.19479 0.00005 0.00001 0.00035 0.00036 2.19514

A60 2.21702 -0.00005 -0.00011 -0.00044 -0.00054 2.21648

A61 1.87125 0.00000 0.00010 0.00005 0.00014 1.87139

A62 2.21702 -0.00005 -0.00011 -0.00044 -0.00054 2.21648

A63 2.19479 0.00005 0.00001 0.00035 0.00036 2.19514

A64 1.89571 0.00002 -0.00019 0.00003 -0.00015 1.89556

A65 2.18800 -0.00003 0.00001 -0.00025 -0.00024 2.18776

A66 2.19937 0.00001 0.00017 0.00022 0.00039 2.19976

A67 1.89069 -0.00004 0.00017 -0.00007 0.00009 1.89078

A68 2.19414 0.00002 -0.00008 -0.00038 -0.00047 2.19367

A69 2.19414 0.00002 -0.00008 -0.00038 -0.00047 2.19367

A70 2.20313 -0.00007 -0.00016 -0.00032 -0.00047 2.20266

A71 2.04003 0.00003 0.00008 0.00016 0.00023 2.04026

A72 2.04003 0.00003 0.00008 0.00016 0.00023 2.04026

A73 2.10549 0.00005 0.00008 0.00023 0.00032 2.10581

A74 2.10549 0.00005 0.00008 0.00023 0.00032 2.10581

A75 2.07220 -0.00009 -0.00017 -0.00046 -0.00063 2.07156

A76 2.10589 0.00003 0.00008 0.00020 0.00028 2.10617

A77 2.08369 -0.00002 -0.00008 -0.00018 -0.00027 2.08343

A78 2.09358 -0.00001 0.00000 -0.00003 -0.00003 2.09356

A79 2.09716 0.00001 0.00000 0.00003 0.00003 2.09719

A80 2.08920 -0.00000 0.00005 0.00006 0.00011 2.08931

A81 2.09682 -0.00001 -0.00005 -0.00008 -0.00013 2.09668

A82 2.08808 0.00001 -0.00000 0.00001 0.00001 2.08808

A83 2.09756 -0.00001 0.00000 -0.00000 -0.00000 2.09755

A84 2.09756 -0.00001 0.00000 -0.00000 -0.00000 2.09755

A85 2.09716 0.00001 0.00000 0.00003 0.00003 2.09719

A86 2.09682 -0.00001 -0.00005 -0.00008 -0.00013 2.09668

A87 2.08920 -0.00000 0.00005 0.00006 0.00011 2.08931

A88 2.10589 0.00003 0.00008 0.00020 0.00028 2.10617

A89 2.08369 -0.00002 -0.00008 -0.00018 -0.00027 2.08343

A90 2.09358 -0.00001 0.00000 -0.00003 -0.00003 2.09356

A91 2.08808 0.00001 -0.00000 0.00001 0.00001 2.08808

A92 2.09756 -0.00001 0.00000 -0.00000 -0.00000 2.09755

A93 2.09756 -0.00001 0.00000 -0.00000 -0.00000 2.09755

A94 2.09716 0.00001 0.00000 0.00003 0.00003 2.09719

A95 2.09682 -0.00001 -0.00005 -0.00008 -0.00013 2.09668

A96 2.08920 -0.00000 0.00005 0.00006 0.00011 2.08931

A97 2.10589 0.00003 0.00008 0.00020 0.00028 2.10617

A98 2.09358 -0.00001 0.00000 -0.00003 -0.00003 2.09356

A99 2.08369 -0.00002 -0.00008 -0.00018 -0.00027 2.08343

A100 2.10549 0.00005 0.00008 0.00023 0.00032 2.10581

A101 2.10549 0.00005 0.00008 0.00023 0.00032 2.10581

A102 2.07220 -0.00009 -0.00017 -0.00046 -0.00063 2.07156

A103 2.10589 0.00003 0.00008 0.00020 0.00028 2.10617

A104 2.08369 -0.00002 -0.00008 -0.00018 -0.00027 2.08343

A105 2.09358 -0.00001 0.00000 -0.00003 -0.00003 2.09356

A106 2.09716 0.00001 0.00000 0.00003 0.00003 2.09719

A107 2.09682 -0.00001 -0.00005 -0.00008 -0.00013 2.09668

A108 2.08920 -0.00000 0.00005 0.00006 0.00011 2.08931

A109 2.10549 0.00005 0.00008 0.00023 0.00032 2.10581

A110 2.10549 0.00005 0.00008 0.00023 0.00032 2.10581

A111 2.07220 -0.00009 -0.00017 -0.00046 -0.00063 2.07156

A112 2.10589 0.00003 0.00008 0.00020 0.00028 2.10617

A113 2.08369 -0.00002 -0.00008 -0.00018 -0.00027 2.08343

A114 2.09358 -0.00001 0.00000 -0.00003 -0.00003 2.09356

A115 2.09716 0.00001 0.00000 0.00003 0.00003 2.09719

A116 2.08920 -0.00000 0.00005 0.00006 0.00011 2.08931

A117 2.09682 -0.00001 -0.00005 -0.00008 -0.00013 2.09668

A118 2.08808 0.00001 -0.00000 0.00001 0.00001 2.08808

A119 2.09756 -0.00001 0.00000 -0.00000 -0.00000 2.09755

A120 2.09756 -0.00001 0.00000 -0.00000 -0.00000 2.09755

A121 2.09716 0.00001 0.00000 0.00003 0.00003 2.09719

A122 2.09682 -0.00001 -0.00005 -0.00008 -0.00013 2.09668

A123 2.08920 -0.00000 0.00005 0.00006 0.00011 2.08931

A124 2.10589 0.00003 0.00008 0.00020 0.00028 2.10617

A125 2.08369 -0.00002 -0.00008 -0.00018 -0.00027 2.08343

A126 2.09358 -0.00001 0.00000 -0.00003 -0.00003 2.09356

A127 2.10549 0.00005 0.00008 0.00023 0.00032 2.10581

A128 2.10549 0.00005 0.00008 0.00023 0.00032 2.10581

A129 2.07220 -0.00009 -0.00017 -0.00046 -0.00063 2.07156

A130 2.10589 0.00003 0.00008 0.00020 0.00028 2.10617

A131 2.08369 -0.00002 -0.00008 -0.00018 -0.00027 2.08343

A132 2.09358 -0.00001 0.00000 -0.00003 -0.00003 2.09356

A133 2.09716 0.00001 0.00000 0.00003 0.00003 2.09719

A134 2.08920 -0.00000 0.00005 0.00006 0.00011 2.08931

A135 2.09682 -0.00001 -0.00005 -0.00008 -0.00013 2.09668

A136 2.08808 0.00001 -0.00000 0.00001 0.00001 2.08808

A137 2.09756 -0.00001 0.00000 -0.00000 -0.00000 2.09755

A138 2.09756 -0.00001 0.00000 -0.00000 -0.00000 2.09755

A139 2.09716 0.00001 0.00000 0.00003 0.00003 2.09719

A140 2.09682 -0.00001 -0.00005 -0.00008 -0.00013 2.09668

A141 2.08920 -0.00000 0.00005 0.00006 0.00011 2.08931

A142 2.10589 0.00003 0.00008 0.00020 0.00028 2.10617

A143 2.08369 -0.00002 -0.00008 -0.00018 -0.00027 2.08343

A144 2.09358 -0.00001 0.00000 -0.00003 -0.00003 2.09356

A145 1.57091 0.00000 0.00000 0.00006 0.00007 1.57098

A146 1.57091 0.00000 0.00000 0.00006 0.00007 1.57098

A147 1.57091 0.00000 0.00000 0.00006 0.00007 1.57098

A148 1.57091 0.00000 0.00000 0.00006 0.00007 1.57098

A149 3.14181 0.00000 0.00000 0.00013 0.00015 3.14196

A150 3.14181 0.00000 0.00000 0.00013 0.00015 3.14196

A151 3.12064 -0.00008 -0.00001 -0.00611 -0.00612 3.11452

A152 3.12064 -0.00008 -0.00001 -0.00611 -0.00612 3.11452

D1 0.01027 -0.00005 0.00053 -0.00299 -0.00246 0.00780

D2 3.13696 -0.00002 -0.00035 -0.00230 -0.00264 3.13432

D3 -3.11503 -0.00001 0.00082 -0.00077 0.00005 -3.11498

D4 0.01166 0.00001 -0.00006 -0.00007 -0.00013 0.01154

D5 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D6 -3.12503 0.00003 0.00029 0.00225 0.00254 -3.12249

D7 3.12503 -0.00003 -0.00029 -0.00225 -0.00254 3.12249

D8 0.00000 -0.00000 -0.00000 0.00000 0.00000 0.00000

D9 -0.01675 0.00007 -0.00087 0.00489 0.00402 -0.01273

D10 3.03069 -0.00005 -0.00082 -0.00432 -0.00515 3.02554

D11 3.13986 0.00005 0.00002 0.00419 0.00421 -3.13912

D12 -0.09589 -0.00008 0.00006 -0.00502 -0.00496 -0.10085

D13 -3.07158 0.00001 0.00100 0.00196 0.00296 -3.06862

D14 0.07001 0.00001 0.00100 0.00196 0.00296 0.07297

D15 0.05256 0.00004 -0.00003 0.00277 0.00274 0.05531

D16 -3.08903 0.00004 -0.00003 0.00277 0.00274 -3.08628

D17 0.01675 -0.00007 0.00087 -0.00489 -0.00402 0.01273

D18 -3.13986 -0.00005 -0.00002 -0.00419 -0.00421 3.13912

D19 -3.03069 0.00005 0.00082 0.00432 0.00515 -3.02554

D20 0.09589 0.00008 -0.00006 0.00502 0.00496 0.10085

D21 -3.07604 0.00012 -0.00003 0.00844 0.00841 -3.06764

D22 0.04459 0.00004 -0.00004 0.00232 0.00229 0.04688

D23 -0.04459 -0.00004 0.00004 -0.00232 -0.00229 -0.04688

D24 3.07604 -0.00012 0.00003 -0.00844 -0.00841 3.06764

D25 -0.01027 0.00005 -0.00053 0.00299 0.00246 -0.00780

D26 3.11503 0.00001 -0.00082 0.00077 -0.00005 3.11498

D27 -3.13696 0.00002 0.00035 0.00230 0.00264 -3.13432

D28 -0.01166 -0.00001 0.00006 0.00007 0.00013 -0.01154

D29 -0.05256 -0.00004 0.00003 -0.00277 -0.00274 -0.05531

D30 3.08903 -0.00004 0.00003 -0.00277 -0.00274 3.08628

D31 3.07158 -0.00001 -0.00100 -0.00196 -0.00296 3.06862

D32 -0.07001 -0.00001 -0.00100 -0.00196 -0.00296 -0.07297

D33 -0.05256 -0.00004 0.00003 -0.00277 -0.00274 -0.05531

D34 3.07158 -0.00001 -0.00100 -0.00196 -0.00296 3.06862

D35 3.08903 -0.00004 0.00003 -0.00277 -0.00274 3.08628

D36 -0.07001 -0.00001 -0.00100 -0.00196 -0.00296 -0.07297

D37 -1.13169 0.00003 0.00165 0.00728 0.00893 -1.12276

D38 2.00990 0.00003 0.00165 0.00728 0.00893 2.01883

D39 2.00990 0.00003 0.00165 0.00728 0.00893 2.01883

D40 -1.13169 0.00003 0.00165 0.00728 0.00893 -1.12276

D41 -3.13986 -0.00005 -0.00002 -0.00419 -0.00421 3.13912

D42 0.09589 0.00008 -0.00006 0.00502 0.00496 0.10085

D43 0.01675 -0.00007 0.00087 -0.00489 -0.00402 0.01273

D44 -3.03069 0.00005 0.00082 0.00432 0.00515 -3.02554

D45 -3.13696 0.00002 0.00035 0.00230 0.00264 -3.13432

D46 -0.01166 -0.00001 0.00006 0.00007 0.00013 -0.01154

D47 -0.01027 0.00005 -0.00053 0.00299 0.00246 -0.00780

D48 3.11503 0.00001 -0.00082 0.00077 -0.00005 3.11498

D49 -0.01675 0.00007 -0.00087 0.00489 0.00402 -0.01273

D50 3.13986 0.00005 0.00002 0.00419 0.00421 -3.13912

D51 3.03069 -0.00005 -0.00082 -0.00432 -0.00515 3.02554

D52 -0.09589 -0.00008 0.00006 -0.00502 -0.00496 -0.10085

D53 -0.04459 -0.00004 0.00004 -0.00232 -0.00229 -0.04688

D54 3.07604 -0.00012 0.00003 -0.00844 -0.00841 3.06764

D55 -3.07604 0.00012 -0.00003 0.00844 0.00841 -3.06764

D56 0.04459 0.00004 -0.00004 0.00232 0.00229 0.04688

D57 0.01027 -0.00005 0.00053 -0.00299 -0.00246 0.00780

D58 -3.11503 -0.00001 0.00082 -0.00077 0.00005 -3.11498

D59 3.13696 -0.00002 -0.00035 -0.00230 -0.00264 3.13432

D60 0.01166 0.00001 -0.00006 -0.00007 -0.00013 0.01154

D61 0.05256 0.00004 -0.00003 0.00277 0.00274 0.05531

D62 -3.08903 0.00004 -0.00003 0.00277 0.00274 -3.08628

D63 -3.07158 0.00001 0.00100 0.00196 0.00296 -3.06862

D64 0.07001 0.00001 0.00100 0.00196 0.00296 0.07297

D65 -0.00000 0.00000 0.00000 -0.00000 -0.00000 -0.00000

D66 -3.12503 0.00003 0.00029 0.00225 0.00254 -3.12249

D67 3.12503 -0.00003 -0.00029 -0.00225 -0.00254 3.12249

D68 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D69 -3.07158 0.00001 0.00100 0.00196 0.00296 -3.06862

D70 0.05256 0.00004 -0.00003 0.00277 0.00274 0.05531

D71 0.07001 0.00001 0.00100 0.00196 0.00296 0.07297

D72 -3.08903 0.00004 -0.00003 0.00277 0.00274 -3.08628

D73 1.13169 -0.00003 -0.00165 -0.00728 -0.00893 1.12276

D74 -2.00990 -0.00003 -0.00165 -0.00728 -0.00893 -2.01883

D75 -2.00990 -0.00003 -0.00165 -0.00728 -0.00893 -2.01883

D76 1.13169 -0.00003 -0.00165 -0.00728 -0.00893 1.12276

D77 3.13696 -0.00002 -0.00035 -0.00230 -0.00264 3.13432

D78 0.01166 0.00001 -0.00006 -0.00007 -0.00013 0.01154

D79 0.01027 -0.00004 0.00053 -0.00299 -0.00246 0.00780

D80 -3.11503 -0.00001 0.00082 -0.00077 0.00005 -3.11498

D81 3.13986 0.00005 0.00002 0.00419 0.00421 -3.13912

D82 -0.09589 -0.00008 0.00006 -0.00502 -0.00496 -0.10085

D83 -0.01675 0.00007 -0.00087 0.00489 0.00402 -0.01273

D84 3.03069 -0.00005 -0.00082 -0.00432 -0.00515 3.02554

D85 -0.00000 -0.00000 0.00000 0.00000 -0.00000 -0.00000

D86 -3.12503 0.00003 0.00029 0.00225 0.00254 -3.12249

D87 3.12503 -0.00003 -0.00029 -0.00225 -0.00254 3.12249

D88 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D89 -0.01027 0.00004 -0.00053 0.00299 0.00246 -0.00780

D90 -3.13696 0.00002 0.00035 0.00230 0.00264 -3.13432

D91 3.11503 0.00001 -0.00082 0.00077 -0.00005 3.11498

D92 -0.01166 -0.00001 0.00006 0.00007 0.00013 -0.01154

D93 0.01675 -0.00007 0.00087 -0.00489 -0.00402 0.01273

D94 -3.03069 0.00005 0.00082 0.00432 0.00515 -3.02554

D95 -3.13986 -0.00005 -0.00002 -0.00419 -0.00421 3.13912

D96 0.09589 0.00008 -0.00006 0.00502 0.00496 0.10085

D97 3.07158 -0.00001 -0.00100 -0.00196 -0.00296 3.06862

D98 -0.07001 -0.00001 -0.00100 -0.00196 -0.00296 -0.07297

D99 -0.05256 -0.00004 0.00003 -0.00277 -0.00274 -0.05531

D100 3.08903 -0.00004 0.00003 -0.00277 -0.00274 3.08628

D101 0.04459 0.00004 -0.00004 0.00232 0.00229 0.04688

D102 -3.07604 0.00012 -0.00003 0.00844 0.00841 -3.06764

D103 3.07604 -0.00012 0.00003 -0.00844 -0.00841 3.06764

D104 -0.04459 -0.00004 0.00004 -0.00232 -0.00229 -0.04688

D105 3.07158 -0.00001 -0.00100 -0.00196 -0.00296 3.06862

D106 -0.05256 -0.00004 0.00003 -0.00277 -0.00274 -0.05531

D107 -0.07001 -0.00001 -0.00100 -0.00196 -0.00296 -0.07297

D108 3.08903 -0.00004 0.00003 -0.00277 -0.00274 3.08628

D109 -1.13169 0.00003 0.00165 0.00728 0.00893 -1.12276

D110 2.00990 0.00003 0.00165 0.00728 0.00893 2.01883

D111 2.00990 0.00003 0.00165 0.00728 0.00893 2.01883

D112 -1.13169 0.00003 0.00165 0.00728 0.00893 -1.12276

D113 -3.13696 0.00002 0.00035 0.00230 0.00264 -3.13432

D114 -0.01166 -0.00001 0.00006 0.00007 0.00013 -0.01154

D115 -0.01027 0.00004 -0.00053 0.00299 0.00246 -0.00780

D116 3.11503 0.00001 -0.00082 0.00077 -0.00005 3.11498

D117 -3.13986 -0.00005 -0.00002 -0.00419 -0.00421 3.13912

D118 0.09589 0.00008 -0.00006 0.00502 0.00496 0.10085

D119 0.01675 -0.00007 0.00087 -0.00489 -0.00402 0.01273

D120 -3.03069 0.00005 0.00082 0.00432 0.00515 -3.02554

D121 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D122 3.12503 -0.00003 -0.00029 -0.00225 -0.00254 3.12249

D123 -3.12503 0.00003 0.00029 0.00225 0.00254 -3.12249

D124 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D125 0.01027 -0.00004 0.00053 -0.00299 -0.00246 0.00780

D126 3.13696 -0.00002 -0.00035 -0.00230 -0.00264 3.13432

D127 -3.11503 -0.00001 0.00082 -0.00077 0.00005 -3.11498

D128 0.01166 0.00001 -0.00006 -0.00007 -0.00013 0.01154

D129 -0.01675 0.00007 -0.00087 0.00489 0.00402 -0.01273

D130 3.03069 -0.00005 -0.00082 -0.00432 -0.00515 3.02554

D131 3.13986 0.00005 0.00002 0.00419 0.00421 -3.13912

D132 -0.09589 -0.00008 0.00006 -0.00502 -0.00496 -0.10085

D133 -3.07158 0.00001 0.00100 0.00196 0.00296 -3.06862

D134 0.07001 0.00001 0.00100 0.00196 0.00296 0.07297

D135 0.05256 0.00004 -0.00003 0.00277 0.00274 0.05531

D136 -3.08903 0.00004 -0.00003 0.00277 0.00274 -3.08628

D137 3.07604 -0.00012 0.00003 -0.00844 -0.00841 3.06764

D138 -0.04459 -0.00004 0.00004 -0.00232 -0.00229 -0.04688

D139 0.04459 0.00004 -0.00004 0.00232 0.00229 0.04688

D140 -3.07604 0.00012 -0.00003 0.00844 0.00841 -3.06764

D141 1.13169 -0.00003 -0.00165 -0.00728 -0.00893 1.12276

D142 -2.00990 -0.00003 -0.00165 -0.00728 -0.00893 -2.01883

D143 -2.00990 -0.00003 -0.00165 -0.00728 -0.00893 -2.01883

D144 1.13169 -0.00003 -0.00165 -0.00728 -0.00893 1.12276

D145 -3.14010 0.00000 0.00001 0.00016 0.00017 -3.13993

D146 -0.00595 -0.00002 -0.00019 -0.00104 -0.00123 -0.00718

D147 0.00149 0.00000 0.00001 0.00016 0.00017 0.00166

D148 3.13564 -0.00002 -0.00019 -0.00104 -0.00123 3.13441

D149 -3.14010 0.00000 0.00001 0.00016 0.00017 -3.13993

D150 -0.00595 -0.00002 -0.00019 -0.00104 -0.00123 -0.00718

D151 0.00149 0.00000 0.00001 0.00016 0.00017 0.00166

D152 3.13564 -0.00002 -0.00019 -0.00104 -0.00123 3.13441

D153 -0.00299 -0.00001 -0.00003 -0.00032 -0.00035 -0.00333

D154 3.13580 -0.00001 -0.00008 -0.00041 -0.00049 3.13531

D155 -3.13710 0.00001 0.00018 0.00089 0.00107 -3.13603

D156 0.00169 0.00001 0.00013 0.00080 0.00093 0.00262

D157 0.00148 0.00000 0.00001 0.00016 0.00017 0.00165

D158 -3.14011 0.00000 0.00001 0.00016 0.00017 -3.13994

D159 -3.13729 0.00000 0.00006 0.00025 0.00031 -3.13698

D160 0.00430 0.00000 0.00006 0.00025 0.00031 0.00461

D161 0.00148 0.00000 0.00001 0.00016 0.00017 0.00165

D162 -3.13729 0.00000 0.00006 0.00025 0.00031 -3.13698

D163 -3.14011 0.00000 0.00001 0.00016 0.00017 -3.13994

D164 0.00430 0.00000 0.00006 0.00025 0.00031 0.00461

D165 -0.00299 -0.00001 -0.00003 -0.00032 -0.00035 -0.00333

D166 -3.13710 0.00001 0.00018 0.00089 0.00107 -3.13603

D167 3.13580 -0.00001 -0.00008 -0.00041 -0.00049 3.13531

D168 0.00169 0.00001 0.00013 0.00080 0.00093 0.00262

D169 -0.00148 -0.00000 -0.00001 -0.00016 -0.00017 -0.00165

D170 3.13729 -0.00000 -0.00006 -0.00025 -0.00031 3.13698

D171 3.14011 -0.00000 -0.00001 -0.00016 -0.00017 3.13994

D172 -0.00430 -0.00000 -0.00006 -0.00025 -0.00031 -0.00461

D173 -0.00148 -0.00000 -0.00001 -0.00016 -0.00017 -0.00165

D174 3.13729 -0.00000 -0.00006 -0.00025 -0.00031 3.13698

D175 3.14011 -0.00000 -0.00001 -0.00016 -0.00017 3.13994

D176 -0.00430 -0.00000 -0.00006 -0.00025 -0.00031 -0.00461

D177 0.00299 0.00001 0.00003 0.00032 0.00035 0.00333

D178 3.13710 -0.00001 -0.00018 -0.00089 -0.00107 3.13603

D179 -3.13580 0.00001 0.00008 0.00041 0.00049 -3.13531

D180 -0.00169 -0.00001 -0.00013 -0.00080 -0.00093 -0.00262

D181 3.14010 -0.00000 -0.00001 -0.00016 -0.00017 3.13993

D182 -0.00149 -0.00000 -0.00001 -0.00016 -0.00017 -0.00166

D183 0.00595 0.00002 0.00019 0.00104 0.00123 0.00718

D184 -3.13564 0.00002 0.00019 0.00104 0.00123 -3.13441

D185 3.14010 -0.00000 -0.00001 -0.00016 -0.00017 3.13993

D186 0.00595 0.00002 0.00019 0.00104 0.00123 0.00718

D187 -0.00149 -0.00000 -0.00001 -0.00016 -0.00017 -0.00166

D188 -3.13564 0.00002 0.00019 0.00104 0.00123 -3.13441

D189 0.00299 0.00001 0.00003 0.00032 0.00035 0.00333

D190 -3.13580 0.00001 0.00008 0.00041 0.00049 -3.13531

D191 3.13710 -0.00001 -0.00018 -0.00089 -0.00107 3.13603

D192 -0.00169 -0.00001 -0.00013 -0.00080 -0.00093 -0.00262

D193 3.14010 -0.00000 -0.00001 -0.00016 -0.00017 3.13993

D194 0.00595 0.00002 0.00019 0.00104 0.00123 0.00718

D195 -0.00149 -0.00000 -0.00001 -0.00016 -0.00017 -0.00166

D196 -3.13564 0.00002 0.00019 0.00104 0.00123 -3.13441

D197 3.14010 -0.00000 -0.00001 -0.00016 -0.00017 3.13993

D198 0.00595 0.00002 0.00019 0.00104 0.00123 0.00718

D199 -0.00149 -0.00000 -0.00001 -0.00016 -0.00017 -0.00166

D200 -3.13564 0.00002 0.00019 0.00104 0.00123 -3.13441

D201 0.00299 0.00001 0.00003 0.00032 0.00035 0.00333

D202 -3.13580 0.00001 0.00008 0.00041 0.00049 -3.13531

D203 3.13710 -0.00001 -0.00018 -0.00089 -0.00107 3.13603

D204 -0.00169 -0.00001 -0.00013 -0.00080 -0.00093 -0.00262

D205 -0.00148 -0.00000 -0.00001 -0.00016 -0.00017 -0.00165

D206 3.14011 -0.00000 -0.00001 -0.00016 -0.00017 3.13994

D207 3.13729 -0.00000 -0.00006 -0.00025 -0.00031 3.13698

D208 -0.00430 -0.00000 -0.00006 -0.00025 -0.00031 -0.00461

D209 -0.00148 -0.00000 -0.00001 -0.00016 -0.00017 -0.00165

D210 3.13729 -0.00000 -0.00006 -0.00025 -0.00031 3.13698

D211 3.14011 -0.00000 -0.00001 -0.00016 -0.00017 3.13994

D212 -0.00430 -0.00000 -0.00006 -0.00025 -0.00031 -0.00461

D213 0.00299 0.00001 0.00003 0.00032 0.00035 0.00333

D214 3.13710 -0.00001 -0.00018 -0.00089 -0.00107 3.13603

D215 -3.13580 0.00001 0.00008 0.00041 0.00049 -3.13531

D216 -0.00169 -0.00001 -0.00013 -0.00080 -0.00093 -0.00262

D217 -3.14010 0.00000 0.00001 0.00016 0.00017 -3.13993

D218 -0.00595 -0.00002 -0.00019 -0.00104 -0.00123 -0.00718

D219 0.00149 0.00000 0.00001 0.00016 0.00017 0.00166

D220 3.13564 -0.00002 -0.00019 -0.00104 -0.00123 3.13441

D221 -3.14010 0.00000 0.00001 0.00016 0.00017 -3.13993

D222 -0.00595 -0.00002 -0.00019 -0.00104 -0.00123 -0.00718

D223 0.00149 0.00000 0.00001 0.00016 0.00017 0.00166

D224 3.13564 -0.00002 -0.00019 -0.00104 -0.00123 3.13441

D225 -0.00299 -0.00001 -0.00003 -0.00032 -0.00035 -0.00333

D226 3.13580 -0.00001 -0.00008 -0.00041 -0.00049 3.13531

D227 -3.13710 0.00001 0.00018 0.00089 0.00107 -3.13603

D228 0.00169 0.00001 0.00013 0.00080 0.00093 0.00262

D229 0.00148 0.00000 0.00001 0.00016 0.00017 0.00165

D230 -3.14011 0.00000 0.00001 0.00016 0.00017 -3.13994

D231 -3.13729 0.00000 0.00006 0.00025 0.00031 -3.13698

D232 0.00430 0.00000 0.00006 0.00025 0.00031 0.00461

D233 0.00148 0.00000 0.00001 0.00016 0.00017 0.00165

D234 -3.13729 0.00000 0.00006 0.00025 0.00031 -3.13698

D235 -3.14011 0.00000 0.00001 0.00016 0.00017 -3.13994

D236 0.00430 0.00000 0.00006 0.00025 0.00031 0.00461

D237 -0.00299 -0.00001 -0.00003 -0.00032 -0.00035 -0.00333

D238 -3.13710 0.00001 0.00018 0.00089 0.00107 -3.13603

D239 3.13580 -0.00001 -0.00008 -0.00041 -0.00049 3.13531

D240 0.00169 0.00001 0.00013 0.00080 0.00093 0.00262

Item Value Threshold Converged?

Maximum Force 0.000285 0.000450 YES

RMS Force 0.000070 0.000300 YES

Maximum Displacement 0.018497 0.001800 NO

RMS Displacement 0.005607 0.001200 NO

Predicted change in Energy=-1.780758D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Aug 13 18:23:04 2019, MaxMem= 671088640 cpu: 1.2

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

Stoichiometry C44H28N4Zn

Framework group D2D[O(Zn),2SGD(N2),X(C44H28)]

Deg. of freedom 29

Full point group D2D NOp 8

RotChk: IX=0 Diff= 0.00D+00

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681414 4.271168 0.142832

2 6 0 -1.110766 2.890872 0.028056

3 7 0 0.000000 2.090768 -0.028308

4 6 0 1.110766 2.890872 0.028056

5 6 0 0.681414 4.271168 0.142832

6 6 0 2.452451 2.452451 0.000000

7 6 0 2.890872 1.110766 -0.028056

8 7 0 2.090768 -0.000000 0.028308

9 6 0 2.890872 -1.110766 -0.028056

10 6 0 4.271168 -0.681414 -0.142832

11 6 0 4.271168 0.681414 -0.142832

12 6 0 -2.452451 2.452451 0.000000

13 6 0 -2.890872 1.110766 -0.028056

14 6 0 -4.271168 0.681414 -0.142832

15 6 0 -4.271168 -0.681414 -0.142832

16 6 0 -2.890872 -1.110766 -0.028056

17 7 0 -2.090768 0.000000 0.028308

18 6 0 -2.452451 -2.452451 0.000000

19 6 0 -1.110766 -2.890872 0.028056

20 6 0 -0.681414 -4.271168 0.142832

21 6 0 0.681414 -4.271168 0.142832

22 6 0 1.110766 -2.890872 0.028056

23 7 0 -0.000000 -2.090768 -0.028308

24 6 0 2.452451 -2.452451 0.000000

25 6 0 3.508995 3.508995 -0.000000

26 6 0 3.627837 4.399949 -1.073960

27 6 0 4.613954 5.383874 -1.075310

28 6 0 5.494557 5.494557 -0.000000

29 6 0 5.383874 4.613954 1.075310

30 6 0 4.399949 3.627837 1.073960

31 6 0 -5.494557 5.494557 -0.000000

32 6 0 -4.613954 5.383874 -1.075310

33 6 0 -3.627837 4.399949 -1.073960

34 6 0 -3.508995 3.508995 -0.000000

35 6 0 -4.399949 3.627837 1.073960

36 6 0 -5.383874 4.613954 1.075310

37 6 0 3.508995 -3.508995 -0.000000

38 6 0 4.399949 -3.627837 1.073960

39 6 0 5.383874 -4.613954 1.075310

40 6 0 5.494557 -5.494557 -0.000000

41 6 0 4.613954 -5.383874 -1.075310

42 6 0 3.627837 -4.399949 -1.073960

43 6 0 -3.508995 -3.508995 -0.000000

44 6 0 -4.399949 -3.627837 1.073960

45 6 0 -5.383874 -4.613954 1.075310

46 6 0 -5.494557 -5.494557 -0.000000

47 6 0 -4.613954 -5.383874 -1.075310

48 6 0 -3.627837 -4.399949 -1.073960

49 1 0 -1.330728 5.128509 0.230643

50 1 0 1.330728 5.128509 0.230643

51 1 0 5.128509 -1.330728 -0.230643

52 1 0 5.128509 1.330728 -0.230643

53 1 0 -5.128509 1.330728 -0.230643

54 1 0 -5.128509 -1.330728 -0.230643

55 1 0 -1.330728 -5.128509 0.230643

56 1 0 1.330728 -5.128509 0.230643

57 1 0 2.947942 4.313581 -1.914500

58 1 0 4.695612 6.062217 -1.918255

59 1 0 6.261761 6.261761 0.000000

60 1 0 6.062217 4.695612 1.918255

61 1 0 4.313581 2.947942 1.914500

62 1 0 -6.261761 6.261761 0.000000

63 1 0 -4.695612 6.062217 -1.918255

64 1 0 -2.947942 4.313581 -1.914500

65 1 0 -4.313581 2.947942 1.914500

66 1 0 -6.062217 4.695612 1.918255

67 1 0 4.313581 -2.947942 1.914500

68 1 0 6.062217 -4.695612 1.918255

69 1 0 6.261761 -6.261761 0.000000

70 1 0 4.695612 -6.062217 -1.918255

71 1 0 2.947942 -4.313581 -1.914500

72 1 0 -4.313581 -2.947942 1.914500

73 1 0 -6.062217 -4.695612 1.918255

74 1 0 -6.261761 -6.261761 0.000000

75 1 0 -4.695612 -6.062217 -1.918255

76 1 0 -2.947942 -4.313581 -1.914500

77 30 0 0.000000 0.000000 0.000000

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

Rotational constants (GHZ): 0.0581863 0.0581863 0.0300746

Leave Link 202 at Tue Aug 13 18:23:04 2019, MaxMem= 671088640 cpu: 0.1

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

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

Pseudo-potential data read from rwf file.

There are 272 symmetry adapted cartesian basis functions of A1 symmetry.

There are 243 symmetry adapted cartesian basis functions of A2 symmetry.

There are 254 symmetry adapted cartesian basis functions of B1 symmetry.

There are 254 symmetry adapted cartesian basis functions of B2 symmetry.

There are 256 symmetry adapted basis functions of A1 symmetry.

There are 232 symmetry adapted basis functions of A2 symmetry.

There are 242 symmetry adapted basis functions of B1 symmetry.

There are 242 symmetry adapted basis functions of B2 symmetry.

972 basis functions, 1715 primitive gaussians, 1023 cartesian basis functions

166 alpha electrons 166 beta electrons

nuclear repulsion energy 5737.6745839920 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= 77 NActive= 77 NUniq= 13 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T 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= -0.2224027818 Hartrees.

Nuclear repulsion after empirical dispersion term = 5737.4521812101 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 77.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 77

GePol: Total number of spheres = 77

GePol: Number of exposed spheres = 77 (100.00%)

GePol: Number of points = 5650

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.55D-10

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 248

GePol: Fraction of low-weight points (<1% of avg) = 4.39%

GePol: Cavity surface area = 614.052 Ang\*\*2

GePol: Cavity volume = 630.345 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021393202 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5737.4500418900 Hartrees.

Leave Link 301 at Tue Aug 13 18:23:04 2019, MaxMem= 671088640 cpu: 0.8

(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

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36749 LenP2D= 95258.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 972 RedAO= T EigKep= 6.35D-05 NBF= 256 232 242 242

NBsUse= 972 1.00D-06 EigRej= -1.00D+00 NBFU= 256 232 242 242

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= 952 960 976 976 976 MxSgAt= 77 MxSgA2= 77.

Leave Link 302 at Tue Aug 13 18:23:07 2019, MaxMem= 671088640 cpu: 11.1

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Aug 13 18:23:07 2019, MaxMem= 671088640 cpu: 0.9

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

Initial guess from the checkpoint file: "ZnTPP0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000000 0.000000 -0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

Leave Link 401 at Tue Aug 13 18:23:11 2019, MaxMem= 671088640 cpu: 15.1

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3177123 IEndB= 3177123 NGot= 671088640 MDV= 668975710

LenX= 668975710 LenY= 667928158

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= 530000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 95767500.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.11D-15 for 5642.

Iteration 1 A\*A^-1 deviation from orthogonality is 6.66D-15 for 5634 1298.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.88D-15 for 5642.

Iteration 1 A^-1\*A deviation from orthogonality is 7.67D-14 for 5100 5081.

E= -1978.90401051155

DIIS: error= 7.46D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1978.90401051155 IErMin= 1 ErrMin= 7.46D-04

ErrMax= 7.46D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.55D-04 BMatP= 1.55D-04

IDIUse=3 WtCom= 9.93D-01 WtEn= 7.46D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.443 Goal= None Shift= 0.000

RMSDP=2.21D-05 MaxDP=6.50D-04 OVMax= 3.11D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.21D-05 CP: 1.00D+00

E= -1978.90433328218 Delta-E= -0.000322770629 Rises=F Damp=F

DIIS: error= 1.01D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1978.90433328218 IErMin= 2 ErrMin= 1.01D-04

ErrMax= 1.01D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.20D-06 BMatP= 1.55D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.01D-03

Coeff-Com: -0.676D-01 0.107D+01

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

Coeff: -0.676D-01 0.107D+01

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=3.22D-06 MaxDP=7.52D-05 DE=-3.23D-04 OVMax= 4.94D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.79D-06 CP: 1.00D+00 1.07D+00

E= -1978.90433841381 Delta-E= -0.000005131634 Rises=F Damp=F

DIIS: error= 6.23D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1978.90433841381 IErMin= 3 ErrMin= 6.23D-05

ErrMax= 6.23D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.64D-07 BMatP= 2.20D-06

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

Coeff-Com: -0.313D-01 0.394D+00 0.637D+00

Coeff: -0.313D-01 0.394D+00 0.637D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.11D-06 MaxDP=4.55D-05 DE=-5.13D-06 OVMax= 1.70D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.00D-06 CP: 1.00D+00 1.08D+00 8.34D-01

E= -1978.90433887655 Delta-E= -0.000000462739 Rises=F Damp=F

DIIS: error= 3.18D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1978.90433887655 IErMin= 4 ErrMin= 3.18D-05

ErrMax= 3.18D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.91D-07 BMatP= 6.64D-07

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

Coeff-Com: -0.858D-02 0.832D-01 0.354D+00 0.572D+00

Coeff: -0.858D-02 0.832D-01 0.354D+00 0.572D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=4.31D-07 MaxDP=3.10D-05 DE=-4.63D-07 OVMax= 8.69D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.37D-07 CP: 1.00D+00 1.08D+00 8.82D-01 7.74D-01

E= -1978.90433902174 Delta-E= -0.000000145182 Rises=F Damp=F

DIIS: error= 7.72D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1978.90433902174 IErMin= 5 ErrMin= 7.72D-06

ErrMax= 7.72D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.34D-08 BMatP= 1.91D-07

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

Coeff-Com: -0.988D-03-0.304D-02 0.117D+00 0.314D+00 0.572D+00

Coeff: -0.988D-03-0.304D-02 0.117D+00 0.314D+00 0.572D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.74D-07 MaxDP=1.29D-05 DE=-1.45D-07 OVMax= 3.34D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.24D-07 CP: 1.00D+00 1.08D+00 8.95D-01 8.05D-01 6.69D-01

E= -1978.90433904067 Delta-E= -0.000000018930 Rises=F Damp=F

DIIS: error= 3.70D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1978.90433904067 IErMin= 6 ErrMin= 3.70D-06

ErrMax= 3.70D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.24D-09 BMatP= 2.34D-08

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

Coeff-Com: 0.680D-03-0.146D-01 0.112D-01 0.880D-01 0.324D+00 0.591D+00

Coeff: 0.680D-03-0.146D-01 0.112D-01 0.880D-01 0.324D+00 0.591D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=6.16D-08 MaxDP=3.44D-06 DE=-1.89D-08 OVMax= 7.69D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.28D-08 CP: 1.00D+00 1.08D+00 9.03D-01 8.14D-01 7.16D-01

CP: 6.02D-01

E= -1978.90433904300 Delta-E= -0.000000002333 Rises=F Damp=F

DIIS: error= 7.41D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1978.90433904300 IErMin= 7 ErrMin= 7.41D-07

ErrMax= 7.41D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.27D-10 BMatP= 3.24D-09

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

Coeff-Com: 0.383D-03-0.747D-02 0.196D-02 0.358D-01 0.153D+00 0.311D+00

Coeff-Com: 0.506D+00

Coeff: 0.383D-03-0.747D-02 0.196D-02 0.358D-01 0.153D+00 0.311D+00

Coeff: 0.506D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.13D-08 MaxDP=7.55D-07 DE=-2.33D-09 OVMax= 2.52D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 9.92D-09 CP: 1.00D+00 1.08D+00 9.03D-01 8.17D-01 7.15D-01

CP: 6.06D-01 8.05D-01

E= -1978.90433904325 Delta-E= -0.000000000255 Rises=F Damp=F

DIIS: error= 1.86D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1978.90433904325 IErMin= 8 ErrMin= 1.86D-07

ErrMax= 1.86D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.22D-12 BMatP= 1.27D-10

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

Coeff-Com: 0.623D-04-0.985D-03-0.978D-03 0.199D-02 0.181D-01 0.471D-01

Coeff-Com: 0.208D+00 0.727D+00

Coeff: 0.623D-04-0.985D-03-0.978D-03 0.199D-02 0.181D-01 0.471D-01

Coeff: 0.208D+00 0.727D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=3.53D-09 MaxDP=1.82D-07 DE=-2.55D-10 OVMax= 7.56D-07

Error on total polarization charges = 0.08499

SCF Done: E(RB3LYP) = -1978.90433904 A.U. after 8 cycles

NFock= 8 Conv=0.35D-08 -V/T= 1.9793

KE= 2.020692814015D+03 PE=-1.615699921292D+04 EE= 6.419952017969D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.34

(included in total energy above)

Leave Link 502 at Tue Aug 13 18:28:40 2019, MaxMem= 671088640 cpu: 1314.5

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36749 LenP2D= 95258.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 178

Leave Link 701 at Tue Aug 13 18:29:27 2019, MaxMem= 671088640 cpu: 187.2

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

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

Leave Link 702 at Tue Aug 13 18:29:27 2019, MaxMem= 671088640 cpu: 0.1

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 0 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Tue Aug 13 18:30:18 2019, MaxMem= 671088640 cpu: 203.8

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

Dipole =-6.63469280D-13 9.11271059D-13 7.14983628D-14

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000106944 -0.000099148 0.000112971

2 6 0.000161756 0.000001967 -0.000048262

3 7 0.000000000 -0.000018881 -0.000009245

4 6 -0.000161756 0.000001967 -0.000048262

5 6 0.000106944 -0.000099148 0.000112971

6 6 0.000168987 0.000168987 -0.000000000

7 6 0.000001967 -0.000161756 0.000048262

8 7 -0.000018881 0.000000000 0.000009245

9 6 0.000001967 0.000161756 0.000048262

10 6 -0.000099148 -0.000106944 -0.000112971

11 6 -0.000099148 0.000106944 -0.000112971

12 6 -0.000168987 0.000168987 -0.000000000

13 6 -0.000001967 -0.000161756 0.000048262

14 6 0.000099148 0.000106944 -0.000112971

15 6 0.000099148 -0.000106944 -0.000112971

16 6 -0.000001967 0.000161756 0.000048262

17 7 0.000018881 0.000000000 0.000009245

18 6 -0.000168987 -0.000168987 0.000000000

19 6 0.000161756 -0.000001967 -0.000048262

20 6 -0.000106944 0.000099148 0.000112971

21 6 0.000106944 0.000099148 0.000112971

22 6 -0.000161756 -0.000001967 -0.000048262

23 7 -0.000000000 0.000018881 -0.000009245

24 6 0.000168987 -0.000168987 -0.000000000

25 6 -0.000136927 -0.000136927 -0.000000000

26 6 0.000078037 0.000007020 0.000048901

27 6 -0.000039137 -0.000069236 0.000034798

28 6 -0.000004063 -0.000004063 0.000000000

29 6 -0.000069236 -0.000039137 -0.000034798

30 6 0.000007020 0.000078037 -0.000048901

31 6 0.000004063 -0.000004063 0.000000000

32 6 0.000039137 -0.000069236 0.000034798

33 6 -0.000078037 0.000007020 0.000048901

34 6 0.000136927 -0.000136927 0.000000000

35 6 -0.000007020 0.000078037 -0.000048901

36 6 0.000069236 -0.000039137 -0.000034798

37 6 -0.000136927 0.000136927 0.000000000

38 6 0.000007020 -0.000078037 -0.000048901

39 6 -0.000069236 0.000039137 -0.000034798

40 6 -0.000004063 0.000004063 0.000000000

41 6 -0.000039137 0.000069236 0.000034798

42 6 0.000078037 -0.000007020 0.000048901

43 6 0.000136927 0.000136927 -0.000000000

44 6 -0.000007020 -0.000078037 -0.000048901

45 6 0.000069236 0.000039137 -0.000034798

46 6 0.000004063 0.000004063 -0.000000000

47 6 0.000039137 0.000069236 0.000034798

48 6 -0.000078037 -0.000007020 0.000048901

49 1 -0.000008080 0.000022149 -0.000007694

50 1 0.000008080 0.000022149 -0.000007694

51 1 0.000022149 -0.000008080 0.000007694

52 1 0.000022149 0.000008080 0.000007694

53 1 -0.000022149 0.000008080 0.000007694

54 1 -0.000022149 -0.000008080 0.000007694

55 1 -0.000008080 -0.000022149 -0.000007694

56 1 0.000008080 -0.000022149 -0.000007694

57 1 -0.000001776 0.000007566 -0.000011208

58 1 -0.000013320 -0.000012959 0.000004063

59 1 -0.000010025 -0.000010025 0.000000000

60 1 -0.000012959 -0.000013320 -0.000004063

61 1 0.000007566 -0.000001776 0.000011208

62 1 0.000010025 -0.000010025 -0.000000000

63 1 0.000013320 -0.000012959 0.000004063

64 1 0.000001776 0.000007566 -0.000011208

65 1 -0.000007566 -0.000001776 0.000011208

66 1 0.000012959 -0.000013320 -0.000004063

67 1 0.000007566 0.000001776 0.000011208

68 1 -0.000012959 0.000013320 -0.000004063

69 1 -0.000010025 0.000010025 -0.000000000

70 1 -0.000013320 0.000012959 0.000004063

71 1 -0.000001776 -0.000007566 -0.000011208

72 1 -0.000007566 0.000001776 0.000011208

73 1 0.000012959 0.000013320 -0.000004063

74 1 0.000010025 0.000010025 -0.000000000

75 1 0.000013320 0.000012959 0.000004063

76 1 0.000001776 -0.000007566 -0.000011208

77 30 -0.000000000 -0.000000000 0.000000000

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

Cartesian Forces: Max 0.000168987 RMS 0.000066424

Leave Link 716 at Tue Aug 13 18:30:18 2019, MaxMem= 671088640 cpu: 0.1

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.000275519 RMS 0.000048184

Search for a local minimum.

Step number 4 out of a maximum of 462

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

RMS Force = .48184D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4

DE= -1.48D-05 DEPred=-1.78D-05 R= 8.31D-01

TightC=F SS= 1.41D+00 RLast= 5.60D-02 DXNew= 8.4853D-01 1.6815D-01

Trust test= 8.31D-01 RLast= 5.60D-02 DXMaxT set to 5.05D-01

ITU= 1 1 1 0

Eigenvalues --- 0.00527 0.00755 0.00755 0.00755 0.01174

Eigenvalues --- 0.01176 0.01318 0.01473 0.01473 0.01554

Eigenvalues --- 0.01582 0.01583 0.01583 0.01595 0.01623

Eigenvalues --- 0.01623 0.01623 0.01623 0.01680 0.01703

Eigenvalues --- 0.01703 0.01708 0.01783 0.01783 0.01785

Eigenvalues --- 0.01812 0.01815 0.01815 0.01822 0.01879

Eigenvalues --- 0.01880 0.01880 0.01886 0.01899 0.01899

Eigenvalues --- 0.01917 0.02006 0.02025 0.02025 0.02025

Eigenvalues --- 0.02025 0.02058 0.02058 0.02058 0.02066

Eigenvalues --- 0.02066 0.02066 0.02066 0.02074 0.02089

Eigenvalues --- 0.02089 0.02089 0.02090 0.02101 0.02101

Eigenvalues --- 0.02101 0.02101 0.02104 0.02104 0.02104

Eigenvalues --- 0.02104 0.02106 0.02106 0.02106 0.02107

Eigenvalues --- 0.02107 0.02107 0.02107 0.02107 0.02123

Eigenvalues --- 0.02129 0.02129 0.02131 0.02964 0.12211

Eigenvalues --- 0.12211 0.14170 0.15905 0.15994 0.15994

Eigenvalues --- 0.15994 0.15994 0.15996 0.15996 0.15997

Eigenvalues --- 0.15997 0.15999 0.15999 0.15999 0.15999

Eigenvalues --- 0.15999 0.15999 0.15999 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16012

Eigenvalues --- 0.17292 0.21787 0.21788 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22009 0.22824 0.22856 0.22887 0.22887

Eigenvalues --- 0.23329 0.23474 0.23474 0.23474 0.24749

Eigenvalues --- 0.24767 0.24767 0.24787 0.24795 0.24928

Eigenvalues --- 0.24928 0.24934 0.24984 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.32293 0.32293 0.32293 0.33748

Eigenvalues --- 0.35010 0.35010 0.35102 0.35135 0.35154

Eigenvalues --- 0.35181 0.35181 0.35181 0.35181 0.35181

Eigenvalues --- 0.35181 0.35181 0.35189 0.35193 0.35193

Eigenvalues --- 0.35193 0.35202 0.35202 0.35202 0.35202

Eigenvalues --- 0.35202 0.35202 0.35202 0.35231 0.35559

Eigenvalues --- 0.35883 0.35883 0.35883 0.35883 0.35883

Eigenvalues --- 0.35883 0.35883 0.36071 0.36239 0.37148

Eigenvalues --- 0.37148 0.38141 0.38999 0.40017 0.40017

Eigenvalues --- 0.41219 0.41219 0.41221 0.41299 0.41299

Eigenvalues --- 0.41299 0.41374 0.41374 0.41374 0.41374

Eigenvalues --- 0.41579 0.42293 0.43125 0.43326 0.43326

Eigenvalues --- 0.44669 0.44942 0.44942 0.44942 0.44942

Eigenvalues --- 0.45178 0.45296 0.45296 0.45296 0.45804

Eigenvalues --- 0.45804 0.45804 0.45804 0.45893 0.45893

Eigenvalues --- 0.45893 0.46889 0.47944 0.47944 0.48485

Eigenvalues --- 0.48889 0.50572 0.50966 0.50966 0.51719

En-DIIS/RFO-DIIS IScMMF= 0 using points: 4 3 2

RFO step: Lambda=-3.07691739D-06.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=F DC= 9.29D-05 SmlDif= 1.00D-05

RMS Error= 0.1755723129D-03 NUsed= 3 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.80473 0.29894 -0.10367

Iteration 1 RMS(Cart)= 0.00512205 RMS(Int)= 0.00000544

Iteration 2 RMS(Cart)= 0.00001031 RMS(Int)= 0.00000090

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000090

ITry= 1 IFail=0 DXMaxC= 2.55D-02 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.65D-06 for atom 69.

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

(Linear) (Quad) (Total)

R1 2.74025 -0.00009 -0.00003 0.00014 0.00011 2.74036

R2 2.57537 0.00003 0.00007 -0.00028 -0.00021 2.57516

R3 2.03911 0.00002 -0.00004 0.00005 0.00001 2.03912

R4 2.58909 -0.00014 0.00009 -0.00026 -0.00017 2.58892

R5 2.66788 -0.00005 0.00003 0.00000 0.00004 2.66791

R6 2.58909 -0.00014 0.00009 -0.00026 -0.00017 2.58892

R7 3.95134 -0.00012 0.00012 -0.00036 -0.00024 3.95110

R8 2.74025 -0.00009 -0.00003 0.00014 0.00011 2.74036

R9 2.66788 -0.00005 0.00003 0.00000 0.00004 2.66791

R10 2.03911 0.00002 -0.00004 0.00005 0.00001 2.03912

R11 2.66788 -0.00005 0.00003 0.00000 0.00004 2.66791

R12 2.82359 -0.00028 0.00029 -0.00102 -0.00073 2.82286

R13 2.58909 -0.00014 0.00009 -0.00026 -0.00017 2.58892

R14 2.74025 -0.00009 -0.00003 0.00014 0.00011 2.74036

R15 2.58909 -0.00014 0.00009 -0.00026 -0.00017 2.58892

R16 3.95134 -0.00012 0.00012 -0.00036 -0.00024 3.95110

R17 2.74025 -0.00009 -0.00003 0.00014 0.00011 2.74036

R18 2.66788 -0.00005 0.00003 0.00000 0.00004 2.66791

R19 2.57537 0.00003 0.00007 -0.00028 -0.00021 2.57516

R20 2.03911 0.00002 -0.00004 0.00005 0.00001 2.03912

R21 2.03911 0.00002 -0.00004 0.00005 0.00001 2.03912

R22 2.66788 -0.00005 0.00003 0.00000 0.00004 2.66791

R23 2.82359 -0.00028 0.00029 -0.00102 -0.00073 2.82286

R24 2.74025 -0.00009 -0.00003 0.00014 0.00011 2.74036

R25 2.58909 -0.00014 0.00009 -0.00026 -0.00017 2.58892

R26 2.57537 0.00004 0.00007 -0.00028 -0.00021 2.57516

R27 2.03911 0.00002 -0.00004 0.00005 0.00001 2.03912

R28 2.74025 -0.00009 -0.00003 0.00014 0.00011 2.74036

R29 2.03911 0.00002 -0.00004 0.00005 0.00001 2.03912

R30 2.58909 -0.00014 0.00009 -0.00026 -0.00017 2.58892

R31 2.66788 -0.00005 0.00003 0.00000 0.00004 2.66791

R32 3.95134 -0.00012 0.00012 -0.00036 -0.00024 3.95110

R33 2.66788 -0.00005 0.00003 0.00000 0.00004 2.66791

R34 2.82359 -0.00028 0.00029 -0.00102 -0.00073 2.82286

R35 2.74025 -0.00009 -0.00003 0.00014 0.00011 2.74036

R36 2.58909 -0.00014 0.00009 -0.00026 -0.00017 2.58892

R37 2.57537 0.00004 0.00007 -0.00028 -0.00021 2.57516

R38 2.03911 0.00002 -0.00004 0.00005 0.00001 2.03912

R39 2.74025 -0.00009 -0.00003 0.00014 0.00011 2.74036

R40 2.03911 0.00002 -0.00004 0.00005 0.00001 2.03912

R41 2.58909 -0.00014 0.00009 -0.00026 -0.00017 2.58892

R42 2.66788 -0.00005 0.00003 0.00000 0.00004 2.66791

R43 3.95134 -0.00012 0.00012 -0.00036 -0.00024 3.95110

R44 2.82359 -0.00028 0.00029 -0.00102 -0.00073 2.82286

R45 2.64650 -0.00007 -0.00001 0.00015 0.00014 2.64664

R46 2.64650 -0.00007 -0.00001 0.00015 0.00014 2.64664

R47 2.63245 -0.00011 0.00005 -0.00024 -0.00018 2.63227

R48 2.04948 0.00001 -0.00002 0.00001 -0.00001 2.04948

R49 2.63480 -0.00004 -0.00002 0.00001 -0.00000 2.63480

R50 2.05048 -0.00001 -0.00000 -0.00001 -0.00001 2.05047

R51 2.63480 -0.00004 -0.00002 0.00001 -0.00000 2.63480

R52 2.05033 -0.00001 -0.00000 -0.00001 -0.00001 2.05033

R53 2.63245 -0.00011 0.00005 -0.00024 -0.00018 2.63227

R54 2.05048 -0.00001 -0.00000 -0.00001 -0.00001 2.05047

R55 2.04948 0.00001 -0.00002 0.00001 -0.00001 2.04948

R56 2.63480 -0.00004 -0.00002 0.00001 -0.00000 2.63480

R57 2.63480 -0.00004 -0.00002 0.00001 -0.00000 2.63480

R58 2.05033 -0.00001 -0.00000 -0.00001 -0.00001 2.05033

R59 2.63245 -0.00011 0.00005 -0.00024 -0.00018 2.63227

R60 2.05048 -0.00001 -0.00000 -0.00001 -0.00001 2.05047

R61 2.64650 -0.00007 -0.00001 0.00015 0.00014 2.64664

R62 2.04948 0.00001 -0.00002 0.00001 -0.00001 2.04948

R63 2.64650 -0.00007 -0.00001 0.00015 0.00014 2.64664

R64 2.63245 -0.00011 0.00005 -0.00024 -0.00018 2.63227

R65 2.04948 0.00001 -0.00002 0.00001 -0.00001 2.04948

R66 2.05048 -0.00001 -0.00000 -0.00001 -0.00001 2.05047

R67 2.64650 -0.00007 -0.00001 0.00015 0.00014 2.64664

R68 2.64650 -0.00007 -0.00001 0.00015 0.00014 2.64664

R69 2.63245 -0.00011 0.00005 -0.00024 -0.00018 2.63227

R70 2.04948 0.00001 -0.00002 0.00001 -0.00001 2.04948

R71 2.63480 -0.00004 -0.00002 0.00001 -0.00000 2.63480

R72 2.05048 -0.00001 -0.00000 -0.00001 -0.00001 2.05047

R73 2.63480 -0.00004 -0.00002 0.00001 -0.00000 2.63480

R74 2.05033 -0.00001 -0.00000 -0.00001 -0.00001 2.05033

R75 2.63245 -0.00011 0.00005 -0.00024 -0.00018 2.63227

R76 2.05048 -0.00001 -0.00000 -0.00001 -0.00001 2.05047

R77 2.04948 0.00001 -0.00002 0.00001 -0.00001 2.04948

R78 2.64650 -0.00007 -0.00001 0.00015 0.00014 2.64664

R79 2.64650 -0.00007 -0.00001 0.00015 0.00014 2.64664

R80 2.63245 -0.00011 0.00005 -0.00024 -0.00018 2.63227

R81 2.04948 0.00001 -0.00002 0.00001 -0.00001 2.04948

R82 2.63480 -0.00004 -0.00002 0.00001 -0.00000 2.63480

R83 2.05048 -0.00001 -0.00000 -0.00001 -0.00001 2.05047

R84 2.63480 -0.00004 -0.00002 0.00001 -0.00000 2.63480

R85 2.05033 -0.00001 -0.00000 -0.00001 -0.00001 2.05033

R86 2.63245 -0.00011 0.00005 -0.00024 -0.00018 2.63227

R87 2.05048 -0.00001 -0.00000 -0.00001 -0.00001 2.05047

R88 2.04948 0.00001 -0.00002 0.00001 -0.00001 2.04948

A1 1.87139 -0.00004 0.00006 -0.00009 -0.00003 1.87136

A2 2.19514 0.00003 -0.00006 0.00025 0.00019 2.19533

A3 2.21648 0.00002 0.00001 -0.00016 -0.00015 2.21633

A4 1.89556 0.00005 -0.00014 0.00015 0.00001 1.89557

A5 2.18776 -0.00003 0.00006 -0.00011 -0.00005 2.18771

A6 2.19976 -0.00001 0.00007 -0.00004 0.00003 2.19978

A7 1.89078 -0.00001 0.00014 -0.00015 -0.00001 1.89077

A8 2.19367 0.00001 0.00002 -0.00012 -0.00011 2.19356

A9 2.19367 0.00001 0.00002 -0.00012 -0.00011 2.19356

A10 1.89556 0.00005 -0.00014 0.00015 0.00001 1.89557

A11 2.19976 -0.00001 0.00007 -0.00004 0.00003 2.19978

A12 2.18776 -0.00003 0.00006 -0.00011 -0.00005 2.18771

A13 1.87139 -0.00004 0.00006 -0.00009 -0.00003 1.87136

A14 2.21648 0.00002 0.00001 -0.00016 -0.00015 2.21633

A15 2.19514 0.00003 -0.00006 0.00025 0.00019 2.19533

A16 2.20266 0.00001 -0.00005 -0.00026 -0.00031 2.20235

A17 2.04026 -0.00000 0.00002 0.00013 0.00016 2.04042

A18 2.04026 -0.00000 0.00002 0.00013 0.00016 2.04042

A19 2.19976 -0.00001 0.00007 -0.00004 0.00003 2.19978

A20 2.18776 -0.00003 0.00006 -0.00011 -0.00005 2.18771

A21 1.89556 0.00005 -0.00014 0.00015 0.00001 1.89557

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A152 3.11452 0.00007 0.00119 0.00002 0.00121 3.11573

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D2 3.13432 0.00004 0.00020 0.00077 0.00097 3.13530

D3 -3.11498 0.00001 0.00073 0.00032 0.00105 -3.11393

D4 0.01154 0.00001 -0.00003 0.00061 0.00058 0.01212

D5 0.00000 -0.00000 0.00000 0.00000 -0.00000 0.00000

D6 -3.12249 -0.00003 -0.00023 -0.00017 -0.00040 -3.12289

D7 3.12249 0.00003 0.00023 0.00017 0.00040 3.12289

D8 -0.00000 0.00000 -0.00000 -0.00000 0.00000 0.00000

D9 -0.01273 -0.00008 -0.00157 -0.00079 -0.00236 -0.01509

D10 3.02554 -0.00007 0.00026 -0.00484 -0.00458 3.02096

D11 -3.13912 -0.00007 -0.00081 -0.00108 -0.00188 -3.14100

D12 -0.10085 -0.00007 0.00102 -0.00513 -0.00410 -0.10495

D13 -3.06862 0.00004 0.00033 0.00248 0.00280 -3.06582

D14 0.07297 0.00004 0.00033 0.00248 0.00280 0.07578

D15 0.05531 0.00004 -0.00056 0.00281 0.00225 0.05756

D16 -3.08628 0.00004 -0.00056 0.00281 0.00225 -3.08403

D17 0.01273 0.00008 0.00157 0.00079 0.00236 0.01509

D18 3.13912 0.00007 0.00081 0.00108 0.00188 3.14100

D19 -3.02554 0.00007 -0.00026 0.00484 0.00458 -3.02096

D20 0.10085 0.00007 -0.00102 0.00513 0.00410 0.10495

D21 -3.06764 -0.00003 -0.00167 0.00236 0.00069 -3.06695

D22 0.04688 0.00003 -0.00048 0.00238 0.00190 0.04878

D23 -0.04688 -0.00003 0.00048 -0.00238 -0.00190 -0.04878

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D25 -0.00780 -0.00005 -0.00096 -0.00049 -0.00145 -0.00925

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D27 -3.13432 -0.00004 -0.00020 -0.00077 -0.00097 -3.13530

D28 -0.01154 -0.00001 0.00003 -0.00061 -0.00058 -0.01212

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D30 3.08628 -0.00004 0.00056 -0.00281 -0.00225 3.08403

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D35 3.08628 -0.00004 0.00056 -0.00281 -0.00225 3.08403

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D37 -1.12276 -0.00002 -0.00026 0.00133 0.00107 -1.12169

D38 2.01883 -0.00002 -0.00026 0.00133 0.00107 2.01990

D39 2.01883 -0.00002 -0.00026 0.00133 0.00107 2.01990

D40 -1.12276 -0.00002 -0.00026 0.00133 0.00107 -1.12169

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D42 0.10085 0.00007 -0.00102 0.00513 0.00410 0.10495

D43 0.01273 0.00008 0.00157 0.00079 0.00236 0.01509

D44 -3.02554 0.00007 -0.00026 0.00484 0.00458 -3.02096

D45 -3.13432 -0.00004 -0.00020 -0.00077 -0.00097 -3.13530

D46 -0.01154 -0.00001 0.00003 -0.00061 -0.00058 -0.01212

D47 -0.00780 -0.00005 -0.00096 -0.00049 -0.00145 -0.00925

D48 3.11498 -0.00001 -0.00073 -0.00032 -0.00105 3.11393

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D51 3.02554 -0.00007 0.00026 -0.00484 -0.00458 3.02096

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D54 3.06764 0.00003 0.00167 -0.00236 -0.00069 3.06695

D55 -3.06764 -0.00003 -0.00167 0.00236 0.00069 -3.06695

D56 0.04688 0.00003 -0.00048 0.00238 0.00190 0.04878

D57 0.00780 0.00005 0.00096 0.00049 0.00145 0.00925

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D62 -3.08628 0.00004 -0.00056 0.00281 0.00225 -3.08403

D63 -3.06862 0.00004 0.00033 0.00248 0.00280 -3.06582

D64 0.07297 0.00004 0.00033 0.00248 0.00280 0.07578

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D68 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D69 -3.06862 0.00004 0.00033 0.00248 0.00280 -3.06582

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D71 0.07297 0.00004 0.00033 0.00248 0.00280 0.07578

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D74 -2.01883 0.00002 0.00026 -0.00133 -0.00107 -2.01990

D75 -2.01883 0.00002 0.00026 -0.00133 -0.00107 -2.01990

D76 1.12276 0.00002 0.00026 -0.00133 -0.00107 1.12169

D77 3.13432 0.00004 0.00020 0.00077 0.00097 3.13530

D78 0.01154 0.00001 -0.00003 0.00061 0.00058 0.01212

D79 0.00780 0.00005 0.00096 0.00049 0.00145 0.00925

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D83 -0.01273 -0.00008 -0.00157 -0.00079 -0.00236 -0.01509

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D88 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

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D90 -3.13432 -0.00004 -0.00020 -0.00077 -0.00097 -3.13530

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D95 3.13912 0.00007 0.00081 0.00108 0.00188 3.14100

D96 0.10085 0.00007 -0.00102 0.00513 0.00410 0.10495

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D104 -0.04688 -0.00003 0.00048 -0.00238 -0.00190 -0.04878

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D107 -0.07297 -0.00004 -0.00033 -0.00248 -0.00280 -0.07578

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D119 0.01273 0.00008 0.00157 0.00079 0.00236 0.01509

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D136 -3.08628 0.00004 -0.00056 0.00281 0.00225 -3.08403

D137 3.06764 0.00003 0.00167 -0.00236 -0.00069 3.06695

D138 -0.04688 -0.00003 0.00048 -0.00238 -0.00190 -0.04878

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D141 1.12276 0.00002 0.00026 -0.00133 -0.00107 1.12169

D142 -2.01883 0.00002 0.00026 -0.00133 -0.00107 -2.01990

D143 -2.01883 0.00002 0.00026 -0.00133 -0.00107 -2.01990

D144 1.12276 0.00002 0.00026 -0.00133 -0.00107 1.12169

D145 -3.13993 -0.00000 -0.00002 0.00007 0.00005 -3.13988

D146 -0.00718 0.00000 0.00007 -0.00047 -0.00040 -0.00758

D147 0.00166 -0.00000 -0.00002 0.00007 0.00005 0.00171

D148 3.13441 0.00000 0.00007 -0.00047 -0.00040 3.13401

D149 -3.13993 -0.00000 -0.00002 0.00007 0.00005 -3.13988

D150 -0.00718 0.00000 0.00007 -0.00047 -0.00040 -0.00758

D151 0.00166 -0.00000 -0.00002 0.00007 0.00005 0.00171

D152 3.13441 0.00000 0.00007 -0.00047 -0.00040 3.13401

D153 -0.00333 0.00000 0.00004 -0.00013 -0.00009 -0.00342

D154 3.13531 0.00000 0.00002 -0.00015 -0.00012 3.13519

D155 -3.13603 -0.00000 -0.00005 0.00040 0.00035 -3.13567

D156 0.00262 0.00000 -0.00007 0.00039 0.00032 0.00294

D157 0.00165 -0.00000 -0.00002 0.00007 0.00004 0.00170

D158 -3.13994 -0.00000 -0.00002 0.00007 0.00004 -3.13989

D159 -3.13698 -0.00000 -0.00000 0.00008 0.00008 -3.13690

D160 0.00461 -0.00000 -0.00000 0.00008 0.00008 0.00469

D161 0.00165 -0.00000 -0.00002 0.00007 0.00004 0.00170

D162 -3.13698 -0.00000 -0.00000 0.00008 0.00008 -3.13690

D163 -3.13994 -0.00000 -0.00002 0.00007 0.00004 -3.13989

D164 0.00461 -0.00000 -0.00000 0.00008 0.00008 0.00469

D165 -0.00333 0.00000 0.00004 -0.00013 -0.00009 -0.00342

D166 -3.13603 -0.00000 -0.00005 0.00040 0.00035 -3.13567

D167 3.13531 0.00000 0.00002 -0.00015 -0.00012 3.13519

D168 0.00262 0.00000 -0.00007 0.00039 0.00032 0.00294

D169 -0.00165 0.00000 0.00002 -0.00007 -0.00004 -0.00170

D170 3.13698 0.00000 0.00000 -0.00008 -0.00008 3.13690

D171 3.13994 0.00000 0.00002 -0.00007 -0.00004 3.13989

D172 -0.00461 0.00000 0.00000 -0.00008 -0.00008 -0.00469

D173 -0.00165 0.00000 0.00002 -0.00007 -0.00004 -0.00170

D174 3.13698 0.00000 0.00000 -0.00008 -0.00008 3.13690

D175 3.13994 0.00000 0.00002 -0.00007 -0.00004 3.13989

D176 -0.00461 0.00000 0.00000 -0.00008 -0.00008 -0.00469

D177 0.00333 -0.00000 -0.00004 0.00013 0.00009 0.00342

D178 3.13603 0.00000 0.00005 -0.00040 -0.00035 3.13567

D179 -3.13531 -0.00000 -0.00002 0.00015 0.00012 -3.13519

D180 -0.00262 -0.00000 0.00007 -0.00039 -0.00032 -0.00294

D181 3.13993 0.00000 0.00002 -0.00007 -0.00005 3.13988

D182 -0.00166 0.00000 0.00002 -0.00007 -0.00005 -0.00171

D183 0.00718 -0.00000 -0.00007 0.00047 0.00040 0.00758

D184 -3.13441 -0.00000 -0.00007 0.00047 0.00040 -3.13401

D185 3.13993 0.00000 0.00002 -0.00007 -0.00005 3.13988

D186 0.00718 -0.00000 -0.00007 0.00047 0.00040 0.00758

D187 -0.00166 0.00000 0.00002 -0.00007 -0.00005 -0.00171

D188 -3.13441 -0.00000 -0.00007 0.00047 0.00040 -3.13401

D189 0.00333 -0.00000 -0.00004 0.00013 0.00009 0.00342

D190 -3.13531 -0.00000 -0.00002 0.00015 0.00012 -3.13519

D191 3.13603 0.00000 0.00005 -0.00040 -0.00035 3.13567

D192 -0.00262 -0.00000 0.00007 -0.00039 -0.00032 -0.00294

D193 3.13993 0.00000 0.00002 -0.00007 -0.00005 3.13988

D194 0.00718 -0.00000 -0.00007 0.00047 0.00040 0.00758

D195 -0.00166 0.00000 0.00002 -0.00007 -0.00005 -0.00171

D196 -3.13441 -0.00000 -0.00007 0.00047 0.00040 -3.13401

D197 3.13993 0.00000 0.00002 -0.00007 -0.00005 3.13988

D198 0.00718 -0.00000 -0.00007 0.00047 0.00040 0.00758

D199 -0.00166 0.00000 0.00002 -0.00007 -0.00005 -0.00171

D200 -3.13441 -0.00000 -0.00007 0.00047 0.00040 -3.13401

D201 0.00333 -0.00000 -0.00004 0.00013 0.00009 0.00342

D202 -3.13531 -0.00000 -0.00002 0.00015 0.00012 -3.13519

D203 3.13603 0.00000 0.00005 -0.00040 -0.00035 3.13567

D204 -0.00262 -0.00000 0.00007 -0.00039 -0.00032 -0.00294

D205 -0.00165 0.00000 0.00002 -0.00007 -0.00004 -0.00170

D206 3.13994 0.00000 0.00002 -0.00007 -0.00004 3.13989

D207 3.13698 0.00000 0.00000 -0.00008 -0.00008 3.13690

D208 -0.00461 0.00000 0.00000 -0.00008 -0.00008 -0.00469

D209 -0.00165 0.00000 0.00002 -0.00007 -0.00004 -0.00170

D210 3.13698 0.00000 0.00000 -0.00008 -0.00008 3.13690

D211 3.13994 0.00000 0.00002 -0.00007 -0.00004 3.13989

D212 -0.00461 0.00000 0.00000 -0.00008 -0.00008 -0.00469

D213 0.00333 -0.00000 -0.00004 0.00013 0.00009 0.00342

D214 3.13603 0.00000 0.00005 -0.00040 -0.00035 3.13567

D215 -3.13531 -0.00000 -0.00002 0.00015 0.00012 -3.13519

D216 -0.00262 -0.00000 0.00007 -0.00039 -0.00032 -0.00294

D217 -3.13993 -0.00000 -0.00002 0.00007 0.00005 -3.13988

D218 -0.00718 0.00000 0.00007 -0.00047 -0.00040 -0.00758

D219 0.00166 -0.00000 -0.00002 0.00007 0.00005 0.00171

D220 3.13441 0.00000 0.00007 -0.00047 -0.00040 3.13401

D221 -3.13993 -0.00000 -0.00002 0.00007 0.00005 -3.13988

D222 -0.00718 0.00000 0.00007 -0.00047 -0.00040 -0.00758

D223 0.00166 -0.00000 -0.00002 0.00007 0.00005 0.00171

D224 3.13441 0.00000 0.00007 -0.00047 -0.00040 3.13401

D225 -0.00333 0.00000 0.00004 -0.00013 -0.00009 -0.00342

D226 3.13531 0.00000 0.00002 -0.00015 -0.00012 3.13519

D227 -3.13603 -0.00000 -0.00005 0.00040 0.00035 -3.13567

D228 0.00262 0.00000 -0.00007 0.00039 0.00032 0.00294

D229 0.00165 -0.00000 -0.00002 0.00007 0.00004 0.00170

D230 -3.13994 -0.00000 -0.00002 0.00007 0.00004 -3.13989

D231 -3.13698 -0.00000 -0.00000 0.00008 0.00008 -3.13690

D232 0.00461 -0.00000 -0.00000 0.00008 0.00008 0.00469

D233 0.00165 -0.00000 -0.00002 0.00007 0.00004 0.00170

D234 -3.13698 -0.00000 -0.00000 0.00008 0.00008 -3.13690

D235 -3.13994 -0.00000 -0.00002 0.00007 0.00004 -3.13989

D236 0.00461 -0.00000 -0.00000 0.00008 0.00008 0.00469

D237 -0.00333 0.00000 0.00004 -0.00013 -0.00009 -0.00342

D238 -3.13603 -0.00000 -0.00005 0.00040 0.00035 -3.13567

D239 3.13531 0.00000 0.00002 -0.00015 -0.00012 3.13519

D240 0.00262 0.00000 -0.00007 0.00039 0.00032 0.00294

Item Value Threshold Converged?

Maximum Force 0.000276 0.000450 YES

RMS Force 0.000048 0.000300 YES

Maximum Displacement 0.025519 0.001800 NO

RMS Displacement 0.005122 0.001200 NO

Predicted change in Energy=-7.289353D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Aug 13 18:30:18 2019, MaxMem= 671088640 cpu: 1.5

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

Stoichiometry C44H28N4Zn

Framework group D2D[O(Zn),2SGD(N2),X(C44H28)]

Deg. of freedom 29

Full point group D2D NOp 8

RotChk: IX=0 Diff= 0.00D+00

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681358 4.270371 0.152597

2 6 0 -1.110689 2.890571 0.031255

3 7 0 0.000000 2.090656 -0.027037

4 6 0 1.110689 2.890571 0.031255

5 6 0 0.681358 4.270371 0.152597

6 6 0 2.452408 2.452408 0.000000

7 6 0 2.890571 1.110689 -0.031255

8 7 0 2.090656 -0.000000 0.027037

9 6 0 2.890571 -1.110689 -0.031255

10 6 0 4.270371 -0.681358 -0.152597

11 6 0 4.270371 0.681358 -0.152597

12 6 0 -2.452408 2.452408 0.000000

13 6 0 -2.890571 1.110689 -0.031255

14 6 0 -4.270371 0.681358 -0.152597

15 6 0 -4.270371 -0.681358 -0.152597

16 6 0 -2.890571 -1.110689 -0.031255

17 7 0 -2.090656 0.000000 0.027037

18 6 0 -2.452408 -2.452408 0.000000

19 6 0 -1.110689 -2.890571 0.031255

20 6 0 -0.681358 -4.270371 0.152597

21 6 0 0.681358 -4.270371 0.152597

22 6 0 1.110689 -2.890571 0.031255

23 7 0 -0.000000 -2.090656 -0.027037

24 6 0 2.452408 -2.452408 0.000000

25 6 0 3.508679 3.508679 -0.000000

26 6 0 3.624897 4.402486 -1.071972

27 6 0 4.610980 5.386310 -1.073343

28 6 0 5.494310 5.494310 -0.000000

29 6 0 5.386310 4.610980 1.073343

30 6 0 4.402486 3.624897 1.071972

31 6 0 -5.494310 5.494310 -0.000000

32 6 0 -4.610980 5.386310 -1.073343

33 6 0 -3.624897 4.402486 -1.071972

34 6 0 -3.508679 3.508679 -0.000000

35 6 0 -4.402486 3.624897 1.071972

36 6 0 -5.386310 4.610980 1.073343

37 6 0 3.508679 -3.508679 -0.000000

38 6 0 4.402486 -3.624897 1.071972

39 6 0 5.386310 -4.610980 1.073343

40 6 0 5.494310 -5.494310 -0.000000

41 6 0 4.610980 -5.386310 -1.073343

42 6 0 3.624897 -4.402486 -1.071972

43 6 0 -3.508679 -3.508679 -0.000000

44 6 0 -4.402486 -3.624897 1.071972

45 6 0 -5.386310 -4.610980 1.073343

46 6 0 -5.494310 -5.494310 -0.000000

47 6 0 -4.610980 -5.386310 -1.073343

48 6 0 -3.624897 -4.402486 -1.071972

49 1 0 -1.330544 5.127425 0.244147

50 1 0 1.330544 5.127425 0.244147

51 1 0 5.127425 -1.330544 -0.244147

52 1 0 5.127425 1.330544 -0.244147

53 1 0 -5.127425 1.330544 -0.244147

54 1 0 -5.127425 -1.330544 -0.244147

55 1 0 -1.330544 -5.127425 0.244147

56 1 0 1.330544 -5.127425 0.244147

57 1 0 2.943115 4.318061 -1.911177

58 1 0 4.690535 6.066715 -1.914819

59 1 0 6.261510 6.261510 -0.000000

60 1 0 6.066715 4.690535 1.914819

61 1 0 4.318061 2.943115 1.911177

62 1 0 -6.261510 6.261510 -0.000000

63 1 0 -4.690535 6.066715 -1.914819

64 1 0 -2.943115 4.318061 -1.911177

65 1 0 -4.318061 2.943115 1.911177

66 1 0 -6.066715 4.690535 1.914819

67 1 0 4.318061 -2.943115 1.911177

68 1 0 6.066715 -4.690535 1.914819

69 1 0 6.261510 -6.261510 -0.000000

70 1 0 4.690535 -6.066715 -1.914819

71 1 0 2.943115 -4.318061 -1.911177

72 1 0 -4.318061 -2.943115 1.911177

73 1 0 -6.066715 -4.690535 1.914819

74 1 0 -6.261510 -6.261510 -0.000000

75 1 0 -4.690535 -6.066715 -1.914819

76 1 0 -2.943115 -4.318061 -1.911177

77 30 0 0.000000 0.000000 0.000000

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

Rotational constants (GHZ): 0.0581954 0.0581954 0.0300771

Leave Link 202 at Tue Aug 13 18:30:19 2019, MaxMem= 671088640 cpu: 0.1

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

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

Pseudo-potential data read from rwf file.

There are 272 symmetry adapted cartesian basis functions of A1 symmetry.

There are 243 symmetry adapted cartesian basis functions of A2 symmetry.

There are 254 symmetry adapted cartesian basis functions of B1 symmetry.

There are 254 symmetry adapted cartesian basis functions of B2 symmetry.

There are 256 symmetry adapted basis functions of A1 symmetry.

There are 232 symmetry adapted basis functions of A2 symmetry.

There are 242 symmetry adapted basis functions of B1 symmetry.

There are 242 symmetry adapted basis functions of B2 symmetry.

972 basis functions, 1715 primitive gaussians, 1023 cartesian basis functions

166 alpha electrons 166 beta electrons

nuclear repulsion energy 5737.9517347930 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= 77 NActive= 77 NUniq= 13 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T 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= -0.2224007858 Hartrees.

Nuclear repulsion after empirical dispersion term = 5737.7293340073 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 77.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 77

GePol: Total number of spheres = 77

GePol: Number of exposed spheres = 77 (100.00%)

GePol: Number of points = 5658

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.58D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 264

GePol: Fraction of low-weight points (<1% of avg) = 4.67%

GePol: Cavity surface area = 614.240 Ang\*\*2

GePol: Cavity volume = 630.333 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021402758 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5737.7271937315 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

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36749 LenP2D= 95258.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 972 RedAO= T EigKep= 6.36D-05 NBF= 256 232 242 242

NBsUse= 972 1.00D-06 EigRej= -1.00D+00 NBFU= 256 232 242 242

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= 952 960 976 976 976 MxSgAt= 77 MxSgA2= 77.

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Aug 13 18:30:23 2019, MaxMem= 671088640 cpu: 1.3

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

Initial guess from the checkpoint file: "ZnTPP0.chk"

B after Tr= -0.000000 -0.000000 0.000000

Rot= 1.000000 -0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

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

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

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

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

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

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

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

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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= -1979.25494726007

Leave Link 401 at Tue Aug 13 18:30:33 2019, MaxMem= 671088640 cpu: 40.2

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3177123 IEndB= 3177123 NGot= 671088640 MDV= 668975710

LenX= 668975710 LenY= 667928158

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= 530000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 96038892.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.66D-15 for 5655.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.55D-15 for 5642 1282.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.44D-15 for 5655.

Iteration 1 A^-1\*A deviation from orthogonality is 2.01D-13 for 5133 5086.

E= -1978.90416063916

DIIS: error= 4.19D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1978.90416063916 IErMin= 1 ErrMin= 4.19D-04

ErrMax= 4.19D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.87D-05 BMatP= 8.87D-05

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.19D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.443 Goal= None Shift= 0.000

RMSDP=1.29D-05 MaxDP=3.95D-04 OVMax= 1.94D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.29D-05 CP: 1.00D+00

E= -1978.90434455454 Delta-E= -0.000183915373 Rises=F Damp=F

DIIS: error= 5.83D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1978.90434455454 IErMin= 2 ErrMin= 5.83D-05

ErrMax= 5.83D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.20D-06 BMatP= 8.87D-05

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

Coeff-Com: -0.701D-01 0.107D+01

Coeff: -0.701D-01 0.107D+01

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=2.30D-06 MaxDP=5.64D-05 DE=-1.84D-04 OVMax= 2.98D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.92D-06 CP: 1.00D+00 1.10D+00

E= -1978.90434746781 Delta-E= -0.000002913273 Rises=F Damp=F

DIIS: error= 1.45D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1978.90434746781 IErMin= 3 ErrMin= 1.45D-05

ErrMax= 1.45D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.84D-07 BMatP= 1.20D-06

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

Coeff-Com: -0.242D-01 0.294D+00 0.730D+00

Coeff: -0.242D-01 0.294D+00 0.730D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=6.43D-07 MaxDP=4.09D-05 DE=-2.91D-06 OVMax= 7.89D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.77D-07 CP: 1.00D+00 1.11D+00 8.81D-01

E= -1978.90434757089 Delta-E= -0.000000103082 Rises=F Damp=F

DIIS: error= 1.64D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1978.90434757089 IErMin= 3 ErrMin= 1.45D-05

ErrMax= 1.64D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.46D-08 BMatP= 1.84D-07

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

Coeff-Com: -0.780D-02 0.757D-01 0.422D+00 0.510D+00

Coeff: -0.780D-02 0.757D-01 0.422D+00 0.510D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=2.95D-07 MaxDP=2.50D-05 DE=-1.03D-07 OVMax= 5.43D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.36D-07 CP: 1.00D+00 1.11D+00 9.08D-01 7.12D-01

E= -1978.90434764627 Delta-E= -0.000000075381 Rises=F Damp=F

DIIS: error= 4.46D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1978.90434764627 IErMin= 5 ErrMin= 4.46D-06

ErrMax= 4.46D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.53D-09 BMatP= 9.46D-08

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

Coeff-Com: -0.163D-03-0.109D-01 0.949D-01 0.263D+00 0.653D+00

Coeff: -0.163D-03-0.109D-01 0.949D-01 0.263D+00 0.653D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.17D-07 MaxDP=5.91D-06 DE=-7.54D-08 OVMax= 2.17D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.75D-08 CP: 1.00D+00 1.11D+00 9.31D-01 7.75D-01 6.75D-01

E= -1978.90434765265 Delta-E= -0.000000006378 Rises=F Damp=F

DIIS: error= 1.58D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1978.90434765265 IErMin= 6 ErrMin= 1.58D-06

ErrMax= 1.58D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.62D-09 BMatP= 8.53D-09

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

Coeff-Com: 0.679D-03-0.145D-01 0.136D-01 0.105D+00 0.396D+00 0.500D+00

Coeff: 0.679D-03-0.145D-01 0.136D-01 0.105D+00 0.396D+00 0.500D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=3.77D-08 MaxDP=1.94D-06 DE=-6.38D-09 OVMax= 7.17D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.34D-08 CP: 1.00D+00 1.11D+00 9.34D-01 7.70D-01 7.25D-01

CP: 5.23D-01

E= -1978.90434765421 Delta-E= -0.000000001563 Rises=F Damp=F

DIIS: error= 2.39D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1978.90434765421 IErMin= 7 ErrMin= 2.39D-07

ErrMax= 2.39D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.75D-11 BMatP= 1.62D-09

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

Coeff-Com: 0.269D-03-0.529D-02 0.208D-02 0.329D-01 0.137D+00 0.195D+00

Coeff-Com: 0.638D+00

Coeff: 0.269D-03-0.529D-02 0.208D-02 0.329D-01 0.137D+00 0.195D+00

Coeff: 0.638D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=5.30D-09 MaxDP=3.93D-07 DE=-1.56D-09 OVMax= 6.20D-07

Error on total polarization charges = 0.08496

SCF Done: E(RB3LYP) = -1978.90434765 A.U. after 7 cycles

NFock= 7 Conv=0.53D-08 -V/T= 1.9793

KE= 2.020697744816D+03 PE=-1.615755794871D+04 EE= 6.420228662508D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.34

(included in total energy above)

Leave Link 502 at Tue Aug 13 18:35:17 2019, MaxMem= 671088640 cpu: 1133.9

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36749 LenP2D= 95258.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 180

Leave Link 701 at Tue Aug 13 18:36:04 2019, MaxMem= 671088640 cpu: 187.1

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

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

Leave Link 702 at Tue Aug 13 18:36:04 2019, MaxMem= 671088640 cpu: 0.1

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 0 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Tue Aug 13 18:36:52 2019, MaxMem= 671088640 cpu: 191.5

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

Dipole = 6.03961325D-13-1.17239551D-12-5.01820807D-14

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000207590 -0.000107955 0.000006596

2 6 0.000084050 0.000070661 0.000158052

3 7 -0.000000000 -0.000008002 -0.000242868

4 6 -0.000084050 0.000070661 0.000158052

5 6 0.000207590 -0.000107955 0.000006596

6 6 0.000024186 0.000024186 0.000000000

7 6 0.000070661 -0.000084050 -0.000158052

8 7 -0.000008002 0.000000000 0.000242868

9 6 0.000070661 0.000084050 -0.000158052

10 6 -0.000107955 -0.000207590 -0.000006596

11 6 -0.000107955 0.000207590 -0.000006596

12 6 -0.000024186 0.000024186 -0.000000000

13 6 -0.000070661 -0.000084050 -0.000158052

14 6 0.000107955 0.000207590 -0.000006596

15 6 0.000107955 -0.000207590 -0.000006596

16 6 -0.000070661 0.000084050 -0.000158052

17 7 0.000008002 -0.000000000 0.000242868

18 6 -0.000024186 -0.000024186 -0.000000000

19 6 0.000084050 -0.000070661 0.000158052

20 6 -0.000207590 0.000107955 0.000006596

21 6 0.000207590 0.000107955 0.000006596

22 6 -0.000084050 -0.000070661 0.000158052

23 7 0.000000000 0.000008002 -0.000242868

24 6 0.000024186 -0.000024186 -0.000000000

25 6 0.000028925 0.000028925 0.000000000

26 6 0.000017093 -0.000084629 0.000061313

27 6 0.000009819 -0.000020628 0.000031445

28 6 -0.000005573 -0.000005573 -0.000000000

29 6 -0.000020628 0.000009819 -0.000031445

30 6 -0.000084629 0.000017093 -0.000061313

31 6 0.000005573 -0.000005573 -0.000000000

32 6 -0.000009819 -0.000020628 0.000031445

33 6 -0.000017093 -0.000084629 0.000061313

34 6 -0.000028925 0.000028925 -0.000000000

35 6 0.000084629 0.000017093 -0.000061313

36 6 0.000020628 0.000009819 -0.000031445

37 6 0.000028925 -0.000028925 -0.000000000

38 6 -0.000084629 -0.000017093 -0.000061313

39 6 -0.000020628 -0.000009819 -0.000031445

40 6 -0.000005573 0.000005573 -0.000000000

41 6 0.000009819 0.000020628 0.000031445

42 6 0.000017093 0.000084629 0.000061313

43 6 -0.000028925 -0.000028925 -0.000000000

44 6 0.000084629 -0.000017093 -0.000061313

45 6 0.000020628 -0.000009819 -0.000031445

46 6 0.000005573 0.000005573 0.000000000

47 6 -0.000009819 0.000020628 0.000031445

48 6 -0.000017093 0.000084629 0.000061313

49 1 -0.000033818 0.000009517 -0.000012606

50 1 0.000033818 0.000009517 -0.000012606

51 1 0.000009517 -0.000033818 0.000012606

52 1 0.000009517 0.000033818 0.000012606

53 1 -0.000009517 0.000033818 0.000012606

54 1 -0.000009517 -0.000033818 0.000012606

55 1 -0.000033818 -0.000009517 -0.000012606

56 1 0.000033818 -0.000009517 -0.000012606

57 1 -0.000017522 0.000014622 -0.000005291

58 1 -0.000010274 -0.000008888 0.000001114

59 1 -0.000008833 -0.000008833 0.000000000

60 1 -0.000008888 -0.000010274 -0.000001114

61 1 0.000014622 -0.000017522 0.000005291

62 1 0.000008833 -0.000008833 -0.000000000

63 1 0.000010274 -0.000008888 0.000001114

64 1 0.000017522 0.000014622 -0.000005291

65 1 -0.000014622 -0.000017522 0.000005291

66 1 0.000008888 -0.000010274 -0.000001114

67 1 0.000014622 0.000017522 0.000005291

68 1 -0.000008888 0.000010274 -0.000001114

69 1 -0.000008833 0.000008833 0.000000000

70 1 -0.000010274 0.000008888 0.000001114

71 1 -0.000017522 -0.000014622 -0.000005291

72 1 -0.000014622 0.000017522 0.000005291

73 1 0.000008888 0.000010274 -0.000001114

74 1 0.000008833 0.000008833 -0.000000000

75 1 0.000010274 0.000008888 0.000001114

76 1 0.000017522 -0.000014622 -0.000005291

77 30 0.000000000 -0.000000000 -0.000000000

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

Cartesian Forces: Max 0.000242868 RMS 0.000069066

Leave Link 716 at Tue Aug 13 18:36:52 2019, MaxMem= 671088640 cpu: 0.1

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.000170438 RMS 0.000036242

Search for a local minimum.

Step number 5 out of a maximum of 462

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

RMS Force = .36242D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

DE= -8.61D-06 DEPred=-7.29D-06 R= 1.18D+00

TightC=F SS= 1.41D+00 RLast= 2.61D-02 DXNew= 8.4853D-01 7.8393D-02

Trust test= 1.18D+00 RLast= 2.61D-02 DXMaxT set to 5.05D-01

ITU= 1 1 1 1 0

Eigenvalues --- 0.00429 0.00755 0.00755 0.00755 0.00957

Eigenvalues --- 0.01174 0.01318 0.01474 0.01474 0.01556

Eigenvalues --- 0.01582 0.01583 0.01583 0.01595 0.01623

Eigenvalues --- 0.01623 0.01623 0.01623 0.01668 0.01680

Eigenvalues --- 0.01704 0.01704 0.01783 0.01783 0.01785

Eigenvalues --- 0.01812 0.01815 0.01815 0.01822 0.01879

Eigenvalues --- 0.01880 0.01880 0.01886 0.01899 0.01899

Eigenvalues --- 0.01917 0.01931 0.02025 0.02025 0.02025

Eigenvalues --- 0.02025 0.02058 0.02058 0.02058 0.02066

Eigenvalues --- 0.02066 0.02066 0.02066 0.02089 0.02089

Eigenvalues --- 0.02089 0.02089 0.02099 0.02101 0.02101

Eigenvalues --- 0.02101 0.02101 0.02104 0.02104 0.02104

Eigenvalues --- 0.02104 0.02106 0.02106 0.02106 0.02106

Eigenvalues --- 0.02107 0.02107 0.02107 0.02107 0.02123

Eigenvalues --- 0.02129 0.02129 0.02131 0.03616 0.12211

Eigenvalues --- 0.12211 0.14170 0.15993 0.15994 0.15994

Eigenvalues --- 0.15994 0.15994 0.15997 0.15997 0.15997

Eigenvalues --- 0.15999 0.15999 0.15999 0.15999 0.15999

Eigenvalues --- 0.15999 0.15999 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16013 0.16178

Eigenvalues --- 0.17076 0.21778 0.21778 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22004 0.22822 0.22855 0.22886 0.22886

Eigenvalues --- 0.23474 0.23474 0.23474 0.23532 0.24747

Eigenvalues --- 0.24762 0.24762 0.24776 0.24784 0.24924

Eigenvalues --- 0.24924 0.24983 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25256 0.32293 0.32293 0.32293 0.33204

Eigenvalues --- 0.35009 0.35009 0.35133 0.35153 0.35159

Eigenvalues --- 0.35181 0.35181 0.35181 0.35181 0.35181

Eigenvalues --- 0.35181 0.35181 0.35191 0.35193 0.35193

Eigenvalues --- 0.35193 0.35202 0.35202 0.35202 0.35202

Eigenvalues --- 0.35202 0.35202 0.35202 0.35217 0.35779

Eigenvalues --- 0.35883 0.35883 0.35883 0.35883 0.35883

Eigenvalues --- 0.35883 0.35883 0.35997 0.36239 0.37148

Eigenvalues --- 0.37148 0.38351 0.38997 0.40016 0.40016

Eigenvalues --- 0.41217 0.41217 0.41299 0.41299 0.41299

Eigenvalues --- 0.41373 0.41373 0.41373 0.41373 0.41556

Eigenvalues --- 0.41578 0.42292 0.43125 0.43326 0.43326

Eigenvalues --- 0.44873 0.44942 0.44942 0.44942 0.44942

Eigenvalues --- 0.45296 0.45296 0.45296 0.45804 0.45804

Eigenvalues --- 0.45804 0.45804 0.45893 0.45893 0.45893

Eigenvalues --- 0.45970 0.46888 0.47939 0.47939 0.48490

Eigenvalues --- 0.48887 0.50571 0.50965 0.50965 0.52687

En-DIIS/RFO-DIIS IScMMF= 0 using points: 5 4 3 2

RFO step: Lambda=-1.42895045D-06.

NNeg= 0 NP= 4 Switch= 2.50D-03 Rises=F DC= 9.29D-05 SmlDif= 1.00D-05

RMS Error= 0.1265730740D-03 NUsed= 4 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.77427 -0.58579 -0.32331 0.13483

Iteration 1 RMS(Cart)= 0.00532274 RMS(Int)= 0.00000651

Iteration 2 RMS(Cart)= 0.00001165 RMS(Int)= 0.00000228

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000228

ITry= 1 IFail=0 DXMaxC= 2.41D-02 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.24D-06 for atom 69.

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

(Linear) (Quad) (Total)

R1 2.74036 -0.00012 0.00007 -0.00027 -0.00020 2.74016

R2 2.57516 0.00017 -0.00020 0.00051 0.00031 2.57547

R3 2.03912 0.00003 0.00005 0.00001 0.00007 2.03919

R4 2.58892 -0.00007 -0.00026 0.00009 -0.00017 2.58875

R5 2.66791 -0.00006 -0.00006 0.00002 -0.00004 2.66787

R6 2.58892 -0.00007 -0.00026 0.00009 -0.00017 2.58875

R7 3.95110 -0.00006 -0.00044 0.00036 -0.00008 3.95102

R8 2.74036 -0.00012 0.00007 -0.00027 -0.00020 2.74016

R9 2.66791 -0.00006 -0.00006 0.00002 -0.00004 2.66787

R10 2.03912 0.00003 0.00005 0.00001 0.00007 2.03919

R11 2.66791 -0.00006 -0.00006 0.00002 -0.00004 2.66787

R12 2.82286 -0.00012 -0.00093 0.00029 -0.00064 2.82222

R13 2.58892 -0.00007 -0.00026 0.00009 -0.00017 2.58875

R14 2.74036 -0.00012 0.00007 -0.00027 -0.00020 2.74016

R15 2.58892 -0.00007 -0.00026 0.00009 -0.00017 2.58875

R16 3.95110 -0.00006 -0.00044 0.00036 -0.00008 3.95102

R17 2.74036 -0.00012 0.00007 -0.00027 -0.00020 2.74016

R18 2.66791 -0.00006 -0.00006 0.00002 -0.00004 2.66787

R19 2.57516 0.00017 -0.00020 0.00051 0.00031 2.57547

R20 2.03912 0.00003 0.00005 0.00001 0.00007 2.03919

R21 2.03912 0.00003 0.00005 0.00001 0.00007 2.03919

R22 2.66791 -0.00006 -0.00006 0.00002 -0.00004 2.66787

R23 2.82286 -0.00012 -0.00093 0.00029 -0.00064 2.82222

R24 2.74036 -0.00012 0.00007 -0.00027 -0.00020 2.74016

R25 2.58892 -0.00007 -0.00026 0.00009 -0.00017 2.58875

R26 2.57516 0.00017 -0.00020 0.00051 0.00031 2.57547

R27 2.03912 0.00003 0.00005 0.00001 0.00007 2.03919

R28 2.74036 -0.00012 0.00007 -0.00027 -0.00020 2.74016

R29 2.03912 0.00003 0.00005 0.00001 0.00007 2.03919

R30 2.58892 -0.00007 -0.00026 0.00009 -0.00017 2.58875

R31 2.66791 -0.00006 -0.00006 0.00002 -0.00004 2.66787

R32 3.95110 -0.00006 -0.00044 0.00036 -0.00008 3.95102

R33 2.66791 -0.00006 -0.00006 0.00002 -0.00004 2.66787

R34 2.82286 -0.00012 -0.00093 0.00029 -0.00064 2.82222

R35 2.74036 -0.00012 0.00007 -0.00027 -0.00020 2.74016

R36 2.58892 -0.00007 -0.00026 0.00009 -0.00017 2.58875

R37 2.57516 0.00017 -0.00020 0.00051 0.00031 2.57547

R38 2.03912 0.00003 0.00005 0.00001 0.00007 2.03919

R39 2.74036 -0.00012 0.00007 -0.00027 -0.00020 2.74016

R40 2.03912 0.00003 0.00005 0.00001 0.00007 2.03919

R41 2.58892 -0.00007 -0.00026 0.00009 -0.00017 2.58875

R42 2.66791 -0.00006 -0.00006 0.00002 -0.00004 2.66787

R43 3.95110 -0.00006 -0.00044 0.00036 -0.00008 3.95102

R44 2.82286 -0.00012 -0.00093 0.00029 -0.00064 2.82222

R45 2.64664 -0.00011 0.00006 -0.00015 -0.00009 2.64655

R46 2.64664 -0.00011 0.00006 -0.00015 -0.00009 2.64655

R47 2.63227 -0.00003 -0.00022 0.00012 -0.00010 2.63217

R48 2.04948 0.00001 0.00002 0.00002 0.00004 2.04951

R49 2.63480 -0.00003 -0.00000 -0.00003 -0.00003 2.63476

R50 2.05047 -0.00001 -0.00001 0.00001 -0.00001 2.05047

R51 2.63480 -0.00003 -0.00000 -0.00003 -0.00003 2.63476

R52 2.05033 -0.00001 -0.00001 -0.00002 -0.00003 2.05030

R53 2.63227 -0.00003 -0.00022 0.00012 -0.00010 2.63217

R54 2.05047 -0.00001 -0.00001 0.00001 -0.00001 2.05047

R55 2.04948 0.00001 0.00002 0.00002 0.00004 2.04951

R56 2.63480 -0.00003 -0.00000 -0.00003 -0.00003 2.63476

R57 2.63480 -0.00003 -0.00000 -0.00003 -0.00003 2.63476

R58 2.05033 -0.00001 -0.00001 -0.00002 -0.00003 2.05030

R59 2.63227 -0.00003 -0.00022 0.00012 -0.00010 2.63217

R60 2.05047 -0.00001 -0.00001 0.00001 -0.00001 2.05047

R61 2.64664 -0.00011 0.00006 -0.00015 -0.00009 2.64655

R62 2.04948 0.00001 0.00002 0.00002 0.00004 2.04951

R63 2.64664 -0.00011 0.00006 -0.00015 -0.00009 2.64655

R64 2.63227 -0.00003 -0.00022 0.00012 -0.00010 2.63217

R65 2.04948 0.00001 0.00002 0.00002 0.00004 2.04951

R66 2.05047 -0.00001 -0.00001 0.00001 -0.00001 2.05047

R67 2.64664 -0.00011 0.00006 -0.00015 -0.00009 2.64655

R68 2.64664 -0.00011 0.00006 -0.00015 -0.00009 2.64655

R69 2.63227 -0.00003 -0.00022 0.00012 -0.00010 2.63217

R70 2.04948 0.00001 0.00002 0.00002 0.00004 2.04951

R71 2.63480 -0.00003 -0.00000 -0.00003 -0.00003 2.63476

R72 2.05047 -0.00001 -0.00001 0.00001 -0.00001 2.05047

R73 2.63480 -0.00003 -0.00000 -0.00003 -0.00003 2.63476

R74 2.05033 -0.00001 -0.00001 -0.00002 -0.00003 2.05030

R75 2.63227 -0.00003 -0.00022 0.00012 -0.00010 2.63217

R76 2.05047 -0.00001 -0.00001 0.00001 -0.00001 2.05047

R77 2.04948 0.00001 0.00002 0.00002 0.00004 2.04951

R78 2.64664 -0.00011 0.00006 -0.00015 -0.00009 2.64655

R79 2.64664 -0.00011 0.00006 -0.00015 -0.00009 2.64655

R80 2.63227 -0.00003 -0.00022 0.00012 -0.00010 2.63217

R81 2.04948 0.00001 0.00002 0.00002 0.00004 2.04951

R82 2.63480 -0.00003 -0.00000 -0.00003 -0.00003 2.63476

R83 2.05047 -0.00001 -0.00001 0.00001 -0.00001 2.05047

R84 2.63480 -0.00003 -0.00000 -0.00003 -0.00003 2.63476

R85 2.05033 -0.00001 -0.00001 -0.00002 -0.00003 2.05030

R86 2.63227 -0.00003 -0.00022 0.00012 -0.00010 2.63217

R87 2.05047 -0.00001 -0.00001 0.00001 -0.00001 2.05047

R88 2.04948 0.00001 0.00002 0.00002 0.00004 2.04951

A1 1.87136 -0.00004 -0.00011 0.00001 -0.00009 1.87127

A2 2.19533 -0.00000 0.00021 -0.00023 -0.00002 2.19531

A3 2.21633 0.00004 -0.00010 0.00022 0.00012 2.21645

A4 1.89557 0.00004 0.00020 -0.00010 0.00011 1.89568

A5 2.18771 -0.00002 -0.00010 0.00003 -0.00006 2.18765

A6 2.19978 -0.00002 -0.00010 0.00008 -0.00002 2.19976

A7 1.89077 -0.00000 -0.00019 0.00018 -0.00002 1.89076

A8 2.19356 -0.00000 -0.00007 -0.00020 -0.00028 2.19328

A9 2.19356 -0.00000 -0.00007 -0.00020 -0.00028 2.19328

A10 1.89557 0.00004 0.00020 -0.00010 0.00011 1.89568

A11 2.19978 -0.00002 -0.00010 0.00008 -0.00002 2.19976

A12 2.18771 -0.00002 -0.00010 0.00003 -0.00006 2.18765

A13 1.87136 -0.00004 -0.00011 0.00001 -0.00009 1.87127

A14 2.21633 0.00004 -0.00010 0.00022 0.00012 2.21645

A15 2.19533 -0.00000 0.00021 -0.00023 -0.00002 2.19531

A16 2.20235 0.00004 -0.00015 -0.00011 -0.00027 2.20208

A17 2.04042 -0.00002 0.00007 0.00006 0.00013 2.04055

A18 2.04042 -0.00002 0.00007 0.00006 0.00013 2.04055

A19 2.19978 -0.00002 -0.00010 0.00008 -0.00002 2.19976

A20 2.18771 -0.00002 -0.00010 0.00003 -0.00006 2.18765

A21 1.89557 0.00004 0.00020 -0.00010 0.00011 1.89568

A22 1.89077 -0.00000 -0.00019 0.00018 -0.00002 1.89076

A23 2.19356 -0.00000 -0.00007 -0.00020 -0.00028 2.19328

A24 2.19356 -0.00000 -0.00007 -0.00020 -0.00028 2.19328

A25 1.89557 0.00004 0.00020 -0.00010 0.00011 1.89568

A26 2.19978 -0.00002 -0.00010 0.00008 -0.00002 2.19976

A27 2.18771 -0.00002 -0.00010 0.00003 -0.00006 2.18765

A28 1.87136 -0.00004 -0.00011 0.00001 -0.00009 1.87127

A29 2.19533 -0.00000 0.00021 -0.00023 -0.00002 2.19531

A30 2.21633 0.00004 -0.00010 0.00022 0.00012 2.21645

A31 1.87136 -0.00004 -0.00011 0.00001 -0.00009 1.87127

A32 2.19533 -0.00000 0.00021 -0.00023 -0.00002 2.19531

A33 2.21633 0.00004 -0.00010 0.00022 0.00012 2.21645

A34 2.20235 0.00004 -0.00015 -0.00011 -0.00027 2.20208

A35 2.04042 -0.00002 0.00007 0.00006 0.00013 2.04055

A36 2.04042 -0.00002 0.00007 0.00006 0.00013 2.04055

A37 2.18771 -0.00002 -0.00010 0.00003 -0.00006 2.18765

A38 2.19978 -0.00002 -0.00010 0.00008 -0.00002 2.19976

A39 1.89557 0.00004 0.00020 -0.00010 0.00011 1.89568

A40 1.87136 -0.00004 -0.00011 0.00001 -0.00009 1.87127

A41 2.19533 -0.00000 0.00021 -0.00023 -0.00002 2.19531

A42 2.21633 0.00004 -0.00010 0.00022 0.00012 2.21645

A43 1.87136 -0.00004 -0.00011 0.00001 -0.00009 1.87127

A44 2.21633 0.00004 -0.00010 0.00022 0.00012 2.21645

A45 2.19533 -0.00000 0.00021 -0.00023 -0.00002 2.19531

A46 1.89557 0.00004 0.00020 -0.00010 0.00011 1.89568

A47 2.18771 -0.00002 -0.00010 0.00003 -0.00006 2.18765

A48 2.19978 -0.00002 -0.00010 0.00008 -0.00002 2.19976

A49 1.89077 -0.00000 -0.00019 0.00018 -0.00002 1.89076

A50 2.19356 -0.00000 -0.00007 -0.00020 -0.00028 2.19328

A51 2.19356 -0.00000 -0.00007 -0.00020 -0.00028 2.19328

A52 2.20235 0.00004 -0.00015 -0.00011 -0.00027 2.20208

A53 2.04042 -0.00002 0.00007 0.00006 0.00013 2.04055

A54 2.04042 -0.00002 0.00007 0.00006 0.00013 2.04055

A55 2.18771 -0.00002 -0.00010 0.00003 -0.00006 2.18765

A56 2.19978 -0.00002 -0.00010 0.00008 -0.00002 2.19976

A57 1.89557 0.00004 0.00020 -0.00010 0.00011 1.89568

A58 1.87136 -0.00004 -0.00011 0.00001 -0.00009 1.87127

A59 2.19533 -0.00000 0.00021 -0.00023 -0.00002 2.19531

A60 2.21633 0.00004 -0.00010 0.00022 0.00012 2.21645

A61 1.87136 -0.00004 -0.00011 0.00001 -0.00009 1.87127

A62 2.21633 0.00004 -0.00010 0.00022 0.00012 2.21645

A63 2.19533 -0.00000 0.00021 -0.00023 -0.00002 2.19531

A64 1.89557 0.00004 0.00020 -0.00010 0.00011 1.89568

A65 2.18771 -0.00002 -0.00010 0.00003 -0.00006 2.18765

A66 2.19978 -0.00002 -0.00010 0.00008 -0.00002 2.19976

A67 1.89077 -0.00000 -0.00019 0.00018 -0.00002 1.89076

A68 2.19356 -0.00000 -0.00007 -0.00020 -0.00028 2.19328

A69 2.19356 -0.00000 -0.00007 -0.00020 -0.00028 2.19328

A70 2.20235 0.00004 -0.00015 -0.00011 -0.00027 2.20208

A71 2.04042 -0.00002 0.00007 0.00006 0.00013 2.04055

A72 2.04042 -0.00002 0.00007 0.00006 0.00013 2.04055

A73 2.10591 -0.00002 0.00004 0.00001 0.00005 2.10596

A74 2.10591 -0.00002 0.00004 0.00001 0.00005 2.10596

A75 2.07136 0.00004 -0.00008 -0.00001 -0.00009 2.07127

A76 2.10626 -0.00001 0.00003 0.00003 0.00006 2.10632

A77 2.08336 0.00001 -0.00000 -0.00005 -0.00005 2.08332

A78 2.09352 -0.00000 -0.00003 0.00002 -0.00001 2.09351

A79 2.09722 -0.00000 0.00003 0.00001 0.00004 2.09726

A80 2.08927 -0.00001 -0.00007 -0.00001 -0.00007 2.08920

A81 2.09668 0.00001 0.00004 -0.00000 0.00003 2.09672

A82 2.08803 -0.00002 -0.00004 -0.00007 -0.00011 2.08792

A83 2.09758 0.00001 0.00002 0.00003 0.00005 2.09763

A84 2.09758 0.00001 0.00002 0.00003 0.00005 2.09763

A85 2.09722 -0.00000 0.00003 0.00001 0.00004 2.09726

A86 2.09668 0.00001 0.00004 -0.00000 0.00003 2.09672

A87 2.08927 -0.00001 -0.00007 -0.00001 -0.00007 2.08920

A88 2.10626 -0.00001 0.00003 0.00003 0.00006 2.10632

A89 2.08336 0.00001 -0.00000 -0.00005 -0.00005 2.08332

A90 2.09352 -0.00000 -0.00003 0.00002 -0.00001 2.09351

A91 2.08803 -0.00002 -0.00004 -0.00007 -0.00011 2.08792

A92 2.09758 0.00001 0.00002 0.00003 0.00005 2.09763

A93 2.09758 0.00001 0.00002 0.00003 0.00005 2.09763

A94 2.09722 -0.00000 0.00003 0.00001 0.00004 2.09726

A95 2.09668 0.00001 0.00004 -0.00000 0.00003 2.09672

A96 2.08927 -0.00001 -0.00007 -0.00001 -0.00007 2.08920

A97 2.10626 -0.00001 0.00003 0.00003 0.00006 2.10632

A98 2.09352 -0.00000 -0.00003 0.00002 -0.00001 2.09351

A99 2.08336 0.00001 -0.00000 -0.00005 -0.00005 2.08332

A100 2.10591 -0.00002 0.00004 0.00001 0.00005 2.10596

A101 2.10591 -0.00002 0.00004 0.00001 0.00005 2.10596

A102 2.07136 0.00004 -0.00008 -0.00001 -0.00009 2.07127

A103 2.10626 -0.00001 0.00003 0.00003 0.00006 2.10632

A104 2.08336 0.00001 -0.00000 -0.00005 -0.00005 2.08332

A105 2.09352 -0.00000 -0.00003 0.00002 -0.00001 2.09351

A106 2.09722 -0.00000 0.00003 0.00001 0.00004 2.09726

A107 2.09668 0.00001 0.00004 -0.00000 0.00003 2.09672

A108 2.08927 -0.00001 -0.00007 -0.00001 -0.00007 2.08920

A109 2.10591 -0.00002 0.00004 0.00001 0.00005 2.10596

A110 2.10591 -0.00002 0.00004 0.00001 0.00005 2.10596

A111 2.07136 0.00004 -0.00008 -0.00001 -0.00009 2.07127

A112 2.10626 -0.00001 0.00003 0.00003 0.00006 2.10632

A113 2.08336 0.00001 -0.00000 -0.00005 -0.00005 2.08332

A114 2.09352 -0.00000 -0.00003 0.00002 -0.00001 2.09351

A115 2.09722 -0.00000 0.00003 0.00001 0.00004 2.09726

A116 2.08927 -0.00001 -0.00007 -0.00001 -0.00007 2.08920

A117 2.09668 0.00001 0.00004 -0.00000 0.00003 2.09672

A118 2.08803 -0.00002 -0.00004 -0.00007 -0.00011 2.08792

A119 2.09758 0.00001 0.00002 0.00003 0.00005 2.09763

A120 2.09758 0.00001 0.00002 0.00003 0.00005 2.09763

A121 2.09722 -0.00000 0.00003 0.00001 0.00004 2.09726

A122 2.09668 0.00001 0.00004 -0.00000 0.00003 2.09672

A123 2.08927 -0.00001 -0.00007 -0.00001 -0.00007 2.08920

A124 2.10626 -0.00001 0.00003 0.00003 0.00006 2.10632

A125 2.08336 0.00001 -0.00000 -0.00005 -0.00005 2.08332

A126 2.09352 -0.00000 -0.00003 0.00002 -0.00001 2.09351

A127 2.10591 -0.00002 0.00004 0.00001 0.00005 2.10596

A128 2.10591 -0.00002 0.00004 0.00001 0.00005 2.10596

A129 2.07136 0.00004 -0.00008 -0.00001 -0.00009 2.07127

A130 2.10626 -0.00001 0.00003 0.00003 0.00006 2.10632

A131 2.08336 0.00001 -0.00000 -0.00005 -0.00005 2.08332

A132 2.09352 -0.00000 -0.00003 0.00002 -0.00001 2.09351

A133 2.09722 -0.00000 0.00003 0.00001 0.00004 2.09726

A134 2.08927 -0.00001 -0.00007 -0.00001 -0.00007 2.08920

A135 2.09668 0.00001 0.00004 -0.00000 0.00003 2.09672

A136 2.08803 -0.00002 -0.00004 -0.00007 -0.00011 2.08792

A137 2.09758 0.00001 0.00002 0.00003 0.00005 2.09763

A138 2.09758 0.00001 0.00002 0.00003 0.00005 2.09763

A139 2.09722 -0.00000 0.00003 0.00001 0.00004 2.09726

A140 2.09668 0.00001 0.00004 -0.00000 0.00003 2.09672

A141 2.08927 -0.00001 -0.00007 -0.00001 -0.00007 2.08920

A142 2.10626 -0.00001 0.00003 0.00003 0.00006 2.10632

A143 2.08336 0.00001 -0.00000 -0.00005 -0.00005 2.08332

A144 2.09352 -0.00000 -0.00003 0.00002 -0.00001 2.09351

A145 1.57096 -0.00000 0.00000 -0.00000 0.00000 1.57097

A146 1.57096 -0.00000 0.00000 -0.00000 0.00000 1.57097

A147 1.57096 -0.00000 0.00000 -0.00000 0.00000 1.57097

A148 1.57096 -0.00000 0.00000 -0.00000 0.00000 1.57097

A149 3.14193 -0.00000 0.00000 -0.00000 0.00000 3.14193

A150 3.14193 -0.00000 0.00000 -0.00000 0.00000 3.14193

A151 3.11573 0.00001 -0.00021 0.00007 -0.00013 3.11560

A152 3.11573 0.00001 -0.00021 0.00007 -0.00013 3.11560

D1 0.00925 -0.00001 0.00003 -0.00019 -0.00016 0.00909

D2 3.13530 0.00002 0.00066 0.00075 0.00141 3.13670

D3 -3.11393 -0.00002 -0.00014 -0.00043 -0.00057 -3.11450

D4 0.01212 0.00001 0.00049 0.00050 0.00099 0.01311

D5 0.00000 -0.00000 -0.00000 -0.00000 0.00000 0.00000

D6 -3.12289 -0.00001 -0.00018 -0.00024 -0.00042 -3.12331

D7 3.12289 0.00001 0.00018 0.00024 0.00042 3.12331

D8 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D9 -0.01509 0.00001 -0.00005 0.00030 0.00025 -0.01484

D10 3.02096 -0.00003 -0.00355 -0.00188 -0.00543 3.01553

D11 -3.14100 -0.00002 -0.00068 -0.00064 -0.00132 3.14086

D12 -0.10495 -0.00005 -0.00418 -0.00282 -0.00700 -0.11196

D13 -3.06582 -0.00000 0.00155 0.00046 0.00202 -3.06380

D14 0.07578 -0.00000 0.00155 0.00046 0.00202 0.07779

D15 0.05756 0.00003 0.00229 0.00155 0.00385 0.06141

D16 -3.08403 0.00003 0.00229 0.00155 0.00385 -3.08019

D17 0.01509 -0.00001 0.00005 -0.00030 -0.00025 0.01484

D18 3.14100 0.00002 0.00068 0.00064 0.00132 -3.14086

D19 -3.02096 0.00003 0.00355 0.00188 0.00543 -3.01553

D20 0.10495 0.00005 0.00418 0.00282 0.00700 0.11196

D21 -3.06695 0.00002 0.00215 0.00123 0.00338 -3.06357

D22 0.04878 0.00003 0.00195 0.00130 0.00325 0.05203

D23 -0.04878 -0.00003 -0.00195 -0.00130 -0.00325 -0.05203

D24 3.06695 -0.00002 -0.00215 -0.00123 -0.00338 3.06357

D25 -0.00925 0.00001 -0.00003 0.00019 0.00016 -0.00909

D26 3.11393 0.00002 0.00014 0.00043 0.00057 3.11450

D27 -3.13530 -0.00002 -0.00066 -0.00075 -0.00141 -3.13670

D28 -0.01212 -0.00001 -0.00049 -0.00050 -0.00099 -0.01311

D29 -0.05756 -0.00003 -0.00229 -0.00155 -0.00385 -0.06141

D30 3.08403 -0.00003 -0.00229 -0.00155 -0.00385 3.08019

D31 3.06582 0.00000 -0.00155 -0.00046 -0.00202 3.06380

D32 -0.07578 0.00000 -0.00155 -0.00046 -0.00202 -0.07779

D33 -0.05756 -0.00003 -0.00229 -0.00155 -0.00385 -0.06141

D34 3.06582 0.00000 -0.00155 -0.00046 -0.00202 3.06380

D35 3.08403 -0.00003 -0.00229 -0.00155 -0.00385 3.08019

D36 -0.07578 0.00000 -0.00155 -0.00046 -0.00202 -0.07779

D37 -1.12169 -0.00001 0.00058 0.00075 0.00133 -1.12036

D38 2.01990 -0.00001 0.00058 0.00075 0.00133 2.02123

D39 2.01990 -0.00001 0.00058 0.00075 0.00133 2.02123

D40 -1.12169 -0.00001 0.00058 0.00075 0.00133 -1.12036

D41 3.14100 0.00002 0.00068 0.00064 0.00132 -3.14086

D42 0.10495 0.00005 0.00418 0.00282 0.00700 0.11196

D43 0.01509 -0.00001 0.00005 -0.00030 -0.00025 0.01484

D44 -3.02096 0.00003 0.00355 0.00188 0.00543 -3.01553

D45 -3.13530 -0.00002 -0.00066 -0.00075 -0.00141 -3.13670

D46 -0.01212 -0.00001 -0.00049 -0.00050 -0.00099 -0.01311

D47 -0.00925 0.00001 -0.00003 0.00019 0.00016 -0.00909

D48 3.11393 0.00002 0.00014 0.00043 0.00057 3.11450

D49 -0.01509 0.00001 -0.00005 0.00030 0.00025 -0.01484

D50 -3.14100 -0.00002 -0.00068 -0.00064 -0.00132 3.14086

D51 3.02096 -0.00003 -0.00355 -0.00188 -0.00543 3.01553

D52 -0.10495 -0.00005 -0.00418 -0.00282 -0.00700 -0.11196

D53 -0.04878 -0.00003 -0.00195 -0.00130 -0.00325 -0.05203

D54 3.06695 -0.00002 -0.00215 -0.00123 -0.00338 3.06357

D55 -3.06695 0.00002 0.00215 0.00123 0.00338 -3.06357

D56 0.04878 0.00003 0.00195 0.00130 0.00325 0.05203

D57 0.00925 -0.00001 0.00003 -0.00019 -0.00016 0.00909

D58 -3.11393 -0.00002 -0.00014 -0.00043 -0.00057 -3.11450

D59 3.13530 0.00002 0.00066 0.00075 0.00141 3.13670

D60 0.01212 0.00001 0.00049 0.00050 0.00099 0.01311

D61 0.05756 0.00003 0.00229 0.00155 0.00385 0.06141

D62 -3.08403 0.00003 0.00229 0.00155 0.00385 -3.08019

D63 -3.06582 -0.00000 0.00155 0.00046 0.00202 -3.06380

D64 0.07578 -0.00000 0.00155 0.00046 0.00202 0.07779

D65 -0.00000 -0.00000 -0.00000 0.00000 -0.00000 -0.00000

D66 -3.12289 -0.00001 -0.00018 -0.00024 -0.00042 -3.12331

D67 3.12289 0.00001 0.00018 0.00024 0.00042 3.12331

D68 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D69 -3.06582 -0.00000 0.00155 0.00046 0.00202 -3.06380

D70 0.05756 0.00003 0.00229 0.00155 0.00385 0.06141

D71 0.07578 -0.00000 0.00155 0.00046 0.00202 0.07779

D72 -3.08403 0.00003 0.00229 0.00155 0.00385 -3.08019

D73 1.12169 0.00001 -0.00058 -0.00075 -0.00133 1.12036

D74 -2.01990 0.00001 -0.00058 -0.00075 -0.00133 -2.02123

D75 -2.01990 0.00001 -0.00058 -0.00075 -0.00133 -2.02123

D76 1.12169 0.00001 -0.00058 -0.00075 -0.00133 1.12036

D77 3.13530 0.00002 0.00066 0.00075 0.00141 3.13670

D78 0.01212 0.00001 0.00049 0.00050 0.00099 0.01311

D79 0.00925 -0.00001 0.00003 -0.00019 -0.00016 0.00909

D80 -3.11393 -0.00002 -0.00014 -0.00043 -0.00057 -3.11450

D81 -3.14100 -0.00002 -0.00068 -0.00064 -0.00132 3.14086

D82 -0.10495 -0.00005 -0.00418 -0.00282 -0.00700 -0.11196

D83 -0.01509 0.00001 -0.00005 0.00030 0.00025 -0.01484

D84 3.02096 -0.00003 -0.00355 -0.00188 -0.00543 3.01553

D85 -0.00000 0.00000 -0.00000 -0.00000 -0.00000 -0.00000

D86 -3.12289 -0.00001 -0.00018 -0.00024 -0.00042 -3.12331

D87 3.12289 0.00001 0.00018 0.00024 0.00042 3.12331

D88 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D89 -0.00925 0.00001 -0.00003 0.00019 0.00016 -0.00909

D90 -3.13530 -0.00002 -0.00066 -0.00075 -0.00141 -3.13670

D91 3.11393 0.00002 0.00014 0.00043 0.00057 3.11450

D92 -0.01212 -0.00001 -0.00049 -0.00050 -0.00099 -0.01311

D93 0.01509 -0.00001 0.00005 -0.00030 -0.00025 0.01484

D94 -3.02096 0.00003 0.00355 0.00188 0.00543 -3.01553

D95 3.14100 0.00002 0.00068 0.00064 0.00132 -3.14086

D96 0.10495 0.00005 0.00418 0.00282 0.00700 0.11196

D97 3.06582 0.00000 -0.00155 -0.00046 -0.00202 3.06380

D98 -0.07578 0.00000 -0.00155 -0.00046 -0.00202 -0.07779

D99 -0.05756 -0.00003 -0.00229 -0.00155 -0.00385 -0.06141

D100 3.08403 -0.00003 -0.00229 -0.00155 -0.00385 3.08019

D101 0.04878 0.00003 0.00195 0.00130 0.00325 0.05203

D102 -3.06695 0.00002 0.00215 0.00123 0.00338 -3.06357

D103 3.06695 -0.00002 -0.00215 -0.00123 -0.00338 3.06357

D104 -0.04878 -0.00003 -0.00195 -0.00130 -0.00325 -0.05203

D105 3.06582 0.00000 -0.00155 -0.00046 -0.00202 3.06380

D106 -0.05756 -0.00003 -0.00229 -0.00155 -0.00385 -0.06141

D107 -0.07578 0.00000 -0.00155 -0.00046 -0.00202 -0.07779

D108 3.08403 -0.00003 -0.00229 -0.00155 -0.00385 3.08019

D109 -1.12169 -0.00001 0.00058 0.00075 0.00133 -1.12036

D110 2.01990 -0.00001 0.00058 0.00075 0.00133 2.02123

D111 2.01990 -0.00001 0.00058 0.00075 0.00133 2.02123

D112 -1.12169 -0.00001 0.00058 0.00075 0.00133 -1.12036

D113 -3.13530 -0.00002 -0.00066 -0.00075 -0.00141 -3.13670

D114 -0.01212 -0.00001 -0.00049 -0.00050 -0.00099 -0.01311

D115 -0.00925 0.00001 -0.00003 0.00019 0.00016 -0.00909

D116 3.11393 0.00002 0.00014 0.00043 0.00057 3.11450

D117 3.14100 0.00002 0.00068 0.00064 0.00132 -3.14086

D118 0.10495 0.00005 0.00418 0.00282 0.00700 0.11196

D119 0.01509 -0.00001 0.00005 -0.00030 -0.00025 0.01484

D120 -3.02096 0.00003 0.00355 0.00188 0.00543 -3.01553

D121 0.00000 0.00000 -0.00000 -0.00000 0.00000 0.00000

D122 3.12289 0.00001 0.00018 0.00024 0.00042 3.12331

D123 -3.12289 -0.00001 -0.00018 -0.00024 -0.00042 -3.12331

D124 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D125 0.00925 -0.00001 0.00003 -0.00019 -0.00016 0.00909

D126 3.13530 0.00002 0.00066 0.00075 0.00141 3.13670

D127 -3.11393 -0.00002 -0.00014 -0.00043 -0.00057 -3.11450

D128 0.01212 0.00001 0.00049 0.00050 0.00099 0.01311

D129 -0.01509 0.00001 -0.00005 0.00030 0.00025 -0.01484

D130 3.02096 -0.00003 -0.00355 -0.00188 -0.00543 3.01553

D131 -3.14100 -0.00002 -0.00068 -0.00064 -0.00132 3.14086

D132 -0.10495 -0.00005 -0.00418 -0.00282 -0.00700 -0.11196

D133 -3.06582 -0.00000 0.00155 0.00046 0.00202 -3.06380

D134 0.07578 -0.00000 0.00155 0.00046 0.00202 0.07779

D135 0.05756 0.00003 0.00229 0.00155 0.00385 0.06141

D136 -3.08403 0.00003 0.00229 0.00155 0.00385 -3.08019

D137 3.06695 -0.00002 -0.00215 -0.00123 -0.00338 3.06357

D138 -0.04878 -0.00003 -0.00195 -0.00130 -0.00325 -0.05203

D139 0.04878 0.00003 0.00195 0.00130 0.00325 0.05203

D140 -3.06695 0.00002 0.00215 0.00123 0.00338 -3.06357

D141 1.12169 0.00001 -0.00058 -0.00075 -0.00133 1.12036

D142 -2.01990 0.00001 -0.00058 -0.00075 -0.00133 -2.02123

D143 -2.01990 0.00001 -0.00058 -0.00075 -0.00133 -2.02123

D144 1.12169 0.00001 -0.00058 -0.00075 -0.00133 1.12036

D145 -3.13988 -0.00000 0.00005 0.00000 0.00005 -3.13983

D146 -0.00758 0.00001 -0.00032 0.00053 0.00021 -0.00737

D147 0.00171 -0.00000 0.00005 0.00000 0.00005 0.00176

D148 3.13401 0.00001 -0.00032 0.00053 0.00021 3.13422

D149 -3.13988 -0.00000 0.00005 0.00000 0.00005 -3.13983

D150 -0.00758 0.00001 -0.00032 0.00053 0.00021 -0.00737

D151 0.00171 -0.00000 0.00005 0.00000 0.00005 0.00176

D152 3.13401 0.00001 -0.00032 0.00053 0.00021 3.13422

D153 -0.00342 0.00000 -0.00010 -0.00000 -0.00010 -0.00353

D154 3.13519 0.00000 -0.00009 0.00013 0.00003 3.13523

D155 -3.13567 -0.00001 0.00027 -0.00053 -0.00026 -3.13594

D156 0.00294 -0.00001 0.00028 -0.00040 -0.00013 0.00281

D157 0.00170 -0.00000 0.00005 0.00000 0.00005 0.00175

D158 -3.13989 -0.00000 0.00005 0.00000 0.00005 -3.13984

D159 -3.13690 -0.00000 0.00004 -0.00013 -0.00009 -3.13699

D160 0.00469 -0.00000 0.00004 -0.00013 -0.00009 0.00460

D161 0.00170 -0.00000 0.00005 0.00000 0.00005 0.00175

D162 -3.13690 -0.00000 0.00004 -0.00013 -0.00009 -3.13699

D163 -3.13989 -0.00000 0.00005 0.00000 0.00005 -3.13984

D164 0.00469 -0.00000 0.00004 -0.00013 -0.00009 0.00460

D165 -0.00342 0.00000 -0.00010 -0.00000 -0.00010 -0.00353

D166 -3.13567 -0.00001 0.00027 -0.00053 -0.00026 -3.13594

D167 3.13519 0.00000 -0.00009 0.00013 0.00003 3.13523

D168 0.00294 -0.00001 0.00028 -0.00040 -0.00013 0.00281

D169 -0.00170 0.00000 -0.00005 -0.00000 -0.00005 -0.00175

D170 3.13690 0.00000 -0.00004 0.00013 0.00009 3.13699

D171 3.13989 0.00000 -0.00005 -0.00000 -0.00005 3.13984

D172 -0.00469 0.00000 -0.00004 0.00013 0.00009 -0.00460

D173 -0.00170 0.00000 -0.00005 -0.00000 -0.00005 -0.00175

D174 3.13690 0.00000 -0.00004 0.00013 0.00009 3.13699

D175 3.13989 0.00000 -0.00005 -0.00000 -0.00005 3.13984

D176 -0.00469 0.00000 -0.00004 0.00013 0.00009 -0.00460

D177 0.00342 -0.00000 0.00010 0.00000 0.00010 0.00353

D178 3.13567 0.00001 -0.00027 0.00053 0.00026 3.13594

D179 -3.13519 -0.00000 0.00009 -0.00013 -0.00003 -3.13523

D180 -0.00294 0.00001 -0.00028 0.00040 0.00013 -0.00281

D181 3.13988 0.00000 -0.00005 -0.00000 -0.00005 3.13983

D182 -0.00171 0.00000 -0.00005 -0.00000 -0.00005 -0.00176

D183 0.00758 -0.00001 0.00032 -0.00053 -0.00021 0.00737

D184 -3.13401 -0.00001 0.00032 -0.00053 -0.00021 -3.13422

D185 3.13988 0.00000 -0.00005 -0.00000 -0.00005 3.13983

D186 0.00758 -0.00001 0.00032 -0.00053 -0.00021 0.00737

D187 -0.00171 0.00000 -0.00005 -0.00000 -0.00005 -0.00176

D188 -3.13401 -0.00001 0.00032 -0.00053 -0.00021 -3.13422

D189 0.00342 -0.00000 0.00010 0.00000 0.00010 0.00353

D190 -3.13519 -0.00000 0.00009 -0.00013 -0.00003 -3.13523

D191 3.13567 0.00001 -0.00027 0.00053 0.00026 3.13594

D192 -0.00294 0.00001 -0.00028 0.00040 0.00013 -0.00281

D193 3.13988 0.00000 -0.00005 -0.00000 -0.00005 3.13983

D194 0.00758 -0.00001 0.00032 -0.00053 -0.00021 0.00737

D195 -0.00171 0.00000 -0.00005 -0.00000 -0.00005 -0.00176

D196 -3.13401 -0.00001 0.00032 -0.00053 -0.00021 -3.13422

D197 3.13988 0.00000 -0.00005 -0.00000 -0.00005 3.13983

D198 0.00758 -0.00001 0.00032 -0.00053 -0.00021 0.00737

D199 -0.00171 0.00000 -0.00005 -0.00000 -0.00005 -0.00176

D200 -3.13401 -0.00001 0.00032 -0.00053 -0.00021 -3.13422

D201 0.00342 -0.00000 0.00010 0.00000 0.00010 0.00353

D202 -3.13519 -0.00000 0.00009 -0.00013 -0.00003 -3.13523

D203 3.13567 0.00001 -0.00027 0.00053 0.00026 3.13594

D204 -0.00294 0.00001 -0.00028 0.00040 0.00013 -0.00281

D205 -0.00170 0.00000 -0.00005 -0.00000 -0.00005 -0.00175

D206 3.13989 0.00000 -0.00005 -0.00000 -0.00005 3.13984

D207 3.13690 0.00000 -0.00004 0.00013 0.00009 3.13699

D208 -0.00469 0.00000 -0.00004 0.00013 0.00009 -0.00460

D209 -0.00170 0.00000 -0.00005 -0.00000 -0.00005 -0.00175

D210 3.13690 0.00000 -0.00004 0.00013 0.00009 3.13699

D211 3.13989 0.00000 -0.00005 -0.00000 -0.00005 3.13984

D212 -0.00469 0.00000 -0.00004 0.00013 0.00009 -0.00460

D213 0.00342 -0.00000 0.00010 0.00000 0.00010 0.00353

D214 3.13567 0.00001 -0.00027 0.00053 0.00026 3.13594

D215 -3.13519 -0.00000 0.00009 -0.00013 -0.00003 -3.13523

D216 -0.00294 0.00001 -0.00028 0.00040 0.00013 -0.00281

D217 -3.13988 -0.00000 0.00005 0.00000 0.00005 -3.13983

D218 -0.00758 0.00001 -0.00032 0.00053 0.00021 -0.00737

D219 0.00171 -0.00000 0.00005 0.00000 0.00005 0.00176

D220 3.13401 0.00001 -0.00032 0.00053 0.00021 3.13422

D221 -3.13988 -0.00000 0.00005 0.00000 0.00005 -3.13983

D222 -0.00758 0.00001 -0.00032 0.00053 0.00021 -0.00737

D223 0.00171 -0.00000 0.00005 0.00000 0.00005 0.00176

D224 3.13401 0.00001 -0.00032 0.00053 0.00021 3.13422

D225 -0.00342 0.00000 -0.00010 -0.00000 -0.00010 -0.00353

D226 3.13519 0.00000 -0.00009 0.00013 0.00003 3.13523

D227 -3.13567 -0.00001 0.00027 -0.00053 -0.00026 -3.13594

D228 0.00294 -0.00001 0.00028 -0.00040 -0.00013 0.00281

D229 0.00170 -0.00000 0.00005 0.00000 0.00005 0.00175

D230 -3.13989 -0.00000 0.00005 0.00000 0.00005 -3.13984

D231 -3.13690 -0.00000 0.00004 -0.00013 -0.00009 -3.13699

D232 0.00469 -0.00000 0.00004 -0.00013 -0.00009 0.00460

D233 0.00170 -0.00000 0.00005 0.00000 0.00005 0.00175

D234 -3.13690 -0.00000 0.00004 -0.00013 -0.00009 -3.13699

D235 -3.13989 -0.00000 0.00005 0.00000 0.00005 -3.13984

D236 0.00469 -0.00000 0.00004 -0.00013 -0.00009 0.00460

D237 -0.00342 0.00000 -0.00010 -0.00000 -0.00010 -0.00353

D238 -3.13567 -0.00001 0.00027 -0.00053 -0.00026 -3.13594

D239 3.13519 0.00000 -0.00009 0.00013 0.00003 3.13523

D240 0.00294 -0.00001 0.00028 -0.00040 -0.00013 0.00281

Item Value Threshold Converged?

Maximum Force 0.000170 0.000450 YES

RMS Force 0.000036 0.000300 YES

Maximum Displacement 0.024111 0.001800 NO

RMS Displacement 0.005323 0.001200 NO

Predicted change in Energy=-3.736965D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Aug 13 18:36:52 2019, MaxMem= 671088640 cpu: 0.8

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

Stoichiometry C44H28N4Zn

Framework group D2D[O(Zn),2SGD(N2),X(C44H28)]

Deg. of freedom 29

Full point group D2D NOp 8

RotChk: IX=0 Diff= 0.00D+00

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681441 4.269416 0.162031

2 6 0 -1.110610 2.890213 0.034757

3 7 0 0.000000 2.090613 -0.027175

4 6 0 1.110610 2.890213 0.034757

5 6 0 0.681441 4.269416 0.162031

6 6 0 2.452301 2.452301 0.000000

7 6 0 2.890213 1.110610 -0.034757

8 7 0 2.090613 -0.000000 0.027175

9 6 0 2.890213 -1.110610 -0.034757

10 6 0 4.269416 -0.681441 -0.162031

11 6 0 4.269416 0.681441 -0.162031

12 6 0 -2.452301 2.452301 0.000000

13 6 0 -2.890213 1.110610 -0.034757

14 6 0 -4.269416 0.681441 -0.162031

15 6 0 -4.269416 -0.681441 -0.162031

16 6 0 -2.890213 -1.110610 -0.034757

17 7 0 -2.090613 0.000000 0.027175

18 6 0 -2.452301 -2.452301 0.000000

19 6 0 -1.110610 -2.890213 0.034757

20 6 0 -0.681441 -4.269416 0.162031

21 6 0 0.681441 -4.269416 0.162031

22 6 0 1.110610 -2.890213 0.034757

23 7 0 -0.000000 -2.090613 -0.027175

24 6 0 2.452301 -2.452301 0.000000

25 6 0 3.508334 3.508334 -0.000000

26 6 0 3.621481 4.405256 -1.069635

27 6 0 4.607556 5.389014 -1.071058

28 6 0 5.493990 5.493990 -0.000000

29 6 0 5.389014 4.607556 1.071058

30 6 0 4.405256 3.621481 1.069635

31 6 0 -5.493990 5.493990 -0.000000

32 6 0 -4.607556 5.389014 -1.071058

33 6 0 -3.621481 4.405256 -1.069635

34 6 0 -3.508334 3.508334 -0.000000

35 6 0 -4.405256 3.621481 1.069635

36 6 0 -5.389014 4.607556 1.071058

37 6 0 3.508334 -3.508334 -0.000000

38 6 0 4.405256 -3.621481 1.069635

39 6 0 5.389014 -4.607556 1.071058

40 6 0 5.493990 -5.493990 -0.000000

41 6 0 4.607556 -5.389014 -1.071058

42 6 0 3.621481 -4.405256 -1.069635

43 6 0 -3.508334 -3.508334 -0.000000

44 6 0 -4.405256 -3.621481 1.069635

45 6 0 -5.389014 -4.607556 1.071058

46 6 0 -5.493990 -5.493990 -0.000000

47 6 0 -4.607556 -5.389014 -1.071058

48 6 0 -3.621481 -4.405256 -1.069635

49 1 0 -1.330754 5.126056 0.256906

50 1 0 1.330754 5.126056 0.256906

51 1 0 5.126056 -1.330754 -0.256906

52 1 0 5.126056 1.330754 -0.256906

53 1 0 -5.126056 1.330754 -0.256906

54 1 0 -5.126056 -1.330754 -0.256906

55 1 0 -1.330754 -5.126056 0.256906

56 1 0 1.330754 -5.126056 0.256906

57 1 0 2.937121 4.323394 -1.907018

58 1 0 4.684569 6.071842 -1.910802

59 1 0 6.261179 6.261179 0.000000

60 1 0 6.071842 4.684569 1.910802

61 1 0 4.323394 2.937121 1.907018

62 1 0 -6.261179 6.261179 0.000000

63 1 0 -4.684569 6.071842 -1.910802

64 1 0 -2.937121 4.323394 -1.907018

65 1 0 -4.323394 2.937121 1.907018

66 1 0 -6.071842 4.684569 1.910802

67 1 0 4.323394 -2.937121 1.907018

68 1 0 6.071842 -4.684569 1.910802

69 1 0 6.261179 -6.261179 0.000000

70 1 0 4.684569 -6.071842 -1.910802

71 1 0 2.937121 -4.323394 -1.907018

72 1 0 -4.323394 -2.937121 1.907018

73 1 0 -6.071842 -4.684569 1.910802

74 1 0 -6.261179 -6.261179 0.000000

75 1 0 -4.684569 -6.071842 -1.910802

76 1 0 -2.937121 -4.323394 -1.907018

77 30 0 0.000000 0.000000 0.000000

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

Rotational constants (GHZ): 0.0582074 0.0582074 0.0300805

Leave Link 202 at Tue Aug 13 18:36:52 2019, MaxMem= 671088640 cpu: 0.0

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

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

Pseudo-potential data read from rwf file.

There are 272 symmetry adapted cartesian basis functions of A1 symmetry.

There are 243 symmetry adapted cartesian basis functions of A2 symmetry.

There are 254 symmetry adapted cartesian basis functions of B1 symmetry.

There are 254 symmetry adapted cartesian basis functions of B2 symmetry.

There are 256 symmetry adapted basis functions of A1 symmetry.

There are 232 symmetry adapted basis functions of A2 symmetry.

There are 242 symmetry adapted basis functions of B1 symmetry.

There are 242 symmetry adapted basis functions of B2 symmetry.

972 basis functions, 1715 primitive gaussians, 1023 cartesian basis functions

166 alpha electrons 166 beta electrons

nuclear repulsion energy 5738.3633463528 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= 77 NActive= 77 NUniq= 13 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T 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= -0.2224158405 Hartrees.

Nuclear repulsion after empirical dispersion term = 5738.1409305122 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 77.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 77

GePol: Total number of spheres = 77

GePol: Number of exposed spheres = 77 (100.00%)

GePol: Number of points = 5690

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.17D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 272

GePol: Fraction of low-weight points (<1% of avg) = 4.78%

GePol: Cavity surface area = 614.307 Ang\*\*2

GePol: Cavity volume = 630.255 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021402349 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5738.1387902773 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

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36757 LenP2D= 95282.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 972 RedAO= T EigKep= 6.36D-05 NBF= 256 232 242 242

NBsUse= 972 1.00D-06 EigRej= -1.00D+00 NBFU= 256 232 242 242

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= 952 960 976 976 976 MxSgAt= 77 MxSgA2= 77.

Leave Link 302 at Tue Aug 13 18:36:55 2019, MaxMem= 671088640 cpu: 9.4

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Aug 13 18:36:55 2019, MaxMem= 671088640 cpu: 0.8

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

Initial guess from the checkpoint file: "ZnTPP0.chk"

B after Tr= -0.000000 -0.000000 0.000000

Rot= 1.000000 -0.000000 -0.000000 -0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

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

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

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

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

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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= -1979.25505334454

Leave Link 401 at Tue Aug 13 18:37:03 2019, MaxMem= 671088640 cpu: 32.7

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3177123 IEndB= 3177123 NGot= 671088640 MDV= 668975710

LenX= 668975710 LenY= 667928158

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= 530000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 97128300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.66D-15 for 5683.

Iteration 1 A\*A^-1 deviation from orthogonality is 7.55D-15 for 5674 1282.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.77D-15 for 5683.

Iteration 1 A^-1\*A deviation from orthogonality is 3.66D-12 for 4805 4795.

E= -1978.90412564854

DIIS: error= 4.78D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1978.90412564854 IErMin= 1 ErrMin= 4.78D-04

ErrMax= 4.78D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.08D-04 BMatP= 1.08D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.78D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.443 Goal= None Shift= 0.000

RMSDP=1.49D-05 MaxDP=4.00D-04 OVMax= 2.22D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.49D-05 CP: 1.00D+00

E= -1978.90434909473 Delta-E= -0.000223446194 Rises=F Damp=F

DIIS: error= 6.57D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1978.90434909473 IErMin= 2 ErrMin= 6.57D-05

ErrMax= 6.57D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.50D-06 BMatP= 1.08D-04

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

Coeff-Com: -0.713D-01 0.107D+01

Coeff: -0.713D-01 0.107D+01

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=2.58D-06 MaxDP=5.55D-05 DE=-2.23D-04 OVMax= 3.41D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.30D-06 CP: 1.00D+00 1.08D+00

E= -1978.90435265006 Delta-E= -0.000003555325 Rises=F Damp=F

DIIS: error= 1.31D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1978.90435265006 IErMin= 3 ErrMin= 1.31D-05

ErrMax= 1.31D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.89D-07 BMatP= 1.50D-06

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

Coeff-Com: -0.227D-01 0.272D+00 0.751D+00

Coeff: -0.227D-01 0.272D+00 0.751D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=7.26D-07 MaxDP=3.56D-05 DE=-3.56D-06 OVMax= 1.02D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.35D-07 CP: 1.00D+00 1.09D+00 8.80D-01

E= -1978.90435276632 Delta-E= -0.000000116263 Rises=F Damp=F

DIIS: error= 1.27D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1978.90435276632 IErMin= 4 ErrMin= 1.27D-05

ErrMax= 1.27D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.29D-08 BMatP= 1.89D-07

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

Coeff-Com: -0.745D-02 0.726D-01 0.420D+00 0.515D+00

Coeff: -0.745D-02 0.726D-01 0.420D+00 0.515D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=3.04D-07 MaxDP=2.38D-05 DE=-1.16D-07 OVMax= 6.44D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.40D-07 CP: 1.00D+00 1.10D+00 9.14D-01 7.36D-01

E= -1978.90435284720 Delta-E= -0.000000080883 Rises=F Damp=F

DIIS: error= 4.46D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1978.90435284720 IErMin= 5 ErrMin= 4.46D-06

ErrMax= 4.46D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.15D-09 BMatP= 9.29D-08

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

Coeff-Com: 0.237D-03-0.146D-01 0.719D-01 0.253D+00 0.689D+00

Coeff: 0.237D-03-0.146D-01 0.719D-01 0.253D+00 0.689D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.13D-07 MaxDP=7.35D-06 DE=-8.09D-08 OVMax= 2.56D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.52D-08 CP: 1.00D+00 1.10D+00 9.35D-01 7.84D-01 7.03D-01

E= -1978.90435285270 Delta-E= -0.000000005495 Rises=F Damp=F

DIIS: error= 2.10D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1978.90435285270 IErMin= 6 ErrMin= 2.10D-06

ErrMax= 2.10D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.88D-09 BMatP= 8.15D-09

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

Coeff-Com: 0.716D-03-0.149D-01 0.119D-01 0.119D+00 0.435D+00 0.449D+00

Coeff: 0.716D-03-0.149D-01 0.119D-01 0.119D+00 0.435D+00 0.449D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=3.73D-08 MaxDP=2.09D-06 DE=-5.50D-09 OVMax= 8.25D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.39D-08 CP: 1.00D+00 1.10D+00 9.37D-01 7.87D-01 7.38D-01

CP: 4.91D-01

E= -1978.90435285450 Delta-E= -0.000000001797 Rises=F Damp=F

DIIS: error= 1.70D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1978.90435285450 IErMin= 7 ErrMin= 1.70D-07

ErrMax= 1.70D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.77D-11 BMatP= 1.88D-09

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

Coeff-Com: 0.259D-03-0.501D-02 0.142D-02 0.352D-01 0.140D+00 0.166D+00

Coeff-Com: 0.662D+00

Coeff: 0.259D-03-0.501D-02 0.142D-02 0.352D-01 0.140D+00 0.166D+00

Coeff: 0.662D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=6.07D-09 MaxDP=4.57D-07 DE=-1.80D-09 OVMax= 1.21D-06

Error on total polarization charges = 0.08494

SCF Done: E(RB3LYP) = -1978.90435285 A.U. after 7 cycles

NFock= 7 Conv=0.61D-08 -V/T= 1.9793

KE= 2.020704418371D+03 PE=-1.615838641243D+04 EE= 6.420638850931D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.34

(included in total energy above)

Leave Link 502 at Tue Aug 13 18:41:53 2019, MaxMem= 671088640 cpu: 1159.7

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36757 LenP2D= 95282.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 182

Leave Link 701 at Tue Aug 13 18:42:39 2019, MaxMem= 671088640 cpu: 183.1

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

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

Leave Link 702 at Tue Aug 13 18:42:39 2019, MaxMem= 671088640 cpu: 0.1

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 0 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Tue Aug 13 18:43:26 2019, MaxMem= 671088640 cpu: 187.1

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

Dipole = 5.72875081D-13 8.81072992D-13 1.86517468D-14

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000078279 -0.000039260 -0.000010837

2 6 0.000026131 0.000099295 0.000061504

3 7 0.000000000 -0.000080111 -0.000086809

4 6 -0.000026131 0.000099295 0.000061504

5 6 0.000078279 -0.000039260 -0.000010837

6 6 -0.000077752 -0.000077752 -0.000000000

7 6 0.000099295 -0.000026131 -0.000061504

8 7 -0.000080111 0.000000000 0.000086809

9 6 0.000099295 0.000026131 -0.000061504

10 6 -0.000039260 -0.000078279 0.000010837

11 6 -0.000039260 0.000078279 0.000010837

12 6 0.000077752 -0.000077752 -0.000000000

13 6 -0.000099295 -0.000026131 -0.000061504

14 6 0.000039260 0.000078279 0.000010837

15 6 0.000039260 -0.000078279 0.000010837

16 6 -0.000099295 0.000026131 -0.000061504

17 7 0.000080111 -0.000000000 0.000086809

18 6 0.000077752 0.000077752 0.000000000

19 6 0.000026131 -0.000099295 0.000061504

20 6 -0.000078279 0.000039260 -0.000010837

21 6 0.000078279 0.000039260 -0.000010837

22 6 -0.000026131 -0.000099295 0.000061504

23 7 -0.000000000 0.000080111 -0.000086809

24 6 -0.000077752 0.000077752 -0.000000000

25 6 0.000100223 0.000100223 0.000000000

26 6 -0.000032342 -0.000062117 0.000014894

27 6 0.000018560 0.000017094 0.000005974

28 6 -0.000013380 -0.000013380 0.000000000

29 6 0.000017094 0.000018560 -0.000005974

30 6 -0.000062117 -0.000032342 -0.000014894

31 6 0.000013380 -0.000013380 0.000000000

32 6 -0.000018560 0.000017094 0.000005974

33 6 0.000032342 -0.000062117 0.000014894

34 6 -0.000100223 0.000100223 -0.000000000

35 6 0.000062117 -0.000032342 -0.000014894

36 6 -0.000017094 0.000018560 -0.000005974

37 6 0.000100223 -0.000100223 0.000000000

38 6 -0.000062117 0.000032342 -0.000014894

39 6 0.000017094 -0.000018560 -0.000005974

40 6 -0.000013380 0.000013380 -0.000000000

41 6 0.000018560 -0.000017094 0.000005974

42 6 -0.000032342 0.000062117 0.000014894

43 6 -0.000100223 -0.000100223 0.000000000

44 6 0.000062117 0.000032342 -0.000014894

45 6 -0.000017094 -0.000018560 -0.000005974

46 6 0.000013380 0.000013380 -0.000000000

47 6 -0.000018560 -0.000017094 0.000005974

48 6 0.000032342 0.000062117 0.000014894

49 1 -0.000014307 -0.000005688 -0.000000071

50 1 0.000014307 -0.000005688 -0.000000071

51 1 -0.000005688 -0.000014307 0.000000071

52 1 -0.000005688 0.000014307 0.000000071

53 1 0.000005688 0.000014307 0.000000071

54 1 0.000005688 -0.000014307 0.000000071

55 1 -0.000014307 0.000005688 -0.000000071

56 1 0.000014307 0.000005688 -0.000000071

57 1 -0.000002402 0.000009611 -0.000001258

58 1 -0.000001761 -0.000006410 -0.000002709

59 1 -0.000002354 -0.000002354 0.000000000

60 1 -0.000006410 -0.000001761 0.000002709

61 1 0.000009611 -0.000002402 0.000001258

62 1 0.000002354 -0.000002354 -0.000000000

63 1 0.000001761 -0.000006410 -0.000002709

64 1 0.000002402 0.000009611 -0.000001258

65 1 -0.000009611 -0.000002402 0.000001258

66 1 0.000006410 -0.000001761 0.000002709

67 1 0.000009611 0.000002402 0.000001258

68 1 -0.000006410 0.000001761 0.000002709

69 1 -0.000002354 0.000002354 -0.000000000

70 1 -0.000001761 0.000006410 -0.000002709

71 1 -0.000002402 -0.000009611 -0.000001258

72 1 -0.000009611 0.000002402 0.000001258

73 1 0.000006410 0.000001761 0.000002709

74 1 0.000002354 0.000002354 -0.000000000

75 1 0.000001761 0.000006410 -0.000002709

76 1 0.000002402 -0.000009611 -0.000001258

77 30 -0.000000000 -0.000000000 0.000000000

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

Cartesian Forces: Max 0.000100223 RMS 0.000042252

Leave Link 716 at Tue Aug 13 18:43:26 2019, MaxMem= 671088640 cpu: 0.1

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.000066951 RMS 0.000015851

Search for a local minimum.

Step number 6 out of a maximum of 462

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

RMS Force = .15851D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

6

DE= -5.20D-06 DEPred=-3.74D-06 R= 1.39D+00

TightC=F SS= 1.41D+00 RLast= 3.44D-02 DXNew= 8.4853D-01 1.0315D-01

Trust test= 1.39D+00 RLast= 3.44D-02 DXMaxT set to 5.05D-01

ITU= 1 1 1 1 1 0

Eigenvalues --- 0.00420 0.00755 0.00755 0.00755 0.00805

Eigenvalues --- 0.01174 0.01318 0.01476 0.01476 0.01559

Eigenvalues --- 0.01582 0.01583 0.01583 0.01596 0.01623

Eigenvalues --- 0.01623 0.01623 0.01623 0.01638 0.01681

Eigenvalues --- 0.01705 0.01705 0.01783 0.01783 0.01785

Eigenvalues --- 0.01812 0.01815 0.01815 0.01822 0.01867

Eigenvalues --- 0.01879 0.01880 0.01880 0.01886 0.01900

Eigenvalues --- 0.01900 0.01918 0.02025 0.02025 0.02025

Eigenvalues --- 0.02025 0.02058 0.02058 0.02058 0.02066

Eigenvalues --- 0.02066 0.02066 0.02066 0.02072 0.02089

Eigenvalues --- 0.02089 0.02089 0.02090 0.02101 0.02101

Eigenvalues --- 0.02101 0.02101 0.02104 0.02104 0.02104

Eigenvalues --- 0.02104 0.02106 0.02106 0.02106 0.02107

Eigenvalues --- 0.02107 0.02107 0.02107 0.02110 0.02123

Eigenvalues --- 0.02129 0.02129 0.02131 0.03529 0.12211

Eigenvalues --- 0.12211 0.14169 0.15994 0.15994 0.15994

Eigenvalues --- 0.15994 0.15997 0.15997 0.15997 0.15999

Eigenvalues --- 0.15999 0.15999 0.15999 0.15999 0.15999

Eigenvalues --- 0.15999 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16002 0.16123

Eigenvalues --- 0.17087 0.21765 0.21765 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22011 0.22821 0.22855 0.22886 0.22886

Eigenvalues --- 0.23474 0.23474 0.23474 0.23643 0.24743

Eigenvalues --- 0.24755 0.24755 0.24760 0.24761 0.24918

Eigenvalues --- 0.24918 0.24981 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25595 0.32293 0.32293 0.32293 0.34326

Eigenvalues --- 0.35008 0.35008 0.35131 0.35152 0.35166

Eigenvalues --- 0.35181 0.35181 0.35181 0.35181 0.35181

Eigenvalues --- 0.35181 0.35181 0.35191 0.35193 0.35193

Eigenvalues --- 0.35193 0.35202 0.35202 0.35202 0.35202

Eigenvalues --- 0.35202 0.35202 0.35202 0.35210 0.35827

Eigenvalues --- 0.35883 0.35883 0.35883 0.35883 0.35883

Eigenvalues --- 0.35883 0.35883 0.35915 0.36239 0.37147

Eigenvalues --- 0.37147 0.38406 0.38996 0.40015 0.40015

Eigenvalues --- 0.41213 0.41213 0.41300 0.41300 0.41300

Eigenvalues --- 0.41373 0.41373 0.41373 0.41373 0.41459

Eigenvalues --- 0.41576 0.42291 0.43125 0.43325 0.43325

Eigenvalues --- 0.44514 0.44942 0.44942 0.44942 0.44942

Eigenvalues --- 0.45296 0.45296 0.45296 0.45804 0.45804

Eigenvalues --- 0.45804 0.45804 0.45893 0.45893 0.45893

Eigenvalues --- 0.45894 0.46693 0.46887 0.47932 0.47932

Eigenvalues --- 0.48885 0.50570 0.50965 0.50965 0.53607

En-DIIS/RFO-DIIS IScMMF= 0 using points: 6 5 4 3 2

RFO step: Lambda=-2.53428658D-07.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 9.29D-05 SmlDif= 1.00D-05

RMS Error= 0.4457897010D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.28503 -0.35787 0.05507 0.00144 0.01633

Iteration 1 RMS(Cart)= 0.00091737 RMS(Int)= 0.00000036

Iteration 2 RMS(Cart)= 0.00000054 RMS(Int)= 0.00000027

ITry= 1 IFail=0 DXMaxC= 5.52D-03 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 5.13D-08 for atom 55.

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

(Linear) (Quad) (Total)

R1 2.74016 -0.00005 -0.00010 -0.00006 -0.00016 2.74000

R2 2.57547 0.00007 0.00013 0.00003 0.00016 2.57564

R3 2.03919 0.00000 0.00002 -0.00001 0.00001 2.03920

R4 2.58875 -0.00000 -0.00006 0.00005 -0.00002 2.58874

R5 2.66787 -0.00001 -0.00005 0.00002 -0.00003 2.66784

R6 2.58875 -0.00000 -0.00006 0.00005 -0.00002 2.58874

R7 3.95102 -0.00003 -0.00009 -0.00006 -0.00015 3.95087

R8 2.74016 -0.00005 -0.00010 -0.00006 -0.00016 2.74000

R9 2.66787 -0.00001 -0.00005 0.00002 -0.00003 2.66784

R10 2.03919 0.00000 0.00002 -0.00001 0.00001 2.03920

R11 2.66787 -0.00001 -0.00005 0.00002 -0.00003 2.66784

R12 2.82222 0.00003 -0.00016 0.00023 0.00007 2.82229

R13 2.58875 -0.00000 -0.00006 0.00005 -0.00002 2.58874

R14 2.74016 -0.00005 -0.00010 -0.00006 -0.00016 2.74000

R15 2.58875 -0.00000 -0.00006 0.00005 -0.00002 2.58874

R16 3.95102 -0.00003 -0.00009 -0.00006 -0.00015 3.95087

R17 2.74016 -0.00005 -0.00010 -0.00006 -0.00016 2.74000

R18 2.66787 -0.00001 -0.00005 0.00002 -0.00003 2.66784

R19 2.57547 0.00007 0.00013 0.00003 0.00016 2.57564

R20 2.03919 0.00000 0.00002 -0.00001 0.00001 2.03920

R21 2.03919 0.00000 0.00002 -0.00001 0.00001 2.03920

R22 2.66787 -0.00001 -0.00005 0.00002 -0.00003 2.66784

R23 2.82222 0.00003 -0.00016 0.00023 0.00007 2.82229

R24 2.74016 -0.00005 -0.00010 -0.00006 -0.00016 2.74000

R25 2.58875 -0.00000 -0.00006 0.00005 -0.00002 2.58874

R26 2.57547 0.00007 0.00013 0.00003 0.00016 2.57564

R27 2.03919 0.00000 0.00002 -0.00001 0.00001 2.03920

R28 2.74016 -0.00005 -0.00010 -0.00006 -0.00016 2.74000

R29 2.03919 0.00000 0.00002 -0.00001 0.00001 2.03920

R30 2.58875 -0.00000 -0.00006 0.00005 -0.00002 2.58874

R31 2.66787 -0.00001 -0.00005 0.00002 -0.00003 2.66784

R32 3.95102 -0.00003 -0.00009 -0.00006 -0.00015 3.95087

R33 2.66787 -0.00001 -0.00005 0.00002 -0.00003 2.66784

R34 2.82222 0.00003 -0.00016 0.00023 0.00007 2.82229

R35 2.74016 -0.00005 -0.00010 -0.00006 -0.00016 2.74000

R36 2.58875 -0.00000 -0.00006 0.00005 -0.00002 2.58874

R37 2.57547 0.00007 0.00013 0.00003 0.00016 2.57564

R38 2.03919 0.00000 0.00002 -0.00001 0.00001 2.03920

R39 2.74016 -0.00005 -0.00010 -0.00006 -0.00016 2.74000

R40 2.03919 0.00000 0.00002 -0.00001 0.00001 2.03920

R41 2.58875 -0.00000 -0.00006 0.00005 -0.00002 2.58874

R42 2.66787 -0.00001 -0.00005 0.00002 -0.00003 2.66784

R43 3.95102 -0.00003 -0.00009 -0.00006 -0.00015 3.95087

R44 2.82222 0.00003 -0.00016 0.00023 0.00007 2.82229

R45 2.64655 -0.00005 -0.00008 -0.00002 -0.00010 2.64645

R46 2.64655 -0.00005 -0.00008 -0.00002 -0.00010 2.64645

R47 2.63217 0.00001 -0.00003 0.00004 0.00001 2.63218

R48 2.04951 0.00000 0.00001 -0.00001 0.00001 2.04952

R49 2.63476 -0.00001 -0.00002 0.00002 -0.00001 2.63475

R50 2.05047 -0.00000 -0.00001 0.00000 -0.00000 2.05046

R51 2.63476 -0.00001 -0.00002 0.00002 -0.00001 2.63475

R52 2.05030 -0.00000 -0.00001 0.00000 -0.00001 2.05028

R53 2.63217 0.00001 -0.00003 0.00004 0.00001 2.63218

R54 2.05047 -0.00000 -0.00001 0.00000 -0.00000 2.05046

R55 2.04951 0.00000 0.00001 -0.00001 0.00001 2.04952

R56 2.63476 -0.00001 -0.00002 0.00002 -0.00001 2.63475

R57 2.63476 -0.00001 -0.00002 0.00002 -0.00001 2.63475

R58 2.05030 -0.00000 -0.00001 0.00000 -0.00001 2.05028

R59 2.63217 0.00001 -0.00003 0.00004 0.00001 2.63218

R60 2.05047 -0.00000 -0.00001 0.00000 -0.00000 2.05046

R61 2.64655 -0.00005 -0.00008 -0.00002 -0.00010 2.64645

R62 2.04951 0.00000 0.00001 -0.00001 0.00001 2.04952

R63 2.64655 -0.00005 -0.00008 -0.00002 -0.00010 2.64645

R64 2.63217 0.00001 -0.00003 0.00004 0.00001 2.63218

R65 2.04951 0.00000 0.00001 -0.00001 0.00001 2.04952

R66 2.05047 -0.00000 -0.00001 0.00000 -0.00000 2.05046

R67 2.64655 -0.00005 -0.00008 -0.00002 -0.00010 2.64645

R68 2.64655 -0.00005 -0.00008 -0.00002 -0.00010 2.64645

R69 2.63217 0.00001 -0.00003 0.00004 0.00001 2.63218

R70 2.04951 0.00000 0.00001 -0.00001 0.00001 2.04952

R71 2.63476 -0.00001 -0.00002 0.00002 -0.00001 2.63475

R72 2.05047 -0.00000 -0.00001 0.00000 -0.00000 2.05046

R73 2.63476 -0.00001 -0.00002 0.00002 -0.00001 2.63475

R74 2.05030 -0.00000 -0.00001 0.00000 -0.00001 2.05028

R75 2.63217 0.00001 -0.00003 0.00004 0.00001 2.63218

R76 2.05047 -0.00000 -0.00001 0.00000 -0.00000 2.05046

R77 2.04951 0.00000 0.00001 -0.00001 0.00001 2.04952

R78 2.64655 -0.00005 -0.00008 -0.00002 -0.00010 2.64645

R79 2.64655 -0.00005 -0.00008 -0.00002 -0.00010 2.64645

R80 2.63217 0.00001 -0.00003 0.00004 0.00001 2.63218

R81 2.04951 0.00000 0.00001 -0.00001 0.00001 2.04952

R82 2.63476 -0.00001 -0.00002 0.00002 -0.00001 2.63475

R83 2.05047 -0.00000 -0.00001 0.00000 -0.00000 2.05046

R84 2.63476 -0.00001 -0.00002 0.00002 -0.00001 2.63475

R85 2.05030 -0.00000 -0.00001 0.00000 -0.00001 2.05028

R86 2.63217 0.00001 -0.00003 0.00004 0.00001 2.63218

R87 2.05047 -0.00000 -0.00001 0.00000 -0.00000 2.05046

R88 2.04951 0.00000 0.00001 -0.00001 0.00001 2.04952

A1 1.87127 -0.00002 -0.00004 -0.00002 -0.00006 1.87121

A2 2.19531 -0.00001 -0.00003 -0.00005 -0.00007 2.19523

A3 2.21645 0.00002 0.00007 0.00006 0.00013 2.21659

A4 1.89568 0.00003 0.00006 0.00008 0.00014 1.89582

A5 2.18765 0.00000 -0.00001 0.00003 0.00001 2.18767

A6 2.19976 -0.00003 -0.00004 -0.00011 -0.00015 2.19961

A7 1.89076 -0.00002 -0.00003 -0.00012 -0.00015 1.89060

A8 2.19328 0.00001 -0.00005 0.00004 -0.00002 2.19326

A9 2.19328 0.00001 -0.00005 0.00004 -0.00002 2.19326

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D3 -3.11450 -0.00000 -0.00036 0.00022 -0.00013 -3.11463

D4 0.01311 0.00000 0.00025 0.00009 0.00034 0.01346

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D7 3.12331 -0.00000 0.00018 -0.00025 -0.00007 3.12324

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D12 -0.11196 -0.00001 -0.00162 -0.00028 -0.00190 -0.11386

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D14 0.07779 -0.00000 0.00018 0.00030 0.00048 0.07827

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D16 -3.08019 0.00001 0.00089 0.00015 0.00104 -3.07915

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D39 2.02123 -0.00001 -0.00009 -0.00056 -0.00066 2.02057

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D75 -2.02123 0.00001 0.00009 0.00056 0.00066 -2.02057

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D132 -0.11196 -0.00001 -0.00162 -0.00028 -0.00190 -0.11386

D133 -3.06380 -0.00000 0.00018 0.00030 0.00048 -3.06332

D134 0.07779 -0.00000 0.00018 0.00030 0.00048 0.07827

D135 0.06141 0.00001 0.00089 0.00015 0.00104 0.06245

D136 -3.08019 0.00001 0.00089 0.00015 0.00104 -3.07915

D137 3.06357 -0.00001 -0.00077 -0.00039 -0.00116 3.06241

D138 -0.05203 -0.00001 -0.00075 -0.00014 -0.00089 -0.05292

D139 0.05203 0.00001 0.00075 0.00014 0.00089 0.05292

D140 -3.06357 0.00001 0.00077 0.00039 0.00116 -3.06241

D141 1.12036 0.00001 0.00009 0.00056 0.00066 1.12102

D142 -2.02123 0.00001 0.00009 0.00056 0.00066 -2.02057

D143 -2.02123 0.00001 0.00009 0.00056 0.00066 -2.02057

D144 1.12036 0.00001 0.00009 0.00056 0.00066 1.12102

D145 -3.13983 0.00000 0.00001 0.00006 0.00007 -3.13977

D146 -0.00737 0.00000 0.00014 -0.00002 0.00012 -0.00725

D147 0.00176 0.00000 0.00001 0.00006 0.00007 0.00183

D148 3.13422 0.00000 0.00014 -0.00002 0.00012 3.13434

D149 -3.13983 0.00000 0.00001 0.00006 0.00007 -3.13977

D150 -0.00737 0.00000 0.00014 -0.00002 0.00012 -0.00725

D151 0.00176 0.00000 0.00001 0.00006 0.00007 0.00183

D152 3.13422 0.00000 0.00014 -0.00002 0.00012 3.13434

D153 -0.00353 -0.00000 -0.00001 -0.00012 -0.00013 -0.00366

D154 3.13523 -0.00000 0.00004 -0.00017 -0.00013 3.13509

D155 -3.13594 -0.00000 -0.00015 -0.00004 -0.00018 -3.13612

D156 0.00281 -0.00000 -0.00009 -0.00009 -0.00018 0.00263

D157 0.00175 0.00000 0.00001 0.00006 0.00007 0.00182

D158 -3.13984 0.00000 0.00001 0.00006 0.00007 -3.13978

D159 -3.13699 0.00000 -0.00005 0.00011 0.00007 -3.13692

D160 0.00460 0.00000 -0.00005 0.00011 0.00007 0.00467

D161 0.00175 0.00000 0.00001 0.00006 0.00007 0.00182

D162 -3.13699 0.00000 -0.00005 0.00011 0.00007 -3.13692

D163 -3.13984 0.00000 0.00001 0.00006 0.00007 -3.13978

D164 0.00460 0.00000 -0.00005 0.00011 0.00007 0.00467

D165 -0.00353 -0.00000 -0.00001 -0.00012 -0.00013 -0.00366

D166 -3.13594 -0.00000 -0.00015 -0.00004 -0.00018 -3.13612

D167 3.13523 -0.00000 0.00004 -0.00017 -0.00013 3.13509

D168 0.00281 -0.00000 -0.00009 -0.00009 -0.00018 0.00263

D169 -0.00175 -0.00000 -0.00001 -0.00006 -0.00007 -0.00182

D170 3.13699 -0.00000 0.00005 -0.00011 -0.00007 3.13692

D171 3.13984 -0.00000 -0.00001 -0.00006 -0.00007 3.13978

D172 -0.00460 -0.00000 0.00005 -0.00011 -0.00007 -0.00467

D173 -0.00175 -0.00000 -0.00001 -0.00006 -0.00007 -0.00182

D174 3.13699 -0.00000 0.00005 -0.00011 -0.00007 3.13692

D175 3.13984 -0.00000 -0.00001 -0.00006 -0.00007 3.13978

D176 -0.00460 -0.00000 0.00005 -0.00011 -0.00007 -0.00467

D177 0.00353 0.00000 0.00001 0.00012 0.00013 0.00366

D178 3.13594 0.00000 0.00015 0.00004 0.00018 3.13612

D179 -3.13523 0.00000 -0.00004 0.00017 0.00013 -3.13509

D180 -0.00281 0.00000 0.00009 0.00009 0.00018 -0.00263

D181 3.13983 -0.00000 -0.00001 -0.00006 -0.00007 3.13977

D182 -0.00176 -0.00000 -0.00001 -0.00006 -0.00007 -0.00183

D183 0.00737 -0.00000 -0.00014 0.00002 -0.00012 0.00725

D184 -3.13422 -0.00000 -0.00014 0.00002 -0.00012 -3.13434

D185 3.13983 -0.00000 -0.00001 -0.00006 -0.00007 3.13977

D186 0.00737 -0.00000 -0.00014 0.00002 -0.00012 0.00725

D187 -0.00176 -0.00000 -0.00001 -0.00006 -0.00007 -0.00183

D188 -3.13422 -0.00000 -0.00014 0.00002 -0.00012 -3.13434

D189 0.00353 0.00000 0.00001 0.00012 0.00013 0.00366

D190 -3.13523 0.00000 -0.00004 0.00017 0.00013 -3.13509

D191 3.13594 0.00000 0.00015 0.00004 0.00018 3.13612

D192 -0.00281 0.00000 0.00009 0.00009 0.00018 -0.00263

D193 3.13983 -0.00000 -0.00001 -0.00006 -0.00007 3.13977

D194 0.00737 -0.00000 -0.00014 0.00002 -0.00012 0.00725

D195 -0.00176 -0.00000 -0.00001 -0.00006 -0.00007 -0.00183

D196 -3.13422 -0.00000 -0.00014 0.00002 -0.00012 -3.13434

D197 3.13983 -0.00000 -0.00001 -0.00006 -0.00007 3.13977

D198 0.00737 -0.00000 -0.00014 0.00002 -0.00012 0.00725

D199 -0.00176 -0.00000 -0.00001 -0.00006 -0.00007 -0.00183

D200 -3.13422 -0.00000 -0.00014 0.00002 -0.00012 -3.13434

D201 0.00353 0.00000 0.00001 0.00012 0.00013 0.00366

D202 -3.13523 0.00000 -0.00004 0.00017 0.00013 -3.13509

D203 3.13594 0.00000 0.00015 0.00004 0.00018 3.13612

D204 -0.00281 0.00000 0.00009 0.00009 0.00018 -0.00263

D205 -0.00175 -0.00000 -0.00001 -0.00006 -0.00007 -0.00182

D206 3.13984 -0.00000 -0.00001 -0.00006 -0.00007 3.13978

D207 3.13699 -0.00000 0.00005 -0.00011 -0.00007 3.13692

D208 -0.00460 -0.00000 0.00005 -0.00011 -0.00007 -0.00467

D209 -0.00175 -0.00000 -0.00001 -0.00006 -0.00007 -0.00182

D210 3.13699 -0.00000 0.00005 -0.00011 -0.00007 3.13692

D211 3.13984 -0.00000 -0.00001 -0.00006 -0.00007 3.13978

D212 -0.00460 -0.00000 0.00005 -0.00011 -0.00007 -0.00467

D213 0.00353 0.00000 0.00001 0.00012 0.00013 0.00366

D214 3.13594 0.00000 0.00015 0.00004 0.00018 3.13612

D215 -3.13523 0.00000 -0.00004 0.00017 0.00013 -3.13509

D216 -0.00281 0.00000 0.00009 0.00009 0.00018 -0.00263

D217 -3.13983 0.00000 0.00001 0.00006 0.00007 -3.13977

D218 -0.00737 0.00000 0.00014 -0.00002 0.00012 -0.00725

D219 0.00176 0.00000 0.00001 0.00006 0.00007 0.00183

D220 3.13422 0.00000 0.00014 -0.00002 0.00012 3.13434

D221 -3.13983 0.00000 0.00001 0.00006 0.00007 -3.13977

D222 -0.00737 0.00000 0.00014 -0.00002 0.00012 -0.00725

D223 0.00176 0.00000 0.00001 0.00006 0.00007 0.00183

D224 3.13422 0.00000 0.00014 -0.00002 0.00012 3.13434

D225 -0.00353 -0.00000 -0.00001 -0.00012 -0.00013 -0.00366

D226 3.13523 -0.00000 0.00004 -0.00017 -0.00013 3.13509

D227 -3.13594 -0.00000 -0.00015 -0.00004 -0.00018 -3.13612

D228 0.00281 -0.00000 -0.00009 -0.00009 -0.00018 0.00263

D229 0.00175 0.00000 0.00001 0.00006 0.00007 0.00182

D230 -3.13984 0.00000 0.00001 0.00006 0.00007 -3.13978

D231 -3.13699 0.00000 -0.00005 0.00011 0.00007 -3.13692

D232 0.00460 0.00000 -0.00005 0.00011 0.00007 0.00467

D233 0.00175 0.00000 0.00001 0.00006 0.00007 0.00182

D234 -3.13699 0.00000 -0.00005 0.00011 0.00007 -3.13692

D235 -3.13984 0.00000 0.00001 0.00006 0.00007 -3.13978

D236 0.00460 0.00000 -0.00005 0.00011 0.00007 0.00467

D237 -0.00353 -0.00000 -0.00001 -0.00012 -0.00013 -0.00366

D238 -3.13594 -0.00000 -0.00015 -0.00004 -0.00018 -3.13612

D239 3.13523 -0.00000 0.00004 -0.00017 -0.00013 3.13509

D240 0.00281 -0.00000 -0.00009 -0.00009 -0.00018 0.00263

Item Value Threshold Converged?

Maximum Force 0.000067 0.000450 YES

RMS Force 0.000016 0.000300 YES

Maximum Displacement 0.005523 0.001800 NO

RMS Displacement 0.000917 0.001200 YES

Predicted change in Energy=-4.742471D-07

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

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

Stoichiometry C44H28N4Zn

Framework group D2D[O(Zn),2SGD(N2),X(C44H28)]

Deg. of freedom 29

Full point group D2D NOp 8

RotChk: IX=0 Diff= 0.00D+00

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681484 4.269157 0.164086

2 6 0 -1.110541 2.890129 0.035503

3 7 0 0.000000 2.090529 -0.027459

4 6 0 1.110541 2.890129 0.035503

5 6 0 0.681484 4.269157 0.164086

6 6 0 2.452183 2.452183 0.000000

7 6 0 2.890129 1.110541 -0.035503

8 7 0 2.090529 -0.000000 0.027459

9 6 0 2.890129 -1.110541 -0.035503

10 6 0 4.269157 -0.681484 -0.164086

11 6 0 4.269157 0.681484 -0.164086

12 6 0 -2.452183 2.452183 0.000000

13 6 0 -2.890129 1.110541 -0.035503

14 6 0 -4.269157 0.681484 -0.164086

15 6 0 -4.269157 -0.681484 -0.164086

16 6 0 -2.890129 -1.110541 -0.035503

17 7 0 -2.090529 0.000000 0.027459

18 6 0 -2.452183 -2.452183 0.000000

19 6 0 -1.110541 -2.890129 0.035503

20 6 0 -0.681484 -4.269157 0.164086

21 6 0 0.681484 -4.269157 0.164086

22 6 0 1.110541 -2.890129 0.035503

23 7 0 -0.000000 -2.090529 -0.027459

24 6 0 2.452183 -2.452183 0.000000

25 6 0 3.508242 3.508242 -0.000000

26 6 0 3.621357 4.405038 -1.069674

27 6 0 4.607485 5.388753 -1.071137

28 6 0 5.493806 5.493806 0.000000

29 6 0 5.388753 4.607485 1.071137

30 6 0 4.405038 3.621357 1.069674

31 6 0 -5.493806 5.493806 0.000000

32 6 0 -4.607485 5.388753 -1.071137

33 6 0 -3.621357 4.405038 -1.069674

34 6 0 -3.508242 3.508242 -0.000000

35 6 0 -4.405038 3.621357 1.069674

36 6 0 -5.388753 4.607485 1.071137

37 6 0 3.508242 -3.508242 -0.000000

38 6 0 4.405038 -3.621357 1.069674

39 6 0 5.388753 -4.607485 1.071137

40 6 0 5.493806 -5.493806 0.000000

41 6 0 4.607485 -5.388753 -1.071137

42 6 0 3.621357 -4.405038 -1.069674

43 6 0 -3.508242 -3.508242 -0.000000

44 6 0 -4.405038 -3.621357 1.069674

45 6 0 -5.388753 -4.607485 1.071137

46 6 0 -5.493806 -5.493806 0.000000

47 6 0 -4.607485 -5.388753 -1.071137

48 6 0 -3.621357 -4.405038 -1.069674

49 1 0 -1.330917 5.125618 0.259828

50 1 0 1.330917 5.125618 0.259828

51 1 0 5.125618 -1.330917 -0.259828

52 1 0 5.125618 1.330917 -0.259828

53 1 0 -5.125618 1.330917 -0.259828

54 1 0 -5.125618 -1.330917 -0.259828

55 1 0 -1.330917 -5.125618 0.259828

56 1 0 1.330917 -5.125618 0.259828

57 1 0 2.936967 4.323214 -1.907040

58 1 0 4.684584 6.071446 -1.910980

59 1 0 6.260992 6.260992 0.000000

60 1 0 6.071446 4.684584 1.910980

61 1 0 4.323214 2.936967 1.907040

62 1 0 -6.260992 6.260992 0.000000

63 1 0 -4.684584 6.071446 -1.910980

64 1 0 -2.936967 4.323214 -1.907040

65 1 0 -4.323214 2.936967 1.907040

66 1 0 -6.071446 4.684584 1.910980

67 1 0 4.323214 -2.936967 1.907040

68 1 0 6.071446 -4.684584 1.910980

69 1 0 6.260992 -6.260992 0.000000

70 1 0 4.684584 -6.071446 -1.910980

71 1 0 2.936967 -4.323214 -1.907040

72 1 0 -4.323214 -2.936967 1.907040

73 1 0 -6.071446 -4.684584 1.910980

74 1 0 -6.260992 -6.260992 0.000000

75 1 0 -4.684584 -6.071446 -1.910980

76 1 0 -2.936967 -4.323214 -1.907040

77 30 0 0.000000 0.000000 0.000000

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

Rotational constants (GHZ): 0.0582110 0.0582110 0.0300828

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

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

Pseudo-potential data read from rwf file.

There are 272 symmetry adapted cartesian basis functions of A1 symmetry.

There are 243 symmetry adapted cartesian basis functions of A2 symmetry.

There are 254 symmetry adapted cartesian basis functions of B1 symmetry.

There are 254 symmetry adapted cartesian basis functions of B2 symmetry.

There are 256 symmetry adapted basis functions of A1 symmetry.

There are 232 symmetry adapted basis functions of A2 symmetry.

There are 242 symmetry adapted basis functions of B1 symmetry.

There are 242 symmetry adapted basis functions of B2 symmetry.

972 basis functions, 1715 primitive gaussians, 1023 cartesian basis functions

166 alpha electrons 166 beta electrons

nuclear repulsion energy 5738.4943395508 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= 77 NActive= 77 NUniq= 13 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T 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= -0.2224135280 Hartrees.

Nuclear repulsion after empirical dispersion term = 5738.2719260228 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 77.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 77

GePol: Total number of spheres = 77

GePol: Number of exposed spheres = 77 (100.00%)

GePol: Number of points = 5690

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.75D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 272

GePol: Fraction of low-weight points (<1% of avg) = 4.78%

GePol: Cavity surface area = 614.366 Ang\*\*2

GePol: Cavity volume = 630.258 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021384217 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5738.2697876011 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

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36757 LenP2D= 95282.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 972 RedAO= T EigKep= 6.36D-05 NBF= 256 232 242 242

NBsUse= 972 1.00D-06 EigRej= -1.00D+00 NBFU= 256 232 242 242

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= 952 960 976 976 976 MxSgAt= 77 MxSgA2= 77.

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

DipDrv: MaxL=1.

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

Initial guess from the checkpoint file: "ZnTPP0.chk"

B after Tr= 0.000000 0.000000 -0.000000

Rot= 1.000000 0.000000 -0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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Virtual (A1) (B2) (B2) (A1) (B2) (A1) (A1) (A1) (B2) (B2)

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

Leave Link 401 at Tue Aug 13 18:43:32 2019, MaxMem= 671088640 cpu: 10.9

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3177123 IEndB= 3177123 NGot= 671088640 MDV= 668975710

LenX= 668975710 LenY= 667928158

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= 530000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 97128300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.22D-15 for 1281.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.44D-15 for 5674 1282.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.00D-15 for 5676.

Iteration 1 A^-1\*A deviation from orthogonality is 6.13D-12 for 3423 3413.

E= -1978.90434665113

DIIS: error= 7.60D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1978.90434665113 IErMin= 1 ErrMin= 7.60D-05

ErrMax= 7.60D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.43D-06 BMatP= 3.43D-06

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

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.443 Goal= None Shift= 0.000

RMSDP=3.27D-06 MaxDP=1.21D-04 OVMax= 5.49D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.27D-06 CP: 1.00D+00

E= -1978.90435326742 Delta-E= -0.000006616294 Rises=F Damp=F

DIIS: error= 1.25D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1978.90435326742 IErMin= 2 ErrMin= 1.25D-05

ErrMax= 1.25D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.41D-08 BMatP= 3.43D-06

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

Coeff-Com: -0.646D-01 0.106D+01

Coeff: -0.646D-01 0.106D+01

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=4.88D-07 MaxDP=1.47D-05 DE=-6.62D-06 OVMax= 8.50D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.52D-07 CP: 1.00D+00 1.06D+00

E= -1978.90435335557 Delta-E= -0.000000088146 Rises=F Damp=F

DIIS: error= 6.41D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1978.90435335557 IErMin= 3 ErrMin= 6.41D-06

ErrMax= 6.41D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.46D-08 BMatP= 5.41D-08

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

Coeff-Com: -0.332D-01 0.450D+00 0.583D+00

Coeff: -0.332D-01 0.450D+00 0.583D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.87D-07 MaxDP=1.45D-05 DE=-8.81D-08 OVMax= 3.94D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.62D-07 CP: 1.00D+00 1.07D+00 8.08D-01

E= -1978.90435337223 Delta-E= -0.000000016656 Rises=F Damp=F

DIIS: error= 4.10D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1978.90435337223 IErMin= 4 ErrMin= 4.10D-06

ErrMax= 4.10D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.20D-09 BMatP= 2.46D-08

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

Coeff-Com: -0.944D-02 0.108D+00 0.355D+00 0.547D+00

Coeff: -0.944D-02 0.108D+00 0.355D+00 0.547D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=7.86D-08 MaxDP=5.35D-06 DE=-1.67D-08 OVMax= 1.68D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 5.67D-08 CP: 1.00D+00 1.07D+00 8.58D-01 6.98D-01

E= -1978.90435337824 Delta-E= -0.000000006015 Rises=F Damp=F

DIIS: error= 1.00D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1978.90435337824 IErMin= 5 ErrMin= 1.00D-06

ErrMax= 1.00D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.96D-10 BMatP= 7.20D-09

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

Coeff-Com: -0.179D-02 0.112D-01 0.123D+00 0.263D+00 0.605D+00

Coeff: -0.179D-02 0.112D-01 0.123D+00 0.263D+00 0.605D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=2.57D-08 MaxDP=1.47D-06 DE=-6.02D-09 OVMax= 5.16D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.87D-08 CP: 1.00D+00 1.07D+00 8.72D-01 7.55D-01 7.61D-01

E= -1978.90435337873 Delta-E= -0.000000000485 Rises=F Damp=F

DIIS: error= 5.02D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1978.90435337873 IErMin= 6 ErrMin= 5.02D-07

ErrMax= 5.02D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-10 BMatP= 3.96D-10

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

Coeff-Com: 0.620D-03-0.145D-01 0.772D-02 0.572D-01 0.374D+00 0.575D+00

Coeff: 0.620D-03-0.145D-01 0.772D-02 0.572D-01 0.374D+00 0.575D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=9.43D-09 MaxDP=4.92D-07 DE=-4.85D-10 OVMax= 1.89D-06

Error on total polarization charges = 0.08494

SCF Done: E(RB3LYP) = -1978.90435338 A.U. after 6 cycles

NFock= 6 Conv=0.94D-08 -V/T= 1.9793

KE= 2.020706227707D+03 PE=-1.615865197217D+04 EE= 6.420771603479D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.34

(included in total energy above)

Leave Link 502 at Tue Aug 13 18:47:43 2019, MaxMem= 671088640 cpu: 1004.5

(Enter /home/kira/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

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

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36757 LenP2D= 95282.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 182

Leave Link 701 at Tue Aug 13 18:48:31 2019, MaxMem= 671088640 cpu: 190.1

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

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

Leave Link 702 at Tue Aug 13 18:48:31 2019, MaxMem= 671088640 cpu: 0.1

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 0 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Tue Aug 13 18:49:21 2019, MaxMem= 671088640 cpu: 198.1

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

Dipole = 3.11750625D-13-2.13162821D-13 9.32587341D-15

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000008595 -0.000009629 -0.000003289

2 6 -0.000023972 0.000034840 0.000010350

3 7 0.000000000 -0.000028509 -0.000005082

4 6 0.000023972 0.000034840 0.000010350

5 6 0.000008595 -0.000009629 -0.000003289

6 6 -0.000041663 -0.000041663 -0.000000000

7 6 0.000034840 0.000023972 -0.000010350

8 7 -0.000028509 -0.000000000 0.000005082

9 6 0.000034840 -0.000023972 -0.000010350

10 6 -0.000009629 -0.000008595 0.000003289

11 6 -0.000009629 0.000008595 0.000003289

12 6 0.000041663 -0.000041663 -0.000000000

13 6 -0.000034840 0.000023972 -0.000010350

14 6 0.000009629 0.000008595 0.000003289

15 6 0.000009629 -0.000008595 0.000003289

16 6 -0.000034840 -0.000023972 -0.000010350

17 7 0.000028509 -0.000000000 0.000005082

18 6 0.000041663 0.000041663 0.000000000

19 6 -0.000023972 -0.000034840 0.000010350

20 6 -0.000008595 0.000009629 -0.000003289

21 6 0.000008595 0.000009629 -0.000003289

22 6 0.000023972 -0.000034840 0.000010350

23 7 0.000000000 0.000028509 -0.000005082

24 6 -0.000041663 0.000041663 -0.000000000

25 6 0.000043752 0.000043752 -0.000000000

26 6 -0.000018053 -0.000024362 0.000000574

27 6 0.000010198 0.000011602 0.000001541

28 6 -0.000005715 -0.000005715 0.000000000

29 6 0.000011602 0.000010198 -0.000001541

30 6 -0.000024362 -0.000018053 -0.000000574

31 6 0.000005715 -0.000005715 -0.000000000

32 6 -0.000010198 0.000011602 0.000001541

33 6 0.000018053 -0.000024362 0.000000574

34 6 -0.000043752 0.000043752 0.000000000

35 6 0.000024362 -0.000018053 -0.000000574

36 6 -0.000011602 0.000010198 -0.000001541

37 6 0.000043752 -0.000043752 0.000000000

38 6 -0.000024362 0.000018053 -0.000000574

39 6 0.000011602 -0.000010198 -0.000001541

40 6 -0.000005715 0.000005715 -0.000000000

41 6 0.000010198 -0.000011602 0.000001541

42 6 -0.000018053 0.000024362 0.000000574

43 6 -0.000043752 -0.000043752 -0.000000000

44 6 0.000024362 0.000018053 -0.000000574

45 6 -0.000011602 -0.000010198 -0.000001541

46 6 0.000005715 0.000005715 0.000000000

47 6 -0.000010198 -0.000011602 0.000001541

48 6 0.000018053 0.000024362 0.000000574

49 1 -0.000006006 -0.000003083 -0.000001809

50 1 0.000006006 -0.000003083 -0.000001809

51 1 -0.000003083 -0.000006006 0.000001809

52 1 -0.000003083 0.000006006 0.000001809

53 1 0.000003083 0.000006006 0.000001809

54 1 0.000003083 -0.000006006 0.000001809

55 1 -0.000006006 0.000003083 -0.000001809

56 1 0.000006006 0.000003083 -0.000001809

57 1 -0.000001757 0.000002596 0.000001941

58 1 0.000000881 0.000000021 0.000000612

59 1 0.000001280 0.000001280 0.000000000

60 1 0.000000021 0.000000881 -0.000000612

61 1 0.000002596 -0.000001757 -0.000001941

62 1 -0.000001280 0.000001280 -0.000000000

63 1 -0.000000881 0.000000021 0.000000612

64 1 0.000001757 0.000002596 0.000001941

65 1 -0.000002596 -0.000001757 -0.000001941

66 1 -0.000000021 0.000000881 -0.000000612

67 1 0.000002596 0.000001757 -0.000001941

68 1 0.000000021 -0.000000881 -0.000000612

69 1 0.000001280 -0.000001280 0.000000000

70 1 0.000000881 -0.000000021 0.000000612

71 1 -0.000001757 -0.000002596 0.000001941

72 1 -0.000002596 0.000001757 -0.000001941

73 1 -0.000000021 -0.000000881 -0.000000612

74 1 -0.000001280 -0.000001280 -0.000000000

75 1 -0.000000881 -0.000000021 0.000000612

76 1 0.000001757 -0.000002596 0.000001941

77 30 -0.000000000 0.000000000 -0.000000000

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

Cartesian Forces: Max 0.000043752 RMS 0.000016010

Leave Link 716 at Tue Aug 13 18:49:21 2019, MaxMem= 671088640 cpu: 0.1

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.000028908 RMS 0.000005785

Search for a local minimum.

Step number 7 out of a maximum of 462

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

RMS Force = .57849D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

6 7

DE= -5.24D-07 DEPred=-4.74D-07 R= 1.11D+00

Trust test= 1.11D+00 RLast= 9.79D-03 DXMaxT set to 5.05D-01

ITU= 0 1 1 1 1 1 0

Eigenvalues --- 0.00365 0.00755 0.00755 0.00755 0.00972

Eigenvalues --- 0.01174 0.01318 0.01477 0.01477 0.01560

Eigenvalues --- 0.01583 0.01583 0.01583 0.01596 0.01619

Eigenvalues --- 0.01623 0.01623 0.01623 0.01623 0.01681

Eigenvalues --- 0.01705 0.01705 0.01783 0.01783 0.01785

Eigenvalues --- 0.01812 0.01815 0.01815 0.01823 0.01865

Eigenvalues --- 0.01879 0.01880 0.01880 0.01886 0.01900

Eigenvalues --- 0.01900 0.01918 0.02025 0.02025 0.02025

Eigenvalues --- 0.02025 0.02055 0.02058 0.02058 0.02058

Eigenvalues --- 0.02066 0.02066 0.02066 0.02066 0.02089

Eigenvalues --- 0.02089 0.02089 0.02095 0.02101 0.02101

Eigenvalues --- 0.02101 0.02101 0.02104 0.02104 0.02104

Eigenvalues --- 0.02104 0.02106 0.02106 0.02106 0.02107

Eigenvalues --- 0.02107 0.02107 0.02107 0.02116 0.02123

Eigenvalues --- 0.02129 0.02129 0.02132 0.03469 0.12210

Eigenvalues --- 0.12210 0.14169 0.15562 0.15994 0.15994

Eigenvalues --- 0.15994 0.15994 0.15997 0.15997 0.15997

Eigenvalues --- 0.15999 0.15999 0.15999 0.15999 0.15999

Eigenvalues --- 0.15999 0.15999 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16005 0.16041

Eigenvalues --- 0.17180 0.21761 0.21761 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22000 0.22000 0.22000

Eigenvalues --- 0.22011 0.22509 0.22821 0.22855 0.22886

Eigenvalues --- 0.22886 0.23474 0.23474 0.23474 0.24325

Eigenvalues --- 0.24741 0.24752 0.24752 0.24754 0.24755

Eigenvalues --- 0.24916 0.24916 0.24981 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.32293 0.32293 0.32293 0.34526

Eigenvalues --- 0.35007 0.35007 0.35131 0.35152 0.35160

Eigenvalues --- 0.35181 0.35181 0.35181 0.35181 0.35181

Eigenvalues --- 0.35181 0.35181 0.35193 0.35193 0.35193

Eigenvalues --- 0.35193 0.35202 0.35202 0.35202 0.35202

Eigenvalues --- 0.35202 0.35202 0.35202 0.35263 0.35734

Eigenvalues --- 0.35883 0.35883 0.35883 0.35883 0.35883

Eigenvalues --- 0.35883 0.35883 0.36033 0.36239 0.37147

Eigenvalues --- 0.37147 0.37843 0.38996 0.40015 0.40015

Eigenvalues --- 0.40999 0.41212 0.41212 0.41299 0.41299

Eigenvalues --- 0.41299 0.41373 0.41373 0.41373 0.41373

Eigenvalues --- 0.41576 0.42291 0.43125 0.43324 0.43324

Eigenvalues --- 0.44408 0.44942 0.44942 0.44942 0.44942

Eigenvalues --- 0.45296 0.45296 0.45296 0.45307 0.45804

Eigenvalues --- 0.45804 0.45804 0.45804 0.45893 0.45893

Eigenvalues --- 0.45893 0.46885 0.47317 0.47929 0.47929

Eigenvalues --- 0.48884 0.50569 0.50965 0.50965 0.53190

En-DIIS/RFO-DIIS IScMMF= 0 using points: 7 6 5 4 3

RFO step: Lambda=-3.37711404D-08.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 1.48D-05 SmlDif= 1.00D-05

RMS Error= 0.1481690666D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.89521 0.20178 -0.17136 0.05636 0.01801

Iteration 1 RMS(Cart)= 0.00048527 RMS(Int)= 0.00000012

Iteration 2 RMS(Cart)= 0.00000013 RMS(Int)= 0.00000009

ITry= 1 IFail=0 DXMaxC= 1.49D-03 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.40D-07 for atom 69.

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

(Linear) (Quad) (Total)

R1 2.74000 -0.00001 -0.00003 -0.00001 -0.00004 2.73996

R2 2.57564 0.00002 0.00004 -0.00000 0.00004 2.57568

R3 2.03920 0.00000 0.00000 0.00000 0.00000 2.03921

R4 2.58874 0.00002 -0.00001 0.00003 0.00003 2.58876

R5 2.66784 -0.00001 -0.00001 -0.00000 -0.00002 2.66782

R6 2.58874 0.00002 -0.00001 0.00003 0.00003 2.58876

R7 3.95087 -0.00000 0.00000 -0.00003 -0.00003 3.95084

R8 2.74000 -0.00001 -0.00003 -0.00001 -0.00004 2.73996

R9 2.66784 -0.00001 -0.00001 -0.00000 -0.00002 2.66782

R10 2.03920 0.00000 0.00000 0.00000 0.00000 2.03921

R11 2.66784 -0.00001 -0.00001 -0.00000 -0.00002 2.66782

R12 2.82229 0.00003 -0.00001 0.00010 0.00009 2.82238

R13 2.58874 0.00002 -0.00001 0.00003 0.00003 2.58876

R14 2.74000 -0.00001 -0.00003 -0.00001 -0.00004 2.73996

R15 2.58874 0.00002 -0.00001 0.00003 0.00003 2.58876

R16 3.95087 -0.00000 0.00000 -0.00003 -0.00003 3.95084

R17 2.74000 -0.00001 -0.00003 -0.00001 -0.00004 2.73996

R18 2.66784 -0.00001 -0.00001 -0.00000 -0.00002 2.66782

R19 2.57564 0.00002 0.00004 -0.00000 0.00004 2.57568

R20 2.03920 0.00000 0.00000 0.00000 0.00000 2.03921

R21 2.03920 0.00000 0.00000 0.00000 0.00000 2.03921

R22 2.66784 -0.00001 -0.00001 -0.00000 -0.00002 2.66782

R23 2.82229 0.00003 -0.00001 0.00010 0.00009 2.82238

R24 2.74000 -0.00001 -0.00003 -0.00001 -0.00004 2.73996

R25 2.58874 0.00002 -0.00001 0.00003 0.00003 2.58876

R26 2.57564 0.00002 0.00004 -0.00000 0.00004 2.57568

R27 2.03920 0.00000 0.00000 0.00000 0.00000 2.03921

R28 2.74000 -0.00001 -0.00003 -0.00001 -0.00004 2.73996

R29 2.03920 0.00000 0.00000 0.00000 0.00000 2.03921

R30 2.58874 0.00002 -0.00001 0.00003 0.00003 2.58876

R31 2.66784 -0.00001 -0.00001 -0.00000 -0.00002 2.66782

R32 3.95087 -0.00000 0.00000 -0.00003 -0.00003 3.95084

R33 2.66784 -0.00001 -0.00001 -0.00000 -0.00002 2.66782

R34 2.82229 0.00003 -0.00001 0.00010 0.00009 2.82238

R35 2.74000 -0.00001 -0.00003 -0.00001 -0.00004 2.73996

R36 2.58874 0.00002 -0.00001 0.00003 0.00003 2.58876

R37 2.57564 0.00002 0.00004 -0.00000 0.00004 2.57568

R38 2.03920 0.00000 0.00000 0.00000 0.00000 2.03921

R39 2.74000 -0.00001 -0.00003 -0.00001 -0.00004 2.73996

R40 2.03920 0.00000 0.00000 0.00000 0.00000 2.03921

R41 2.58874 0.00002 -0.00001 0.00003 0.00003 2.58876

R42 2.66784 -0.00001 -0.00001 -0.00000 -0.00002 2.66782

R43 3.95087 -0.00000 0.00000 -0.00003 -0.00003 3.95084

R44 2.82229 0.00003 -0.00001 0.00010 0.00009 2.82238

R45 2.64645 -0.00001 -0.00003 -0.00000 -0.00003 2.64643

R46 2.64645 -0.00001 -0.00003 -0.00000 -0.00003 2.64643

R47 2.63218 0.00001 0.00000 0.00003 0.00003 2.63221

R48 2.04952 -0.00000 0.00000 -0.00000 0.00000 2.04952

R49 2.63475 -0.00000 -0.00001 0.00001 0.00000 2.63475

R50 2.05046 -0.00000 -0.00000 0.00000 -0.00000 2.05046

R51 2.63475 -0.00000 -0.00001 0.00001 0.00000 2.63475

R52 2.05028 0.00000 -0.00000 0.00001 0.00001 2.05029

R53 2.63218 0.00001 0.00000 0.00003 0.00003 2.63221

R54 2.05046 -0.00000 -0.00000 0.00000 -0.00000 2.05046

R55 2.04952 -0.00000 0.00000 -0.00000 0.00000 2.04952

R56 2.63475 -0.00000 -0.00001 0.00001 0.00000 2.63475

R57 2.63475 -0.00000 -0.00001 0.00001 0.00000 2.63475

R58 2.05028 0.00000 -0.00000 0.00001 0.00001 2.05029

R59 2.63218 0.00001 0.00000 0.00003 0.00003 2.63221

R60 2.05046 -0.00000 -0.00000 0.00000 -0.00000 2.05046

R61 2.64645 -0.00001 -0.00003 -0.00000 -0.00003 2.64643

R62 2.04952 -0.00000 0.00000 -0.00000 0.00000 2.04952

R63 2.64645 -0.00001 -0.00003 -0.00000 -0.00003 2.64643

R64 2.63218 0.00001 0.00000 0.00003 0.00003 2.63221

R65 2.04952 -0.00000 0.00000 -0.00000 0.00000 2.04952

R66 2.05046 -0.00000 -0.00000 0.00000 -0.00000 2.05046

R67 2.64645 -0.00001 -0.00003 -0.00000 -0.00003 2.64643

R68 2.64645 -0.00001 -0.00003 -0.00000 -0.00003 2.64643

R69 2.63218 0.00001 0.00000 0.00003 0.00003 2.63221

R70 2.04952 -0.00000 0.00000 -0.00000 0.00000 2.04952

R71 2.63475 -0.00000 -0.00001 0.00001 0.00000 2.63475

R72 2.05046 -0.00000 -0.00000 0.00000 -0.00000 2.05046

R73 2.63475 -0.00000 -0.00001 0.00001 0.00000 2.63475

R74 2.05028 0.00000 -0.00000 0.00001 0.00001 2.05029

R75 2.63218 0.00001 0.00000 0.00003 0.00003 2.63221

R76 2.05046 -0.00000 -0.00000 0.00000 -0.00000 2.05046

R77 2.04952 -0.00000 0.00000 -0.00000 0.00000 2.04952

R78 2.64645 -0.00001 -0.00003 -0.00000 -0.00003 2.64643

R79 2.64645 -0.00001 -0.00003 -0.00000 -0.00003 2.64643

R80 2.63218 0.00001 0.00000 0.00003 0.00003 2.63221

R81 2.04952 -0.00000 0.00000 -0.00000 0.00000 2.04952

R82 2.63475 -0.00000 -0.00001 0.00001 0.00000 2.63475

R83 2.05046 -0.00000 -0.00000 0.00000 -0.00000 2.05046

R84 2.63475 -0.00000 -0.00001 0.00001 0.00000 2.63475

R85 2.05028 0.00000 -0.00000 0.00001 0.00001 2.05029

R86 2.63218 0.00001 0.00000 0.00003 0.00003 2.63221

R87 2.05046 -0.00000 -0.00000 0.00000 -0.00000 2.05046

R88 2.04952 -0.00000 0.00000 -0.00000 0.00000 2.04952

A1 1.87121 0.00000 -0.00000 -0.00000 -0.00000 1.87120

A2 2.19523 -0.00001 -0.00001 -0.00003 -0.00004 2.19519

A3 2.21659 0.00001 0.00002 0.00003 0.00005 2.21663

A4 1.89582 -0.00000 -0.00000 0.00002 0.00002 1.89584

A5 2.18767 0.00001 0.00000 0.00003 0.00003 2.18770

A6 2.19961 -0.00001 0.00000 -0.00005 -0.00005 2.19956

A7 1.89060 -0.00000 0.00001 -0.00004 -0.00003 1.89057

A8 2.19326 0.00000 -0.00001 0.00002 0.00001 2.19327

A9 2.19326 0.00000 -0.00001 0.00002 0.00001 2.19327

A10 1.89582 -0.00000 -0.00000 0.00002 0.00002 1.89584

A11 2.19961 -0.00001 0.00000 -0.00005 -0.00005 2.19956

A12 2.18767 0.00001 0.00000 0.00003 0.00003 2.18770

A13 1.87121 0.00000 -0.00000 -0.00000 -0.00000 1.87120

A14 2.21659 0.00001 0.00002 0.00003 0.00005 2.21663

A15 2.19523 -0.00001 -0.00001 -0.00003 -0.00004 2.19519

A16 2.20216 0.00001 -0.00000 0.00005 0.00005 2.20220

A17 2.04051 -0.00001 0.00000 -0.00002 -0.00002 2.04049

A18 2.04051 -0.00001 0.00000 -0.00002 -0.00002 2.04049

A19 2.19961 -0.00001 0.00000 -0.00005 -0.00005 2.19956

A20 2.18767 0.00001 0.00000 0.00003 0.00003 2.18770

A21 1.89582 -0.00000 -0.00000 0.00002 0.00002 1.89584

A22 1.89060 -0.00000 0.00001 -0.00004 -0.00003 1.89057

A23 2.19326 0.00000 -0.00001 0.00002 0.00001 2.19327

A24 2.19326 0.00000 -0.00001 0.00002 0.00001 2.19327

A25 1.89582 -0.00000 -0.00000 0.00002 0.00002 1.89584

A26 2.19961 -0.00001 0.00000 -0.00005 -0.00005 2.19956

A27 2.18767 0.00001 0.00000 0.00003 0.00003 2.18770

A28 1.87121 0.00000 -0.00000 -0.00000 -0.00000 1.87120

A29 2.19523 -0.00001 -0.00001 -0.00003 -0.00004 2.19519

A30 2.21659 0.00001 0.00002 0.00003 0.00005 2.21663

A31 1.87121 0.00000 -0.00000 -0.00000 -0.00000 1.87120

A32 2.19523 -0.00001 -0.00001 -0.00003 -0.00004 2.19519

A33 2.21659 0.00001 0.00002 0.00003 0.00005 2.21663

A34 2.20216 0.00001 -0.00000 0.00005 0.00005 2.20220

A35 2.04051 -0.00001 0.00000 -0.00002 -0.00002 2.04049

A36 2.04051 -0.00001 0.00000 -0.00002 -0.00002 2.04049

A37 2.18767 0.00001 0.00000 0.00003 0.00003 2.18770

A38 2.19961 -0.00001 0.00000 -0.00005 -0.00005 2.19956

A39 1.89582 -0.00000 -0.00000 0.00002 0.00002 1.89584

A40 1.87121 0.00000 -0.00000 -0.00000 -0.00000 1.87120

A41 2.19523 -0.00001 -0.00001 -0.00003 -0.00004 2.19519

A42 2.21659 0.00001 0.00002 0.00003 0.00005 2.21663

A43 1.87121 0.00000 -0.00000 -0.00000 -0.00000 1.87120

A44 2.21659 0.00001 0.00002 0.00003 0.00005 2.21663

A45 2.19523 -0.00001 -0.00001 -0.00003 -0.00004 2.19519

A46 1.89582 -0.00000 -0.00000 0.00002 0.00002 1.89584

A47 2.18767 0.00001 0.00000 0.00003 0.00003 2.18770

A48 2.19961 -0.00001 0.00000 -0.00005 -0.00005 2.19956

A49 1.89060 -0.00000 0.00001 -0.00004 -0.00003 1.89057

A50 2.19326 0.00000 -0.00001 0.00002 0.00001 2.19327

A51 2.19326 0.00000 -0.00001 0.00002 0.00001 2.19327

A52 2.20216 0.00001 -0.00000 0.00005 0.00005 2.20220

A53 2.04051 -0.00001 0.00000 -0.00002 -0.00002 2.04049

A54 2.04051 -0.00001 0.00000 -0.00002 -0.00002 2.04049

A55 2.18767 0.00001 0.00000 0.00003 0.00003 2.18770

A56 2.19961 -0.00001 0.00000 -0.00005 -0.00005 2.19956

A57 1.89582 -0.00000 -0.00000 0.00002 0.00002 1.89584

A58 1.87121 0.00000 -0.00000 -0.00000 -0.00000 1.87120

A59 2.19523 -0.00001 -0.00001 -0.00003 -0.00004 2.19519

A60 2.21659 0.00001 0.00002 0.00003 0.00005 2.21663

A61 1.87121 0.00000 -0.00000 -0.00000 -0.00000 1.87120

A62 2.21659 0.00001 0.00002 0.00003 0.00005 2.21663

A63 2.19523 -0.00001 -0.00001 -0.00003 -0.00004 2.19519

A64 1.89582 -0.00000 -0.00000 0.00002 0.00002 1.89584

A65 2.18767 0.00001 0.00000 0.00003 0.00003 2.18770

A66 2.19961 -0.00001 0.00000 -0.00005 -0.00005 2.19956

A67 1.89060 -0.00000 0.00001 -0.00004 -0.00003 1.89057

A68 2.19326 0.00000 -0.00001 0.00002 0.00001 2.19327

A69 2.19326 0.00000 -0.00001 0.00002 0.00001 2.19327

A70 2.20216 0.00001 -0.00000 0.00005 0.00005 2.20220

A71 2.04051 -0.00001 0.00000 -0.00002 -0.00002 2.04049

A72 2.04051 -0.00001 0.00000 -0.00002 -0.00002 2.04049

A73 2.10589 -0.00001 -0.00000 -0.00003 -0.00003 2.10586

A74 2.10589 -0.00001 -0.00000 -0.00003 -0.00003 2.10586

A75 2.07141 0.00001 0.00000 0.00006 0.00006 2.07147

A76 2.10626 -0.00001 0.00000 -0.00003 -0.00003 2.10623

A77 2.08339 0.00000 -0.00000 0.00003 0.00002 2.08342

A78 2.09350 0.00000 0.00000 0.00000 0.00001 2.09351

A79 2.09724 -0.00000 0.00000 -0.00001 -0.00001 2.09723

A80 2.08917 0.00000 -0.00000 0.00001 0.00001 2.08918

A81 2.09677 0.00000 0.00000 0.00000 0.00000 2.09677

A82 2.08796 0.00000 -0.00001 0.00003 0.00002 2.08798

A83 2.09761 -0.00000 0.00001 -0.00002 -0.00001 2.09760

A84 2.09761 -0.00000 0.00001 -0.00002 -0.00001 2.09760

A85 2.09724 -0.00000 0.00000 -0.00001 -0.00001 2.09723

A86 2.09677 0.00000 0.00000 0.00000 0.00000 2.09677

A87 2.08917 0.00000 -0.00000 0.00001 0.00001 2.08918

A88 2.10626 -0.00001 0.00000 -0.00003 -0.00003 2.10623

A89 2.08339 0.00000 -0.00000 0.00003 0.00002 2.08342

A90 2.09350 0.00000 0.00000 0.00000 0.00001 2.09351

A91 2.08796 0.00000 -0.00001 0.00003 0.00002 2.08798

A92 2.09761 -0.00000 0.00001 -0.00002 -0.00001 2.09760

A93 2.09761 -0.00000 0.00001 -0.00002 -0.00001 2.09760

A94 2.09724 -0.00000 0.00000 -0.00001 -0.00001 2.09723

A95 2.09677 0.00000 0.00000 0.00000 0.00000 2.09677

A96 2.08917 0.00000 -0.00000 0.00001 0.00001 2.08918

A97 2.10626 -0.00001 0.00000 -0.00003 -0.00003 2.10623

A98 2.09350 0.00000 0.00000 0.00000 0.00001 2.09351

A99 2.08339 0.00000 -0.00000 0.00003 0.00002 2.08342

A100 2.10589 -0.00001 -0.00000 -0.00003 -0.00003 2.10586

A101 2.10589 -0.00001 -0.00000 -0.00003 -0.00003 2.10586

A102 2.07141 0.00001 0.00000 0.00006 0.00006 2.07147

A103 2.10626 -0.00001 0.00000 -0.00003 -0.00003 2.10623

A104 2.08339 0.00000 -0.00000 0.00003 0.00002 2.08342

A105 2.09350 0.00000 0.00000 0.00000 0.00001 2.09351

A106 2.09724 -0.00000 0.00000 -0.00001 -0.00001 2.09723

A107 2.09677 0.00000 0.00000 0.00000 0.00000 2.09677

A108 2.08917 0.00000 -0.00000 0.00001 0.00001 2.08918

A109 2.10589 -0.00001 -0.00000 -0.00003 -0.00003 2.10586

A110 2.10589 -0.00001 -0.00000 -0.00003 -0.00003 2.10586

A111 2.07141 0.00001 0.00000 0.00006 0.00006 2.07147

A112 2.10626 -0.00001 0.00000 -0.00003 -0.00003 2.10623

A113 2.08339 0.00000 -0.00000 0.00003 0.00002 2.08342

A114 2.09350 0.00000 0.00000 0.00000 0.00001 2.09351

A115 2.09724 -0.00000 0.00000 -0.00001 -0.00001 2.09723

A116 2.08917 0.00000 -0.00000 0.00001 0.00001 2.08918

A117 2.09677 0.00000 0.00000 0.00000 0.00000 2.09677

A118 2.08796 0.00000 -0.00001 0.00003 0.00002 2.08798

A119 2.09761 -0.00000 0.00001 -0.00002 -0.00001 2.09760

A120 2.09761 -0.00000 0.00001 -0.00002 -0.00001 2.09760

A121 2.09724 -0.00000 0.00000 -0.00001 -0.00001 2.09723

A122 2.09677 0.00000 0.00000 0.00000 0.00000 2.09677

A123 2.08917 0.00000 -0.00000 0.00001 0.00001 2.08918

A124 2.10626 -0.00001 0.00000 -0.00003 -0.00003 2.10623

A125 2.08339 0.00000 -0.00000 0.00003 0.00002 2.08342

A126 2.09350 0.00000 0.00000 0.00000 0.00001 2.09351

A127 2.10589 -0.00001 -0.00000 -0.00003 -0.00003 2.10586

A128 2.10589 -0.00001 -0.00000 -0.00003 -0.00003 2.10586

A129 2.07141 0.00001 0.00000 0.00006 0.00006 2.07147

A130 2.10626 -0.00001 0.00000 -0.00003 -0.00003 2.10623

A131 2.08339 0.00000 -0.00000 0.00003 0.00002 2.08342

A132 2.09350 0.00000 0.00000 0.00000 0.00001 2.09351

A133 2.09724 -0.00000 0.00000 -0.00001 -0.00001 2.09723

A134 2.08917 0.00000 -0.00000 0.00001 0.00001 2.08918

A135 2.09677 0.00000 0.00000 0.00000 0.00000 2.09677

A136 2.08796 0.00000 -0.00001 0.00003 0.00002 2.08798

A137 2.09761 -0.00000 0.00001 -0.00002 -0.00001 2.09760

A138 2.09761 -0.00000 0.00001 -0.00002 -0.00001 2.09760

A139 2.09724 -0.00000 0.00000 -0.00001 -0.00001 2.09723

A140 2.09677 0.00000 0.00000 0.00000 0.00000 2.09677

A141 2.08917 0.00000 -0.00000 0.00001 0.00001 2.08918

A142 2.10626 -0.00001 0.00000 -0.00003 -0.00003 2.10623

A143 2.08339 0.00000 -0.00000 0.00003 0.00002 2.08342

A144 2.09350 0.00000 0.00000 0.00000 0.00001 2.09351

A145 1.57097 -0.00000 -0.00000 -0.00000 -0.00000 1.57097

A146 1.57097 -0.00000 -0.00000 -0.00000 -0.00000 1.57097

A147 1.57097 -0.00000 -0.00000 -0.00000 -0.00000 1.57097

A148 1.57097 -0.00000 -0.00000 -0.00000 -0.00000 1.57097

A149 3.14194 -0.00000 -0.00000 -0.00000 -0.00000 3.14193

A150 3.14194 -0.00000 -0.00000 -0.00000 -0.00000 3.14193

A151 3.11533 0.00000 0.00004 0.00008 0.00011 3.11544

A152 3.11533 0.00000 0.00004 0.00008 0.00011 3.11544

D1 0.00889 -0.00000 -0.00006 0.00004 -0.00001 0.00888

D2 3.13698 0.00000 0.00008 0.00006 0.00014 3.13713

D3 -3.11463 -0.00000 -0.00012 0.00004 -0.00008 -3.11471

D4 0.01346 0.00000 0.00002 0.00006 0.00008 0.01353

D5 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D6 -3.12324 -0.00000 -0.00006 -0.00000 -0.00006 -3.12330

D7 3.12324 0.00000 0.00006 0.00000 0.00006 3.12330

D8 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D9 -0.01451 0.00000 0.00009 -0.00007 0.00002 -0.01449

D10 3.01412 0.00000 0.00006 -0.00010 -0.00005 3.01407

D11 3.14070 -0.00000 -0.00005 -0.00009 -0.00014 3.14057

D12 -0.11386 -0.00000 -0.00009 -0.00012 -0.00020 -0.11406

D13 -3.06332 -0.00000 -0.00012 0.00004 -0.00007 -3.06340

D14 0.07827 -0.00000 -0.00012 0.00004 -0.00007 0.07820

D15 0.06245 0.00000 0.00005 0.00006 0.00011 0.06256

D16 -3.07915 0.00000 0.00005 0.00006 0.00011 -3.07904

D17 0.01451 -0.00000 -0.00009 0.00007 -0.00002 0.01449

D18 -3.14070 0.00000 0.00005 0.00009 0.00014 -3.14057

D19 -3.01412 -0.00000 -0.00006 0.00010 0.00005 -3.01407

D20 0.11386 0.00000 0.00009 0.00012 0.00020 0.11406

D21 -3.06241 -0.00000 0.00000 -0.00002 -0.00002 -3.06243

D22 0.05292 0.00000 0.00004 0.00006 0.00010 0.05301

D23 -0.05292 -0.00000 -0.00004 -0.00006 -0.00010 -0.05301

D24 3.06241 0.00000 -0.00000 0.00002 0.00002 3.06243

D25 -0.00889 0.00000 0.00006 -0.00004 0.00001 -0.00888

D26 3.11463 0.00000 0.00012 -0.00004 0.00008 3.11471

D27 -3.13698 -0.00000 -0.00008 -0.00006 -0.00014 -3.13713

D28 -0.01346 -0.00000 -0.00002 -0.00006 -0.00008 -0.01353

D29 -0.06245 -0.00000 -0.00005 -0.00006 -0.00011 -0.06256

D30 3.07915 -0.00000 -0.00005 -0.00006 -0.00011 3.07904

D31 3.06332 0.00000 0.00012 -0.00004 0.00007 3.06340

D32 -0.07827 0.00000 0.00012 -0.00004 0.00007 -0.07820

D33 -0.06245 -0.00000 -0.00005 -0.00006 -0.00011 -0.06256

D34 3.06332 0.00000 0.00012 -0.00004 0.00007 3.06340

D35 3.07915 -0.00000 -0.00005 -0.00006 -0.00011 3.07904

D36 -0.07827 0.00000 0.00012 -0.00004 0.00007 -0.07820

D37 -1.12102 0.00000 -0.00004 0.00041 0.00037 -1.12065

D38 2.02057 0.00000 -0.00004 0.00041 0.00037 2.02094

D39 2.02057 0.00000 -0.00004 0.00041 0.00037 2.02094

D40 -1.12102 0.00000 -0.00004 0.00041 0.00037 -1.12065

D41 -3.14070 0.00000 0.00005 0.00009 0.00014 -3.14057

D42 0.11386 0.00000 0.00009 0.00012 0.00020 0.11406

D43 0.01451 -0.00000 -0.00009 0.00007 -0.00002 0.01449

D44 -3.01412 -0.00000 -0.00006 0.00010 0.00005 -3.01407

D45 -3.13698 -0.00000 -0.00008 -0.00006 -0.00014 -3.13713

D46 -0.01346 -0.00000 -0.00002 -0.00006 -0.00008 -0.01353

D47 -0.00889 0.00000 0.00006 -0.00004 0.00001 -0.00888

D48 3.11463 0.00000 0.00012 -0.00004 0.00008 3.11471

D49 -0.01451 0.00000 0.00009 -0.00007 0.00002 -0.01449

D50 3.14070 -0.00000 -0.00005 -0.00009 -0.00014 3.14057

D51 3.01412 0.00000 0.00006 -0.00010 -0.00005 3.01407

D52 -0.11386 -0.00000 -0.00009 -0.00012 -0.00020 -0.11406

D53 -0.05292 -0.00000 -0.00004 -0.00006 -0.00010 -0.05301

D54 3.06241 0.00000 -0.00000 0.00002 0.00002 3.06243

D55 -3.06241 -0.00000 0.00000 -0.00002 -0.00002 -3.06243

D56 0.05292 0.00000 0.00004 0.00006 0.00010 0.05301

D57 0.00889 -0.00000 -0.00006 0.00004 -0.00001 0.00888

D58 -3.11463 -0.00000 -0.00012 0.00004 -0.00008 -3.11471

D59 3.13698 0.00000 0.00008 0.00006 0.00014 3.13713

D60 0.01346 0.00000 0.00002 0.00006 0.00008 0.01353

D61 0.06245 0.00000 0.00005 0.00006 0.00011 0.06256

D62 -3.07915 0.00000 0.00005 0.00006 0.00011 -3.07904

D63 -3.06332 -0.00000 -0.00012 0.00004 -0.00007 -3.06340

D64 0.07827 -0.00000 -0.00012 0.00004 -0.00007 0.07820

D65 -0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D66 -3.12324 -0.00000 -0.00006 -0.00000 -0.00006 -3.12330

D67 3.12324 0.00000 0.00006 0.00000 0.00006 3.12330

D68 0.00000 0.00000 -0.00000 0.00000 -0.00000 0.00000

D69 -3.06332 -0.00000 -0.00012 0.00004 -0.00007 -3.06340

D70 0.06245 0.00000 0.00005 0.00006 0.00011 0.06256

D71 0.07827 -0.00000 -0.00012 0.00004 -0.00007 0.07820

D72 -3.07915 0.00000 0.00005 0.00006 0.00011 -3.07904

D73 1.12102 -0.00000 0.00004 -0.00041 -0.00037 1.12065

D74 -2.02057 -0.00000 0.00004 -0.00041 -0.00037 -2.02094

D75 -2.02057 -0.00000 0.00004 -0.00041 -0.00037 -2.02094

D76 1.12102 -0.00000 0.00004 -0.00041 -0.00037 1.12065

D77 3.13698 0.00000 0.00008 0.00006 0.00014 3.13713

D78 0.01346 0.00000 0.00002 0.00006 0.00008 0.01353

D79 0.00889 -0.00000 -0.00006 0.00004 -0.00001 0.00888

D80 -3.11463 -0.00000 -0.00012 0.00004 -0.00008 -3.11471

D81 3.14070 -0.00000 -0.00005 -0.00009 -0.00014 3.14057

D82 -0.11386 -0.00000 -0.00009 -0.00012 -0.00020 -0.11406

D83 -0.01451 0.00000 0.00009 -0.00007 0.00002 -0.01449

D84 3.01412 0.00000 0.00006 -0.00010 -0.00005 3.01407

D85 -0.00000 0.00000 -0.00000 0.00000 0.00000 0.00000

D86 -3.12324 -0.00000 -0.00006 -0.00000 -0.00006 -3.12330

D87 3.12324 0.00000 0.00006 0.00000 0.00006 3.12330

D88 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D89 -0.00889 0.00000 0.00006 -0.00004 0.00001 -0.00888

D90 -3.13698 -0.00000 -0.00008 -0.00006 -0.00014 -3.13713

D91 3.11463 0.00000 0.00012 -0.00004 0.00008 3.11471

D92 -0.01346 -0.00000 -0.00002 -0.00006 -0.00008 -0.01353

D93 0.01451 -0.00000 -0.00009 0.00007 -0.00002 0.01449

D94 -3.01412 -0.00000 -0.00006 0.00010 0.00005 -3.01407

D95 -3.14070 0.00000 0.00005 0.00009 0.00014 -3.14057

D96 0.11386 0.00000 0.00009 0.00012 0.00020 0.11406

D97 3.06332 0.00000 0.00012 -0.00004 0.00007 3.06340

D98 -0.07827 0.00000 0.00012 -0.00004 0.00007 -0.07820

D99 -0.06245 -0.00000 -0.00005 -0.00006 -0.00011 -0.06256

D100 3.07915 -0.00000 -0.00005 -0.00006 -0.00011 3.07904

D101 0.05292 0.00000 0.00004 0.00006 0.00010 0.05301

D102 -3.06241 -0.00000 0.00000 -0.00002 -0.00002 -3.06243

D103 3.06241 0.00000 -0.00000 0.00002 0.00002 3.06243

D104 -0.05292 -0.00000 -0.00004 -0.00006 -0.00010 -0.05301

D105 3.06332 0.00000 0.00012 -0.00004 0.00007 3.06340

D106 -0.06245 -0.00000 -0.00005 -0.00006 -0.00011 -0.06256

D107 -0.07827 0.00000 0.00012 -0.00004 0.00007 -0.07820

D108 3.07915 -0.00000 -0.00005 -0.00006 -0.00011 3.07904

D109 -1.12102 0.00000 -0.00004 0.00041 0.00037 -1.12065

D110 2.02057 0.00000 -0.00004 0.00041 0.00037 2.02094

D111 2.02057 0.00000 -0.00004 0.00041 0.00037 2.02094

D112 -1.12102 0.00000 -0.00004 0.00041 0.00037 -1.12065

D113 -3.13698 -0.00000 -0.00008 -0.00006 -0.00014 -3.13713

D114 -0.01346 -0.00000 -0.00002 -0.00006 -0.00008 -0.01353

D115 -0.00889 0.00000 0.00006 -0.00004 0.00001 -0.00888

D116 3.11463 0.00000 0.00012 -0.00004 0.00008 3.11471

D117 -3.14070 0.00000 0.00005 0.00009 0.00014 -3.14057

D118 0.11386 0.00000 0.00009 0.00012 0.00020 0.11406

D119 0.01451 -0.00000 -0.00009 0.00007 -0.00002 0.01449

D120 -3.01412 -0.00000 -0.00006 0.00010 0.00005 -3.01407

D121 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D122 3.12324 0.00000 0.00006 0.00000 0.00006 3.12330

D123 -3.12324 -0.00000 -0.00006 -0.00000 -0.00006 -3.12330

D124 0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D125 0.00889 -0.00000 -0.00006 0.00004 -0.00001 0.00888

D126 3.13698 0.00000 0.00008 0.00006 0.00014 3.13713

D127 -3.11463 -0.00000 -0.00012 0.00004 -0.00008 -3.11471

D128 0.01346 0.00000 0.00002 0.00006 0.00008 0.01353

D129 -0.01451 0.00000 0.00009 -0.00007 0.00002 -0.01449

D130 3.01412 0.00000 0.00006 -0.00010 -0.00005 3.01407

D131 3.14070 -0.00000 -0.00005 -0.00009 -0.00014 3.14057

D132 -0.11386 -0.00000 -0.00009 -0.00012 -0.00020 -0.11406

D133 -3.06332 -0.00000 -0.00012 0.00004 -0.00007 -3.06340

D134 0.07827 -0.00000 -0.00012 0.00004 -0.00007 0.07820

D135 0.06245 0.00000 0.00005 0.00006 0.00011 0.06256

D136 -3.07915 0.00000 0.00005 0.00006 0.00011 -3.07904

D137 3.06241 0.00000 -0.00000 0.00002 0.00002 3.06243

D138 -0.05292 -0.00000 -0.00004 -0.00006 -0.00010 -0.05301

D139 0.05292 0.00000 0.00004 0.00006 0.00010 0.05301

D140 -3.06241 -0.00000 0.00000 -0.00002 -0.00002 -3.06243

D141 1.12102 -0.00000 0.00004 -0.00041 -0.00037 1.12065

D142 -2.02057 -0.00000 0.00004 -0.00041 -0.00037 -2.02094

D143 -2.02057 -0.00000 0.00004 -0.00041 -0.00037 -2.02094

D144 1.12102 -0.00000 0.00004 -0.00041 -0.00037 1.12065

D145 -3.13977 -0.00000 -0.00001 -0.00000 -0.00001 -3.13978

D146 -0.00725 0.00000 0.00006 0.00002 0.00008 -0.00717

D147 0.00183 -0.00000 -0.00001 -0.00000 -0.00001 0.00182

D148 3.13434 0.00000 0.00006 0.00002 0.00008 3.13442

D149 -3.13977 -0.00000 -0.00001 -0.00000 -0.00001 -3.13978

D150 -0.00725 0.00000 0.00006 0.00002 0.00008 -0.00717

D151 0.00183 -0.00000 -0.00001 -0.00000 -0.00001 0.00182

D152 3.13434 0.00000 0.00006 0.00002 0.00008 3.13442

D153 -0.00366 0.00000 0.00002 0.00000 0.00002 -0.00364

D154 3.13509 0.00000 0.00004 -0.00002 0.00001 3.13510

D155 -3.13612 -0.00000 -0.00005 -0.00002 -0.00007 -3.13619

D156 0.00263 -0.00000 -0.00003 -0.00004 -0.00008 0.00255

D157 0.00182 -0.00000 -0.00001 -0.00000 -0.00001 0.00181

D158 -3.13978 -0.00000 -0.00001 -0.00000 -0.00001 -3.13979

D159 -3.13692 -0.00000 -0.00003 0.00003 -0.00000 -3.13693

D160 0.00467 -0.00000 -0.00003 0.00003 -0.00000 0.00467

D161 0.00182 -0.00000 -0.00001 -0.00000 -0.00001 0.00181

D162 -3.13692 -0.00000 -0.00003 0.00003 -0.00000 -3.13693

D163 -3.13978 -0.00000 -0.00001 -0.00000 -0.00001 -3.13979

D164 0.00467 -0.00000 -0.00003 0.00003 -0.00000 0.00467

D165 -0.00366 0.00000 0.00002 0.00000 0.00002 -0.00364

D166 -3.13612 -0.00000 -0.00005 -0.00002 -0.00007 -3.13619

D167 3.13509 0.00000 0.00004 -0.00002 0.00001 3.13510

D168 0.00263 -0.00000 -0.00003 -0.00004 -0.00008 0.00255

D169 -0.00182 0.00000 0.00001 0.00000 0.00001 -0.00181

D170 3.13692 0.00000 0.00003 -0.00003 0.00000 3.13693

D171 3.13978 0.00000 0.00001 0.00000 0.00001 3.13979

D172 -0.00467 0.00000 0.00003 -0.00003 0.00000 -0.00467

D173 -0.00182 0.00000 0.00001 0.00000 0.00001 -0.00181

D174 3.13692 0.00000 0.00003 -0.00003 0.00000 3.13693

D175 3.13978 0.00000 0.00001 0.00000 0.00001 3.13979

D176 -0.00467 0.00000 0.00003 -0.00003 0.00000 -0.00467

D177 0.00366 -0.00000 -0.00002 -0.00000 -0.00002 0.00364

D178 3.13612 0.00000 0.00005 0.00002 0.00007 3.13619

D179 -3.13509 -0.00000 -0.00004 0.00002 -0.00001 -3.13510

D180 -0.00263 0.00000 0.00003 0.00004 0.00008 -0.00255

D181 3.13977 0.00000 0.00001 0.00000 0.00001 3.13978

D182 -0.00183 0.00000 0.00001 0.00000 0.00001 -0.00182

D183 0.00725 -0.00000 -0.00006 -0.00002 -0.00008 0.00717

D184 -3.13434 -0.00000 -0.00006 -0.00002 -0.00008 -3.13442

D185 3.13977 0.00000 0.00001 0.00000 0.00001 3.13978

D186 0.00725 -0.00000 -0.00006 -0.00002 -0.00008 0.00717

D187 -0.00183 0.00000 0.00001 0.00000 0.00001 -0.00182

D188 -3.13434 -0.00000 -0.00006 -0.00002 -0.00008 -3.13442

D189 0.00366 -0.00000 -0.00002 -0.00000 -0.00002 0.00364

D190 -3.13509 -0.00000 -0.00004 0.00002 -0.00001 -3.13510

D191 3.13612 0.00000 0.00005 0.00002 0.00007 3.13619

D192 -0.00263 0.00000 0.00003 0.00004 0.00008 -0.00255

D193 3.13977 0.00000 0.00001 0.00000 0.00001 3.13978

D194 0.00725 -0.00000 -0.00006 -0.00002 -0.00008 0.00717

D195 -0.00183 0.00000 0.00001 0.00000 0.00001 -0.00182

D196 -3.13434 -0.00000 -0.00006 -0.00002 -0.00008 -3.13442

D197 3.13977 0.00000 0.00001 0.00000 0.00001 3.13978

D198 0.00725 -0.00000 -0.00006 -0.00002 -0.00008 0.00717

D199 -0.00183 0.00000 0.00001 0.00000 0.00001 -0.00182

D200 -3.13434 -0.00000 -0.00006 -0.00002 -0.00008 -3.13442

D201 0.00366 -0.00000 -0.00002 -0.00000 -0.00002 0.00364

D202 -3.13509 -0.00000 -0.00004 0.00002 -0.00001 -3.13510

D203 3.13612 0.00000 0.00005 0.00002 0.00007 3.13619

D204 -0.00263 0.00000 0.00003 0.00004 0.00008 -0.00255

D205 -0.00182 0.00000 0.00001 0.00000 0.00001 -0.00181

D206 3.13978 0.00000 0.00001 0.00000 0.00001 3.13979

D207 3.13692 0.00000 0.00003 -0.00003 0.00000 3.13693

D208 -0.00467 0.00000 0.00003 -0.00003 0.00000 -0.00467

D209 -0.00182 0.00000 0.00001 0.00000 0.00001 -0.00181

D210 3.13692 0.00000 0.00003 -0.00003 0.00000 3.13693

D211 3.13978 0.00000 0.00001 0.00000 0.00001 3.13979

D212 -0.00467 0.00000 0.00003 -0.00003 0.00000 -0.00467

D213 0.00366 -0.00000 -0.00002 -0.00000 -0.00002 0.00364

D214 3.13612 0.00000 0.00005 0.00002 0.00007 3.13619

D215 -3.13509 -0.00000 -0.00004 0.00002 -0.00001 -3.13510

D216 -0.00263 0.00000 0.00003 0.00004 0.00008 -0.00255

D217 -3.13977 -0.00000 -0.00001 -0.00000 -0.00001 -3.13978

D218 -0.00725 0.00000 0.00006 0.00002 0.00008 -0.00717

D219 0.00183 -0.00000 -0.00001 -0.00000 -0.00001 0.00182

D220 3.13434 0.00000 0.00006 0.00002 0.00008 3.13442

D221 -3.13977 -0.00000 -0.00001 -0.00000 -0.00001 -3.13978

D222 -0.00725 0.00000 0.00006 0.00002 0.00008 -0.00717

D223 0.00183 -0.00000 -0.00001 -0.00000 -0.00001 0.00182

D224 3.13434 0.00000 0.00006 0.00002 0.00008 3.13442

D225 -0.00366 0.00000 0.00002 0.00000 0.00002 -0.00364

D226 3.13509 0.00000 0.00004 -0.00002 0.00001 3.13510

D227 -3.13612 -0.00000 -0.00005 -0.00002 -0.00007 -3.13619

D228 0.00263 -0.00000 -0.00003 -0.00004 -0.00008 0.00255

D229 0.00182 -0.00000 -0.00001 -0.00000 -0.00001 0.00181

D230 -3.13978 -0.00000 -0.00001 -0.00000 -0.00001 -3.13979

D231 -3.13692 -0.00000 -0.00003 0.00003 -0.00000 -3.13693

D232 0.00467 -0.00000 -0.00003 0.00003 -0.00000 0.00467

D233 0.00182 -0.00000 -0.00001 -0.00000 -0.00001 0.00181

D234 -3.13692 -0.00000 -0.00003 0.00003 -0.00000 -3.13693

D235 -3.13978 -0.00000 -0.00001 -0.00000 -0.00001 -3.13979

D236 0.00467 -0.00000 -0.00003 0.00003 -0.00000 0.00467

D237 -0.00366 0.00000 0.00002 0.00000 0.00002 -0.00364

D238 -3.13612 -0.00000 -0.00005 -0.00002 -0.00007 -3.13619

D239 3.13509 0.00000 0.00004 -0.00002 0.00001 3.13510

D240 0.00263 -0.00000 -0.00003 -0.00004 -0.00008 0.00255

Item Value Threshold Converged?

Maximum Force 0.000029 0.000450 YES

RMS Force 0.000006 0.000300 YES

Maximum Displacement 0.001494 0.001800 YES

RMS Displacement 0.000485 0.001200 YES

Predicted change in Energy=-5.162924D-08

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) 1.4499 -DE/DX = 0.0 !

! R2 R(1,5) 1.363 -DE/DX = 0.0 !

! R3 R(1,49) 1.0791 -DE/DX = 0.0 !

! R4 R(2,3) 1.3699 -DE/DX = 0.0 !

! R5 R(2,12) 1.4118 -DE/DX = 0.0 !

! R6 R(3,4) 1.3699 -DE/DX = 0.0 !

! R7 R(3,77) 2.0907 -DE/DX = 0.0 !

! R8 R(4,5) 1.4499 -DE/DX = 0.0 !

! R9 R(4,6) 1.4118 -DE/DX = 0.0 !

! R10 R(5,50) 1.0791 -DE/DX = 0.0 !

! R11 R(6,7) 1.4118 -DE/DX = 0.0 !

! R12 R(6,25) 1.4935 -DE/DX = 0.0 !

! R13 R(7,8) 1.3699 -DE/DX = 0.0 !

! R14 R(7,11) 1.4499 -DE/DX = 0.0 !

! R15 R(8,9) 1.3699 -DE/DX = 0.0 !

! R16 R(8,77) 2.0907 -DE/DX = 0.0 !

! R17 R(9,10) 1.4499 -DE/DX = 0.0 !

! R18 R(9,24) 1.4118 -DE/DX = 0.0 !

! R19 R(10,11) 1.363 -DE/DX = 0.0 !

! R20 R(10,51) 1.0791 -DE/DX = 0.0 !

! R21 R(11,52) 1.0791 -DE/DX = 0.0 !

! R22 R(12,13) 1.4118 -DE/DX = 0.0 !

! R23 R(12,34) 1.4935 -DE/DX = 0.0 !

! R24 R(13,14) 1.4499 -DE/DX = 0.0 !

! R25 R(13,17) 1.3699 -DE/DX = 0.0 !

! R26 R(14,15) 1.363 -DE/DX = 0.0 !

! R27 R(14,53) 1.0791 -DE/DX = 0.0 !

! R28 R(15,16) 1.4499 -DE/DX = 0.0 !

! R29 R(15,54) 1.0791 -DE/DX = 0.0 !

! R30 R(16,17) 1.3699 -DE/DX = 0.0 !

! R31 R(16,18) 1.4118 -DE/DX = 0.0 !

! R32 R(17,77) 2.0907 -DE/DX = 0.0 !

! R33 R(18,19) 1.4118 -DE/DX = 0.0 !

! R34 R(18,43) 1.4935 -DE/DX = 0.0 !

! R35 R(19,20) 1.4499 -DE/DX = 0.0 !

! R36 R(19,23) 1.3699 -DE/DX = 0.0 !

! R37 R(20,21) 1.363 -DE/DX = 0.0 !

! R38 R(20,55) 1.0791 -DE/DX = 0.0 !

! R39 R(21,22) 1.4499 -DE/DX = 0.0 !

! R40 R(21,56) 1.0791 -DE/DX = 0.0 !

! R41 R(22,23) 1.3699 -DE/DX = 0.0 !

! R42 R(22,24) 1.4118 -DE/DX = 0.0 !

! R43 R(23,77) 2.0907 -DE/DX = 0.0 !

! R44 R(24,37) 1.4935 -DE/DX = 0.0 !

! R45 R(25,26) 1.4004 -DE/DX = 0.0 !

! R46 R(25,30) 1.4004 -DE/DX = 0.0 !

! R47 R(26,27) 1.3929 -DE/DX = 0.0 !

! R48 R(26,57) 1.0846 -DE/DX = 0.0 !

! R49 R(27,28) 1.3943 -DE/DX = 0.0 !

! R50 R(27,58) 1.0851 -DE/DX = 0.0 !

! R51 R(28,29) 1.3943 -DE/DX = 0.0 !

! R52 R(28,59) 1.085 -DE/DX = 0.0 !

! R53 R(29,30) 1.3929 -DE/DX = 0.0 !

! R54 R(29,60) 1.0851 -DE/DX = 0.0 !

! R55 R(30,61) 1.0846 -DE/DX = 0.0 !

! R56 R(31,32) 1.3943 -DE/DX = 0.0 !

! R57 R(31,36) 1.3943 -DE/DX = 0.0 !

! R58 R(31,62) 1.085 -DE/DX = 0.0 !

! R59 R(32,33) 1.3929 -DE/DX = 0.0 !

! R60 R(32,63) 1.0851 -DE/DX = 0.0 !

! R61 R(33,34) 1.4004 -DE/DX = 0.0 !

! R62 R(33,64) 1.0846 -DE/DX = 0.0 !

! R63 R(34,35) 1.4004 -DE/DX = 0.0 !

! R64 R(35,36) 1.3929 -DE/DX = 0.0 !

! R65 R(35,65) 1.0846 -DE/DX = 0.0 !

! R66 R(36,66) 1.0851 -DE/DX = 0.0 !

! R67 R(37,38) 1.4004 -DE/DX = 0.0 !

! R68 R(37,42) 1.4004 -DE/DX = 0.0 !

! R69 R(38,39) 1.3929 -DE/DX = 0.0 !

! R70 R(38,67) 1.0846 -DE/DX = 0.0 !

! R71 R(39,40) 1.3943 -DE/DX = 0.0 !

! R72 R(39,68) 1.0851 -DE/DX = 0.0 !

! R73 R(40,41) 1.3943 -DE/DX = 0.0 !

! R74 R(40,69) 1.085 -DE/DX = 0.0 !

! R75 R(41,42) 1.3929 -DE/DX = 0.0 !

! R76 R(41,70) 1.0851 -DE/DX = 0.0 !

! R77 R(42,71) 1.0846 -DE/DX = 0.0 !

! R78 R(43,44) 1.4004 -DE/DX = 0.0 !

! R79 R(43,48) 1.4004 -DE/DX = 0.0 !

! R80 R(44,45) 1.3929 -DE/DX = 0.0 !

! R81 R(44,72) 1.0846 -DE/DX = 0.0 !

! R82 R(45,46) 1.3943 -DE/DX = 0.0 !

! R83 R(45,73) 1.0851 -DE/DX = 0.0 !

! R84 R(46,47) 1.3943 -DE/DX = 0.0 !

! R85 R(46,74) 1.085 -DE/DX = 0.0 !

! R86 R(47,48) 1.3929 -DE/DX = 0.0 !

! R87 R(47,75) 1.0851 -DE/DX = 0.0 !

! R88 R(48,76) 1.0846 -DE/DX = 0.0 !

! A1 A(2,1,5) 107.2123 -DE/DX = 0.0 !

! A2 A(2,1,49) 125.7776 -DE/DX = 0.0 !

! A3 A(5,1,49) 127.001 -DE/DX = 0.0 !

! A4 A(1,2,3) 108.6225 -DE/DX = 0.0 !

! A5 A(1,2,12) 125.3442 -DE/DX = 0.0 !

! A6 A(3,2,12) 126.0283 -DE/DX = 0.0 !

! A7 A(2,3,4) 108.3234 -DE/DX = 0.0 !

! A8 A(2,3,77) 125.6646 -DE/DX = 0.0 !

! A9 A(4,3,77) 125.6646 -DE/DX = 0.0 !

! A10 A(3,4,5) 108.6225 -DE/DX = 0.0 !

! A11 A(3,4,6) 126.0283 -DE/DX = 0.0 !

! A12 A(5,4,6) 125.3442 -DE/DX = 0.0 !

! A13 A(1,5,4) 107.2123 -DE/DX = 0.0 !

! A14 A(1,5,50) 127.001 -DE/DX = 0.0 !

! A15 A(4,5,50) 125.7776 -DE/DX = 0.0 !

! A16 A(4,6,7) 126.1744 -DE/DX = 0.0 !

! A17 A(4,6,25) 116.9128 -DE/DX = 0.0 !

! A18 A(7,6,25) 116.9128 -DE/DX = 0.0 !

! A19 A(6,7,8) 126.0283 -DE/DX = 0.0 !

! A20 A(6,7,11) 125.3442 -DE/DX = 0.0 !

! A21 A(8,7,11) 108.6225 -DE/DX = 0.0 !

! A22 A(7,8,9) 108.3234 -DE/DX = 0.0 !

! A23 A(7,8,77) 125.6646 -DE/DX = 0.0 !

! A24 A(9,8,77) 125.6646 -DE/DX = 0.0 !

! A25 A(8,9,10) 108.6225 -DE/DX = 0.0 !

! A26 A(8,9,24) 126.0283 -DE/DX = 0.0 !

! A27 A(10,9,24) 125.3442 -DE/DX = 0.0 !

! A28 A(9,10,11) 107.2123 -DE/DX = 0.0 !

! A29 A(9,10,51) 125.7776 -DE/DX = 0.0 !

! A30 A(11,10,51) 127.001 -DE/DX = 0.0 !

! A31 A(7,11,10) 107.2123 -DE/DX = 0.0 !

! A32 A(7,11,52) 125.7776 -DE/DX = 0.0 !

! A33 A(10,11,52) 127.001 -DE/DX = 0.0 !

! A34 A(2,12,13) 126.1744 -DE/DX = 0.0 !

! A35 A(2,12,34) 116.9128 -DE/DX = 0.0 !

! A36 A(13,12,34) 116.9128 -DE/DX = 0.0 !

! A37 A(12,13,14) 125.3442 -DE/DX = 0.0 !

! A38 A(12,13,17) 126.0283 -DE/DX = 0.0 !

! A39 A(14,13,17) 108.6225 -DE/DX = 0.0 !

! A40 A(13,14,15) 107.2123 -DE/DX = 0.0 !

! A41 A(13,14,53) 125.7776 -DE/DX = 0.0 !

! A42 A(15,14,53) 127.001 -DE/DX = 0.0 !

! A43 A(14,15,16) 107.2123 -DE/DX = 0.0 !

! A44 A(14,15,54) 127.001 -DE/DX = 0.0 !

! A45 A(16,15,54) 125.7776 -DE/DX = 0.0 !

! A46 A(15,16,17) 108.6225 -DE/DX = 0.0 !

! A47 A(15,16,18) 125.3442 -DE/DX = 0.0 !

! A48 A(17,16,18) 126.0283 -DE/DX = 0.0 !

! A49 A(13,17,16) 108.3234 -DE/DX = 0.0 !

! A50 A(13,17,77) 125.6646 -DE/DX = 0.0 !

! A51 A(16,17,77) 125.6646 -DE/DX = 0.0 !

! A52 A(16,18,19) 126.1744 -DE/DX = 0.0 !

! A53 A(16,18,43) 116.9128 -DE/DX = 0.0 !

! A54 A(19,18,43) 116.9128 -DE/DX = 0.0 !

! A55 A(18,19,20) 125.3442 -DE/DX = 0.0 !

! A56 A(18,19,23) 126.0283 -DE/DX = 0.0 !

! A57 A(20,19,23) 108.6225 -DE/DX = 0.0 !

! A58 A(19,20,21) 107.2123 -DE/DX = 0.0 !

! A59 A(19,20,55) 125.7776 -DE/DX = 0.0 !

! A60 A(21,20,55) 127.001 -DE/DX = 0.0 !

! A61 A(20,21,22) 107.2123 -DE/DX = 0.0 !

! A62 A(20,21,56) 127.001 -DE/DX = 0.0 !

! A63 A(22,21,56) 125.7776 -DE/DX = 0.0 !

! A64 A(21,22,23) 108.6225 -DE/DX = 0.0 !

! A65 A(21,22,24) 125.3442 -DE/DX = 0.0 !

! A66 A(23,22,24) 126.0283 -DE/DX = 0.0 !

! A67 A(19,23,22) 108.3234 -DE/DX = 0.0 !

! A68 A(19,23,77) 125.6646 -DE/DX = 0.0 !

! A69 A(22,23,77) 125.6646 -DE/DX = 0.0 !

! A70 A(9,24,22) 126.1744 -DE/DX = 0.0 !

! A71 A(9,24,37) 116.9128 -DE/DX = 0.0 !

! A72 A(22,24,37) 116.9128 -DE/DX = 0.0 !

! A73 A(6,25,26) 120.6585 -DE/DX = 0.0 !

! A74 A(6,25,30) 120.6585 -DE/DX = 0.0 !

! A75 A(26,25,30) 118.6829 -DE/DX = 0.0 !

! A76 A(25,26,27) 120.6797 -DE/DX = 0.0 !

! A77 A(25,26,57) 119.3697 -DE/DX = 0.0 !

! A78 A(27,26,57) 119.9486 -DE/DX = 0.0 !

! A79 A(26,27,28) 120.163 -DE/DX = 0.0 !

! A80 A(26,27,58) 119.7006 -DE/DX = 0.0 !

! A81 A(28,27,58) 120.1361 -DE/DX = 0.0 !

! A82 A(27,28,29) 119.6312 -DE/DX = 0.0 !

! A83 A(27,28,59) 120.1844 -DE/DX = 0.0 !

! A84 A(29,28,59) 120.1844 -DE/DX = 0.0 !

! A85 A(28,29,30) 120.163 -DE/DX = 0.0 !

! A86 A(28,29,60) 120.1361 -DE/DX = 0.0 !

! A87 A(30,29,60) 119.7006 -DE/DX = 0.0 !

! A88 A(25,30,29) 120.6797 -DE/DX = 0.0 !

! A89 A(25,30,61) 119.3697 -DE/DX = 0.0 !

! A90 A(29,30,61) 119.9486 -DE/DX = 0.0 !

! A91 A(32,31,36) 119.6312 -DE/DX = 0.0 !

! A92 A(32,31,62) 120.1844 -DE/DX = 0.0 !

! A93 A(36,31,62) 120.1844 -DE/DX = 0.0 !

! A94 A(31,32,33) 120.163 -DE/DX = 0.0 !

! A95 A(31,32,63) 120.1361 -DE/DX = 0.0 !

! A96 A(33,32,63) 119.7006 -DE/DX = 0.0 !

! A97 A(32,33,34) 120.6797 -DE/DX = 0.0 !

! A98 A(32,33,64) 119.9486 -DE/DX = 0.0 !

! A99 A(34,33,64) 119.3697 -DE/DX = 0.0 !

! A100 A(12,34,33) 120.6585 -DE/DX = 0.0 !

! A101 A(12,34,35) 120.6585 -DE/DX = 0.0 !

! A102 A(33,34,35) 118.6829 -DE/DX = 0.0 !

! A103 A(34,35,36) 120.6797 -DE/DX = 0.0 !

! A104 A(34,35,65) 119.3697 -DE/DX = 0.0 !

! A105 A(36,35,65) 119.9486 -DE/DX = 0.0 !

! A106 A(31,36,35) 120.163 -DE/DX = 0.0 !

! A107 A(31,36,66) 120.1361 -DE/DX = 0.0 !

! A108 A(35,36,66) 119.7006 -DE/DX = 0.0 !

! A109 A(24,37,38) 120.6585 -DE/DX = 0.0 !

! A110 A(24,37,42) 120.6585 -DE/DX = 0.0 !

! A111 A(38,37,42) 118.6829 -DE/DX = 0.0 !

! A112 A(37,38,39) 120.6797 -DE/DX = 0.0 !

! A113 A(37,38,67) 119.3697 -DE/DX = 0.0 !

! A114 A(39,38,67) 119.9486 -DE/DX = 0.0 !

! A115 A(38,39,40) 120.163 -DE/DX = 0.0 !

! A116 A(38,39,68) 119.7006 -DE/DX = 0.0 !

! A117 A(40,39,68) 120.1361 -DE/DX = 0.0 !

! A118 A(39,40,41) 119.6312 -DE/DX = 0.0 !

! A119 A(39,40,69) 120.1844 -DE/DX = 0.0 !

! A120 A(41,40,69) 120.1844 -DE/DX = 0.0 !

! A121 A(40,41,42) 120.163 -DE/DX = 0.0 !

! A122 A(40,41,70) 120.1361 -DE/DX = 0.0 !

! A123 A(42,41,70) 119.7006 -DE/DX = 0.0 !

! A124 A(37,42,41) 120.6797 -DE/DX = 0.0 !

! A125 A(37,42,71) 119.3697 -DE/DX = 0.0 !

! A126 A(41,42,71) 119.9486 -DE/DX = 0.0 !

! A127 A(18,43,44) 120.6585 -DE/DX = 0.0 !

! A128 A(18,43,48) 120.6585 -DE/DX = 0.0 !

! A129 A(44,43,48) 118.6829 -DE/DX = 0.0 !

! A130 A(43,44,45) 120.6797 -DE/DX = 0.0 !

! A131 A(43,44,72) 119.3697 -DE/DX = 0.0 !

! A132 A(45,44,72) 119.9486 -DE/DX = 0.0 !

! A133 A(44,45,46) 120.163 -DE/DX = 0.0 !

! A134 A(44,45,73) 119.7006 -DE/DX = 0.0 !

! A135 A(46,45,73) 120.1361 -DE/DX = 0.0 !

! A136 A(45,46,47) 119.6312 -DE/DX = 0.0 !

! A137 A(45,46,74) 120.1844 -DE/DX = 0.0 !

! A138 A(47,46,74) 120.1844 -DE/DX = 0.0 !

! A139 A(46,47,48) 120.163 -DE/DX = 0.0 !

! A140 A(46,47,75) 120.1361 -DE/DX = 0.0 !

! A141 A(48,47,75) 119.7006 -DE/DX = 0.0 !

! A142 A(43,48,47) 120.6797 -DE/DX = 0.0 !

! A143 A(43,48,76) 119.3697 -DE/DX = 0.0 !

! A144 A(47,48,76) 119.9486 -DE/DX = 0.0 !

! A145 A(3,77,8) 90.0099 -DE/DX = 0.0 !

! A146 A(3,77,17) 90.0099 -DE/DX = 0.0 !

! A147 A(8,77,23) 90.0099 -DE/DX = 0.0 !

! A148 A(17,77,23) 90.0099 -DE/DX = 0.0 !

! A149 L(3,77,23,17,-1) 180.0198 -DE/DX = 0.0 !

! A150 L(8,77,17,23,-1) 180.0198 -DE/DX = 0.0 !

! A151 L(3,77,23,17,-2) 178.495 -DE/DX = 0.0 !

! A152 L(8,77,17,23,-2) 178.495 -DE/DX = 0.0 !

! D1 D(5,1,2,3) 0.5095 -DE/DX = 0.0 !

! D2 D(5,1,2,12) 179.7358 -DE/DX = 0.0 !

! D3 D(49,1,2,3) -178.4553 -DE/DX = 0.0 !

! D4 D(49,1,2,12) 0.771 -DE/DX = 0.0 !

! D5 D(2,1,5,4) 0.0 -DE/DX = 0.0 !

! D6 D(2,1,5,50) -178.9484 -DE/DX = 0.0 !

! D7 D(49,1,5,4) 178.9484 -DE/DX = 0.0 !

! D8 D(49,1,5,50) 0.0 -DE/DX = 0.0 !

! D9 D(1,2,3,4) -0.8313 -DE/DX = 0.0 !

! D10 D(1,2,3,77) 172.6961 -DE/DX = 0.0 !

! D11 D(12,2,3,4) 179.9491 -DE/DX = 0.0 !

! D12 D(12,2,3,77) -6.5236 -DE/DX = 0.0 !

! D13 D(1,2,12,13) -175.5155 -DE/DX = 0.0 !

! D14 D(1,2,12,34) 4.4845 -DE/DX = 0.0 !

! D15 D(3,2,12,13) 3.5779 -DE/DX = 0.0 !

! D16 D(3,2,12,34) -176.4221 -DE/DX = 0.0 !

! D17 D(2,3,4,5) 0.8313 -DE/DX = 0.0 !

! D18 D(2,3,4,6) -179.9491 -DE/DX = 0.0 !

! D19 D(77,3,4,5) -172.6961 -DE/DX = 0.0 !

! D20 D(77,3,4,6) 6.5236 -DE/DX = 0.0 !

! D21 D(2,3,77,8) -175.4631 -DE/DX = 0.0 !

! D22 D(2,3,77,17) 3.0319 -DE/DX = 0.0 !

! D23 D(4,3,77,8) -3.0319 -DE/DX = 0.0 !

! D24 D(4,3,77,17) 175.4631 -DE/DX = 0.0 !

! D25 D(3,4,5,1) -0.5095 -DE/DX = 0.0 !

! D26 D(3,4,5,50) 178.4553 -DE/DX = 0.0 !

! D27 D(6,4,5,1) -179.7358 -DE/DX = 0.0 !

! D28 D(6,4,5,50) -0.771 -DE/DX = 0.0 !

! D29 D(3,4,6,7) -3.5779 -DE/DX = 0.0 !

! D30 D(3,4,6,25) 176.4221 -DE/DX = 0.0 !

! D31 D(5,4,6,7) 175.5155 -DE/DX = 0.0 !

! D32 D(5,4,6,25) -4.4845 -DE/DX = 0.0 !

! D33 D(4,6,7,8) -3.5779 -DE/DX = 0.0 !

! D34 D(4,6,7,11) 175.5155 -DE/DX = 0.0 !

! D35 D(25,6,7,8) 176.4221 -DE/DX = 0.0 !

! D36 D(25,6,7,11) -4.4845 -DE/DX = 0.0 !

! D37 D(4,6,25,26) -64.2296 -DE/DX = 0.0 !

! D38 D(4,6,25,30) 115.7704 -DE/DX = 0.0 !

! D39 D(7,6,25,26) 115.7704 -DE/DX = 0.0 !

! D40 D(7,6,25,30) -64.2296 -DE/DX = 0.0 !

! D41 D(6,7,8,9) -179.9491 -DE/DX = 0.0 !

! D42 D(6,7,8,77) 6.5236 -DE/DX = 0.0 !

! D43 D(11,7,8,9) 0.8313 -DE/DX = 0.0 !

! D44 D(11,7,8,77) -172.6961 -DE/DX = 0.0 !

! D45 D(6,7,11,10) -179.7358 -DE/DX = 0.0 !

! D46 D(6,7,11,52) -0.771 -DE/DX = 0.0 !

! D47 D(8,7,11,10) -0.5095 -DE/DX = 0.0 !

! D48 D(8,7,11,52) 178.4553 -DE/DX = 0.0 !

! D49 D(7,8,9,10) -0.8313 -DE/DX = 0.0 !

! D50 D(7,8,9,24) 179.9491 -DE/DX = 0.0 !

! D51 D(77,8,9,10) 172.6961 -DE/DX = 0.0 !

! D52 D(77,8,9,24) -6.5236 -DE/DX = 0.0 !

! D53 D(7,8,77,3) -3.0319 -DE/DX = 0.0 !

! D54 D(7,8,77,23) 175.4631 -DE/DX = 0.0 !

! D55 D(9,8,77,3) -175.4631 -DE/DX = 0.0 !

! D56 D(9,8,77,23) 3.0319 -DE/DX = 0.0 !

! D57 D(8,9,10,11) 0.5095 -DE/DX = 0.0 !

! D58 D(8,9,10,51) -178.4553 -DE/DX = 0.0 !

! D59 D(24,9,10,11) 179.7358 -DE/DX = 0.0 !

! D60 D(24,9,10,51) 0.771 -DE/DX = 0.0 !

! D61 D(8,9,24,22) 3.5779 -DE/DX = 0.0 !

! D62 D(8,9,24,37) -176.4221 -DE/DX = 0.0 !

! D63 D(10,9,24,22) -175.5155 -DE/DX = 0.0 !

! D64 D(10,9,24,37) 4.4845 -DE/DX = 0.0 !

! D65 D(9,10,11,7) 0.0 -DE/DX = 0.0 !

! D66 D(9,10,11,52) -178.9484 -DE/DX = 0.0 !

! D67 D(51,10,11,7) 178.9484 -DE/DX = 0.0 !

! D68 D(51,10,11,52) 0.0 -DE/DX = 0.0 !

! D69 D(2,12,13,14) -175.5155 -DE/DX = 0.0 !

! D70 D(2,12,13,17) 3.5779 -DE/DX = 0.0 !

! D71 D(34,12,13,14) 4.4845 -DE/DX = 0.0 !

! D72 D(34,12,13,17) -176.4221 -DE/DX = 0.0 !

! D73 D(2,12,34,33) 64.2296 -DE/DX = 0.0 !

! D74 D(2,12,34,35) -115.7704 -DE/DX = 0.0 !

! D75 D(13,12,34,33) -115.7704 -DE/DX = 0.0 !

! D76 D(13,12,34,35) 64.2296 -DE/DX = 0.0 !

! D77 D(12,13,14,15) 179.7358 -DE/DX = 0.0 !

! D78 D(12,13,14,53) 0.771 -DE/DX = 0.0 !

! D79 D(17,13,14,15) 0.5095 -DE/DX = 0.0 !

! D80 D(17,13,14,53) -178.4553 -DE/DX = 0.0 !

! D81 D(12,13,17,16) 179.9491 -DE/DX = 0.0 !

! D82 D(12,13,17,77) -6.5236 -DE/DX = 0.0 !

! D83 D(14,13,17,16) -0.8313 -DE/DX = 0.0 !

! D84 D(14,13,17,77) 172.6961 -DE/DX = 0.0 !

! D85 D(13,14,15,16) 0.0 -DE/DX = 0.0 !

! D86 D(13,14,15,54) -178.9484 -DE/DX = 0.0 !

! D87 D(53,14,15,16) 178.9484 -DE/DX = 0.0 !

! D88 D(53,14,15,54) 0.0 -DE/DX = 0.0 !

! D89 D(14,15,16,17) -0.5095 -DE/DX = 0.0 !

! D90 D(14,15,16,18) -179.7358 -DE/DX = 0.0 !

! D91 D(54,15,16,17) 178.4553 -DE/DX = 0.0 !

! D92 D(54,15,16,18) -0.771 -DE/DX = 0.0 !

! D93 D(15,16,17,13) 0.8313 -DE/DX = 0.0 !

! D94 D(15,16,17,77) -172.6961 -DE/DX = 0.0 !

! D95 D(18,16,17,13) -179.9491 -DE/DX = 0.0 !

! D96 D(18,16,17,77) 6.5236 -DE/DX = 0.0 !

! D97 D(15,16,18,19) 175.5155 -DE/DX = 0.0 !

! D98 D(15,16,18,43) -4.4845 -DE/DX = 0.0 !

! D99 D(17,16,18,19) -3.5779 -DE/DX = 0.0 !

! D100 D(17,16,18,43) 176.4221 -DE/DX = 0.0 !

! D101 D(13,17,77,3) 3.0319 -DE/DX = 0.0 !

! D102 D(13,17,77,23) -175.4631 -DE/DX = 0.0 !

! D103 D(16,17,77,3) 175.4631 -DE/DX = 0.0 !

! D104 D(16,17,77,23) -3.0319 -DE/DX = 0.0 !

! D105 D(16,18,19,20) 175.5155 -DE/DX = 0.0 !

! D106 D(16,18,19,23) -3.5779 -DE/DX = 0.0 !

! D107 D(43,18,19,20) -4.4845 -DE/DX = 0.0 !

! D108 D(43,18,19,23) 176.4221 -DE/DX = 0.0 !

! D109 D(16,18,43,44) -64.2296 -DE/DX = 0.0 !

! D110 D(16,18,43,48) 115.7704 -DE/DX = 0.0 !

! D111 D(19,18,43,44) 115.7704 -DE/DX = 0.0 !

! D112 D(19,18,43,48) -64.2296 -DE/DX = 0.0 !

! D113 D(18,19,20,21) -179.7358 -DE/DX = 0.0 !

! D114 D(18,19,20,55) -0.771 -DE/DX = 0.0 !

! D115 D(23,19,20,21) -0.5095 -DE/DX = 0.0 !

! D116 D(23,19,20,55) 178.4553 -DE/DX = 0.0 !

! D117 D(18,19,23,22) -179.9491 -DE/DX = 0.0 !

! D118 D(18,19,23,77) 6.5236 -DE/DX = 0.0 !

! D119 D(20,19,23,22) 0.8313 -DE/DX = 0.0 !

! D120 D(20,19,23,77) -172.6961 -DE/DX = 0.0 !

! D121 D(19,20,21,22) 0.0 -DE/DX = 0.0 !

! D122 D(19,20,21,56) 178.9484 -DE/DX = 0.0 !

! D123 D(55,20,21,22) -178.9484 -DE/DX = 0.0 !

! D124 D(55,20,21,56) 0.0 -DE/DX = 0.0 !

! D125 D(20,21,22,23) 0.5095 -DE/DX = 0.0 !

! D126 D(20,21,22,24) 179.7358 -DE/DX = 0.0 !

! D127 D(56,21,22,23) -178.4553 -DE/DX = 0.0 !

! D128 D(56,21,22,24) 0.771 -DE/DX = 0.0 !

! D129 D(21,22,23,19) -0.8313 -DE/DX = 0.0 !

! D130 D(21,22,23,77) 172.6961 -DE/DX = 0.0 !

! D131 D(24,22,23,19) 179.9491 -DE/DX = 0.0 !

! D132 D(24,22,23,77) -6.5236 -DE/DX = 0.0 !

! D133 D(21,22,24,9) -175.5155 -DE/DX = 0.0 !

! D134 D(21,22,24,37) 4.4845 -DE/DX = 0.0 !

! D135 D(23,22,24,9) 3.5779 -DE/DX = 0.0 !

! D136 D(23,22,24,37) -176.4221 -DE/DX = 0.0 !

! D137 D(19,23,77,8) 175.4631 -DE/DX = 0.0 !

! D138 D(19,23,77,17) -3.0319 -DE/DX = 0.0 !

! D139 D(22,23,77,8) 3.0319 -DE/DX = 0.0 !

! D140 D(22,23,77,17) -175.4631 -DE/DX = 0.0 !

! D141 D(9,24,37,38) 64.2296 -DE/DX = 0.0 !

! D142 D(9,24,37,42) -115.7704 -DE/DX = 0.0 !

! D143 D(22,24,37,38) -115.7704 -DE/DX = 0.0 !

! D144 D(22,24,37,42) 64.2296 -DE/DX = 0.0 !

! D145 D(6,25,26,27) -179.8953 -DE/DX = 0.0 !

! D146 D(6,25,26,57) -0.4155 -DE/DX = 0.0 !

! D147 D(30,25,26,27) 0.1047 -DE/DX = 0.0 !

! D148 D(30,25,26,57) 179.5845 -DE/DX = 0.0 !

! D149 D(6,25,30,29) -179.8953 -DE/DX = 0.0 !

! D150 D(6,25,30,61) -0.4155 -DE/DX = 0.0 !

! D151 D(26,25,30,29) 0.1047 -DE/DX = 0.0 !

! D152 D(26,25,30,61) 179.5845 -DE/DX = 0.0 !

! D153 D(25,26,27,28) -0.2097 -DE/DX = 0.0 !

! D154 D(25,26,27,58) 179.6276 -DE/DX = 0.0 !

! D155 D(57,26,27,28) -179.6865 -DE/DX = 0.0 !

! D156 D(57,26,27,58) 0.1508 -DE/DX = 0.0 !

! D157 D(26,27,28,29) 0.1041 -DE/DX = 0.0 !

! D158 D(26,27,28,59) -179.8959 -DE/DX = 0.0 !

! D159 D(58,27,28,29) -179.7325 -DE/DX = 0.0 !

! D160 D(58,27,28,59) 0.2675 -DE/DX = 0.0 !

! D161 D(27,28,29,30) 0.1041 -DE/DX = 0.0 !

! D162 D(27,28,29,60) -179.7325 -DE/DX = 0.0 !

! D163 D(59,28,29,30) -179.8959 -DE/DX = 0.0 !

! D164 D(59,28,29,60) 0.2675 -DE/DX = 0.0 !

! D165 D(28,29,30,25) -0.2097 -DE/DX = 0.0 !

! D166 D(28,29,30,61) -179.6865 -DE/DX = 0.0 !

! D167 D(60,29,30,25) 179.6276 -DE/DX = 0.0 !

! D168 D(60,29,30,61) 0.1508 -DE/DX = 0.0 !

! D169 D(36,31,32,33) -0.1041 -DE/DX = 0.0 !

! D170 D(36,31,32,63) 179.7325 -DE/DX = 0.0 !

! D171 D(62,31,32,33) 179.8959 -DE/DX = 0.0 !

! D172 D(62,31,32,63) -0.2675 -DE/DX = 0.0 !

! D173 D(32,31,36,35) -0.1041 -DE/DX = 0.0 !

! D174 D(32,31,36,66) 179.7325 -DE/DX = 0.0 !

! D175 D(62,31,36,35) 179.8959 -DE/DX = 0.0 !

! D176 D(62,31,36,66) -0.2675 -DE/DX = 0.0 !

! D177 D(31,32,33,34) 0.2097 -DE/DX = 0.0 !

! D178 D(31,32,33,64) 179.6865 -DE/DX = 0.0 !

! D179 D(63,32,33,34) -179.6276 -DE/DX = 0.0 !

! D180 D(63,32,33,64) -0.1508 -DE/DX = 0.0 !

! D181 D(32,33,34,12) 179.8953 -DE/DX = 0.0 !

! D182 D(32,33,34,35) -0.1047 -DE/DX = 0.0 !

! D183 D(64,33,34,12) 0.4155 -DE/DX = 0.0 !

! D184 D(64,33,34,35) -179.5845 -DE/DX = 0.0 !

! D185 D(12,34,35,36) 179.8953 -DE/DX = 0.0 !

! D186 D(12,34,35,65) 0.4155 -DE/DX = 0.0 !

! D187 D(33,34,35,36) -0.1047 -DE/DX = 0.0 !

! D188 D(33,34,35,65) -179.5845 -DE/DX = 0.0 !

! D189 D(34,35,36,31) 0.2097 -DE/DX = 0.0 !

! D190 D(34,35,36,66) -179.6276 -DE/DX = 0.0 !

! D191 D(65,35,36,31) 179.6865 -DE/DX = 0.0 !

! D192 D(65,35,36,66) -0.1508 -DE/DX = 0.0 !

! D193 D(24,37,38,39) 179.8953 -DE/DX = 0.0 !

! D194 D(24,37,38,67) 0.4155 -DE/DX = 0.0 !

! D195 D(42,37,38,39) -0.1047 -DE/DX = 0.0 !

! D196 D(42,37,38,67) -179.5845 -DE/DX = 0.0 !

! D197 D(24,37,42,41) 179.8953 -DE/DX = 0.0 !

! D198 D(24,37,42,71) 0.4155 -DE/DX = 0.0 !

! D199 D(38,37,42,41) -0.1047 -DE/DX = 0.0 !

! D200 D(38,37,42,71) -179.5845 -DE/DX = 0.0 !

! D201 D(37,38,39,40) 0.2097 -DE/DX = 0.0 !

! D202 D(37,38,39,68) -179.6276 -DE/DX = 0.0 !

! D203 D(67,38,39,40) 179.6865 -DE/DX = 0.0 !

! D204 D(67,38,39,68) -0.1508 -DE/DX = 0.0 !

! D205 D(38,39,40,41) -0.1041 -DE/DX = 0.0 !

! D206 D(38,39,40,69) 179.8959 -DE/DX = 0.0 !

! D207 D(68,39,40,41) 179.7325 -DE/DX = 0.0 !

! D208 D(68,39,40,69) -0.2675 -DE/DX = 0.0 !

! D209 D(39,40,41,42) -0.1041 -DE/DX = 0.0 !

! D210 D(39,40,41,70) 179.7325 -DE/DX = 0.0 !

! D211 D(69,40,41,42) 179.8959 -DE/DX = 0.0 !

! D212 D(69,40,41,70) -0.2675 -DE/DX = 0.0 !

! D213 D(40,41,42,37) 0.2097 -DE/DX = 0.0 !

! D214 D(40,41,42,71) 179.6865 -DE/DX = 0.0 !

! D215 D(70,41,42,37) -179.6276 -DE/DX = 0.0 !

! D216 D(70,41,42,71) -0.1508 -DE/DX = 0.0 !

! D217 D(18,43,44,45) -179.8953 -DE/DX = 0.0 !

! D218 D(18,43,44,72) -0.4155 -DE/DX = 0.0 !

! D219 D(48,43,44,45) 0.1047 -DE/DX = 0.0 !

! D220 D(48,43,44,72) 179.5845 -DE/DX = 0.0 !

! D221 D(18,43,48,47) -179.8953 -DE/DX = 0.0 !

! D222 D(18,43,48,76) -0.4155 -DE/DX = 0.0 !

! D223 D(44,43,48,47) 0.1047 -DE/DX = 0.0 !

! D224 D(44,43,48,76) 179.5845 -DE/DX = 0.0 !

! D225 D(43,44,45,46) -0.2097 -DE/DX = 0.0 !

! D226 D(43,44,45,73) 179.6276 -DE/DX = 0.0 !

! D227 D(72,44,45,46) -179.6865 -DE/DX = 0.0 !

! D228 D(72,44,45,73) 0.1508 -DE/DX = 0.0 !

! D229 D(44,45,46,47) 0.1041 -DE/DX = 0.0 !

! D230 D(44,45,46,74) -179.8959 -DE/DX = 0.0 !

! D231 D(73,45,46,47) -179.7325 -DE/DX = 0.0 !

! D232 D(73,45,46,74) 0.2675 -DE/DX = 0.0 !

! D233 D(45,46,47,48) 0.1041 -DE/DX = 0.0 !

! D234 D(45,46,47,75) -179.7325 -DE/DX = 0.0 !

! D235 D(74,46,47,48) -179.8959 -DE/DX = 0.0 !

! D236 D(74,46,47,75) 0.2675 -DE/DX = 0.0 !

! D237 D(46,47,48,43) -0.2097 -DE/DX = 0.0 !

! D238 D(46,47,48,76) -179.6865 -DE/DX = 0.0 !

! D239 D(75,47,48,43) 179.6276 -DE/DX = 0.0 !

! D240 D(75,47,48,76) 0.1508 -DE/DX = 0.0 !

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

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Largest change from initial coordinates is atom 60 0.000 Angstoms.

Leave Link 103 at Tue Aug 13 18:49:21 2019, MaxMem= 671088640 cpu: 0.9

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

Stoichiometry C44H28N4Zn

Framework group D2D[O(Zn),2SGD(N2),X(C44H28)]

Deg. of freedom 29

Full point group D2D NOp 8

RotChk: IX=0 Diff= 0.00D+00

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681484 4.269157 0.164086

2 6 0 -1.110541 2.890129 0.035503

3 7 0 0.000000 2.090529 -0.027459

4 6 0 1.110541 2.890129 0.035503

5 6 0 0.681484 4.269157 0.164086

6 6 0 2.452183 2.452183 0.000000

7 6 0 2.890129 1.110541 -0.035503

8 7 0 2.090529 -0.000000 0.027459

9 6 0 2.890129 -1.110541 -0.035503

10 6 0 4.269157 -0.681484 -0.164086

11 6 0 4.269157 0.681484 -0.164086

12 6 0 -2.452183 2.452183 0.000000

13 6 0 -2.890129 1.110541 -0.035503

14 6 0 -4.269157 0.681484 -0.164086

15 6 0 -4.269157 -0.681484 -0.164086

16 6 0 -2.890129 -1.110541 -0.035503

17 7 0 -2.090529 0.000000 0.027459

18 6 0 -2.452183 -2.452183 0.000000

19 6 0 -1.110541 -2.890129 0.035503

20 6 0 -0.681484 -4.269157 0.164086

21 6 0 0.681484 -4.269157 0.164086

22 6 0 1.110541 -2.890129 0.035503

23 7 0 -0.000000 -2.090529 -0.027459

24 6 0 2.452183 -2.452183 0.000000

25 6 0 3.508242 3.508242 -0.000000

26 6 0 3.621357 4.405038 -1.069674

27 6 0 4.607485 5.388753 -1.071137

28 6 0 5.493806 5.493806 0.000000

29 6 0 5.388753 4.607485 1.071137

30 6 0 4.405038 3.621357 1.069674

31 6 0 -5.493806 5.493806 0.000000

32 6 0 -4.607485 5.388753 -1.071137

33 6 0 -3.621357 4.405038 -1.069674

34 6 0 -3.508242 3.508242 -0.000000

35 6 0 -4.405038 3.621357 1.069674

36 6 0 -5.388753 4.607485 1.071137

37 6 0 3.508242 -3.508242 -0.000000

38 6 0 4.405038 -3.621357 1.069674

39 6 0 5.388753 -4.607485 1.071137

40 6 0 5.493806 -5.493806 0.000000

41 6 0 4.607485 -5.388753 -1.071137

42 6 0 3.621357 -4.405038 -1.069674

43 6 0 -3.508242 -3.508242 -0.000000

44 6 0 -4.405038 -3.621357 1.069674

45 6 0 -5.388753 -4.607485 1.071137

46 6 0 -5.493806 -5.493806 0.000000

47 6 0 -4.607485 -5.388753 -1.071137

48 6 0 -3.621357 -4.405038 -1.069674

49 1 0 -1.330917 5.125618 0.259828

50 1 0 1.330917 5.125618 0.259828

51 1 0 5.125618 -1.330917 -0.259828

52 1 0 5.125618 1.330917 -0.259828

53 1 0 -5.125618 1.330917 -0.259828

54 1 0 -5.125618 -1.330917 -0.259828

55 1 0 -1.330917 -5.125618 0.259828

56 1 0 1.330917 -5.125618 0.259828

57 1 0 2.936967 4.323214 -1.907040

58 1 0 4.684584 6.071446 -1.910980

59 1 0 6.260992 6.260992 0.000000

60 1 0 6.071446 4.684584 1.910980

61 1 0 4.323214 2.936967 1.907040

62 1 0 -6.260992 6.260992 0.000000

63 1 0 -4.684584 6.071446 -1.910980

64 1 0 -2.936967 4.323214 -1.907040

65 1 0 -4.323214 2.936967 1.907040

66 1 0 -6.071446 4.684584 1.910980

67 1 0 4.323214 -2.936967 1.907040

68 1 0 6.071446 -4.684584 1.910980

69 1 0 6.260992 -6.260992 0.000000

70 1 0 4.684584 -6.071446 -1.910980

71 1 0 2.936967 -4.323214 -1.907040

72 1 0 -4.323214 -2.936967 1.907040

73 1 0 -6.071446 -4.684584 1.910980

74 1 0 -6.260992 -6.260992 0.000000

75 1 0 -4.684584 -6.071446 -1.910980

76 1 0 -2.936967 -4.323214 -1.907040

77 30 0 0.000000 0.000000 0.000000

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

Rotational constants (GHZ): 0.0582110 0.0582110 0.0300828

Leave Link 202 at Tue Aug 13 18:49:21 2019, MaxMem= 671088640 cpu: 0.0

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

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

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

Population analysis using the SCF density.

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

Orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The electronic state is 1-A1.

Alpha occ. eigenvalues -- -14.30274 -14.30274 -14.30273 -14.30273 -10.20850

Alpha occ. eigenvalues -- -10.20850 -10.20850 -10.20850 -10.20849 -10.20849

Alpha occ. eigenvalues -- -10.20849 -10.20849 -10.19527 -10.19527 -10.19527

Alpha occ. eigenvalues -- -10.19527 -10.18649 -10.18649 -10.18649 -10.18649

Alpha occ. eigenvalues -- -10.17325 -10.17325 -10.17325 -10.17325 -10.17325

Alpha occ. eigenvalues -- -10.17325 -10.17325 -10.17325 -10.17283 -10.17283

Alpha occ. eigenvalues -- -10.17283 -10.17283 -10.17252 -10.17252 -10.17252

Alpha occ. eigenvalues -- -10.17252 -10.17215 -10.17215 -10.17215 -10.17215

Alpha occ. eigenvalues -- -10.16829 -10.16829 -10.16829 -10.16829 -10.16763

Alpha occ. eigenvalues -- -10.16763 -10.16763 -10.16763 -0.96311 -0.95466

Alpha occ. eigenvalues -- -0.95466 -0.94579 -0.86920 -0.86555 -0.86555

Alpha occ. eigenvalues -- -0.86379 -0.82290 -0.80635 -0.80635 -0.78863

Alpha occ. eigenvalues -- -0.76631 -0.76592 -0.76592 -0.76144 -0.74941

Alpha occ. eigenvalues -- -0.74862 -0.74862 -0.74828 -0.74123 -0.73406

Alpha occ. eigenvalues -- -0.73406 -0.71852 -0.70867 -0.66163 -0.66163

Alpha occ. eigenvalues -- -0.62134 -0.61068 -0.60823 -0.60823 -0.60677

Alpha occ. eigenvalues -- -0.59897 -0.59897 -0.59468 -0.59445 -0.58587

Alpha occ. eigenvalues -- -0.57012 -0.56547 -0.56261 -0.56261 -0.56057

Alpha occ. eigenvalues -- -0.55332 -0.55332 -0.54829 -0.54320 -0.52699

Alpha occ. eigenvalues -- -0.52699 -0.52628 -0.51909 -0.51398 -0.51398

Alpha occ. eigenvalues -- -0.49894 -0.49806 -0.49164 -0.49164 -0.46156

Alpha occ. eigenvalues -- -0.46073 -0.45862 -0.45731 -0.45731 -0.44985

Alpha occ. eigenvalues -- -0.44985 -0.44864 -0.44341 -0.42569 -0.42546

Alpha occ. eigenvalues -- -0.42305 -0.42305 -0.42195 -0.42155 -0.42155

Alpha occ. eigenvalues -- -0.42129 -0.41797 -0.41216 -0.40818 -0.40818

Alpha occ. eigenvalues -- -0.40139 -0.40139 -0.39299 -0.39066 -0.38439

Alpha occ. eigenvalues -- -0.38303 -0.37820 -0.37820 -0.36828 -0.36767

Alpha occ. eigenvalues -- -0.36708 -0.36708 -0.35813 -0.35163 -0.34764

Alpha occ. eigenvalues -- -0.34695 -0.34695 -0.34605 -0.34599 -0.34599

Alpha occ. eigenvalues -- -0.33902 -0.31870 -0.31301 -0.31301 -0.28611

Alpha occ. eigenvalues -- -0.28611 -0.26425 -0.26019 -0.25991 -0.25945

Alpha occ. eigenvalues -- -0.25930 -0.25930 -0.25682 -0.25255 -0.25238

Alpha occ. eigenvalues -- -0.25238 -0.24717 -0.24717 -0.24647 -0.20184

Alpha occ. eigenvalues -- -0.18937

Alpha virt. eigenvalues -- -0.09064 -0.09064 -0.03556 -0.01361 -0.01316

Alpha virt. eigenvalues -- -0.01316 -0.01116 -0.01041 -0.01029 -0.00930

Alpha virt. eigenvalues -- -0.00930 0.03358 0.03798 0.04518 0.04646

Alpha virt. eigenvalues -- 0.04646 0.05596 0.05596 0.05822 0.06119

Alpha virt. eigenvalues -- 0.07000 0.07000 0.07197 0.08446 0.08983

Alpha virt. eigenvalues -- 0.08983 0.09147 0.09179 0.09557 0.09557

Alpha virt. eigenvalues -- 0.10009 0.10277 0.10339 0.10376 0.11364

Alpha virt. eigenvalues -- 0.11364 0.11918 0.11918 0.12037 0.12647

Alpha virt. eigenvalues -- 0.13045 0.13045 0.13326 0.13423 0.13695

Alpha virt. eigenvalues -- 0.13695 0.13809 0.14078 0.14170 0.14728

Alpha virt. eigenvalues -- 0.15121 0.15121 0.15773 0.15773 0.16274

Alpha virt. eigenvalues -- 0.16461 0.18510 0.18510 0.20796 0.21632

Alpha virt. eigenvalues -- 0.22463 0.23766 0.23766 0.23814 0.23862

Alpha virt. eigenvalues -- 0.24494 0.25350 0.25688 0.25688 0.26612

Alpha virt. eigenvalues -- 0.26946 0.26946 0.27152 0.27581 0.28038

Alpha virt. eigenvalues -- 0.28054 0.28054 0.28372 0.28519 0.28519

Alpha virt. eigenvalues -- 0.28918 0.29009 0.29009 0.29010 0.29992

Alpha virt. eigenvalues -- 0.29992 0.30039 0.30049 0.30669 0.31413

Alpha virt. eigenvalues -- 0.31413 0.31596 0.32476 0.34392 0.35120

Alpha virt. eigenvalues -- 0.35359 0.35359 0.35508 0.36081 0.36081

Alpha virt. eigenvalues -- 0.36373 0.36473 0.36753 0.36753 0.36852

Alpha virt. eigenvalues -- 0.36852 0.37487 0.37665 0.38134 0.38779

Alpha virt. eigenvalues -- 0.38849 0.39795 0.39795 0.39797 0.39867

Alpha virt. eigenvalues -- 0.39867 0.40128 0.40540 0.40793 0.41155

Alpha virt. eigenvalues -- 0.41200 0.41200 0.41478 0.41535 0.41535

Alpha virt. eigenvalues -- 0.41912 0.41955 0.41990 0.41990 0.42349

Alpha virt. eigenvalues -- 0.42980 0.42980 0.43152 0.43431 0.43431

Alpha virt. eigenvalues -- 0.43723 0.43879 0.44575 0.44575 0.44601

Alpha virt. eigenvalues -- 0.44829 0.45046 0.45147 0.45219 0.45219

Alpha virt. eigenvalues -- 0.45518 0.46539 0.46539 0.46774 0.46774

Alpha virt. eigenvalues -- 0.46835 0.47207 0.47595 0.48416 0.48416

Alpha virt. eigenvalues -- 0.48766 0.48766 0.49664 0.49664 0.49995

Alpha virt. eigenvalues -- 0.49999 0.50136 0.51020 0.51114 0.51349

Alpha virt. eigenvalues -- 0.51782 0.52598 0.52598 0.53594 0.53594

Alpha virt. eigenvalues -- 0.53679 0.54246 0.54246 0.54286 0.54884

Alpha virt. eigenvalues -- 0.55960 0.56631 0.57532 0.57677 0.57677

Alpha virt. eigenvalues -- 0.57715 0.57900 0.58626 0.58626 0.59659

Alpha virt. eigenvalues -- 0.59659 0.60331 0.60460 0.60602 0.60839

Alpha virt. eigenvalues -- 0.60839 0.61152 0.61324 0.61324 0.61386

Alpha virt. eigenvalues -- 0.61510 0.61516 0.61657 0.61657 0.62106

Alpha virt. eigenvalues -- 0.62516 0.62617 0.62617 0.62762 0.63648

Alpha virt. eigenvalues -- 0.63898 0.63898 0.64424 0.64555 0.64836

Alpha virt. eigenvalues -- 0.64836 0.65153 0.65227 0.65335 0.65437

Alpha virt. eigenvalues -- 0.65437 0.65564 0.66823 0.66823 0.66881

Alpha virt. eigenvalues -- 0.67116 0.67968 0.67968 0.68150 0.69635

Alpha virt. eigenvalues -- 0.69635 0.70395 0.70711 0.72180 0.72180

Alpha virt. eigenvalues -- 0.72611 0.72611 0.72694 0.73045 0.73289

Alpha virt. eigenvalues -- 0.73760 0.73787 0.73787 0.74429 0.74493

Alpha virt. eigenvalues -- 0.75337 0.75337 0.75723 0.75848 0.75848

Alpha virt. eigenvalues -- 0.75952 0.76469 0.76469 0.77006 0.78250

Alpha virt. eigenvalues -- 0.78260 0.78869 0.78869 0.79700 0.79743

Alpha virt. eigenvalues -- 0.79990 0.80537 0.80537 0.81093 0.81093

Alpha virt. eigenvalues -- 0.81419 0.81953 0.82369 0.82664 0.82664

Alpha virt. eigenvalues -- 0.84132 0.84615 0.85250 0.85250 0.85690

Alpha virt. eigenvalues -- 0.85794 0.87013 0.87285 0.87285 0.87399

Alpha virt. eigenvalues -- 0.89301 0.89301 0.89302 0.89497 0.90001

Alpha virt. eigenvalues -- 0.90001 0.90117 0.91772 0.92560 0.92684

Alpha virt. eigenvalues -- 0.92684 0.93361 0.93558 0.94473 0.94473

Alpha virt. eigenvalues -- 0.94991 0.96109 0.96620 0.96788 0.96788

Alpha virt. eigenvalues -- 0.98372 0.99146 0.99146 1.00407 1.00505

Alpha virt. eigenvalues -- 1.01503 1.01503 1.02404 1.02469 1.02827

Alpha virt. eigenvalues -- 1.04412 1.04412 1.05228 1.05228 1.05341

Alpha virt. eigenvalues -- 1.05453 1.05932 1.07581 1.08591 1.09226

Alpha virt. eigenvalues -- 1.09226 1.09719 1.11356 1.11356 1.11644

Alpha virt. eigenvalues -- 1.12557 1.13167 1.13167 1.14992 1.14992

Alpha virt. eigenvalues -- 1.15230 1.15462 1.15462 1.16885 1.17514

Alpha virt. eigenvalues -- 1.17514 1.17633 1.17633 1.17867 1.18328

Alpha virt. eigenvalues -- 1.19469 1.20497 1.20497 1.20958 1.21019

Alpha virt. eigenvalues -- 1.21094 1.21438 1.21438 1.21749 1.21749

Alpha virt. eigenvalues -- 1.22277 1.22828 1.22971 1.23975 1.24161

Alpha virt. eigenvalues -- 1.24161 1.24766 1.24766 1.25277 1.25325

Alpha virt. eigenvalues -- 1.25676 1.26445 1.27012 1.27012 1.27775

Alpha virt. eigenvalues -- 1.28532 1.28532 1.28827 1.30246 1.31486

Alpha virt. eigenvalues -- 1.31806 1.32636 1.32636 1.37143 1.38171

Alpha virt. eigenvalues -- 1.38595 1.38595 1.40391 1.40391 1.41032

Alpha virt. eigenvalues -- 1.41255 1.41741 1.43969 1.43969 1.44475

Alpha virt. eigenvalues -- 1.45941 1.47242 1.47242 1.47706 1.47723

Alpha virt. eigenvalues -- 1.48059 1.48534 1.48534 1.48539 1.49294

Alpha virt. eigenvalues -- 1.49994 1.49994 1.50305 1.50690 1.52899

Alpha virt. eigenvalues -- 1.52899 1.53718 1.54174 1.54451 1.54451

Alpha virt. eigenvalues -- 1.55548 1.55548 1.55715 1.56727 1.56727

Alpha virt. eigenvalues -- 1.57149 1.58563 1.59949 1.61260 1.61260

Alpha virt. eigenvalues -- 1.61460 1.61682 1.62535 1.62535 1.64836

Alpha virt. eigenvalues -- 1.64836 1.65259 1.67334 1.68458 1.68666

Alpha virt. eigenvalues -- 1.68666 1.68773 1.70139 1.70207 1.70207

Alpha virt. eigenvalues -- 1.71110 1.71110 1.71694 1.73965 1.74279

Alpha virt. eigenvalues -- 1.74716 1.76064 1.76064 1.76158 1.76287

Alpha virt. eigenvalues -- 1.76357 1.76357 1.77480 1.77480 1.77707

Alpha virt. eigenvalues -- 1.79010 1.79082 1.79905 1.80586 1.80586

Alpha virt. eigenvalues -- 1.81095 1.81289 1.81399 1.81830 1.81830

Alpha virt. eigenvalues -- 1.83685 1.83685 1.84124 1.84128 1.84558

Alpha virt. eigenvalues -- 1.84787 1.85072 1.85222 1.85222 1.86524

Alpha virt. eigenvalues -- 1.87567 1.87567 1.88657 1.88870 1.88870

Alpha virt. eigenvalues -- 1.89088 1.89660 1.89981 1.91737 1.91971

Alpha virt. eigenvalues -- 1.91971 1.92211 1.92565 1.92713 1.92785

Alpha virt. eigenvalues -- 1.92785 1.93158 1.93232 1.93232 1.94017

Alpha virt. eigenvalues -- 1.94080 1.94121 1.94121 1.94591 1.96178

Alpha virt. eigenvalues -- 1.96407 1.96407 1.96689 1.96971 1.96971

Alpha virt. eigenvalues -- 1.98495 1.99902 1.99997 1.99997 2.00084

Alpha virt. eigenvalues -- 2.00213 2.00556 2.00556 2.01260 2.06900

Alpha virt. eigenvalues -- 2.07144 2.08170 2.08170 2.09100 2.09100

Alpha virt. eigenvalues -- 2.09104 2.11700 2.13063 2.13904 2.14304

Alpha virt. eigenvalues -- 2.14304 2.19160 2.22089 2.23720 2.24110

Alpha virt. eigenvalues -- 2.24110 2.25803 2.25876 2.25876 2.26301

Alpha virt. eigenvalues -- 2.26583 2.26836 2.27625 2.27625 2.27835

Alpha virt. eigenvalues -- 2.28125 2.28341 2.28341 2.28682 2.29592

Alpha virt. eigenvalues -- 2.29592 2.29659 2.29877 2.30520 2.30520

Alpha virt. eigenvalues -- 2.32006 2.32115 2.32445 2.33142 2.33142

Alpha virt. eigenvalues -- 2.33973 2.33973 2.35654 2.35762 2.36440

Alpha virt. eigenvalues -- 2.36729 2.36729 2.36832 2.38526 2.38738

Alpha virt. eigenvalues -- 2.39662 2.39662 2.40442 2.40442 2.40919

Alpha virt. eigenvalues -- 2.44253 2.44865 2.44865 2.44970 2.47256

Alpha virt. eigenvalues -- 2.47341 2.49851 2.49851 2.53871 2.54681

Alpha virt. eigenvalues -- 2.54681 2.54903 2.55451 2.57018 2.57718

Alpha virt. eigenvalues -- 2.57972 2.57972 2.59297 2.59374 2.59374

Alpha virt. eigenvalues -- 2.60402 2.61072 2.61072 2.62117 2.62454

Alpha virt. eigenvalues -- 2.62674 2.62770 2.64559 2.64559 2.65206

Alpha virt. eigenvalues -- 2.65206 2.65617 2.65620 2.68503 2.69773

Alpha virt. eigenvalues -- 2.70071 2.70071 2.70289 2.72767 2.72767

Alpha virt. eigenvalues -- 2.73257 2.74889 2.74889 2.75016 2.75043

Alpha virt. eigenvalues -- 2.77012 2.77012 2.78467 2.78610 2.79432

Alpha virt. eigenvalues -- 2.79445 2.79445 2.80399 2.80679 2.82656

Alpha virt. eigenvalues -- 2.82656 2.84183 2.84843 2.85481 2.85481

Alpha virt. eigenvalues -- 2.85969 2.87050 2.89784 2.89784 2.90174

Alpha virt. eigenvalues -- 2.90174 2.90673 2.92973 2.94116 2.95892

Alpha virt. eigenvalues -- 2.95892 2.96850 2.98852 2.98852 2.99046

Alpha virt. eigenvalues -- 2.99721 3.01290 3.02782 3.04316 3.04877

Alpha virt. eigenvalues -- 3.04877 3.06540 3.07481 3.07481 3.07582

Alpha virt. eigenvalues -- 3.08395 3.08395 3.09188 3.11350 3.11687

Alpha virt. eigenvalues -- 3.11860 3.12217 3.12217 3.14525 3.16838

Alpha virt. eigenvalues -- 3.16838 3.16849 3.19546 3.19619 3.19619

Alpha virt. eigenvalues -- 3.19736 3.22486 3.25834 3.25947 3.25947

Alpha virt. eigenvalues -- 3.26087 3.26816 3.26816 3.29255 3.29591

Alpha virt. eigenvalues -- 3.29591 3.29856 3.29976 3.29996 3.30214

Alpha virt. eigenvalues -- 3.30214 3.30436 3.31091 3.31193 3.31272

Alpha virt. eigenvalues -- 3.31272 3.31847 3.32135 3.34686 3.34686

Alpha virt. eigenvalues -- 3.34715 3.35837 3.35837 3.36785 3.38248

Alpha virt. eigenvalues -- 3.38248 3.39729 3.40864 3.42407 3.43091

Alpha virt. eigenvalues -- 3.43091 3.44709 3.50363 3.51898 3.51956

Alpha virt. eigenvalues -- 3.51956 3.56787 3.58143 3.58143 3.58602

Alpha virt. eigenvalues -- 3.58602 3.59419 3.59738 3.61534 3.62677

Alpha virt. eigenvalues -- 3.66704 3.67307 3.67307 3.72803 3.73568

Alpha virt. eigenvalues -- 3.75789 3.75789 3.82769 3.82769 3.82872

Alpha virt. eigenvalues -- 3.85007 3.87457 3.87457 3.89144 3.91617

Alpha virt. eigenvalues -- 3.93980 3.93980 3.95111 3.95447 3.96267

Alpha virt. eigenvalues -- 3.96313 3.96313 3.96391 3.99534 4.01085

Alpha virt. eigenvalues -- 4.01085 4.12026 4.33381 4.35441 4.40179

Alpha virt. eigenvalues -- 4.40179 4.46726 4.49709 4.54091 4.54091

Alpha virt. eigenvalues -- 4.61897 4.66888 4.66888 4.67840 4.78821

Alpha virt. eigenvalues -- 4.78831 4.78831 4.78841 5.11536 5.18916

Alpha virt. eigenvalues -- 5.18916 5.32589 7.77675 7.77675 7.88025

Alpha virt. eigenvalues -- 7.92778 8.13982 11.12048 23.25291 23.28974

Alpha virt. eigenvalues -- 23.28974 23.30653 23.46368 23.53063 23.53063

Alpha virt. eigenvalues -- 23.57714 23.74795 23.75935 23.75935 23.77727

Alpha virt. eigenvalues -- 23.81067 23.81232 23.81232 23.81492 23.85161

Alpha virt. eigenvalues -- 23.86126 23.86126 23.86887 23.92662 23.94755

Alpha virt. eigenvalues -- 23.94755 23.96993 23.98200 23.99159 23.99159

Alpha virt. eigenvalues -- 23.99221 24.04793 24.04950 24.04950 24.05134

Alpha virt. eigenvalues -- 24.08773 24.09280 24.09280 24.09729 24.13357

Alpha virt. eigenvalues -- 24.13718 24.13718 24.14423 24.16343 24.16382

Alpha virt. eigenvalues -- 24.16382 24.16394 35.63343 35.64463 35.66095

Alpha virt. eigenvalues -- 35.66095

Condensed to atoms (all electrons):

Mulliken charges:

1

1 C -0.261142

2 C 0.308668

3 N -0.706255

4 C 0.308668

5 C -0.261142

6 C -0.149008

7 C 0.308668

8 N -0.706255

9 C 0.308668

10 C -0.261142

11 C -0.261142

12 C -0.149008

13 C 0.308668

14 C -0.261142

15 C -0.261142

16 C 0.308668

17 N -0.706255

18 C -0.149008

19 C 0.308668

20 C -0.261142

21 C -0.261142

22 C 0.308668

23 N -0.706255

24 C -0.149008

25 C -0.105848

26 C -0.211897

27 C -0.217879

28 C -0.221700

29 C -0.217879

30 C -0.211897

31 C -0.221700

32 C -0.217879

33 C -0.211897

34 C -0.105848

35 C -0.211897

36 C -0.217879

37 C -0.105848

38 C -0.211897

39 C -0.217879

40 C -0.221700

41 C -0.217879

42 C -0.211897

43 C -0.105848

44 C -0.211897

45 C -0.217879

46 C -0.221700

47 C -0.217879

48 C -0.211897

49 H 0.239146

50 H 0.239146

51 H 0.239146

52 H 0.239146

53 H 0.239146

54 H 0.239146

55 H 0.239146

56 H 0.239146

57 H 0.224238

58 H 0.225860

59 H 0.225720

60 H 0.225860

61 H 0.224238

62 H 0.225720

63 H 0.225860

64 H 0.224238

65 H 0.224238

66 H 0.225860

67 H 0.224238

68 H 0.225860

69 H 0.225720

70 H 0.225860

71 H 0.224238

72 H 0.224238

73 H 0.225860

74 H 0.225720

75 H 0.225860

76 H 0.224238

77 Zn 1.372414

Sum of Mulliken charges = -0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 C -0.021996

2 C 0.308668

3 N -0.706255

4 C 0.308668

5 C -0.021996

6 C -0.149008

7 C 0.308668

8 N -0.706255

9 C 0.308668

10 C -0.021996

11 C -0.021996

12 C -0.149008

13 C 0.308668

14 C -0.021996

15 C -0.021996

16 C 0.308668

17 N -0.706255

18 C -0.149008

19 C 0.308668

20 C -0.021996

21 C -0.021996

22 C 0.308668

23 N -0.706255

24 C -0.149008

25 C -0.105848

26 C 0.012341

27 C 0.007981

28 C 0.004019

29 C 0.007981

30 C 0.012341

31 C 0.004019

32 C 0.007981

33 C 0.012341

34 C -0.105848

35 C 0.012341

36 C 0.007981

37 C -0.105848

38 C 0.012341

39 C 0.007981

40 C 0.004019

41 C 0.007981

42 C 0.012341

43 C -0.105848

44 C 0.012341

45 C 0.007981

46 C 0.004019

47 C 0.007981

48 C 0.012341

77 Zn 1.372414

Electronic spatial extent (au): <R\*\*2>= 33352.9766

Charge= -0.0000 electrons

Dipole moment (field-independent basis, Debye):

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

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

XX= -248.6474 YY= -248.6474 ZZ= -276.6356

XY= 0.0000 XZ= 0.0000 YZ= -0.0000

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

XX= 9.3294 YY= 9.3294 ZZ= -18.6588

XY= 0.0000 XZ= 0.0000 YZ= -0.0000

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

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

XXY= -0.0000 XXZ= 89.9106 XZZ= -0.0000 YZZ= 0.0000

YYZ= -89.9106 XYZ= -0.0000

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

XXXX= -21528.0504 YYYY= -21528.0504 ZZZZ= -1080.9904 XXXY= -0.0000

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

ZZZY= -0.0000 XXYY= -5779.8971 XXZZ= -3834.9829 YYZZ= -3834.9829

XXYZ= -0.0000 YYXZ= 0.0000 ZZXY= -0.0000

N-N= 5.738269787601D+03 E-N=-1.615865197821D+04 KE= 2.020706227707D+03

Symmetry A1 KE= 5.778493066606D+02

Symmetry A2 KE= 4.453814196470D+02

Symmetry B1 KE= 4.987377506994D+02

Symmetry B2 KE= 4.987377506994D+02

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Tue Aug 13 18:49:27 2019, MaxMem= 671088640 cpu: 25.6

(Enter /home/kira/g09/l9999.exe)

1\1\ WCSS.PL-BEM-LOCALHOST\FOpt\RB3LYP\GenECP\C44H28N4Zn1\KIRA\13-Aug-

2019\0\\#p opt freq b3lyp/genecp scrf=(solvent=dmso,smd) empiricaldisp

ersion=gd3bj\\ZnTPP0\\0,1\C,-0.6814836847,4.2691569083,0.1640859429\C,

-1.1105409583,2.8901294306,0.0355027808\N,0.,2.0905285459,-0.027459306

7\C,1.1105409583,2.8901294306,0.0355027808\C,0.6814836847,4.2691569083

,0.1640859429\C,2.4521830609,2.4521830609,0.\C,2.8901294306,1.11054095

83,-0.0355027808\N,2.0905285459,0.,0.0274593067\C,2.8901294306,-1.1105

409583,-0.0355027808\C,4.2691569083,-0.6814836847,-0.1640859429\C,4.26

91569083,0.6814836847,-0.1640859429\C,-2.4521830609,2.4521830609,0.\C,

-2.8901294306,1.1105409583,-0.0355027808\C,-4.2691569083,0.6814836847,

-0.1640859429\C,-4.2691569083,-0.6814836847,-0.1640859429\C,-2.8901294

306,-1.1105409583,-0.0355027808\N,-2.0905285459,0.,0.0274593067\C,-2.4

521830609,-2.4521830609,0.\C,-1.1105409583,-2.8901294306,0.0355027808\

C,-0.6814836847,-4.2691569083,0.1640859429\C,0.6814836847,-4.269156908

3,0.1640859429\C,1.1105409583,-2.8901294306,0.0355027808\N,0.,-2.09052

85459,-0.0274593067\C,2.4521830609,-2.4521830609,0.\C,3.5082420649,3.5

082420649,0.\C,3.621356962,4.4050379303,-1.0696739965\C,4.6074850511,5

.3887527402,-1.0711374359\C,5.4938063781,5.4938063781,0.\C,5.388752740

2,4.6074850511,1.0711374359\C,4.4050379303,3.621356962,1.0696739965\C,

-5.4938063781,5.4938063781,0.\C,-4.6074850511,5.3887527402,-1.07113743

59\C,-3.621356962,4.4050379303,-1.0696739965\C,-3.5082420649,3.5082420

649,0.\C,-4.4050379303,3.621356962,1.0696739965\C,-5.3887527402,4.6074

850511,1.0711374359\C,3.5082420649,-3.5082420649,0.\C,4.4050379303,-3.

621356962,1.0696739965\C,5.3887527402,-4.6074850511,1.0711374359\C,5.4

938063781,-5.4938063781,0.\C,4.6074850511,-5.3887527402,-1.0711374359\

C,3.621356962,-4.4050379303,-1.0696739965\C,-3.5082420649,-3.508242064

9,0.\C,-4.4050379303,-3.621356962,1.0696739965\C,-5.3887527402,-4.6074

850511,1.0711374359\C,-5.4938063781,-5.4938063781,0.\C,-4.6074850511,-

5.3887527402,-1.0711374359\C,-3.621356962,-4.4050379303,-1.0696739965\

H,-1.3309170091,5.1256177951,0.2598284106\H,1.3309170091,5.1256177951,

0.2598284106\H,5.1256177951,-1.3309170091,-0.2598284106\H,5.1256177951

,1.3309170091,-0.2598284106\H,-5.1256177951,1.3309170091,-0.2598284106

\H,-5.1256177951,-1.3309170091,-0.2598284106\H,-1.3309170091,-5.125617

7951,0.2598284106\H,1.3309170091,-5.1256177951,0.2598284106\H,2.936966

8579,4.3232144846,-1.907039927\H,4.6845840293,6.0714462862,-1.91097950

61\H,6.2609915148,6.2609915148,0.\H,6.0714462862,4.6845840293,1.910979

5061\H,4.3232144846,2.9369668579,1.907039927\H,-6.2609915148,6.2609915

148,0.\H,-4.6845840293,6.0714462862,-1.9109795061\H,-2.9369668579,4.32

32144846,-1.907039927\H,-4.3232144846,2.9369668579,1.907039927\H,-6.07

14462862,4.6845840293,1.9109795061\H,4.3232144846,-2.9369668579,1.9070

39927\H,6.0714462862,-4.6845840293,1.9109795061\H,6.2609915148,-6.2609

915148,0.\H,4.6845840293,-6.0714462862,-1.9109795061\H,2.9369668579,-4

.3232144846,-1.907039927\H,-4.3232144846,-2.9369668579,1.907039927\H,-

6.0714462862,-4.6845840293,1.9109795061\H,-6.2609915148,-6.2609915148,

0.\H,-4.6845840293,-6.0714462862,-1.9109795061\H,-2.9369668579,-4.3232

144846,-1.907039927\Zn,0.,0.,0.\\Version=ES64L-G09RevE.01\State=1-A1\H

F=-1978.9043534\RMSD=9.429e-09\RMSF=1.601e-05\Dipole=0.,0.,0.\Quadrupo

le=6.9361771,6.9361771,-13.8723542,0.,0.,0.\PG=D02D [O(Zn1),2SGD(N2),X

(C44H28)]\\@

A people that values its privileges above its principles soon loses both.

-- Dwight D. Eisenhower

Leave Link 9999 at Tue Aug 13 18:49:28 2019, MaxMem= 671088640 cpu: 0.3

Job cpu time: 0 days 3 hours 27 minutes 14.6 seconds.

File lengths (MBytes): RWF= 1603 Int= 0 D2E= 0 Chk= 69 Scr= 1

Normal termination of Gaussian 09 at Tue Aug 13 18:49:28 2019.

(Enter /home/kira/g09/l1.exe)

Link1: Proceeding to internal job step number 2.

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

#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/GenECP Freq

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

1/10=4,29=7,30=1,38=1,40=1/1,3;

2/12=2,40=1/2;

3/5=7,6=2,11=2,14=-4,16=1,17=8,25=1,30=1,70=2,71=2,72=21,74=-5,82=7,116=1,124=41,140=1/1,2,3;

4/5=101/1;

5/5=2,38=6,53=21,98=1/2;

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

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

10/6=1/2;

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

7/8=1,10=1,25=1/1,2,3,16;

1/10=4,30=1/3;

99//99;

Leave Link 1 at Tue Aug 13 18:49:28 2019, MaxMem= 671088640 cpu: 0.2

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

Structure from the checkpoint file: "ZnTPP0.chk"

------

ZnTPP0

------

Charge = 0 Multiplicity = 1

Redundant internal coordinates found in file.

C,0,-0.6814836847,4.2691569083,0.1640859429

C,0,-1.1105409583,2.8901294306,0.0355027808

N,0,0.,2.0905285459,-0.0274593067

C,0,1.1105409583,2.8901294306,0.0355027808

C,0,0.6814836847,4.2691569083,0.1640859429

C,0,2.4521830609,2.4521830609,0.

C,0,2.8901294306,1.1105409583,-0.0355027808

N,0,2.0905285459,0.,0.0274593067

C,0,2.8901294306,-1.1105409583,-0.0355027808

C,0,4.2691569083,-0.6814836847,-0.1640859429

C,0,4.2691569083,0.6814836847,-0.1640859429

C,0,-2.4521830609,2.4521830609,0.

C,0,-2.8901294306,1.1105409583,-0.0355027808

C,0,-4.2691569083,0.6814836847,-0.1640859429

C,0,-4.2691569083,-0.6814836847,-0.1640859429

C,0,-2.8901294306,-1.1105409583,-0.0355027808

N,0,-2.0905285459,0.,0.0274593067

C,0,-2.4521830609,-2.4521830609,0.

C,0,-1.1105409583,-2.8901294306,0.0355027808

C,0,-0.6814836847,-4.2691569083,0.1640859429

C,0,0.6814836847,-4.2691569083,0.1640859429

C,0,1.1105409583,-2.8901294306,0.0355027808

N,0,0.,-2.0905285459,-0.0274593067

C,0,2.4521830609,-2.4521830609,0.

C,0,3.5082420649,3.5082420649,0.

C,0,3.621356962,4.4050379303,-1.0696739965

C,0,4.6074850511,5.3887527402,-1.0711374359

C,0,5.4938063781,5.4938063781,0.

C,0,5.3887527402,4.6074850511,1.0711374359

C,0,4.4050379303,3.621356962,1.0696739965

C,0,-5.4938063781,5.4938063781,0.

C,0,-4.6074850511,5.3887527402,-1.0711374359

C,0,-3.621356962,4.4050379303,-1.0696739965

C,0,-3.5082420649,3.5082420649,0.

C,0,-4.4050379303,3.621356962,1.0696739965

C,0,-5.3887527402,4.6074850511,1.0711374359

C,0,3.5082420649,-3.5082420649,0.

C,0,4.4050379303,-3.621356962,1.0696739965

C,0,5.3887527402,-4.6074850511,1.0711374359

C,0,5.4938063781,-5.4938063781,0.

C,0,4.6074850511,-5.3887527402,-1.0711374359

C,0,3.621356962,-4.4050379303,-1.0696739965

C,0,-3.5082420649,-3.5082420649,0.

C,0,-4.4050379303,-3.621356962,1.0696739965

C,0,-5.3887527402,-4.6074850511,1.0711374359

C,0,-5.4938063781,-5.4938063781,0.

C,0,-4.6074850511,-5.3887527402,-1.0711374359

C,0,-3.621356962,-4.4050379303,-1.0696739965

H,0,-1.3309170091,5.1256177951,0.2598284106

H,0,1.3309170091,5.1256177951,0.2598284106

H,0,5.1256177951,-1.3309170091,-0.2598284106

H,0,5.1256177951,1.3309170091,-0.2598284106

H,0,-5.1256177951,1.3309170091,-0.2598284106

H,0,-5.1256177951,-1.3309170091,-0.2598284106

H,0,-1.3309170091,-5.1256177951,0.2598284106

H,0,1.3309170091,-5.1256177951,0.2598284106

H,0,2.9369668579,4.3232144846,-1.907039927

H,0,4.6845840293,6.0714462862,-1.9109795061

H,0,6.2609915148,6.2609915148,0.

H,0,6.0714462862,4.6845840293,1.9109795061

H,0,4.3232144846,2.9369668579,1.907039927

H,0,-6.2609915148,6.2609915148,0.

H,0,-4.6845840293,6.0714462862,-1.9109795061

H,0,-2.9369668579,4.3232144846,-1.907039927

H,0,-4.3232144846,2.9369668579,1.907039927

H,0,-6.0714462862,4.6845840293,1.9109795061

H,0,4.3232144846,-2.9369668579,1.907039927

H,0,6.0714462862,-4.6845840293,1.9109795061

H,0,6.2609915148,-6.2609915148,0.

H,0,4.6845840293,-6.0714462862,-1.9109795061

H,0,2.9369668579,-4.3232144846,-1.907039927

H,0,-4.3232144846,-2.9369668579,1.907039927

H,0,-6.0714462862,-4.6845840293,1.9109795061

H,0,-6.2609915148,-6.2609915148,0.

H,0,-4.6845840293,-6.0714462862,-1.9109795061

H,0,-2.9369668579,-4.3232144846,-1.907039927

Zn,0,0.,0.,0.

Recover connectivity data from disk.

NAtoms= 77 NQM= 77 NQMF= 0 NMMI= 0 NMMIF= 0

NMic= 0 NMicF= 0.

Isotopes and Nuclear Properties:

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

in nuclear magnetons)

Atom 1 2 3 4 5 6 7 8 9 10

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

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

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

AtZEff= -3.6000000 -3.6000000 -4.5500000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -4.5500000 -3.6000000 -3.6000000

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

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

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

Atom 11 12 13 14 15 16 17 18 19 20

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

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

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

AtZEff= -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -4.5500000 -3.6000000 -3.6000000 -3.6000000

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

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

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

Atom 21 22 23 24 25 26 27 28 29 30

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

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

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

AtZEff= -3.6000000 -3.6000000 -4.5500000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000

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 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

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

Atom 31 32 33 34 35 36 37 38 39 40

IAtWgt= 12 12 12 12 12 12 12 12 12 12

AtmWgt= 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000

NucSpn= 0 0 0 0 0 0 0 0 0 0

AtZEff= -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000

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

NMagM= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

AtZNuc= 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000

Atom 41 42 43 44 45 46 47 48 49 50

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

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

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

AtZEff= -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -3.6000000 -1.0000000 -1.0000000

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

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

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

Atom 51 52 53 54 55 56 57 58 59 60

IAtWgt= 1 1 1 1 1 1 1 1 1 1

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 1 1 1 1 1 1 1 1 1 1

AtZEff= -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000

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

NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Atom 61 62 63 64 65 66 67 68 69 70

IAtWgt= 1 1 1 1 1 1 1 1 1 1

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 1 1 1 1 1 1 1 1 1 1

AtZEff= -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000

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

NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Atom 71 72 73 74 75 76 77

IAtWgt= 1 1 1 1 1 1 64

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 63.9291454

NucSpn= 1 1 1 1 1 1 0

AtZEff= -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000 -1.0000000 -19.0500000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 0.0000000

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 30.0000000

Leave Link 101 at Tue Aug 13 18:49:28 2019, MaxMem= 671088640 cpu: 0.7

(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) 1.4499 calculate D2E/DX2 analytically !

! R2 R(1,5) 1.363 calculate D2E/DX2 analytically !

! R3 R(1,49) 1.0791 calculate D2E/DX2 analytically !

! R4 R(2,3) 1.3699 calculate D2E/DX2 analytically !

! R5 R(2,12) 1.4118 calculate D2E/DX2 analytically !

! R6 R(3,4) 1.3699 calculate D2E/DX2 analytically !

! R7 R(3,77) 2.0907 calculate D2E/DX2 analytically !

! R8 R(4,5) 1.4499 calculate D2E/DX2 analytically !

! R9 R(4,6) 1.4118 calculate D2E/DX2 analytically !

! R10 R(5,50) 1.0791 calculate D2E/DX2 analytically !

! R11 R(6,7) 1.4118 calculate D2E/DX2 analytically !

! R12 R(6,25) 1.4935 calculate D2E/DX2 analytically !

! R13 R(7,8) 1.3699 calculate D2E/DX2 analytically !

! R14 R(7,11) 1.4499 calculate D2E/DX2 analytically !

! R15 R(8,9) 1.3699 calculate D2E/DX2 analytically !

! R16 R(8,77) 2.0907 calculate D2E/DX2 analytically !

! R17 R(9,10) 1.4499 calculate D2E/DX2 analytically !

! R18 R(9,24) 1.4118 calculate D2E/DX2 analytically !

! R19 R(10,11) 1.363 calculate D2E/DX2 analytically !

! R20 R(10,51) 1.0791 calculate D2E/DX2 analytically !

! R21 R(11,52) 1.0791 calculate D2E/DX2 analytically !

! R22 R(12,13) 1.4118 calculate D2E/DX2 analytically !

! R23 R(12,34) 1.4935 calculate D2E/DX2 analytically !

! R24 R(13,14) 1.4499 calculate D2E/DX2 analytically !

! R25 R(13,17) 1.3699 calculate D2E/DX2 analytically !

! R26 R(14,15) 1.363 calculate D2E/DX2 analytically !

! R27 R(14,53) 1.0791 calculate D2E/DX2 analytically !

! R28 R(15,16) 1.4499 calculate D2E/DX2 analytically !

! R29 R(15,54) 1.0791 calculate D2E/DX2 analytically !

! R30 R(16,17) 1.3699 calculate D2E/DX2 analytically !

! R31 R(16,18) 1.4118 calculate D2E/DX2 analytically !

! R32 R(17,77) 2.0907 calculate D2E/DX2 analytically !

! R33 R(18,19) 1.4118 calculate D2E/DX2 analytically !

! R34 R(18,43) 1.4935 calculate D2E/DX2 analytically !

! R35 R(19,20) 1.4499 calculate D2E/DX2 analytically !

! R36 R(19,23) 1.3699 calculate D2E/DX2 analytically !

! R37 R(20,21) 1.363 calculate D2E/DX2 analytically !

! R38 R(20,55) 1.0791 calculate D2E/DX2 analytically !

! R39 R(21,22) 1.4499 calculate D2E/DX2 analytically !

! R40 R(21,56) 1.0791 calculate D2E/DX2 analytically !

! R41 R(22,23) 1.3699 calculate D2E/DX2 analytically !

! R42 R(22,24) 1.4118 calculate D2E/DX2 analytically !

! R43 R(23,77) 2.0907 calculate D2E/DX2 analytically !

! R44 R(24,37) 1.4935 calculate D2E/DX2 analytically !

! R45 R(25,26) 1.4004 calculate D2E/DX2 analytically !

! R46 R(25,30) 1.4004 calculate D2E/DX2 analytically !

! R47 R(26,27) 1.3929 calculate D2E/DX2 analytically !

! R48 R(26,57) 1.0846 calculate D2E/DX2 analytically !

! R49 R(27,28) 1.3943 calculate D2E/DX2 analytically !

! R50 R(27,58) 1.0851 calculate D2E/DX2 analytically !

! R51 R(28,29) 1.3943 calculate D2E/DX2 analytically !

! R52 R(28,59) 1.085 calculate D2E/DX2 analytically !

! R53 R(29,30) 1.3929 calculate D2E/DX2 analytically !

! R54 R(29,60) 1.0851 calculate D2E/DX2 analytically !

! R55 R(30,61) 1.0846 calculate D2E/DX2 analytically !

! R56 R(31,32) 1.3943 calculate D2E/DX2 analytically !

! R57 R(31,36) 1.3943 calculate D2E/DX2 analytically !

! R58 R(31,62) 1.085 calculate D2E/DX2 analytically !

! R59 R(32,33) 1.3929 calculate D2E/DX2 analytically !

! R60 R(32,63) 1.0851 calculate D2E/DX2 analytically !

! R61 R(33,34) 1.4004 calculate D2E/DX2 analytically !

! R62 R(33,64) 1.0846 calculate D2E/DX2 analytically !

! R63 R(34,35) 1.4004 calculate D2E/DX2 analytically !

! R64 R(35,36) 1.3929 calculate D2E/DX2 analytically !

! R65 R(35,65) 1.0846 calculate D2E/DX2 analytically !

! R66 R(36,66) 1.0851 calculate D2E/DX2 analytically !

! R67 R(37,38) 1.4004 calculate D2E/DX2 analytically !

! R68 R(37,42) 1.4004 calculate D2E/DX2 analytically !

! R69 R(38,39) 1.3929 calculate D2E/DX2 analytically !

! R70 R(38,67) 1.0846 calculate D2E/DX2 analytically !

! R71 R(39,40) 1.3943 calculate D2E/DX2 analytically !

! R72 R(39,68) 1.0851 calculate D2E/DX2 analytically !

! R73 R(40,41) 1.3943 calculate D2E/DX2 analytically !

! R74 R(40,69) 1.085 calculate D2E/DX2 analytically !

! R75 R(41,42) 1.3929 calculate D2E/DX2 analytically !

! R76 R(41,70) 1.0851 calculate D2E/DX2 analytically !

! R77 R(42,71) 1.0846 calculate D2E/DX2 analytically !

! R78 R(43,44) 1.4004 calculate D2E/DX2 analytically !

! R79 R(43,48) 1.4004 calculate D2E/DX2 analytically !

! R80 R(44,45) 1.3929 calculate D2E/DX2 analytically !

! R81 R(44,72) 1.0846 calculate D2E/DX2 analytically !

! R82 R(45,46) 1.3943 calculate D2E/DX2 analytically !

! R83 R(45,73) 1.0851 calculate D2E/DX2 analytically !

! R84 R(46,47) 1.3943 calculate D2E/DX2 analytically !

! R85 R(46,74) 1.085 calculate D2E/DX2 analytically !

! R86 R(47,48) 1.3929 calculate D2E/DX2 analytically !

! R87 R(47,75) 1.0851 calculate D2E/DX2 analytically !

! R88 R(48,76) 1.0846 calculate D2E/DX2 analytically !

! A1 A(2,1,5) 107.2123 calculate D2E/DX2 analytically !

! A2 A(2,1,49) 125.7776 calculate D2E/DX2 analytically !

! A3 A(5,1,49) 127.001 calculate D2E/DX2 analytically !

! A4 A(1,2,3) 108.6225 calculate D2E/DX2 analytically !

! A5 A(1,2,12) 125.3442 calculate D2E/DX2 analytically !

! A6 A(3,2,12) 126.0283 calculate D2E/DX2 analytically !

! A7 A(2,3,4) 108.3234 calculate D2E/DX2 analytically !

! A8 A(2,3,77) 125.6646 calculate D2E/DX2 analytically !

! A9 A(4,3,77) 125.6646 calculate D2E/DX2 analytically !

! A10 A(3,4,5) 108.6225 calculate D2E/DX2 analytically !

! A11 A(3,4,6) 126.0283 calculate D2E/DX2 analytically !

! A12 A(5,4,6) 125.3442 calculate D2E/DX2 analytically !

! A13 A(1,5,4) 107.2123 calculate D2E/DX2 analytically !

! A14 A(1,5,50) 127.001 calculate D2E/DX2 analytically !

! A15 A(4,5,50) 125.7776 calculate D2E/DX2 analytically !

! A16 A(4,6,7) 126.1744 calculate D2E/DX2 analytically !

! A17 A(4,6,25) 116.9128 calculate D2E/DX2 analytically !

! A18 A(7,6,25) 116.9128 calculate D2E/DX2 analytically !

! A19 A(6,7,8) 126.0283 calculate D2E/DX2 analytically !

! A20 A(6,7,11) 125.3442 calculate D2E/DX2 analytically !

! A21 A(8,7,11) 108.6225 calculate D2E/DX2 analytically !

! A22 A(7,8,9) 108.3234 calculate D2E/DX2 analytically !

! A23 A(7,8,77) 125.6646 calculate D2E/DX2 analytically !

! A24 A(9,8,77) 125.6646 calculate D2E/DX2 analytically !

! A25 A(8,9,10) 108.6225 calculate D2E/DX2 analytically !

! A26 A(8,9,24) 126.0283 calculate D2E/DX2 analytically !

! A27 A(10,9,24) 125.3442 calculate D2E/DX2 analytically !

! A28 A(9,10,11) 107.2123 calculate D2E/DX2 analytically !

! A29 A(9,10,51) 125.7776 calculate D2E/DX2 analytically !

! A30 A(11,10,51) 127.001 calculate D2E/DX2 analytically !

! A31 A(7,11,10) 107.2123 calculate D2E/DX2 analytically !

! A32 A(7,11,52) 125.7776 calculate D2E/DX2 analytically !

! A33 A(10,11,52) 127.001 calculate D2E/DX2 analytically !

! A34 A(2,12,13) 126.1744 calculate D2E/DX2 analytically !

! A35 A(2,12,34) 116.9128 calculate D2E/DX2 analytically !

! A36 A(13,12,34) 116.9128 calculate D2E/DX2 analytically !

! A37 A(12,13,14) 125.3442 calculate D2E/DX2 analytically !

! A38 A(12,13,17) 126.0283 calculate D2E/DX2 analytically !

! A39 A(14,13,17) 108.6225 calculate D2E/DX2 analytically !

! A40 A(13,14,15) 107.2123 calculate D2E/DX2 analytically !

! A41 A(13,14,53) 125.7776 calculate D2E/DX2 analytically !

! A42 A(15,14,53) 127.001 calculate D2E/DX2 analytically !

! A43 A(14,15,16) 107.2123 calculate D2E/DX2 analytically !

! A44 A(14,15,54) 127.001 calculate D2E/DX2 analytically !

! A45 A(16,15,54) 125.7776 calculate D2E/DX2 analytically !

! A46 A(15,16,17) 108.6225 calculate D2E/DX2 analytically !

! A47 A(15,16,18) 125.3442 calculate D2E/DX2 analytically !

! A48 A(17,16,18) 126.0283 calculate D2E/DX2 analytically !

! A49 A(13,17,16) 108.3234 calculate D2E/DX2 analytically !

! A50 A(13,17,77) 125.6646 calculate D2E/DX2 analytically !

! A51 A(16,17,77) 125.6646 calculate D2E/DX2 analytically !

! A52 A(16,18,19) 126.1744 calculate D2E/DX2 analytically !

! A53 A(16,18,43) 116.9128 calculate D2E/DX2 analytically !

! A54 A(19,18,43) 116.9128 calculate D2E/DX2 analytically !

! A55 A(18,19,20) 125.3442 calculate D2E/DX2 analytically !

! A56 A(18,19,23) 126.0283 calculate D2E/DX2 analytically !

! A57 A(20,19,23) 108.6225 calculate D2E/DX2 analytically !

! A58 A(19,20,21) 107.2123 calculate D2E/DX2 analytically !

! A59 A(19,20,55) 125.7776 calculate D2E/DX2 analytically !

! A60 A(21,20,55) 127.001 calculate D2E/DX2 analytically !

! A61 A(20,21,22) 107.2123 calculate D2E/DX2 analytically !

! A62 A(20,21,56) 127.001 calculate D2E/DX2 analytically !

! A63 A(22,21,56) 125.7776 calculate D2E/DX2 analytically !

! A64 A(21,22,23) 108.6225 calculate D2E/DX2 analytically !

! A65 A(21,22,24) 125.3442 calculate D2E/DX2 analytically !

! A66 A(23,22,24) 126.0283 calculate D2E/DX2 analytically !

! A67 A(19,23,22) 108.3234 calculate D2E/DX2 analytically !

! A68 A(19,23,77) 125.6646 calculate D2E/DX2 analytically !

! A69 A(22,23,77) 125.6646 calculate D2E/DX2 analytically !

! A70 A(9,24,22) 126.1744 calculate D2E/DX2 analytically !

! A71 A(9,24,37) 116.9128 calculate D2E/DX2 analytically !

! A72 A(22,24,37) 116.9128 calculate D2E/DX2 analytically !

! A73 A(6,25,26) 120.6585 calculate D2E/DX2 analytically !

! A74 A(6,25,30) 120.6585 calculate D2E/DX2 analytically !

! A75 A(26,25,30) 118.6829 calculate D2E/DX2 analytically !

! A76 A(25,26,27) 120.6797 calculate D2E/DX2 analytically !

! A77 A(25,26,57) 119.3697 calculate D2E/DX2 analytically !

! A78 A(27,26,57) 119.9486 calculate D2E/DX2 analytically !

! A79 A(26,27,28) 120.163 calculate D2E/DX2 analytically !

! A80 A(26,27,58) 119.7006 calculate D2E/DX2 analytically !

! A81 A(28,27,58) 120.1361 calculate D2E/DX2 analytically !

! A82 A(27,28,29) 119.6312 calculate D2E/DX2 analytically !

! A83 A(27,28,59) 120.1844 calculate D2E/DX2 analytically !

! A84 A(29,28,59) 120.1844 calculate D2E/DX2 analytically !

! A85 A(28,29,30) 120.163 calculate D2E/DX2 analytically !

! A86 A(28,29,60) 120.1361 calculate D2E/DX2 analytically !

! A87 A(30,29,60) 119.7006 calculate D2E/DX2 analytically !

! A88 A(25,30,29) 120.6797 calculate D2E/DX2 analytically !

! A89 A(25,30,61) 119.3697 calculate D2E/DX2 analytically !

! A90 A(29,30,61) 119.9486 calculate D2E/DX2 analytically !

! A91 A(32,31,36) 119.6312 calculate D2E/DX2 analytically !

! A92 A(32,31,62) 120.1844 calculate D2E/DX2 analytically !

! A93 A(36,31,62) 120.1844 calculate D2E/DX2 analytically !

! A94 A(31,32,33) 120.163 calculate D2E/DX2 analytically !

! A95 A(31,32,63) 120.1361 calculate D2E/DX2 analytically !

! A96 A(33,32,63) 119.7006 calculate D2E/DX2 analytically !

! A97 A(32,33,34) 120.6797 calculate D2E/DX2 analytically !

! A98 A(32,33,64) 119.9486 calculate D2E/DX2 analytically !

! A99 A(34,33,64) 119.3697 calculate D2E/DX2 analytically !

! A100 A(12,34,33) 120.6585 calculate D2E/DX2 analytically !

! A101 A(12,34,35) 120.6585 calculate D2E/DX2 analytically !

! A102 A(33,34,35) 118.6829 calculate D2E/DX2 analytically !

! A103 A(34,35,36) 120.6797 calculate D2E/DX2 analytically !

! A104 A(34,35,65) 119.3697 calculate D2E/DX2 analytically !

! A105 A(36,35,65) 119.9486 calculate D2E/DX2 analytically !

! A106 A(31,36,35) 120.163 calculate D2E/DX2 analytically !

! A107 A(31,36,66) 120.1361 calculate D2E/DX2 analytically !

! A108 A(35,36,66) 119.7006 calculate D2E/DX2 analytically !

! A109 A(24,37,38) 120.6585 calculate D2E/DX2 analytically !

! A110 A(24,37,42) 120.6585 calculate D2E/DX2 analytically !

! A111 A(38,37,42) 118.6829 calculate D2E/DX2 analytically !

! A112 A(37,38,39) 120.6797 calculate D2E/DX2 analytically !

! A113 A(37,38,67) 119.3697 calculate D2E/DX2 analytically !

! A114 A(39,38,67) 119.9486 calculate D2E/DX2 analytically !

! A115 A(38,39,40) 120.163 calculate D2E/DX2 analytically !

! A116 A(38,39,68) 119.7006 calculate D2E/DX2 analytically !

! A117 A(40,39,68) 120.1361 calculate D2E/DX2 analytically !

! A118 A(39,40,41) 119.6312 calculate D2E/DX2 analytically !

! A119 A(39,40,69) 120.1844 calculate D2E/DX2 analytically !

! A120 A(41,40,69) 120.1844 calculate D2E/DX2 analytically !

! A121 A(40,41,42) 120.163 calculate D2E/DX2 analytically !

! A122 A(40,41,70) 120.1361 calculate D2E/DX2 analytically !

! A123 A(42,41,70) 119.7006 calculate D2E/DX2 analytically !

! A124 A(37,42,41) 120.6797 calculate D2E/DX2 analytically !

! A125 A(37,42,71) 119.3697 calculate D2E/DX2 analytically !

! A126 A(41,42,71) 119.9486 calculate D2E/DX2 analytically !

! A127 A(18,43,44) 120.6585 calculate D2E/DX2 analytically !

! A128 A(18,43,48) 120.6585 calculate D2E/DX2 analytically !

! A129 A(44,43,48) 118.6829 calculate D2E/DX2 analytically !

! A130 A(43,44,45) 120.6797 calculate D2E/DX2 analytically !

! A131 A(43,44,72) 119.3697 calculate D2E/DX2 analytically !

! A132 A(45,44,72) 119.9486 calculate D2E/DX2 analytically !

! A133 A(44,45,46) 120.163 calculate D2E/DX2 analytically !

! A134 A(44,45,73) 119.7006 calculate D2E/DX2 analytically !

! A135 A(46,45,73) 120.1361 calculate D2E/DX2 analytically !

! A136 A(45,46,47) 119.6312 calculate D2E/DX2 analytically !

! A137 A(45,46,74) 120.1844 calculate D2E/DX2 analytically !

! A138 A(47,46,74) 120.1844 calculate D2E/DX2 analytically !

! A139 A(46,47,48) 120.163 calculate D2E/DX2 analytically !

! A140 A(46,47,75) 120.1361 calculate D2E/DX2 analytically !

! A141 A(48,47,75) 119.7006 calculate D2E/DX2 analytically !

! A142 A(43,48,47) 120.6797 calculate D2E/DX2 analytically !

! A143 A(43,48,76) 119.3697 calculate D2E/DX2 analytically !

! A144 A(47,48,76) 119.9486 calculate D2E/DX2 analytically !

! A145 A(3,77,8) 90.0099 calculate D2E/DX2 analytically !

! A146 A(3,77,17) 90.0099 calculate D2E/DX2 analytically !

! A147 A(8,77,23) 90.0099 calculate D2E/DX2 analytically !

! A148 A(17,77,23) 90.0099 calculate D2E/DX2 analytically !

! A149 L(3,77,23,17,-1) 180.0198 calculate D2E/DX2 analytically !

! A150 L(8,77,17,23,-1) 180.0198 calculate D2E/DX2 analytically !

! A151 L(3,77,23,17,-2) 178.495 calculate D2E/DX2 analytically !

! A152 L(8,77,17,23,-2) 178.495 calculate D2E/DX2 analytically !

! D1 D(5,1,2,3) 0.5095 calculate D2E/DX2 analytically !

! D2 D(5,1,2,12) 179.7358 calculate D2E/DX2 analytically !

! D3 D(49,1,2,3) -178.4553 calculate D2E/DX2 analytically !

! D4 D(49,1,2,12) 0.771 calculate D2E/DX2 analytically !

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

! D6 D(2,1,5,50) -178.9484 calculate D2E/DX2 analytically !

! D7 D(49,1,5,4) 178.9484 calculate D2E/DX2 analytically !

! D8 D(49,1,5,50) 0.0 calculate D2E/DX2 analytically !

! D9 D(1,2,3,4) -0.8313 calculate D2E/DX2 analytically !

! D10 D(1,2,3,77) 172.6961 calculate D2E/DX2 analytically !

! D11 D(12,2,3,4) 179.9491 calculate D2E/DX2 analytically !

! D12 D(12,2,3,77) -6.5236 calculate D2E/DX2 analytically !

! D13 D(1,2,12,13) -175.5155 calculate D2E/DX2 analytically !

! D14 D(1,2,12,34) 4.4845 calculate D2E/DX2 analytically !

! D15 D(3,2,12,13) 3.5779 calculate D2E/DX2 analytically !

! D16 D(3,2,12,34) -176.4221 calculate D2E/DX2 analytically !

! D17 D(2,3,4,5) 0.8313 calculate D2E/DX2 analytically !

! D18 D(2,3,4,6) -179.9491 calculate D2E/DX2 analytically !

! D19 D(77,3,4,5) -172.6961 calculate D2E/DX2 analytically !

! D20 D(77,3,4,6) 6.5236 calculate D2E/DX2 analytically !

! D21 D(2,3,77,8) -175.4631 calculate D2E/DX2 analytically !

! D22 D(2,3,77,17) 3.0319 calculate D2E/DX2 analytically !

! D23 D(4,3,77,8) -3.0319 calculate D2E/DX2 analytically !

! D24 D(4,3,77,17) 175.4631 calculate D2E/DX2 analytically !

! D25 D(3,4,5,1) -0.5095 calculate D2E/DX2 analytically !

! D26 D(3,4,5,50) 178.4553 calculate D2E/DX2 analytically !

! D27 D(6,4,5,1) -179.7358 calculate D2E/DX2 analytically !

! D28 D(6,4,5,50) -0.771 calculate D2E/DX2 analytically !

! D29 D(3,4,6,7) -3.5779 calculate D2E/DX2 analytically !

! D30 D(3,4,6,25) 176.4221 calculate D2E/DX2 analytically !

! D31 D(5,4,6,7) 175.5155 calculate D2E/DX2 analytically !

! D32 D(5,4,6,25) -4.4845 calculate D2E/DX2 analytically !

! D33 D(4,6,7,8) -3.5779 calculate D2E/DX2 analytically !

! D34 D(4,6,7,11) 175.5155 calculate D2E/DX2 analytically !

! D35 D(25,6,7,8) 176.4221 calculate D2E/DX2 analytically !

! D36 D(25,6,7,11) -4.4845 calculate D2E/DX2 analytically !

! D37 D(4,6,25,26) -64.2296 calculate D2E/DX2 analytically !

! D38 D(4,6,25,30) 115.7704 calculate D2E/DX2 analytically !

! D39 D(7,6,25,26) 115.7704 calculate D2E/DX2 analytically !

! D40 D(7,6,25,30) -64.2296 calculate D2E/DX2 analytically !

! D41 D(6,7,8,9) -179.9491 calculate D2E/DX2 analytically !

! D42 D(6,7,8,77) 6.5236 calculate D2E/DX2 analytically !

! D43 D(11,7,8,9) 0.8313 calculate D2E/DX2 analytically !

! D44 D(11,7,8,77) -172.6961 calculate D2E/DX2 analytically !

! D45 D(6,7,11,10) -179.7358 calculate D2E/DX2 analytically !

! D46 D(6,7,11,52) -0.771 calculate D2E/DX2 analytically !

! D47 D(8,7,11,10) -0.5095 calculate D2E/DX2 analytically !

! D48 D(8,7,11,52) 178.4553 calculate D2E/DX2 analytically !

! D49 D(7,8,9,10) -0.8313 calculate D2E/DX2 analytically !

! D50 D(7,8,9,24) 179.9491 calculate D2E/DX2 analytically !

! D51 D(77,8,9,10) 172.6961 calculate D2E/DX2 analytically !

! D52 D(77,8,9,24) -6.5236 calculate D2E/DX2 analytically !

! D53 D(7,8,77,3) -3.0319 calculate D2E/DX2 analytically !

! D54 D(7,8,77,23) 175.4631 calculate D2E/DX2 analytically !

! D55 D(9,8,77,3) -175.4631 calculate D2E/DX2 analytically !

! D56 D(9,8,77,23) 3.0319 calculate D2E/DX2 analytically !

! D57 D(8,9,10,11) 0.5095 calculate D2E/DX2 analytically !

! D58 D(8,9,10,51) -178.4553 calculate D2E/DX2 analytically !

! D59 D(24,9,10,11) 179.7358 calculate D2E/DX2 analytically !

! D60 D(24,9,10,51) 0.771 calculate D2E/DX2 analytically !

! D61 D(8,9,24,22) 3.5779 calculate D2E/DX2 analytically !

! D62 D(8,9,24,37) -176.4221 calculate D2E/DX2 analytically !

! D63 D(10,9,24,22) -175.5155 calculate D2E/DX2 analytically !

! D64 D(10,9,24,37) 4.4845 calculate D2E/DX2 analytically !

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

! D66 D(9,10,11,52) -178.9484 calculate D2E/DX2 analytically !

! D67 D(51,10,11,7) 178.9484 calculate D2E/DX2 analytically !

! D68 D(51,10,11,52) 0.0 calculate D2E/DX2 analytically !

! D69 D(2,12,13,14) -175.5155 calculate D2E/DX2 analytically !

! D70 D(2,12,13,17) 3.5779 calculate D2E/DX2 analytically !

! D71 D(34,12,13,14) 4.4845 calculate D2E/DX2 analytically !

! D72 D(34,12,13,17) -176.4221 calculate D2E/DX2 analytically !

! D73 D(2,12,34,33) 64.2296 calculate D2E/DX2 analytically !

! D74 D(2,12,34,35) -115.7704 calculate D2E/DX2 analytically !

! D75 D(13,12,34,33) -115.7704 calculate D2E/DX2 analytically !

! D76 D(13,12,34,35) 64.2296 calculate D2E/DX2 analytically !

! D77 D(12,13,14,15) 179.7358 calculate D2E/DX2 analytically !

! D78 D(12,13,14,53) 0.771 calculate D2E/DX2 analytically !

! D79 D(17,13,14,15) 0.5095 calculate D2E/DX2 analytically !

! D80 D(17,13,14,53) -178.4553 calculate D2E/DX2 analytically !

! D81 D(12,13,17,16) 179.9491 calculate D2E/DX2 analytically !

! D82 D(12,13,17,77) -6.5236 calculate D2E/DX2 analytically !

! D83 D(14,13,17,16) -0.8313 calculate D2E/DX2 analytically !

! D84 D(14,13,17,77) 172.6961 calculate D2E/DX2 analytically !

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

! D86 D(13,14,15,54) -178.9484 calculate D2E/DX2 analytically !

! D87 D(53,14,15,16) 178.9484 calculate D2E/DX2 analytically !

! D88 D(53,14,15,54) 0.0 calculate D2E/DX2 analytically !

! D89 D(14,15,16,17) -0.5095 calculate D2E/DX2 analytically !

! D90 D(14,15,16,18) -179.7358 calculate D2E/DX2 analytically !

! D91 D(54,15,16,17) 178.4553 calculate D2E/DX2 analytically !

! D92 D(54,15,16,18) -0.771 calculate D2E/DX2 analytically !

! D93 D(15,16,17,13) 0.8313 calculate D2E/DX2 analytically !

! D94 D(15,16,17,77) -172.6961 calculate D2E/DX2 analytically !

! D95 D(18,16,17,13) -179.9491 calculate D2E/DX2 analytically !

! D96 D(18,16,17,77) 6.5236 calculate D2E/DX2 analytically !

! D97 D(15,16,18,19) 175.5155 calculate D2E/DX2 analytically !

! D98 D(15,16,18,43) -4.4845 calculate D2E/DX2 analytically !

! D99 D(17,16,18,19) -3.5779 calculate D2E/DX2 analytically !

! D100 D(17,16,18,43) 176.4221 calculate D2E/DX2 analytically !

! D101 D(13,17,77,3) 3.0319 calculate D2E/DX2 analytically !

! D102 D(13,17,77,23) -175.4631 calculate D2E/DX2 analytically !

! D103 D(16,17,77,3) 175.4631 calculate D2E/DX2 analytically !

! D104 D(16,17,77,23) -3.0319 calculate D2E/DX2 analytically !

! D105 D(16,18,19,20) 175.5155 calculate D2E/DX2 analytically !

! D106 D(16,18,19,23) -3.5779 calculate D2E/DX2 analytically !

! D107 D(43,18,19,20) -4.4845 calculate D2E/DX2 analytically !

! D108 D(43,18,19,23) 176.4221 calculate D2E/DX2 analytically !

! D109 D(16,18,43,44) -64.2296 calculate D2E/DX2 analytically !

! D110 D(16,18,43,48) 115.7704 calculate D2E/DX2 analytically !

! D111 D(19,18,43,44) 115.7704 calculate D2E/DX2 analytically !

! D112 D(19,18,43,48) -64.2296 calculate D2E/DX2 analytically !

! D113 D(18,19,20,21) -179.7358 calculate D2E/DX2 analytically !

! D114 D(18,19,20,55) -0.771 calculate D2E/DX2 analytically !

! D115 D(23,19,20,21) -0.5095 calculate D2E/DX2 analytically !

! D116 D(23,19,20,55) 178.4553 calculate D2E/DX2 analytically !

! D117 D(18,19,23,22) -179.9491 calculate D2E/DX2 analytically !

! D118 D(18,19,23,77) 6.5236 calculate D2E/DX2 analytically !

! D119 D(20,19,23,22) 0.8313 calculate D2E/DX2 analytically !

! D120 D(20,19,23,77) -172.6961 calculate D2E/DX2 analytically !

! D121 D(19,20,21,22) 0.0 calculate D2E/DX2 analytically !

! D122 D(19,20,21,56) 178.9484 calculate D2E/DX2 analytically !

! D123 D(55,20,21,22) -178.9484 calculate D2E/DX2 analytically !

! D124 D(55,20,21,56) 0.0 calculate D2E/DX2 analytically !

! D125 D(20,21,22,23) 0.5095 calculate D2E/DX2 analytically !

! D126 D(20,21,22,24) 179.7358 calculate D2E/DX2 analytically !

! D127 D(56,21,22,23) -178.4553 calculate D2E/DX2 analytically !

! D128 D(56,21,22,24) 0.771 calculate D2E/DX2 analytically !

! D129 D(21,22,23,19) -0.8313 calculate D2E/DX2 analytically !

! D130 D(21,22,23,77) 172.6961 calculate D2E/DX2 analytically !

! D131 D(24,22,23,19) 179.9491 calculate D2E/DX2 analytically !

! D132 D(24,22,23,77) -6.5236 calculate D2E/DX2 analytically !

! D133 D(21,22,24,9) -175.5155 calculate D2E/DX2 analytically !

! D134 D(21,22,24,37) 4.4845 calculate D2E/DX2 analytically !

! D135 D(23,22,24,9) 3.5779 calculate D2E/DX2 analytically !

! D136 D(23,22,24,37) -176.4221 calculate D2E/DX2 analytically !

! D137 D(19,23,77,8) 175.4631 calculate D2E/DX2 analytically !

! D138 D(19,23,77,17) -3.0319 calculate D2E/DX2 analytically !

! D139 D(22,23,77,8) 3.0319 calculate D2E/DX2 analytically !

! D140 D(22,23,77,17) -175.4631 calculate D2E/DX2 analytically !

! D141 D(9,24,37,38) 64.2296 calculate D2E/DX2 analytically !

! D142 D(9,24,37,42) -115.7704 calculate D2E/DX2 analytically !

! D143 D(22,24,37,38) -115.7704 calculate D2E/DX2 analytically !

! D144 D(22,24,37,42) 64.2296 calculate D2E/DX2 analytically !

! D145 D(6,25,26,27) -179.8953 calculate D2E/DX2 analytically !

! D146 D(6,25,26,57) -0.4155 calculate D2E/DX2 analytically !

! D147 D(30,25,26,27) 0.1047 calculate D2E/DX2 analytically !

! D148 D(30,25,26,57) 179.5845 calculate D2E/DX2 analytically !

! D149 D(6,25,30,29) -179.8953 calculate D2E/DX2 analytically !

! D150 D(6,25,30,61) -0.4155 calculate D2E/DX2 analytically !

! D151 D(26,25,30,29) 0.1047 calculate D2E/DX2 analytically !

! D152 D(26,25,30,61) 179.5845 calculate D2E/DX2 analytically !

! D153 D(25,26,27,28) -0.2097 calculate D2E/DX2 analytically !

! D154 D(25,26,27,58) 179.6276 calculate D2E/DX2 analytically !

! D155 D(57,26,27,28) -179.6865 calculate D2E/DX2 analytically !

! D156 D(57,26,27,58) 0.1508 calculate D2E/DX2 analytically !

! D157 D(26,27,28,29) 0.1041 calculate D2E/DX2 analytically !

! D158 D(26,27,28,59) -179.8959 calculate D2E/DX2 analytically !

! D159 D(58,27,28,29) -179.7325 calculate D2E/DX2 analytically !

! D160 D(58,27,28,59) 0.2675 calculate D2E/DX2 analytically !

! D161 D(27,28,29,30) 0.1041 calculate D2E/DX2 analytically !

! D162 D(27,28,29,60) -179.7325 calculate D2E/DX2 analytically !

! D163 D(59,28,29,30) -179.8959 calculate D2E/DX2 analytically !

! D164 D(59,28,29,60) 0.2675 calculate D2E/DX2 analytically !

! D165 D(28,29,30,25) -0.2097 calculate D2E/DX2 analytically !

! D166 D(28,29,30,61) -179.6865 calculate D2E/DX2 analytically !

! D167 D(60,29,30,25) 179.6276 calculate D2E/DX2 analytically !

! D168 D(60,29,30,61) 0.1508 calculate D2E/DX2 analytically !

! D169 D(36,31,32,33) -0.1041 calculate D2E/DX2 analytically !

! D170 D(36,31,32,63) 179.7325 calculate D2E/DX2 analytically !

! D171 D(62,31,32,33) 179.8959 calculate D2E/DX2 analytically !

! D172 D(62,31,32,63) -0.2675 calculate D2E/DX2 analytically !

! D173 D(32,31,36,35) -0.1041 calculate D2E/DX2 analytically !

! D174 D(32,31,36,66) 179.7325 calculate D2E/DX2 analytically !

! D175 D(62,31,36,35) 179.8959 calculate D2E/DX2 analytically !

! D176 D(62,31,36,66) -0.2675 calculate D2E/DX2 analytically !

! D177 D(31,32,33,34) 0.2097 calculate D2E/DX2 analytically !

! D178 D(31,32,33,64) 179.6865 calculate D2E/DX2 analytically !

! D179 D(63,32,33,34) -179.6276 calculate D2E/DX2 analytically !

! D180 D(63,32,33,64) -0.1508 calculate D2E/DX2 analytically !

! D181 D(32,33,34,12) 179.8953 calculate D2E/DX2 analytically !

! D182 D(32,33,34,35) -0.1047 calculate D2E/DX2 analytically !

! D183 D(64,33,34,12) 0.4155 calculate D2E/DX2 analytically !

! D184 D(64,33,34,35) -179.5845 calculate D2E/DX2 analytically !

! D185 D(12,34,35,36) 179.8953 calculate D2E/DX2 analytically !

! D186 D(12,34,35,65) 0.4155 calculate D2E/DX2 analytically !

! D187 D(33,34,35,36) -0.1047 calculate D2E/DX2 analytically !

! D188 D(33,34,35,65) -179.5845 calculate D2E/DX2 analytically !

! D189 D(34,35,36,31) 0.2097 calculate D2E/DX2 analytically !

! D190 D(34,35,36,66) -179.6276 calculate D2E/DX2 analytically !

! D191 D(65,35,36,31) 179.6865 calculate D2E/DX2 analytically !

! D192 D(65,35,36,66) -0.1508 calculate D2E/DX2 analytically !

! D193 D(24,37,38,39) 179.8953 calculate D2E/DX2 analytically !

! D194 D(24,37,38,67) 0.4155 calculate D2E/DX2 analytically !

! D195 D(42,37,38,39) -0.1047 calculate D2E/DX2 analytically !

! D196 D(42,37,38,67) -179.5845 calculate D2E/DX2 analytically !

! D197 D(24,37,42,41) 179.8953 calculate D2E/DX2 analytically !

! D198 D(24,37,42,71) 0.4155 calculate D2E/DX2 analytically !

! D199 D(38,37,42,41) -0.1047 calculate D2E/DX2 analytically !

! D200 D(38,37,42,71) -179.5845 calculate D2E/DX2 analytically !

! D201 D(37,38,39,40) 0.2097 calculate D2E/DX2 analytically !

! D202 D(37,38,39,68) -179.6276 calculate D2E/DX2 analytically !

! D203 D(67,38,39,40) 179.6865 calculate D2E/DX2 analytically !

! D204 D(67,38,39,68) -0.1508 calculate D2E/DX2 analytically !

! D205 D(38,39,40,41) -0.1041 calculate D2E/DX2 analytically !

! D206 D(38,39,40,69) 179.8959 calculate D2E/DX2 analytically !

! D207 D(68,39,40,41) 179.7325 calculate D2E/DX2 analytically !

! D208 D(68,39,40,69) -0.2675 calculate D2E/DX2 analytically !

! D209 D(39,40,41,42) -0.1041 calculate D2E/DX2 analytically !

! D210 D(39,40,41,70) 179.7325 calculate D2E/DX2 analytically !

! D211 D(69,40,41,42) 179.8959 calculate D2E/DX2 analytically !

! D212 D(69,40,41,70) -0.2675 calculate D2E/DX2 analytically !

! D213 D(40,41,42,37) 0.2097 calculate D2E/DX2 analytically !

! D214 D(40,41,42,71) 179.6865 calculate D2E/DX2 analytically !

! D215 D(70,41,42,37) -179.6276 calculate D2E/DX2 analytically !

! D216 D(70,41,42,71) -0.1508 calculate D2E/DX2 analytically !

! D217 D(18,43,44,45) -179.8953 calculate D2E/DX2 analytically !

! D218 D(18,43,44,72) -0.4155 calculate D2E/DX2 analytically !

! D219 D(48,43,44,45) 0.1047 calculate D2E/DX2 analytically !

! D220 D(48,43,44,72) 179.5845 calculate D2E/DX2 analytically !

! D221 D(18,43,48,47) -179.8953 calculate D2E/DX2 analytically !

! D222 D(18,43,48,76) -0.4155 calculate D2E/DX2 analytically !

! D223 D(44,43,48,47) 0.1047 calculate D2E/DX2 analytically !

! D224 D(44,43,48,76) 179.5845 calculate D2E/DX2 analytically !

! D225 D(43,44,45,46) -0.2097 calculate D2E/DX2 analytically !

! D226 D(43,44,45,73) 179.6276 calculate D2E/DX2 analytically !

! D227 D(72,44,45,46) -179.6865 calculate D2E/DX2 analytically !

! D228 D(72,44,45,73) 0.1508 calculate D2E/DX2 analytically !

! D229 D(44,45,46,47) 0.1041 calculate D2E/DX2 analytically !

! D230 D(44,45,46,74) -179.8959 calculate D2E/DX2 analytically !

! D231 D(73,45,46,47) -179.7325 calculate D2E/DX2 analytically !

! D232 D(73,45,46,74) 0.2675 calculate D2E/DX2 analytically !

! D233 D(45,46,47,48) 0.1041 calculate D2E/DX2 analytically !

! D234 D(45,46,47,75) -179.7325 calculate D2E/DX2 analytically !

! D235 D(74,46,47,48) -179.8959 calculate D2E/DX2 analytically !

! D236 D(74,46,47,75) 0.2675 calculate D2E/DX2 analytically !

! D237 D(46,47,48,43) -0.2097 calculate D2E/DX2 analytically !

! D238 D(46,47,48,76) -179.6865 calculate D2E/DX2 analytically !

! D239 D(75,47,48,43) 179.6276 calculate D2E/DX2 analytically !

! D240 D(75,47,48,76) 0.1508 calculate D2E/DX2 analytically !

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

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

Number of steps in this run= 2 maximum allowed number of steps= 2.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Aug 13 18:49:28 2019, MaxMem= 671088640 cpu: 0.1

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

Stoichiometry C44H28N4Zn

Framework group D2D[O(Zn),2SGD(N2),X(C44H28)]

Deg. of freedom 29

Full point group D2D NOp 8

RotChk: IX=0 Diff= 0.00D+00

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681484 4.269157 0.164086

2 6 0 -1.110541 2.890129 0.035503

3 7 0 0.000000 2.090529 -0.027459

4 6 0 1.110541 2.890129 0.035503

5 6 0 0.681484 4.269157 0.164086

6 6 0 2.452183 2.452183 0.000000

7 6 0 2.890129 1.110541 -0.035503

8 7 0 2.090529 -0.000000 0.027459

9 6 0 2.890129 -1.110541 -0.035503

10 6 0 4.269157 -0.681484 -0.164086

11 6 0 4.269157 0.681484 -0.164086

12 6 0 -2.452183 2.452183 0.000000

13 6 0 -2.890129 1.110541 -0.035503

14 6 0 -4.269157 0.681484 -0.164086

15 6 0 -4.269157 -0.681484 -0.164086

16 6 0 -2.890129 -1.110541 -0.035503

17 7 0 -2.090529 0.000000 0.027459

18 6 0 -2.452183 -2.452183 0.000000

19 6 0 -1.110541 -2.890129 0.035503

20 6 0 -0.681484 -4.269157 0.164086

21 6 0 0.681484 -4.269157 0.164086

22 6 0 1.110541 -2.890129 0.035503

23 7 0 -0.000000 -2.090529 -0.027459

24 6 0 2.452183 -2.452183 0.000000

25 6 0 3.508242 3.508242 -0.000000

26 6 0 3.621357 4.405038 -1.069674

27 6 0 4.607485 5.388753 -1.071137

28 6 0 5.493806 5.493806 0.000000

29 6 0 5.388753 4.607485 1.071137

30 6 0 4.405038 3.621357 1.069674

31 6 0 -5.493806 5.493806 0.000000

32 6 0 -4.607485 5.388753 -1.071137

33 6 0 -3.621357 4.405038 -1.069674

34 6 0 -3.508242 3.508242 -0.000000

35 6 0 -4.405038 3.621357 1.069674

36 6 0 -5.388753 4.607485 1.071137

37 6 0 3.508242 -3.508242 -0.000000

38 6 0 4.405038 -3.621357 1.069674

39 6 0 5.388753 -4.607485 1.071137

40 6 0 5.493806 -5.493806 0.000000

41 6 0 4.607485 -5.388753 -1.071137

42 6 0 3.621357 -4.405038 -1.069674

43 6 0 -3.508242 -3.508242 -0.000000

44 6 0 -4.405038 -3.621357 1.069674

45 6 0 -5.388753 -4.607485 1.071137

46 6 0 -5.493806 -5.493806 0.000000

47 6 0 -4.607485 -5.388753 -1.071137

48 6 0 -3.621357 -4.405038 -1.069674

49 1 0 -1.330917 5.125618 0.259828

50 1 0 1.330917 5.125618 0.259828

51 1 0 5.125618 -1.330917 -0.259828

52 1 0 5.125618 1.330917 -0.259828

53 1 0 -5.125618 1.330917 -0.259828

54 1 0 -5.125618 -1.330917 -0.259828

55 1 0 -1.330917 -5.125618 0.259828

56 1 0 1.330917 -5.125618 0.259828

57 1 0 2.936967 4.323214 -1.907040

58 1 0 4.684584 6.071446 -1.910980

59 1 0 6.260992 6.260992 0.000000

60 1 0 6.071446 4.684584 1.910980

61 1 0 4.323214 2.936967 1.907040

62 1 0 -6.260992 6.260992 0.000000

63 1 0 -4.684584 6.071446 -1.910980

64 1 0 -2.936967 4.323214 -1.907040

65 1 0 -4.323214 2.936967 1.907040

66 1 0 -6.071446 4.684584 1.910980

67 1 0 4.323214 -2.936967 1.907040

68 1 0 6.071446 -4.684584 1.910980

69 1 0 6.260992 -6.260992 0.000000

70 1 0 4.684584 -6.071446 -1.910980

71 1 0 2.936967 -4.323214 -1.907040

72 1 0 -4.323214 -2.936967 1.907040

73 1 0 -6.071446 -4.684584 1.910980

74 1 0 -6.260992 -6.260992 0.000000

75 1 0 -4.684584 -6.071446 -1.910980

76 1 0 -2.936967 -4.323214 -1.907040

77 30 0 0.000000 0.000000 0.000000

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

Rotational constants (GHZ): 0.0582110 0.0582110 0.0300828

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

Basis read from chk: "ZnTPP0.chk" (5D, 7F)

Pseudo-potential data read from chk file.

There are 272 symmetry adapted cartesian basis functions of A1 symmetry.

There are 243 symmetry adapted cartesian basis functions of A2 symmetry.

There are 254 symmetry adapted cartesian basis functions of B1 symmetry.

There are 254 symmetry adapted cartesian basis functions of B2 symmetry.

There are 256 symmetry adapted basis functions of A1 symmetry.

There are 232 symmetry adapted basis functions of A2 symmetry.

There are 242 symmetry adapted basis functions of B1 symmetry.

There are 242 symmetry adapted basis functions of B2 symmetry.

972 basis functions, 1715 primitive gaussians, 1023 cartesian basis functions

166 alpha electrons 166 beta electrons

nuclear repulsion energy 5738.4943395508 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= 77 NActive= 77 NUniq= 13 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T 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= -0.2224135280 Hartrees.

Nuclear repulsion after empirical dispersion term = 5738.2719260228 Hartrees.

No density basis found on file 20724.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 77.

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 = 77

GePol: Total number of spheres = 77

GePol: Number of exposed spheres = 77 (100.00%)

GePol: Number of points = 5690

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.75D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 272

GePol: Fraction of low-weight points (<1% of avg) = 4.78%

GePol: Cavity surface area = 614.366 Ang\*\*2

GePol: Cavity volume = 630.258 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021384217 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5738.2697876011 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

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36757 LenP2D= 95282.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 972 RedAO= T EigKep= 6.36D-05 NBF= 256 232 242 242

NBsUse= 972 1.00D-06 EigRej= -1.00D+00 NBFU= 256 232 242 242

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= 952 960 976 976 976 MxSgAt= 77 MxSgA2= 77.

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Aug 13 18:49:31 2019, MaxMem= 671088640 cpu: 0.9

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

Initial guess from the checkpoint file: "ZnTPP0.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 -0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

Leave Link 401 at Tue Aug 13 18:49:35 2019, MaxMem= 671088640 cpu: 15.6

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3177123 IEndB= 3177123 NGot= 671088640 MDV= 668975710

LenX= 668975710 LenY= 667928158

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= 530000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 97128300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.66D-15 for 1281.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.00D-15 for 5674 1282.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.22D-15 for 5676.

Iteration 1 A^-1\*A deviation from orthogonality is 5.52D-12 for 3424 3414.

E= -1978.90435337865

DIIS: error= 5.39D-08 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1978.90435337865 IErMin= 1 ErrMin= 5.39D-08

ErrMax= 5.39D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.10D-12 BMatP= 2.10D-12

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

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=3.02D-09 MaxDP=1.87D-07 OVMax= 6.28D-07

Error on total polarization charges = 0.08494

SCF Done: E(RB3LYP) = -1978.90435338 A.U. after 1 cycles

NFock= 1 Conv=0.30D-08 -V/T= 1.9793

KE= 2.020706256559D+03 PE=-1.615865200707D+04 EE= 6.420771609527D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.34

(included in total energy above)

Leave Link 502 at Tue Aug 13 18:51:27 2019, MaxMem= 671088640 cpu: 447.0

(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: 1 972

NBasis= 972 NAE= 166 NBE= 166 NFC= 0 NFV= 0

NROrb= 972 NOA= 166 NOB= 166 NVA= 806 NVB= 806

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.98725107D-01

Leave Link 801 at Tue Aug 13 18:51:27 2019, MaxMem= 671088640 cpu: 0.2

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

Using compressed storage, NAtomX= 77.

Will process 78 centers per pass.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36757 LenP2D= 95282.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 2 by ecpmxn.

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

Leave Link 1101 at Tue Aug 13 18:51:43 2019, MaxMem= 671088640 cpu: 60.9

(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 Aug 13 18:51:43 2019, MaxMem= 671088640 cpu: 0.7

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

Forming Gx(P) for the SCF density, NAtomX= 77.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 671087920.

G2DrvN: will do 78 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= 2000

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

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

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

Petite list used in FoFCou.

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

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

GePol: Maximum number of non-zero 1st derivatives = 182

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 Aug 13 19:05:58 2019, MaxMem= 671088640 cpu: 3417.2

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

Minotr: Closed shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=111111111111111111111111111

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= 671086894 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 72.

FoF2E skips out because all densities are zero.

CalDSu exits because no D1Ps are significant.

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

IRaf= 630000000 NMat= 39 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

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

42 vectors produced by pass 0 Test12= 3.19D-13 2.38D-09 XBig12= 2.45D+03 3.32D+01.

AX will form 42 AO Fock derivatives at one time.

42 vectors produced by pass 1 Test12= 3.19D-13 2.38D-09 XBig12= 4.23D+02 3.61D+00.

42 vectors produced by pass 2 Test12= 3.19D-13 2.38D-09 XBig12= 6.43D+01 1.51D+00.

42 vectors produced by pass 3 Test12= 3.19D-13 2.38D-09 XBig12= 2.21D+01 6.44D-01.

42 vectors produced by pass 4 Test12= 3.19D-13 2.38D-09 XBig12= 2.52D+00 1.44D-01.

42 vectors produced by pass 5 Test12= 3.19D-13 2.38D-09 XBig12= 2.75D-01 4.66D-02.

42 vectors produced by pass 6 Test12= 3.19D-13 2.38D-09 XBig12= 8.44D-03 9.19D-03.

37 vectors produced by pass 7 Test12= 3.19D-13 2.38D-09 XBig12= 1.53D-04 1.15D-03.

25 vectors produced by pass 8 Test12= 3.19D-13 2.38D-09 XBig12= 2.59D-06 1.23D-04.

15 vectors produced by pass 9 Test12= 3.19D-13 2.38D-09 XBig12= 4.07D-08 1.77D-05.

4 vectors produced by pass 10 Test12= 3.19D-13 2.38D-09 XBig12= 5.32D-10 1.65D-06.

3 vectors produced by pass 11 Test12= 3.19D-13 2.38D-09 XBig12= 9.69D-12 2.59D-07.

2 vectors produced by pass 12 Test12= 3.19D-13 2.38D-09 XBig12= 1.91D-13 2.72D-08.

2 vectors produced by pass 13 Test12= 3.19D-13 2.38D-09 XBig12= 6.11D-15 4.10D-09.

InvSVY: IOpt=1 It= 1 EMax= 1.78D-14

Solved reduced A of dimension 382 with 42 vectors.

FullF1: Do perturbations 1 to 42.

Isotropic polarizability for W= 0.000000 1107.83 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 Aug 13 21:55:19 2019, MaxMem= 671088640 cpu: 40621.7

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

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

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

Population analysis using the SCF density.

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

Orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The electronic state is 1-A1.

Alpha occ. eigenvalues -- -14.30274 -14.30274 -14.30273 -14.30273 -10.20850

Alpha occ. eigenvalues -- -10.20850 -10.20850 -10.20850 -10.20849 -10.20849

Alpha occ. eigenvalues -- -10.20849 -10.20849 -10.19527 -10.19527 -10.19527

Alpha occ. eigenvalues -- -10.19527 -10.18649 -10.18649 -10.18649 -10.18649

Alpha occ. eigenvalues -- -10.17325 -10.17325 -10.17325 -10.17325 -10.17325

Alpha occ. eigenvalues -- -10.17325 -10.17325 -10.17325 -10.17283 -10.17283

Alpha occ. eigenvalues -- -10.17283 -10.17283 -10.17252 -10.17252 -10.17252

Alpha occ. eigenvalues -- -10.17252 -10.17215 -10.17215 -10.17215 -10.17215

Alpha occ. eigenvalues -- -10.16829 -10.16829 -10.16829 -10.16829 -10.16763

Alpha occ. eigenvalues -- -10.16763 -10.16763 -10.16763 -0.96311 -0.95466

Alpha occ. eigenvalues -- -0.95466 -0.94579 -0.86920 -0.86555 -0.86555

Alpha occ. eigenvalues -- -0.86379 -0.82290 -0.80635 -0.80635 -0.78864

Alpha occ. eigenvalues -- -0.76631 -0.76592 -0.76592 -0.76144 -0.74941

Alpha occ. eigenvalues -- -0.74862 -0.74862 -0.74828 -0.74123 -0.73406

Alpha occ. eigenvalues -- -0.73406 -0.71852 -0.70867 -0.66163 -0.66163

Alpha occ. eigenvalues -- -0.62134 -0.61068 -0.60823 -0.60823 -0.60677

Alpha occ. eigenvalues -- -0.59897 -0.59897 -0.59468 -0.59445 -0.58587

Alpha occ. eigenvalues -- -0.57012 -0.56547 -0.56261 -0.56261 -0.56057

Alpha occ. eigenvalues -- -0.55332 -0.55332 -0.54829 -0.54320 -0.52699

Alpha occ. eigenvalues -- -0.52699 -0.52628 -0.51909 -0.51398 -0.51398

Alpha occ. eigenvalues -- -0.49894 -0.49806 -0.49165 -0.49165 -0.46156

Alpha occ. eigenvalues -- -0.46073 -0.45862 -0.45731 -0.45731 -0.44985

Alpha occ. eigenvalues -- -0.44985 -0.44864 -0.44341 -0.42569 -0.42546

Alpha occ. eigenvalues -- -0.42305 -0.42305 -0.42195 -0.42155 -0.42155

Alpha occ. eigenvalues -- -0.42129 -0.41797 -0.41216 -0.40818 -0.40818

Alpha occ. eigenvalues -- -0.40139 -0.40139 -0.39299 -0.39066 -0.38439

Alpha occ. eigenvalues -- -0.38303 -0.37820 -0.37820 -0.36828 -0.36767

Alpha occ. eigenvalues -- -0.36708 -0.36708 -0.35813 -0.35163 -0.34764

Alpha occ. eigenvalues -- -0.34695 -0.34695 -0.34605 -0.34599 -0.34599

Alpha occ. eigenvalues -- -0.33902 -0.31871 -0.31301 -0.31301 -0.28611

Alpha occ. eigenvalues -- -0.28611 -0.26425 -0.26019 -0.25991 -0.25945

Alpha occ. eigenvalues -- -0.25930 -0.25930 -0.25682 -0.25255 -0.25238

Alpha occ. eigenvalues -- -0.25238 -0.24717 -0.24717 -0.24647 -0.20184

Alpha occ. eigenvalues -- -0.18937

Alpha virt. eigenvalues -- -0.09064 -0.09064 -0.03556 -0.01361 -0.01316

Alpha virt. eigenvalues -- -0.01316 -0.01116 -0.01041 -0.01029 -0.00930

Alpha virt. eigenvalues -- -0.00930 0.03358 0.03798 0.04518 0.04646

Alpha virt. eigenvalues -- 0.04646 0.05596 0.05596 0.05822 0.06119

Alpha virt. eigenvalues -- 0.07000 0.07000 0.07197 0.08446 0.08983

Alpha virt. eigenvalues -- 0.08983 0.09147 0.09179 0.09557 0.09557

Alpha virt. eigenvalues -- 0.10009 0.10277 0.10339 0.10376 0.11364

Alpha virt. eigenvalues -- 0.11364 0.11918 0.11918 0.12037 0.12647

Alpha virt. eigenvalues -- 0.13045 0.13045 0.13326 0.13423 0.13695

Alpha virt. eigenvalues -- 0.13695 0.13809 0.14078 0.14170 0.14728

Alpha virt. eigenvalues -- 0.15121 0.15121 0.15773 0.15773 0.16274

Alpha virt. eigenvalues -- 0.16461 0.18510 0.18510 0.20796 0.21632

Alpha virt. eigenvalues -- 0.22463 0.23766 0.23766 0.23814 0.23862

Alpha virt. eigenvalues -- 0.24494 0.25350 0.25688 0.25688 0.26612

Alpha virt. eigenvalues -- 0.26946 0.26946 0.27152 0.27581 0.28038

Alpha virt. eigenvalues -- 0.28054 0.28054 0.28372 0.28519 0.28519

Alpha virt. eigenvalues -- 0.28918 0.29009 0.29009 0.29010 0.29992

Alpha virt. eigenvalues -- 0.29992 0.30039 0.30049 0.30669 0.31413

Alpha virt. eigenvalues -- 0.31413 0.31596 0.32476 0.34392 0.35120

Alpha virt. eigenvalues -- 0.35359 0.35359 0.35508 0.36081 0.36081

Alpha virt. eigenvalues -- 0.36373 0.36473 0.36753 0.36753 0.36852

Alpha virt. eigenvalues -- 0.36852 0.37487 0.37665 0.38134 0.38779

Alpha virt. eigenvalues -- 0.38849 0.39795 0.39795 0.39797 0.39867

Alpha virt. eigenvalues -- 0.39867 0.40128 0.40540 0.40793 0.41155

Alpha virt. eigenvalues -- 0.41200 0.41200 0.41478 0.41535 0.41535

Alpha virt. eigenvalues -- 0.41912 0.41955 0.41990 0.41990 0.42349

Alpha virt. eigenvalues -- 0.42980 0.42980 0.43152 0.43431 0.43431

Alpha virt. eigenvalues -- 0.43723 0.43879 0.44575 0.44575 0.44601

Alpha virt. eigenvalues -- 0.44829 0.45046 0.45147 0.45219 0.45219

Alpha virt. eigenvalues -- 0.45518 0.46539 0.46539 0.46774 0.46774

Alpha virt. eigenvalues -- 0.46835 0.47207 0.47595 0.48416 0.48416

Alpha virt. eigenvalues -- 0.48766 0.48766 0.49664 0.49664 0.49995

Alpha virt. eigenvalues -- 0.49999 0.50136 0.51020 0.51114 0.51349

Alpha virt. eigenvalues -- 0.51782 0.52598 0.52598 0.53594 0.53594

Alpha virt. eigenvalues -- 0.53679 0.54246 0.54246 0.54286 0.54884

Alpha virt. eigenvalues -- 0.55960 0.56631 0.57532 0.57677 0.57677

Alpha virt. eigenvalues -- 0.57715 0.57900 0.58626 0.58626 0.59659

Alpha virt. eigenvalues -- 0.59659 0.60331 0.60460 0.60602 0.60839

Alpha virt. eigenvalues -- 0.60839 0.61152 0.61323 0.61323 0.61386

Alpha virt. eigenvalues -- 0.61510 0.61516 0.61657 0.61657 0.62106

Alpha virt. eigenvalues -- 0.62516 0.62617 0.62617 0.62762 0.63648

Alpha virt. eigenvalues -- 0.63898 0.63898 0.64424 0.64555 0.64836

Alpha virt. eigenvalues -- 0.64836 0.65153 0.65227 0.65335 0.65437

Alpha virt. eigenvalues -- 0.65437 0.65564 0.66823 0.66823 0.66881

Alpha virt. eigenvalues -- 0.67116 0.67968 0.67968 0.68150 0.69635

Alpha virt. eigenvalues -- 0.69635 0.70395 0.70711 0.72180 0.72180

Alpha virt. eigenvalues -- 0.72611 0.72611 0.72694 0.73045 0.73289

Alpha virt. eigenvalues -- 0.73760 0.73787 0.73787 0.74429 0.74493

Alpha virt. eigenvalues -- 0.75337 0.75337 0.75723 0.75848 0.75848

Alpha virt. eigenvalues -- 0.75952 0.76469 0.76469 0.77006 0.78250

Alpha virt. eigenvalues -- 0.78260 0.78869 0.78869 0.79700 0.79743

Alpha virt. eigenvalues -- 0.79990 0.80537 0.80537 0.81093 0.81093

Alpha virt. eigenvalues -- 0.81419 0.81953 0.82369 0.82664 0.82664

Alpha virt. eigenvalues -- 0.84132 0.84615 0.85250 0.85250 0.85690

Alpha virt. eigenvalues -- 0.85794 0.87013 0.87285 0.87285 0.87399

Alpha virt. eigenvalues -- 0.89301 0.89301 0.89302 0.89497 0.90001

Alpha virt. eigenvalues -- 0.90001 0.90117 0.91772 0.92560 0.92684

Alpha virt. eigenvalues -- 0.92684 0.93361 0.93558 0.94473 0.94473

Alpha virt. eigenvalues -- 0.94991 0.96109 0.96620 0.96788 0.96788

Alpha virt. eigenvalues -- 0.98372 0.99146 0.99146 1.00407 1.00505

Alpha virt. eigenvalues -- 1.01503 1.01503 1.02404 1.02469 1.02827

Alpha virt. eigenvalues -- 1.04412 1.04412 1.05228 1.05228 1.05341

Alpha virt. eigenvalues -- 1.05453 1.05932 1.07581 1.08591 1.09226

Alpha virt. eigenvalues -- 1.09226 1.09719 1.11356 1.11356 1.11644

Alpha virt. eigenvalues -- 1.12557 1.13167 1.13167 1.14992 1.14992

Alpha virt. eigenvalues -- 1.15230 1.15462 1.15462 1.16885 1.17514

Alpha virt. eigenvalues -- 1.17514 1.17633 1.17633 1.17867 1.18328

Alpha virt. eigenvalues -- 1.19469 1.20497 1.20497 1.20958 1.21019

Alpha virt. eigenvalues -- 1.21094 1.21438 1.21438 1.21749 1.21749

Alpha virt. eigenvalues -- 1.22277 1.22828 1.22971 1.23975 1.24161

Alpha virt. eigenvalues -- 1.24161 1.24766 1.24766 1.25277 1.25325

Alpha virt. eigenvalues -- 1.25676 1.26445 1.27012 1.27012 1.27775

Alpha virt. eigenvalues -- 1.28532 1.28532 1.28827 1.30246 1.31486

Alpha virt. eigenvalues -- 1.31806 1.32636 1.32636 1.37143 1.38171

Alpha virt. eigenvalues -- 1.38595 1.38595 1.40391 1.40391 1.41032

Alpha virt. eigenvalues -- 1.41255 1.41741 1.43969 1.43969 1.44475

Alpha virt. eigenvalues -- 1.45941 1.47242 1.47242 1.47706 1.47723

Alpha virt. eigenvalues -- 1.48059 1.48534 1.48534 1.48539 1.49294

Alpha virt. eigenvalues -- 1.49994 1.49994 1.50305 1.50690 1.52899

Alpha virt. eigenvalues -- 1.52899 1.53718 1.54174 1.54451 1.54451

Alpha virt. eigenvalues -- 1.55548 1.55548 1.55715 1.56727 1.56727

Alpha virt. eigenvalues -- 1.57149 1.58563 1.59949 1.61260 1.61260

Alpha virt. eigenvalues -- 1.61460 1.61682 1.62535 1.62535 1.64836

Alpha virt. eigenvalues -- 1.64836 1.65259 1.67334 1.68458 1.68666

Alpha virt. eigenvalues -- 1.68666 1.68773 1.70139 1.70207 1.70207

Alpha virt. eigenvalues -- 1.71110 1.71110 1.71694 1.73965 1.74279

Alpha virt. eigenvalues -- 1.74716 1.76064 1.76064 1.76158 1.76287

Alpha virt. eigenvalues -- 1.76357 1.76357 1.77480 1.77480 1.77707

Alpha virt. eigenvalues -- 1.79010 1.79082 1.79905 1.80586 1.80586

Alpha virt. eigenvalues -- 1.81095 1.81289 1.81399 1.81830 1.81830

Alpha virt. eigenvalues -- 1.83685 1.83685 1.84124 1.84128 1.84558

Alpha virt. eigenvalues -- 1.84787 1.85072 1.85222 1.85222 1.86524

Alpha virt. eigenvalues -- 1.87566 1.87566 1.88657 1.88870 1.88870

Alpha virt. eigenvalues -- 1.89088 1.89660 1.89981 1.91737 1.91971

Alpha virt. eigenvalues -- 1.91971 1.92211 1.92565 1.92713 1.92785

Alpha virt. eigenvalues -- 1.92785 1.93158 1.93232 1.93232 1.94017

Alpha virt. eigenvalues -- 1.94080 1.94121 1.94121 1.94591 1.96178

Alpha virt. eigenvalues -- 1.96407 1.96407 1.96689 1.96971 1.96971

Alpha virt. eigenvalues -- 1.98495 1.99902 1.99997 1.99997 2.00083

Alpha virt. eigenvalues -- 2.00213 2.00556 2.00556 2.01260 2.06900

Alpha virt. eigenvalues -- 2.07144 2.08170 2.08170 2.09100 2.09100

Alpha virt. eigenvalues -- 2.09104 2.11700 2.13063 2.13904 2.14304

Alpha virt. eigenvalues -- 2.14304 2.19160 2.22089 2.23720 2.24110

Alpha virt. eigenvalues -- 2.24110 2.25803 2.25876 2.25876 2.26301

Alpha virt. eigenvalues -- 2.26583 2.26836 2.27625 2.27625 2.27835

Alpha virt. eigenvalues -- 2.28125 2.28341 2.28341 2.28682 2.29592

Alpha virt. eigenvalues -- 2.29592 2.29659 2.29877 2.30520 2.30520

Alpha virt. eigenvalues -- 2.32006 2.32115 2.32445 2.33142 2.33142

Alpha virt. eigenvalues -- 2.33973 2.33973 2.35654 2.35762 2.36440

Alpha virt. eigenvalues -- 2.36729 2.36729 2.36832 2.38526 2.38738

Alpha virt. eigenvalues -- 2.39662 2.39662 2.40442 2.40442 2.40919

Alpha virt. eigenvalues -- 2.44253 2.44865 2.44865 2.44970 2.47256

Alpha virt. eigenvalues -- 2.47341 2.49851 2.49851 2.53871 2.54681

Alpha virt. eigenvalues -- 2.54681 2.54903 2.55451 2.57018 2.57718

Alpha virt. eigenvalues -- 2.57972 2.57972 2.59297 2.59374 2.59374

Alpha virt. eigenvalues -- 2.60402 2.61072 2.61072 2.62117 2.62454

Alpha virt. eigenvalues -- 2.62674 2.62770 2.64559 2.64559 2.65206

Alpha virt. eigenvalues -- 2.65206 2.65617 2.65620 2.68503 2.69773

Alpha virt. eigenvalues -- 2.70071 2.70071 2.70289 2.72767 2.72767

Alpha virt. eigenvalues -- 2.73257 2.74889 2.74889 2.75016 2.75043

Alpha virt. eigenvalues -- 2.77012 2.77012 2.78467 2.78610 2.79432

Alpha virt. eigenvalues -- 2.79445 2.79445 2.80399 2.80679 2.82656

Alpha virt. eigenvalues -- 2.82656 2.84183 2.84843 2.85481 2.85481

Alpha virt. eigenvalues -- 2.85969 2.87050 2.89784 2.89784 2.90173

Alpha virt. eigenvalues -- 2.90173 2.90673 2.92973 2.94116 2.95892

Alpha virt. eigenvalues -- 2.95892 2.96850 2.98852 2.98852 2.99046

Alpha virt. eigenvalues -- 2.99721 3.01290 3.02782 3.04316 3.04877

Alpha virt. eigenvalues -- 3.04877 3.06540 3.07481 3.07481 3.07582

Alpha virt. eigenvalues -- 3.08395 3.08395 3.09188 3.11350 3.11687

Alpha virt. eigenvalues -- 3.11860 3.12217 3.12217 3.14525 3.16838

Alpha virt. eigenvalues -- 3.16838 3.16849 3.19546 3.19619 3.19619

Alpha virt. eigenvalues -- 3.19736 3.22486 3.25834 3.25947 3.25947

Alpha virt. eigenvalues -- 3.26087 3.26816 3.26816 3.29255 3.29591

Alpha virt. eigenvalues -- 3.29591 3.29856 3.29976 3.29996 3.30214

Alpha virt. eigenvalues -- 3.30214 3.30436 3.31091 3.31193 3.31272

Alpha virt. eigenvalues -- 3.31272 3.31847 3.32135 3.34686 3.34686

Alpha virt. eigenvalues -- 3.34715 3.35837 3.35837 3.36785 3.38248

Alpha virt. eigenvalues -- 3.38248 3.39729 3.40864 3.42407 3.43091

Alpha virt. eigenvalues -- 3.43091 3.44709 3.50363 3.51898 3.51956

Alpha virt. eigenvalues -- 3.51956 3.56786 3.58143 3.58143 3.58602

Alpha virt. eigenvalues -- 3.58602 3.59419 3.59738 3.61534 3.62677

Alpha virt. eigenvalues -- 3.66704 3.67307 3.67307 3.72803 3.73568

Alpha virt. eigenvalues -- 3.75788 3.75788 3.82769 3.82769 3.82872

Alpha virt. eigenvalues -- 3.85007 3.87457 3.87457 3.89144 3.91616

Alpha virt. eigenvalues -- 3.93980 3.93980 3.95111 3.95447 3.96267

Alpha virt. eigenvalues -- 3.96313 3.96313 3.96391 3.99534 4.01085

Alpha virt. eigenvalues -- 4.01085 4.12026 4.33381 4.35441 4.40178

Alpha virt. eigenvalues -- 4.40178 4.46726 4.49709 4.54091 4.54091

Alpha virt. eigenvalues -- 4.61897 4.66888 4.66888 4.67840 4.78821

Alpha virt. eigenvalues -- 4.78831 4.78831 4.78841 5.11536 5.18916

Alpha virt. eigenvalues -- 5.18916 5.32589 7.77675 7.77675 7.88025

Alpha virt. eigenvalues -- 7.92778 8.13982 11.12048 23.25291 23.28974

Alpha virt. eigenvalues -- 23.28974 23.30653 23.46368 23.53063 23.53063

Alpha virt. eigenvalues -- 23.57714 23.74795 23.75935 23.75935 23.77727

Alpha virt. eigenvalues -- 23.81067 23.81232 23.81232 23.81492 23.85161

Alpha virt. eigenvalues -- 23.86126 23.86126 23.86887 23.92662 23.94755

Alpha virt. eigenvalues -- 23.94755 23.96993 23.98200 23.99159 23.99159

Alpha virt. eigenvalues -- 23.99221 24.04793 24.04950 24.04950 24.05134

Alpha virt. eigenvalues -- 24.08773 24.09280 24.09280 24.09729 24.13357

Alpha virt. eigenvalues -- 24.13718 24.13718 24.14423 24.16343 24.16382

Alpha virt. eigenvalues -- 24.16382 24.16394 35.63343 35.64463 35.66095

Alpha virt. eigenvalues -- 35.66095

Condensed to atoms (all electrons):

Mulliken charges:

1

1 C -0.261141

2 C 0.308668

3 N -0.706255

4 C 0.308668

5 C -0.261141

6 C -0.149009

7 C 0.308668

8 N -0.706255

9 C 0.308668

10 C -0.261141

11 C -0.261141

12 C -0.149009

13 C 0.308668

14 C -0.261141

15 C -0.261141

16 C 0.308668

17 N -0.706255

18 C -0.149009

19 C 0.308668

20 C -0.261141

21 C -0.261141

22 C 0.308668

23 N -0.706255

24 C -0.149009

25 C -0.105849

26 C -0.211896

27 C -0.217880

28 C -0.221702

29 C -0.217880

30 C -0.211896

31 C -0.221702

32 C -0.217880

33 C -0.211896

34 C -0.105849

35 C -0.211896

36 C -0.217880

37 C -0.105849

38 C -0.211896

39 C -0.217880

40 C -0.221702

41 C -0.217880

42 C -0.211896

43 C -0.105849

44 C -0.211896

45 C -0.217880

46 C -0.221702

47 C -0.217880

48 C -0.211896

49 H 0.239146

50 H 0.239146

51 H 0.239146

52 H 0.239146

53 H 0.239146

54 H 0.239146

55 H 0.239146

56 H 0.239146

57 H 0.224238

58 H 0.225860

59 H 0.225720

60 H 0.225860

61 H 0.224238

62 H 0.225720

63 H 0.225860

64 H 0.224238

65 H 0.224238

66 H 0.225860

67 H 0.224238

68 H 0.225860

69 H 0.225720

70 H 0.225860

71 H 0.224238

72 H 0.224238

73 H 0.225860

74 H 0.225720

75 H 0.225860

76 H 0.224238

77 Zn 1.372415

Sum of Mulliken charges = -0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 C -0.021995

2 C 0.308668

3 N -0.706255

4 C 0.308668

5 C -0.021995

6 C -0.149009

7 C 0.308668

8 N -0.706255

9 C 0.308668

10 C -0.021995

11 C -0.021995

12 C -0.149009

13 C 0.308668

14 C -0.021995

15 C -0.021995

16 C 0.308668

17 N -0.706255

18 C -0.149009

19 C 0.308668

20 C -0.021995

21 C -0.021995

22 C 0.308668

23 N -0.706255

24 C -0.149009

25 C -0.105849

26 C 0.012343

27 C 0.007980

28 C 0.004018

29 C 0.007980

30 C 0.012343

31 C 0.004018

32 C 0.007980

33 C 0.012343

34 C -0.105849

35 C 0.012343

36 C 0.007980

37 C -0.105849

38 C 0.012343

39 C 0.007980

40 C 0.004018

41 C 0.007980

42 C 0.012343

43 C -0.105849

44 C 0.012343

45 C 0.007980

46 C 0.004018

47 C 0.007980

48 C 0.012343

77 Zn 1.372415

APT charges:

1

1 C 0.113242

2 C -0.057392

3 N -0.738732

4 C -0.057392

5 C 0.113242

6 C 0.188377

7 C -0.057392

8 N -0.738732

9 C -0.057391

10 C 0.113241

11 C 0.113242

12 C 0.188377

13 C -0.057392

14 C 0.113242

15 C 0.113242

16 C -0.057392

17 N -0.738732

18 C 0.188377

19 C -0.057392

20 C 0.113241

21 C 0.113242

22 C -0.057392

23 N -0.738731

24 C 0.188377

25 C 0.207839

26 C -0.132264

27 C -0.055730

28 C -0.087965

29 C -0.055731

30 C -0.132263

31 C -0.087965

32 C -0.055731

33 C -0.132263

34 C 0.207839

35 C -0.132263

36 C -0.055731

37 C 0.207839

38 C -0.132263

39 C -0.055731

40 C -0.087965

41 C -0.055731

42 C -0.132263

43 C 0.207839

44 C -0.132263

45 C -0.055730

46 C -0.087965

47 C -0.055731

48 C -0.132263

49 H 0.079488

50 H 0.079488

51 H 0.079488

52 H 0.079488

53 H 0.079488

54 H 0.079488

55 H 0.079488

56 H 0.079488

57 H 0.059863

58 H 0.022704

59 H 0.035846

60 H 0.022704

61 H 0.059862

62 H 0.035846

63 H 0.022704

64 H 0.059862

65 H 0.059863

66 H 0.022704

67 H 0.059862

68 H 0.022704

69 H 0.035846

70 H 0.022704

71 H 0.059863

72 H 0.059862

73 H 0.022704

74 H 0.035846

75 H 0.022704

76 H 0.059862

77 Zn 1.339251

Sum of APT charges = 0.00000

APT charges with hydrogens summed into heavy atoms:

1

1 C 0.192730

2 C -0.057392

3 N -0.738732

4 C -0.057392

5 C 0.192730

6 C 0.188377

7 C -0.057392

8 N -0.738732

9 C -0.057391

10 C 0.192730

11 C 0.192730

12 C 0.188377

13 C -0.057392

14 C 0.192730

15 C 0.192730

16 C -0.057392

17 N -0.738732

18 C 0.188377

19 C -0.057392

20 C 0.192730

21 C 0.192730

22 C -0.057392

23 N -0.738731

24 C 0.188377

25 C 0.207839

26 C -0.072401

27 C -0.033026

28 C -0.052119

29 C -0.033026

30 C -0.072401

31 C -0.052119

32 C -0.033027

33 C -0.072401

34 C 0.207839

35 C -0.072401

36 C -0.033027

37 C 0.207839

38 C -0.072401

39 C -0.033027

40 C -0.052119

41 C -0.033027

42 C -0.072401

43 C 0.207839

44 C -0.072401

45 C -0.033027

46 C -0.052119

47 C -0.033027

48 C -0.072400

77 Zn 1.339251

Electronic spatial extent (au): <R\*\*2>= 33352.9765

Charge= -0.0000 electrons

Dipole moment (field-independent basis, Debye):

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

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

XX= -248.6473 YY= -248.6473 ZZ= -276.6355

XY= -0.0000 XZ= 0.0000 YZ= -0.0000

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

XX= 9.3294 YY= 9.3294 ZZ= -18.6588

XY= -0.0000 XZ= 0.0000 YZ= -0.0000

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

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

XXY= 0.0000 XXZ= 89.9108 XZZ= -0.0000 YZZ= 0.0000

YYZ= -89.9108 XYZ= -0.0000

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

XXXX= -21528.0473 YYYY= -21528.0473 ZZZZ= -1080.9900 XXXY= -0.0000

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

ZZZY= -0.0000 XXYY= -5779.9024 XXZZ= -3834.9810 YYZZ= -3834.9810

XXYZ= -0.0000 YYXZ= -0.0000 ZZXY= 0.0000

N-N= 5.738269787601D+03 E-N=-1.615865208060D+04 KE= 2.020706256559D+03

Symmetry A1 KE= 5.778493152223D+02

Symmetry A2 KE= 4.453814259608D+02

Symmetry B1 KE= 4.987377576881D+02

Symmetry B2 KE= 4.987377576881D+02

Exact polarizability:1406.087 0.0001406.087 0.000 0.000 511.312

Approx polarizability:1533.806 -0.0001533.806 0.000 -0.000 597.199

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Tue Aug 13 21:55:28 2019, MaxMem= 671088640 cpu: 36.6

(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.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36757 LenP2D= 95282.

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 = 182

Leave Link 701 at Tue Aug 13 22:00:51 2019, MaxMem= 671088640 cpu: 1287.6

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

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

Leave Link 702 at Tue Aug 13 22:00:51 2019, MaxMem= 671088640 cpu: 0.1

(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= 0 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

wScrn= 0.000000 ICntrl= 100127 IOpCl= 0 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Tue Aug 13 22:09:00 2019, MaxMem= 671088640 cpu: 1955.7

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

Dipole =-1.01535447D-12 1.40082390D-13-5.55666624D-14

Polarizability= 1.40608665D+03 1.09679556D-07 1.40608659D+03

1.74874590D-05 9.22027950D-06 5.11311919D+02

Full mass-weighted force constant matrix:

Low frequencies --- 0.0002 0.0006 0.0007 8.2513 8.7447 8.7447

Low frequencies --- 9.0391 20.2018 39.4198

Diagonal vibrational polarizability:

59.4091676 59.4091507 143.0726411

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 B2 A1

Frequencies -- 8.4611 20.2018 39.4198

Red. masses -- 6.0193 6.2785 4.0512

Frc consts -- 0.0003 0.0015 0.0037

IR Inten -- 0.0000 1.0856 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.01 -0.00 -0.02 -0.00 0.00 0.05 -0.00 -0.01 0.11

2 6 -0.00 -0.00 -0.02 0.00 -0.00 0.07 -0.00 -0.00 0.04

3 7 -0.00 -0.00 0.00 -0.00 -0.00 0.10 0.00 0.00 0.01

4 6 -0.00 0.00 0.02 -0.00 -0.00 0.07 0.00 -0.00 0.04

5 6 -0.01 0.00 0.02 0.00 0.00 0.05 0.00 -0.01 0.11

6 6 -0.00 0.00 0.04 -0.00 0.00 0.06 0.00 0.00 0.00

7 6 -0.00 0.00 0.02 0.00 0.00 0.07 -0.00 0.00 -0.04

8 7 0.00 0.00 0.00 0.00 0.00 0.10 0.00 0.00 -0.01

9 6 0.00 0.00 -0.02 0.00 -0.00 0.07 -0.00 -0.00 -0.04

10 6 0.00 0.01 -0.02 -0.00 0.00 0.05 -0.01 -0.00 -0.11

11 6 -0.00 0.01 0.02 -0.00 -0.00 0.05 -0.01 0.00 -0.11

12 6 -0.00 -0.00 -0.04 0.00 0.00 0.06 -0.00 0.00 0.00

13 6 -0.00 -0.00 -0.02 -0.00 0.00 0.07 0.00 0.00 -0.04

14 6 -0.00 -0.01 -0.02 0.00 -0.00 0.05 0.01 0.00 -0.11

15 6 0.00 -0.01 0.02 0.00 0.00 0.05 0.01 -0.00 -0.11

16 6 0.00 -0.00 0.02 -0.00 -0.00 0.07 0.00 -0.00 -0.04

17 7 -0.00 -0.00 0.00 -0.00 -0.00 0.10 -0.00 -0.00 -0.01

18 6 0.00 -0.00 0.04 0.00 -0.00 0.06 -0.00 -0.00 -0.00

19 6 0.00 -0.00 0.02 0.00 0.00 0.07 -0.00 0.00 0.04

20 6 0.01 -0.00 0.02 -0.00 -0.00 0.05 -0.00 0.01 0.11

21 6 0.01 0.00 -0.02 0.00 -0.00 0.05 0.00 0.01 0.11

22 6 0.00 0.00 -0.02 -0.00 0.00 0.07 0.00 0.00 0.04

23 7 0.00 -0.00 0.00 -0.00 0.00 0.10 0.00 -0.00 0.01

24 6 0.00 0.00 -0.04 -0.00 -0.00 0.06 0.00 -0.00 0.00

25 6 -0.00 0.00 0.08 -0.00 0.00 -0.01 -0.00 -0.00 -0.00

26 6 0.03 0.03 0.11 -0.04 -0.04 -0.05 -0.07 0.07 0.05

27 6 0.03 0.02 0.15 -0.04 -0.04 -0.12 -0.07 0.07 0.05

28 6 0.00 -0.00 0.18 0.00 -0.00 -0.16 0.00 0.00 -0.00

29 6 -0.02 -0.03 0.15 0.04 0.04 -0.12 0.07 -0.07 -0.05

30 6 -0.03 -0.03 0.11 0.04 0.04 -0.05 0.07 -0.07 -0.05

31 6 0.00 0.00 -0.18 -0.00 -0.00 -0.16 -0.00 0.00 -0.00

32 6 0.03 -0.02 -0.15 0.04 -0.04 -0.12 0.07 0.07 0.05

33 6 0.03 -0.03 -0.11 0.04 -0.04 -0.05 0.07 0.07 0.05

34 6 -0.00 -0.00 -0.08 0.00 0.00 -0.01 0.00 -0.00 -0.00

35 6 -0.03 0.03 -0.11 -0.04 0.04 -0.05 -0.07 -0.07 -0.05

36 6 -0.02 0.03 -0.15 -0.04 0.04 -0.12 -0.07 -0.07 -0.05

37 6 0.00 0.00 -0.08 -0.00 -0.00 -0.01 -0.00 0.00 -0.00

38 6 0.03 -0.03 -0.11 0.04 -0.04 -0.05 0.07 0.07 -0.05

39 6 0.02 -0.03 -0.15 0.04 -0.04 -0.12 0.07 0.07 -0.05

40 6 -0.00 -0.00 -0.18 0.00 0.00 -0.16 0.00 -0.00 -0.00

41 6 -0.03 0.02 -0.15 -0.04 0.04 -0.12 -0.07 -0.07 0.05

42 6 -0.03 0.03 -0.11 -0.04 0.04 -0.05 -0.07 -0.07 0.05

43 6 0.00 -0.00 0.08 0.00 -0.00 -0.01 0.00 0.00 0.00

44 6 0.03 0.03 0.11 -0.04 -0.04 -0.05 -0.07 0.07 -0.05

45 6 0.02 0.03 0.15 -0.04 -0.04 -0.12 -0.07 0.07 -0.05

46 6 -0.00 0.00 0.18 -0.00 0.00 -0.16 -0.00 -0.00 0.00

47 6 -0.03 -0.02 0.15 0.04 0.04 -0.12 0.07 -0.07 0.05

48 6 -0.03 -0.03 0.11 0.04 0.04 -0.05 0.07 -0.07 0.05

49 1 -0.01 -0.00 -0.03 -0.00 0.00 0.03 0.00 -0.01 0.15

50 1 -0.01 0.00 0.03 0.00 0.00 0.03 -0.00 -0.01 0.15

51 1 0.00 0.01 -0.03 -0.00 0.00 0.03 -0.01 0.00 -0.15

52 1 -0.00 0.01 0.03 -0.00 -0.00 0.03 -0.01 -0.00 -0.15

53 1 -0.00 -0.01 -0.03 0.00 -0.00 0.03 0.01 -0.00 -0.15

54 1 0.00 -0.01 0.03 0.00 0.00 0.03 0.01 0.00 -0.15

55 1 0.01 -0.00 0.03 -0.00 -0.00 0.03 0.00 0.01 0.15

56 1 0.01 0.00 -0.03 0.00 -0.00 0.03 -0.00 0.01 0.15

57 1 0.05 0.05 0.09 -0.08 -0.07 -0.02 -0.11 0.12 0.08

58 1 0.05 0.04 0.17 -0.07 -0.07 -0.15 -0.12 0.12 0.08

59 1 0.00 -0.00 0.21 0.00 -0.00 -0.22 0.00 0.00 -0.00

60 1 -0.04 -0.05 0.17 0.07 0.07 -0.15 0.12 -0.12 -0.08

61 1 -0.05 -0.05 0.09 0.07 0.08 -0.02 0.12 -0.11 -0.08

62 1 0.00 0.00 -0.21 -0.00 -0.00 -0.22 -0.00 0.00 -0.00

63 1 0.05 -0.04 -0.17 0.07 -0.07 -0.15 0.12 0.12 0.08

64 1 0.05 -0.05 -0.09 0.08 -0.07 -0.02 0.11 0.12 0.08

65 1 -0.05 0.05 -0.09 -0.07 0.08 -0.02 -0.12 -0.11 -0.08

66 1 -0.04 0.05 -0.17 -0.07 0.07 -0.15 -0.12 -0.12 -0.08

67 1 0.05 -0.05 -0.09 0.07 -0.08 -0.02 0.12 0.11 -0.08

68 1 0.04 -0.05 -0.17 0.07 -0.07 -0.15 0.12 0.12 -0.08

69 1 -0.00 -0.00 -0.21 0.00 0.00 -0.22 0.00 -0.00 -0.00

70 1 -0.05 0.04 -0.17 -0.07 0.07 -0.15 -0.12 -0.12 0.08

71 1 -0.05 0.05 -0.09 -0.08 0.07 -0.02 -0.11 -0.12 0.08

72 1 0.05 0.05 0.09 -0.07 -0.08 -0.02 -0.12 0.11 -0.08

73 1 0.04 0.05 0.17 -0.07 -0.07 -0.15 -0.12 0.12 -0.08

74 1 -0.00 0.00 0.21 -0.00 0.00 -0.22 -0.00 -0.00 0.00

75 1 -0.05 -0.04 0.17 0.07 0.07 -0.15 0.12 -0.12 0.08

76 1 -0.05 -0.05 0.09 0.08 0.07 -0.02 0.11 -0.12 0.08

77 30 0.00 -0.00 0.00 -0.00 0.00 0.10 0.00 -0.00 0.00

4 5 6

E E B2

Frequencies -- 43.9680 43.9680 44.0364

Red. masses -- 4.5857 4.5857 5.2777

Frc consts -- 0.0052 0.0052 0.0060

IR Inten -- 0.1800 0.1800 0.2983

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.03 0.13 0.02 -0.00 0.01 -0.00 0.01 -0.02

2 6 -0.00 -0.02 0.06 0.02 -0.00 -0.00 -0.00 0.01 0.00

3 7 -0.00 -0.02 0.02 0.01 -0.00 0.00 -0.00 0.00 0.01

4 6 -0.00 -0.02 0.06 0.02 -0.00 0.02 0.00 0.01 0.00

5 6 -0.00 -0.03 0.13 0.02 -0.00 0.02 0.00 0.01 -0.02

6 6 -0.00 -0.02 0.03 0.02 -0.00 0.03 -0.00 0.00 0.01

7 6 -0.00 -0.02 0.00 0.02 -0.00 0.06 -0.01 -0.00 0.00

8 7 -0.00 -0.01 -0.00 0.02 -0.00 0.02 -0.00 -0.00 0.01

9 6 -0.00 -0.02 -0.02 0.02 -0.00 0.06 -0.01 0.00 0.00

10 6 -0.00 -0.02 -0.02 0.03 -0.00 0.13 -0.01 0.00 -0.02

11 6 -0.00 -0.02 -0.01 0.03 -0.00 0.13 -0.01 -0.00 -0.02

12 6 -0.00 -0.02 0.03 0.02 -0.00 -0.03 0.00 0.00 0.01

13 6 -0.00 -0.02 0.02 0.02 -0.00 -0.06 0.01 -0.00 0.00

14 6 -0.00 -0.02 0.02 0.03 -0.00 -0.13 0.01 -0.00 -0.02

15 6 -0.00 -0.02 0.01 0.03 -0.00 -0.13 0.01 0.00 -0.02

16 6 -0.00 -0.02 -0.00 0.02 -0.00 -0.06 0.01 0.00 0.00

17 7 -0.00 -0.01 0.00 0.02 -0.00 -0.02 0.00 -0.00 0.01

18 6 -0.00 -0.02 -0.03 0.02 -0.00 -0.03 0.00 -0.00 0.01

19 6 -0.00 -0.02 -0.06 0.02 -0.00 -0.02 -0.00 -0.01 0.00

20 6 -0.00 -0.03 -0.13 0.02 -0.00 -0.02 -0.00 -0.01 -0.02

21 6 -0.00 -0.03 -0.13 0.02 -0.00 -0.01 0.00 -0.01 -0.02

22 6 -0.00 -0.02 -0.06 0.02 -0.00 0.00 0.00 -0.01 0.00

23 7 -0.00 -0.02 -0.02 0.01 -0.00 -0.00 -0.00 -0.00 0.01

24 6 -0.00 -0.02 -0.03 0.02 -0.00 0.03 -0.00 -0.00 0.01

25 6 -0.01 -0.01 0.00 0.00 0.01 0.00 0.02 -0.02 0.01

26 6 -0.10 0.04 0.03 -0.00 -0.05 -0.05 0.06 -0.03 0.01

27 6 -0.13 0.06 -0.00 -0.03 -0.02 -0.09 0.12 -0.09 -0.01

28 6 -0.06 0.04 -0.06 -0.06 0.07 -0.07 0.14 -0.14 -0.02

29 6 0.03 -0.00 -0.08 -0.05 0.13 -0.03 0.09 -0.12 -0.01

30 6 0.05 -0.02 -0.05 -0.02 0.10 0.01 0.03 -0.06 0.01

31 6 0.07 0.06 -0.07 -0.04 -0.06 0.06 -0.14 -0.14 -0.02

32 6 0.13 0.05 -0.03 0.00 0.03 0.08 -0.12 -0.09 -0.01

33 6 0.10 0.02 0.01 0.02 0.05 0.05 -0.06 -0.03 0.01

34 6 0.01 -0.00 0.00 0.01 -0.01 -0.00 -0.02 -0.02 0.01

35 6 -0.05 0.00 -0.05 -0.04 -0.10 -0.03 -0.03 -0.06 0.01

36 6 -0.02 0.03 -0.09 -0.06 -0.13 0.00 -0.09 -0.12 -0.01

37 6 0.01 -0.00 -0.00 0.01 -0.01 0.00 0.02 0.02 0.01

38 6 -0.05 0.00 0.05 -0.04 -0.10 0.03 0.03 0.06 0.01

39 6 -0.02 0.03 0.09 -0.06 -0.13 -0.00 0.09 0.12 -0.01

40 6 0.07 0.06 0.07 -0.04 -0.06 -0.06 0.14 0.14 -0.02

41 6 0.13 0.05 0.03 0.00 0.03 -0.08 0.12 0.09 -0.01

42 6 0.10 0.02 -0.01 0.02 0.05 -0.05 0.06 0.03 0.01

43 6 -0.01 -0.01 -0.00 0.00 0.01 -0.00 -0.02 0.02 0.01

44 6 0.05 -0.02 0.05 -0.02 0.10 -0.01 -0.03 0.06 0.01

45 6 0.03 -0.00 0.08 -0.05 0.13 0.03 -0.09 0.12 -0.01

46 6 -0.06 0.04 0.06 -0.06 0.07 0.07 -0.14 0.14 -0.02

47 6 -0.13 0.06 0.00 -0.03 -0.02 0.09 -0.12 0.09 -0.01

48 6 -0.10 0.04 -0.03 -0.00 -0.05 0.05 -0.06 0.03 0.01

49 1 -0.00 -0.03 0.18 0.02 -0.00 0.02 -0.00 0.01 -0.03

50 1 -0.00 -0.03 0.18 0.02 -0.01 0.03 0.00 0.01 -0.03

51 1 -0.01 -0.02 -0.03 0.03 -0.00 0.18 -0.01 0.00 -0.03

52 1 -0.00 -0.02 -0.02 0.03 -0.00 0.18 -0.01 -0.00 -0.03

53 1 -0.01 -0.02 0.03 0.03 -0.00 -0.18 0.01 -0.00 -0.03

54 1 -0.00 -0.02 0.02 0.03 -0.00 -0.18 0.01 0.00 -0.03

55 1 -0.00 -0.03 -0.18 0.02 -0.01 -0.03 -0.00 -0.01 -0.03

56 1 -0.00 -0.03 -0.18 0.02 -0.00 -0.02 0.00 -0.01 -0.03

57 1 -0.15 0.05 0.07 0.01 -0.11 -0.05 0.05 0.00 0.01

58 1 -0.20 0.09 0.02 -0.04 -0.06 -0.12 0.16 -0.10 -0.01

59 1 -0.08 0.06 -0.08 -0.08 0.10 -0.10 0.19 -0.19 -0.03

60 1 0.08 -0.01 -0.12 -0.07 0.20 -0.02 0.10 -0.16 -0.01

61 1 0.12 -0.05 -0.07 -0.02 0.15 0.05 -0.00 -0.05 0.01

62 1 0.10 0.08 -0.10 -0.06 -0.08 0.08 -0.19 -0.19 -0.03

63 1 0.20 0.07 -0.02 0.01 0.08 0.12 -0.16 -0.10 -0.01

64 1 0.15 0.02 0.05 0.05 0.12 0.07 -0.05 0.00 0.01

65 1 -0.11 -0.01 -0.05 -0.05 -0.15 -0.07 0.00 -0.05 0.01

66 1 -0.06 0.04 -0.12 -0.09 -0.20 -0.02 -0.10 -0.16 -0.01

67 1 -0.11 -0.01 0.05 -0.05 -0.15 0.07 -0.00 0.05 0.01

68 1 -0.06 0.04 0.12 -0.09 -0.20 0.02 0.10 0.16 -0.01

69 1 0.10 0.08 0.10 -0.06 -0.08 -0.08 0.19 0.19 -0.03

70 1 0.20 0.07 0.02 0.01 0.08 -0.12 0.16 0.10 -0.01

71 1 0.15 0.02 -0.05 0.05 0.12 -0.07 0.05 -0.00 0.01

72 1 0.12 -0.05 0.07 -0.02 0.15 -0.05 0.00 0.05 0.01

73 1 0.08 -0.01 0.12 -0.07 0.20 0.02 -0.10 0.16 -0.01

74 1 -0.08 0.06 0.08 -0.08 0.10 0.10 -0.19 0.19 -0.03

75 1 -0.20 0.09 -0.02 -0.04 -0.06 0.12 -0.16 0.10 -0.01

76 1 -0.15 0.05 -0.07 0.01 -0.11 0.05 -0.05 -0.00 0.01

77 30 -0.00 -0.02 -0.00 0.02 -0.00 0.00 -0.00 -0.00 0.01

7 8 9

E E B1

Frequencies -- 50.0929 50.0929 57.1435

Red. masses -- 5.0366 5.0366 3.7348

Frc consts -- 0.0074 0.0074 0.0072

IR Inten -- 0.5866 0.5866 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.03 -0.00 -0.00 -0.00 -0.03 -0.06 -0.00 -0.00 -0.00

2 6 0.03 -0.00 0.01 -0.00 -0.03 -0.03 0.01 -0.01 -0.00

3 7 0.03 -0.00 -0.00 -0.00 -0.04 -0.02 0.01 0.00 0.00

4 6 0.03 -0.00 -0.01 -0.00 -0.03 -0.03 0.01 0.01 0.00

5 6 0.03 -0.00 -0.01 -0.00 -0.03 -0.05 -0.00 0.00 0.00

6 6 0.03 -0.00 -0.03 -0.01 -0.03 -0.02 0.01 0.01 0.00

7 6 0.03 -0.00 -0.03 -0.00 -0.03 -0.01 0.01 0.01 -0.00

8 7 0.04 -0.00 -0.02 -0.00 -0.03 0.00 0.00 0.01 -0.00

9 6 0.03 -0.00 -0.03 -0.00 -0.03 0.01 -0.01 0.01 0.00

10 6 0.03 -0.00 -0.05 -0.00 -0.03 0.01 -0.00 -0.00 0.00

11 6 0.03 -0.00 -0.06 -0.00 -0.03 0.00 0.00 -0.00 -0.00

12 6 0.03 -0.01 0.02 -0.00 -0.03 -0.03 0.01 -0.01 0.00

13 6 0.03 -0.00 0.03 -0.00 -0.03 -0.01 0.01 -0.01 0.00

14 6 0.03 -0.00 0.05 -0.00 -0.03 -0.01 0.00 0.00 0.00

15 6 0.03 -0.00 0.06 -0.00 -0.03 -0.00 -0.00 0.00 -0.00

16 6 0.03 -0.00 0.03 -0.00 -0.03 0.01 -0.01 -0.01 -0.00

17 7 0.04 -0.00 0.02 -0.00 -0.03 -0.00 0.00 -0.01 -0.00

18 6 0.03 -0.00 0.03 -0.01 -0.03 0.02 -0.01 -0.01 -0.00

19 6 0.03 -0.00 0.01 -0.00 -0.03 0.03 -0.01 -0.01 0.00

20 6 0.03 -0.00 0.01 -0.00 -0.03 0.05 0.00 -0.00 0.00

21 6 0.03 -0.00 0.00 -0.00 -0.03 0.06 0.00 0.00 -0.00

22 6 0.03 -0.00 -0.01 -0.00 -0.03 0.03 -0.01 0.01 -0.00

23 7 0.03 -0.00 0.00 -0.00 -0.04 0.02 -0.01 0.00 -0.00

24 6 0.03 -0.01 -0.02 -0.00 -0.03 0.03 -0.01 0.01 -0.00

25 6 0.01 0.02 -0.02 -0.02 -0.02 -0.02 0.01 0.01 -0.00

26 6 -0.04 0.07 0.02 -0.01 -0.04 -0.03 -0.07 0.09 0.06

27 6 -0.11 0.14 0.06 -0.06 0.01 0.00 -0.07 0.09 0.06

28 6 -0.11 0.14 0.06 -0.12 0.08 0.05 0.01 0.01 -0.00

29 6 -0.04 0.08 0.02 -0.13 0.09 0.06 0.09 -0.07 -0.06

30 6 0.02 0.01 -0.02 -0.08 0.04 0.03 0.09 -0.07 -0.06

31 6 -0.08 -0.12 -0.05 0.14 0.11 0.06 0.01 -0.01 0.00

32 6 -0.09 -0.13 -0.06 0.08 0.04 0.02 -0.07 -0.09 -0.06

33 6 -0.04 -0.08 -0.03 0.01 -0.02 -0.02 -0.07 -0.09 -0.06

34 6 0.02 -0.02 0.02 0.02 -0.01 -0.02 0.01 -0.01 0.00

35 6 0.04 -0.01 0.03 0.07 0.04 0.02 0.09 0.07 0.06

36 6 -0.01 -0.06 -0.00 0.14 0.11 0.06 0.09 0.07 0.06

37 6 0.02 -0.02 -0.02 0.02 -0.01 0.02 -0.01 0.01 0.00

38 6 0.04 -0.01 -0.03 0.07 0.04 -0.02 -0.09 -0.07 0.06

39 6 -0.01 -0.06 0.00 0.14 0.11 -0.06 -0.09 -0.07 0.06

40 6 -0.08 -0.12 0.05 0.14 0.11 -0.06 -0.01 0.01 0.00

41 6 -0.09 -0.13 0.06 0.08 0.04 -0.02 0.07 0.09 -0.06

42 6 -0.04 -0.08 0.03 0.01 -0.02 0.02 0.07 0.09 -0.06

43 6 0.01 0.02 0.02 -0.02 -0.02 0.02 -0.01 -0.01 -0.00

44 6 0.02 0.01 0.02 -0.08 0.04 -0.03 -0.09 0.07 -0.06

45 6 -0.04 0.08 -0.02 -0.13 0.09 -0.06 -0.09 0.07 -0.06

46 6 -0.11 0.14 -0.06 -0.12 0.08 -0.05 -0.01 -0.01 0.00

47 6 -0.11 0.14 -0.06 -0.06 0.01 -0.00 0.07 -0.09 0.06

48 6 -0.04 0.07 -0.02 -0.01 -0.04 0.03 0.07 -0.09 0.06

49 1 0.02 -0.01 -0.00 -0.00 -0.03 -0.07 -0.01 -0.01 -0.01

50 1 0.02 -0.00 -0.01 -0.00 -0.03 -0.07 -0.01 0.01 0.01

51 1 0.03 -0.00 -0.07 -0.00 -0.02 0.01 -0.01 -0.01 0.01

52 1 0.03 -0.00 -0.07 -0.01 -0.02 0.00 0.01 -0.01 -0.01

53 1 0.03 -0.00 0.07 -0.00 -0.02 -0.01 0.01 0.01 0.01

54 1 0.03 -0.00 0.07 -0.01 -0.02 -0.00 -0.01 0.01 -0.01

55 1 0.02 -0.00 0.01 -0.00 -0.03 0.07 0.01 -0.01 0.01

56 1 0.02 -0.01 0.00 -0.00 -0.03 0.07 0.01 0.01 -0.01

57 1 -0.05 0.07 0.02 0.04 -0.08 -0.06 -0.12 0.14 0.10

58 1 -0.16 0.18 0.10 -0.05 0.00 -0.00 -0.13 0.15 0.10

59 1 -0.16 0.20 0.10 -0.17 0.13 0.08 0.01 0.01 -0.00

60 1 -0.04 0.08 0.02 -0.18 0.15 0.10 0.15 -0.13 -0.10

61 1 0.07 -0.03 -0.05 -0.09 0.05 0.04 0.14 -0.12 -0.10

62 1 -0.13 -0.17 -0.08 0.20 0.16 0.10 0.01 -0.01 0.00

63 1 -0.15 -0.18 -0.10 0.08 0.04 0.02 -0.13 -0.15 -0.10

64 1 -0.05 -0.09 -0.04 -0.03 -0.07 -0.05 -0.12 -0.14 -0.10

65 1 0.08 0.04 0.06 0.07 0.05 0.02 0.14 0.12 0.10

66 1 -0.00 -0.05 0.00 0.18 0.16 0.10 0.15 0.13 0.10

67 1 0.08 0.04 -0.06 0.07 0.05 -0.02 -0.14 -0.12 0.10

68 1 -0.00 -0.05 -0.00 0.18 0.16 -0.10 -0.15 -0.13 0.10

69 1 -0.13 -0.17 0.08 0.20 0.16 -0.10 -0.01 0.01 0.00

70 1 -0.15 -0.18 0.10 0.08 0.04 -0.02 0.13 0.15 -0.10

71 1 -0.05 -0.09 0.04 -0.03 -0.07 0.05 0.12 0.14 -0.10

72 1 0.07 -0.03 0.05 -0.09 0.05 -0.04 -0.14 0.12 -0.10

73 1 -0.04 0.08 -0.02 -0.18 0.15 -0.10 -0.15 0.13 -0.10

74 1 -0.16 0.20 -0.10 -0.17 0.13 -0.08 -0.01 -0.01 0.00

75 1 -0.16 0.18 -0.10 -0.05 0.00 0.00 0.13 -0.15 0.10

76 1 -0.05 0.07 -0.02 0.04 -0.08 0.06 0.12 -0.14 0.10

77 30 0.04 -0.00 0.00 -0.00 -0.04 -0.00 0.00 0.00 -0.00

10 11 12

E E A2

Frequencies -- 65.0991 65.0991 79.3649

Red. masses -- 4.5246 4.5246 5.1805

Frc consts -- 0.0113 0.0113 0.0192

IR Inten -- 0.0729 0.0729 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.00 0.11 -0.01 -0.00 -0.02 -0.10 -0.02 -0.02

2 6 0.00 0.00 0.08 -0.01 -0.00 -0.03 -0.06 -0.03 -0.03

3 7 0.00 0.00 0.06 -0.00 0.00 0.00 -0.04 -0.00 0.00

4 6 -0.00 0.00 0.08 -0.01 0.00 0.03 -0.06 0.03 0.03

5 6 0.00 -0.00 0.11 -0.01 0.00 0.02 -0.10 0.02 0.02

6 6 -0.00 0.00 0.07 -0.00 0.00 0.07 -0.06 0.06 0.05

7 6 -0.00 0.01 0.03 -0.00 0.00 0.08 -0.03 0.06 0.03

8 7 0.00 0.00 -0.00 -0.00 0.00 0.06 -0.00 0.04 -0.00

9 6 0.00 0.01 -0.03 -0.00 -0.00 0.08 0.03 0.06 -0.03

10 6 0.00 0.01 -0.02 0.00 0.00 0.11 0.02 0.10 -0.02

11 6 -0.00 0.01 0.02 0.00 -0.00 0.11 -0.02 0.10 0.02

12 6 0.00 0.00 0.07 -0.00 -0.00 -0.07 -0.06 -0.06 -0.05

13 6 0.00 0.01 0.03 -0.00 -0.00 -0.08 -0.03 -0.06 -0.03

14 6 0.00 0.01 0.02 0.00 0.00 -0.11 -0.02 -0.10 -0.02

15 6 -0.00 0.01 -0.02 0.00 -0.00 -0.11 0.02 -0.10 0.02

16 6 -0.00 0.01 -0.03 -0.00 0.00 -0.08 0.03 -0.06 0.03

17 7 0.00 0.00 0.00 -0.00 0.00 -0.06 0.00 -0.04 -0.00

18 6 -0.00 0.00 -0.07 -0.00 0.00 -0.07 0.06 -0.06 0.05

19 6 -0.00 0.00 -0.08 -0.01 0.00 -0.03 0.06 -0.03 0.03

20 6 0.00 -0.00 -0.11 -0.01 0.00 -0.02 0.10 -0.02 0.02

21 6 -0.00 -0.00 -0.11 -0.01 -0.00 0.02 0.10 0.02 -0.02

22 6 0.00 0.00 -0.08 -0.01 -0.00 0.03 0.06 0.03 -0.03

23 7 0.00 0.00 -0.06 -0.00 0.00 -0.00 0.04 0.00 0.00

24 6 0.00 0.00 -0.07 -0.00 -0.00 0.07 0.06 0.06 -0.05

25 6 -0.00 0.01 0.04 -0.01 0.00 0.04 -0.06 0.06 0.05

26 6 0.03 -0.08 -0.03 -0.08 0.04 0.06 -0.02 0.03 0.03

27 6 0.04 -0.09 -0.08 -0.08 0.03 0.01 0.06 -0.05 -0.02

28 6 0.01 -0.01 -0.06 0.01 -0.01 -0.06 0.10 -0.10 -0.05

29 6 -0.03 0.08 0.01 0.09 -0.04 -0.08 0.05 -0.06 -0.02

30 6 -0.04 0.08 0.06 0.08 -0.03 -0.03 -0.03 0.02 0.03

31 6 -0.01 -0.01 -0.06 0.01 0.01 0.06 0.10 0.10 0.05

32 6 -0.04 -0.09 -0.08 -0.08 -0.03 -0.01 0.06 0.05 0.02

33 6 -0.03 -0.08 -0.03 -0.08 -0.04 -0.06 -0.02 -0.03 -0.03

34 6 0.00 0.01 0.04 -0.01 -0.00 -0.04 -0.06 -0.06 -0.05

35 6 0.04 0.08 0.06 0.08 0.03 0.03 -0.03 -0.02 -0.03

36 6 0.03 0.08 0.01 0.09 0.04 0.08 0.05 0.06 0.02

37 6 0.00 0.01 -0.04 -0.01 -0.00 0.04 0.06 0.06 -0.05

38 6 0.04 0.08 -0.06 0.08 0.03 -0.03 0.03 0.02 -0.03

39 6 0.03 0.08 -0.01 0.09 0.04 -0.08 -0.05 -0.06 0.02

40 6 -0.01 -0.01 0.06 0.01 0.01 -0.06 -0.10 -0.10 0.05

41 6 -0.04 -0.09 0.08 -0.08 -0.03 0.01 -0.06 -0.05 0.02

42 6 -0.03 -0.08 0.03 -0.08 -0.04 0.06 0.02 0.03 -0.03

43 6 -0.00 0.01 -0.04 -0.01 0.00 -0.04 0.06 -0.06 0.05

44 6 -0.04 0.08 -0.06 0.08 -0.03 0.03 0.03 -0.02 0.03

45 6 -0.03 0.08 -0.01 0.09 -0.04 0.08 -0.05 0.06 -0.02

46 6 0.01 -0.01 0.06 0.01 -0.01 0.06 -0.10 0.10 -0.05

47 6 0.04 -0.09 0.08 -0.08 0.03 -0.01 -0.06 0.05 -0.02

48 6 0.03 -0.08 0.03 -0.08 0.04 -0.06 0.02 -0.03 0.03

49 1 -0.00 -0.00 0.13 -0.02 -0.00 -0.04 -0.12 -0.03 -0.03

50 1 0.00 -0.00 0.13 -0.02 0.00 0.05 -0.12 0.03 0.03

51 1 0.00 0.02 -0.05 0.00 0.00 0.13 0.03 0.12 -0.03

52 1 -0.00 0.02 0.04 0.00 -0.00 0.13 -0.03 0.12 0.03

53 1 0.00 0.02 0.05 0.00 0.00 -0.13 -0.03 -0.12 -0.03

54 1 -0.00 0.02 -0.04 0.00 -0.00 -0.13 0.03 -0.12 0.03

55 1 0.00 -0.00 -0.13 -0.02 0.00 -0.05 0.12 -0.03 0.03

56 1 -0.00 -0.00 -0.13 -0.02 -0.00 0.04 0.12 0.03 -0.03

57 1 0.05 -0.14 -0.04 -0.15 0.07 0.11 -0.05 0.05 0.05

58 1 0.08 -0.16 -0.14 -0.14 0.06 0.02 0.09 -0.08 -0.04

59 1 0.02 -0.02 -0.10 0.02 -0.02 -0.10 0.18 -0.18 -0.10

60 1 -0.06 0.14 0.02 0.16 -0.08 -0.14 0.08 -0.09 -0.04

61 1 -0.07 0.15 0.11 0.14 -0.05 -0.04 -0.05 0.05 0.05

62 1 -0.02 -0.02 -0.10 0.02 0.02 0.10 0.18 0.18 0.10

63 1 -0.08 -0.16 -0.14 -0.14 -0.06 -0.02 0.09 0.08 0.04

64 1 -0.05 -0.14 -0.04 -0.15 -0.07 -0.11 -0.05 -0.05 -0.05

65 1 0.07 0.15 0.11 0.14 0.05 0.04 -0.05 -0.05 -0.05

66 1 0.06 0.14 0.02 0.16 0.08 0.14 0.08 0.09 0.04

67 1 0.07 0.15 -0.11 0.14 0.05 -0.04 0.05 0.05 -0.05

68 1 0.06 0.14 -0.02 0.16 0.08 -0.14 -0.08 -0.09 0.04

69 1 -0.02 -0.02 0.10 0.02 0.02 -0.10 -0.18 -0.18 0.10

70 1 -0.08 -0.16 0.14 -0.14 -0.06 0.02 -0.09 -0.08 0.04

71 1 -0.05 -0.14 0.04 -0.15 -0.07 0.11 0.05 0.05 -0.05

72 1 -0.07 0.15 -0.11 0.14 -0.05 0.04 0.05 -0.05 0.05

73 1 -0.06 0.14 -0.02 0.16 -0.08 0.14 -0.08 0.09 -0.04

74 1 0.02 -0.02 0.10 0.02 -0.02 0.10 -0.18 0.18 -0.10

75 1 0.08 -0.16 0.14 -0.14 0.06 -0.02 -0.09 0.08 -0.04

76 1 0.05 -0.14 0.04 -0.15 0.07 -0.11 0.05 -0.05 0.05

77 30 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00

13 14 15

A1 B2 A2

Frequencies -- 85.5263 94.8600 102.3065

Red. masses -- 4.8080 6.2446 5.3056

Frc consts -- 0.0207 0.0331 0.0327

IR Inten -- 0.0000 1.1740 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.01 0.15 0.00 0.02 -0.16 0.03 0.01 -0.06

2 6 0.00 -0.01 0.07 -0.00 0.00 -0.00 0.02 0.01 -0.09

3 7 0.00 -0.00 0.03 0.00 -0.00 0.10 0.02 -0.00 0.00

4 6 -0.00 -0.01 0.07 0.00 0.00 -0.00 0.02 -0.01 0.09

5 6 0.00 -0.01 0.15 -0.00 0.02 -0.16 0.03 -0.01 0.06

6 6 -0.00 -0.00 -0.00 -0.00 0.00 -0.01 0.02 -0.02 0.14

7 6 -0.01 -0.00 -0.07 -0.00 -0.00 -0.00 0.01 -0.02 0.09

8 7 -0.00 -0.00 -0.03 0.00 0.00 0.10 0.00 -0.02 0.00

9 6 -0.01 0.00 -0.07 -0.00 0.00 -0.00 -0.01 -0.02 -0.09

10 6 -0.01 -0.00 -0.15 -0.02 -0.00 -0.16 -0.01 -0.03 -0.06

11 6 -0.01 0.00 -0.15 -0.02 0.00 -0.16 0.01 -0.03 0.06

12 6 0.00 -0.00 0.00 0.00 0.00 -0.01 0.02 0.02 -0.14

13 6 0.01 -0.00 -0.07 0.00 -0.00 -0.00 0.01 0.02 -0.09

14 6 0.01 0.00 -0.15 0.02 0.00 -0.16 0.01 0.03 -0.06

15 6 0.01 -0.00 -0.15 0.02 -0.00 -0.16 -0.01 0.03 0.06

16 6 0.01 0.00 -0.07 0.00 0.00 -0.00 -0.01 0.02 0.09

17 7 0.00 0.00 -0.03 -0.00 -0.00 0.10 -0.00 0.02 0.00

18 6 0.00 0.00 -0.00 0.00 -0.00 -0.01 -0.02 0.02 0.14

19 6 0.00 0.01 0.07 -0.00 -0.00 -0.00 -0.02 0.01 0.09

20 6 -0.00 0.01 0.15 0.00 -0.02 -0.16 -0.03 0.01 0.06

21 6 0.00 0.01 0.15 -0.00 -0.02 -0.16 -0.03 -0.01 -0.06

22 6 -0.00 0.01 0.07 0.00 -0.00 -0.00 -0.02 -0.01 -0.09

23 7 -0.00 0.00 0.03 -0.00 0.00 0.10 -0.02 0.00 0.00

24 6 -0.00 0.00 0.00 -0.00 -0.00 -0.01 -0.02 -0.02 -0.14

25 6 -0.00 -0.00 -0.00 0.00 -0.00 -0.03 0.02 -0.02 0.11

26 6 0.04 -0.06 -0.04 0.01 0.01 -0.01 -0.04 -0.06 0.07

27 6 0.05 -0.06 -0.04 -0.00 0.02 0.02 -0.07 -0.04 -0.02

28 6 -0.01 -0.01 0.00 -0.02 0.02 0.04 -0.03 0.03 -0.06

29 6 -0.06 0.05 0.04 -0.02 0.00 0.02 0.04 0.07 -0.02

30 6 -0.06 0.04 0.04 -0.01 -0.01 -0.01 0.06 0.04 0.07

31 6 0.01 -0.01 -0.00 0.02 0.02 0.04 -0.03 -0.03 0.06

32 6 -0.05 -0.06 -0.04 0.00 0.02 0.02 -0.07 0.04 0.02

33 6 -0.04 -0.06 -0.04 -0.01 0.01 -0.01 -0.04 0.06 -0.07

34 6 0.00 -0.00 0.00 -0.00 -0.00 -0.03 0.02 0.02 -0.11

35 6 0.06 0.04 0.04 0.01 -0.01 -0.01 0.06 -0.04 -0.07

36 6 0.06 0.05 0.04 0.02 0.00 0.02 0.04 -0.07 0.02

37 6 -0.00 0.00 0.00 0.00 0.00 -0.03 -0.02 -0.02 -0.11

38 6 -0.06 -0.04 0.04 -0.01 0.01 -0.01 -0.06 0.04 -0.07

39 6 -0.06 -0.05 0.04 -0.02 -0.00 0.02 -0.04 0.07 0.02

40 6 -0.01 0.01 -0.00 -0.02 -0.02 0.04 0.03 0.03 0.06

41 6 0.05 0.06 -0.04 -0.00 -0.02 0.02 0.07 -0.04 0.02

42 6 0.04 0.06 -0.04 0.01 -0.01 -0.01 0.04 -0.06 -0.07

43 6 0.00 0.00 -0.00 -0.00 0.00 -0.03 -0.02 0.02 0.11

44 6 0.06 -0.04 0.04 0.01 0.01 -0.01 -0.06 -0.04 0.07

45 6 0.06 -0.05 0.04 0.02 -0.00 0.02 -0.04 -0.07 -0.02

46 6 0.01 0.01 0.00 0.02 -0.02 0.04 0.03 -0.03 -0.06

47 6 -0.05 0.06 -0.04 0.00 -0.02 0.02 0.07 0.04 -0.02

48 6 -0.04 0.06 -0.04 -0.01 -0.01 -0.01 0.04 0.06 0.07

49 1 -0.01 -0.02 0.20 0.00 0.03 -0.28 0.03 0.02 -0.12

50 1 0.01 -0.02 0.20 -0.00 0.03 -0.28 0.03 -0.02 0.12

51 1 -0.02 -0.01 -0.20 -0.03 -0.00 -0.28 -0.02 -0.03 -0.12

52 1 -0.02 0.01 -0.20 -0.03 0.00 -0.28 0.02 -0.03 0.12

53 1 0.02 0.01 -0.20 0.03 0.00 -0.28 0.02 0.03 -0.12

54 1 0.02 -0.01 -0.20 0.03 -0.00 -0.28 -0.02 0.03 0.12

55 1 -0.01 0.02 0.20 0.00 -0.03 -0.28 -0.03 0.02 0.12

56 1 0.01 0.02 0.20 -0.00 -0.03 -0.28 -0.03 -0.02 -0.12

57 1 0.08 -0.09 -0.06 0.03 0.01 -0.03 -0.08 -0.11 0.10

58 1 0.09 -0.10 -0.07 0.00 0.04 0.03 -0.12 -0.07 -0.05

59 1 -0.01 -0.01 0.00 -0.04 0.04 0.07 -0.05 0.05 -0.13

60 1 -0.10 0.09 0.07 -0.04 -0.00 0.03 0.07 0.12 -0.05

61 1 -0.09 0.08 0.06 -0.01 -0.03 -0.03 0.11 0.08 0.10

62 1 0.01 -0.01 -0.00 0.04 0.04 0.07 -0.05 -0.05 0.13

63 1 -0.09 -0.10 -0.07 -0.00 0.04 0.03 -0.12 0.07 0.05

64 1 -0.08 -0.09 -0.06 -0.03 0.01 -0.03 -0.08 0.11 -0.10

65 1 0.09 0.08 0.06 0.01 -0.03 -0.03 0.11 -0.08 -0.10

66 1 0.10 0.09 0.07 0.04 -0.00 0.03 0.07 -0.12 0.05

67 1 -0.09 -0.08 0.06 -0.01 0.03 -0.03 -0.11 0.08 -0.10

68 1 -0.10 -0.09 0.07 -0.04 0.00 0.03 -0.07 0.12 0.05

69 1 -0.01 0.01 -0.00 -0.04 -0.04 0.07 0.05 0.05 0.13

70 1 0.09 0.10 -0.07 0.00 -0.04 0.03 0.12 -0.07 0.05

71 1 0.08 0.09 -0.06 0.03 -0.01 -0.03 0.08 -0.11 -0.10

72 1 0.09 -0.08 0.06 0.01 0.03 -0.03 -0.11 -0.08 0.10

73 1 0.10 -0.09 0.07 0.04 0.00 0.03 -0.07 -0.12 -0.05

74 1 0.01 0.01 0.00 0.04 -0.04 0.07 0.05 -0.05 -0.13

75 1 -0.09 0.10 -0.07 -0.00 -0.04 0.03 0.12 0.07 -0.05

76 1 -0.08 0.09 -0.06 -0.03 -0.01 -0.03 0.08 0.11 0.10

77 30 -0.00 0.00 -0.00 0.00 0.00 0.18 -0.00 -0.00 0.00

16 17 18

B1 E E

Frequencies -- 118.5287 141.5601 141.5601

Red. masses -- 7.4463 4.8272 4.8272

Frc consts -- 0.0616 0.0570 0.0570

IR Inten -- 0.0000 0.5878 0.5878

Atom AN X Y Z X Y Z X Y Z

1 6 0.02 -0.02 0.01 -0.00 0.01 -0.08 -0.00 -0.01 0.18

2 6 0.07 -0.04 0.01 -0.00 -0.01 0.08 -0.00 -0.00 0.05

3 7 0.09 0.00 -0.00 -0.00 -0.01 0.07 -0.00 0.01 -0.08

4 6 0.07 0.04 -0.01 -0.00 0.00 -0.05 -0.00 0.01 -0.07

5 6 0.02 0.02 -0.01 -0.00 0.01 -0.17 -0.00 -0.01 0.08

6 6 0.08 0.08 -0.00 0.00 0.00 -0.00 -0.01 0.01 -0.14

7 6 0.04 0.07 0.01 0.00 -0.00 0.05 -0.01 0.00 -0.08

8 7 -0.00 0.09 -0.00 -0.01 -0.00 -0.08 -0.01 0.00 -0.07

9 6 -0.04 0.07 -0.01 -0.01 -0.00 -0.07 0.00 0.00 0.05

10 6 -0.02 0.02 -0.01 0.01 -0.00 0.08 0.01 0.00 0.17

11 6 0.02 0.02 0.01 0.01 -0.00 0.18 0.01 0.00 0.08

12 6 0.08 -0.08 -0.00 -0.01 -0.01 0.14 0.00 -0.00 -0.00

13 6 0.04 -0.07 -0.01 -0.01 -0.00 0.07 0.00 0.00 -0.05

14 6 0.02 -0.02 -0.01 0.01 -0.00 -0.08 0.01 0.00 -0.17

15 6 -0.02 -0.02 0.01 0.01 -0.00 -0.18 0.01 0.00 -0.08

16 6 -0.04 -0.07 0.01 0.00 -0.00 -0.05 -0.01 0.00 0.08

17 7 0.00 -0.09 -0.00 -0.01 -0.00 0.08 -0.01 0.00 0.07

18 6 -0.08 -0.08 0.00 0.00 0.00 0.00 -0.01 0.01 0.14

19 6 -0.07 -0.04 -0.01 -0.00 0.00 0.05 -0.00 0.01 0.07

20 6 -0.02 -0.02 -0.01 -0.00 0.01 0.17 -0.00 -0.01 -0.08

21 6 -0.02 0.02 0.01 -0.00 0.01 0.08 -0.00 -0.01 -0.18

22 6 -0.07 0.04 0.01 -0.00 -0.01 -0.08 -0.00 -0.00 -0.05

23 7 -0.09 0.00 0.00 -0.00 -0.01 -0.07 -0.00 0.01 0.08

24 6 -0.08 0.08 0.00 -0.01 -0.01 -0.14 0.00 -0.00 0.00

25 6 0.09 0.09 -0.00 0.00 0.00 -0.00 -0.00 0.00 -0.12

26 6 0.11 0.08 -0.01 -0.01 0.02 0.01 0.04 0.05 -0.08

27 6 0.11 0.08 -0.01 -0.02 0.02 0.02 0.05 0.04 0.01

28 6 0.10 0.10 0.00 0.00 0.00 0.00 0.01 -0.01 0.05

29 6 0.08 0.11 0.01 0.02 -0.02 -0.02 -0.04 -0.05 0.01

30 6 0.08 0.11 0.01 0.02 -0.01 -0.01 -0.05 -0.04 -0.08

31 6 0.10 -0.10 0.00 0.01 0.01 -0.05 0.00 -0.00 0.00

32 6 0.11 -0.08 0.01 0.05 -0.04 -0.01 -0.02 -0.02 -0.02

33 6 0.11 -0.08 0.01 0.04 -0.05 0.08 -0.01 -0.02 -0.01

34 6 0.09 -0.09 -0.00 -0.00 -0.00 0.12 0.00 -0.00 -0.00

35 6 0.08 -0.11 -0.01 -0.05 0.04 0.08 0.02 0.01 0.01

36 6 0.08 -0.11 -0.01 -0.04 0.05 -0.01 0.02 0.02 0.02

37 6 -0.09 0.09 0.00 -0.00 -0.00 -0.12 0.00 -0.00 0.00

38 6 -0.08 0.11 -0.01 -0.05 0.04 -0.08 0.02 0.01 -0.01

39 6 -0.08 0.11 -0.01 -0.04 0.05 0.01 0.02 0.02 -0.02

40 6 -0.10 0.10 0.00 0.01 0.01 0.05 0.00 -0.00 -0.00

41 6 -0.11 0.08 0.01 0.05 -0.04 0.01 -0.02 -0.02 0.02

42 6 -0.11 0.08 0.01 0.04 -0.05 -0.08 -0.01 -0.02 0.01

43 6 -0.09 -0.09 0.00 0.00 0.00 0.00 -0.00 0.00 0.12

44 6 -0.08 -0.11 0.01 0.02 -0.01 0.01 -0.05 -0.04 0.08

45 6 -0.08 -0.11 0.01 0.02 -0.02 0.02 -0.04 -0.05 -0.01

46 6 -0.10 -0.10 -0.00 0.00 0.00 -0.00 0.01 -0.01 -0.05

47 6 -0.11 -0.08 -0.01 -0.02 0.02 -0.02 0.05 0.04 -0.01

48 6 -0.11 -0.08 -0.01 -0.01 0.02 -0.01 0.04 0.05 0.08

49 1 -0.00 -0.05 0.02 0.01 0.02 -0.12 -0.00 -0.03 0.31

50 1 -0.00 0.05 -0.02 -0.00 0.03 -0.30 0.01 -0.02 0.13

51 1 -0.05 -0.00 -0.02 0.02 0.01 0.13 0.03 0.00 0.30

52 1 0.05 -0.00 0.02 0.03 -0.00 0.31 0.02 -0.01 0.12

53 1 0.05 0.00 -0.02 0.02 0.01 -0.13 0.03 0.00 -0.30

54 1 -0.05 0.00 0.02 0.03 -0.00 -0.31 0.02 -0.01 -0.12

55 1 0.00 -0.05 -0.02 -0.00 0.03 0.30 0.01 -0.02 -0.13

56 1 0.00 0.05 0.02 0.01 0.02 0.12 -0.00 -0.03 -0.31

57 1 0.12 0.07 -0.02 -0.02 0.03 0.01 0.08 0.09 -0.11

58 1 0.12 0.06 -0.02 -0.03 0.04 0.03 0.09 0.08 0.04

59 1 0.10 0.10 0.00 0.00 0.00 0.00 0.01 -0.01 0.12

60 1 0.06 0.12 0.02 0.04 -0.04 -0.03 -0.08 -0.09 0.05

61 1 0.07 0.12 0.02 0.03 -0.02 -0.02 -0.09 -0.07 -0.11

62 1 0.10 -0.10 0.00 0.01 0.01 -0.12 0.00 -0.00 0.00

63 1 0.12 -0.06 0.02 0.09 -0.08 -0.05 -0.04 -0.04 -0.03

64 1 0.12 -0.07 0.02 0.07 -0.09 0.11 -0.02 -0.03 -0.02

65 1 0.07 -0.12 -0.02 -0.09 0.08 0.11 0.03 0.02 0.01

66 1 0.06 -0.12 -0.02 -0.08 0.09 -0.04 0.04 0.03 0.03

67 1 -0.07 0.12 -0.02 -0.09 0.08 -0.11 0.03 0.02 -0.01

68 1 -0.06 0.12 -0.02 -0.08 0.09 0.04 0.04 0.03 -0.03

69 1 -0.10 0.10 -0.00 0.01 0.01 0.12 0.00 -0.00 -0.00

70 1 -0.12 0.06 0.02 0.09 -0.08 0.05 -0.04 -0.04 0.03

71 1 -0.12 0.07 0.02 0.07 -0.09 -0.11 -0.02 -0.03 0.02

72 1 -0.07 -0.12 0.02 0.03 -0.02 0.02 -0.09 -0.07 0.11

73 1 -0.06 -0.12 0.02 0.04 -0.04 0.03 -0.08 -0.09 -0.05

74 1 -0.10 -0.10 -0.00 0.00 0.00 -0.00 0.01 -0.01 -0.12

75 1 -0.12 -0.06 -0.02 -0.03 0.04 -0.03 0.09 0.08 -0.04

76 1 -0.12 -0.07 -0.02 -0.02 0.03 -0.01 0.08 0.09 0.11

77 30 -0.00 0.00 -0.00 -0.01 -0.01 -0.00 -0.01 0.01 -0.00

19 20 21

B2 A1 E

Frequencies -- 199.2900 201.3463 214.4038

Red. masses -- 6.2754 6.8677 10.0673

Frc consts -- 0.1468 0.1640 0.2727

IR Inten -- 31.9059 0.0000 11.5515

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.05 0.11 -0.00 0.03 0.01 0.02 0.07 0.01

2 6 -0.00 -0.03 -0.02 -0.02 0.03 0.03 -0.00 0.08 -0.03

3 7 0.00 -0.03 -0.05 -0.00 0.03 0.04 -0.02 0.09 -0.09

4 6 0.00 -0.03 -0.02 0.02 0.03 0.03 -0.01 0.04 -0.06

5 6 0.00 -0.05 0.11 0.00 0.03 0.01 0.02 0.05 -0.01

6 6 0.01 -0.01 -0.10 0.05 0.05 -0.00 -0.05 -0.04 0.00

7 6 0.03 -0.00 -0.02 0.03 0.02 -0.03 0.02 -0.01 0.05

8 7 0.03 -0.00 -0.05 0.03 -0.00 -0.04 0.07 -0.02 0.08

9 6 0.03 0.00 -0.02 0.03 -0.02 -0.03 0.08 -0.01 0.02

10 6 0.05 0.00 0.11 0.03 -0.00 -0.01 0.07 0.02 -0.01

11 6 0.05 -0.00 0.11 0.03 0.00 -0.01 0.04 0.03 0.01

12 6 -0.01 -0.01 -0.10 -0.05 0.05 -0.00 0.02 0.02 0.02

13 6 -0.03 -0.00 -0.02 -0.03 0.02 -0.03 0.08 -0.01 -0.02

14 6 -0.05 -0.00 0.11 -0.03 0.00 -0.01 0.07 0.02 0.01

15 6 -0.05 0.00 0.11 -0.03 -0.00 -0.01 0.04 0.03 -0.01

16 6 -0.03 0.00 -0.02 -0.03 -0.02 -0.03 0.02 -0.01 -0.05

17 7 -0.03 -0.00 -0.05 -0.03 -0.00 -0.04 0.07 -0.02 -0.08

18 6 -0.01 0.01 -0.10 -0.05 -0.05 -0.00 -0.05 -0.04 -0.00

19 6 -0.00 0.03 -0.02 -0.02 -0.03 0.03 -0.01 0.04 0.06

20 6 -0.00 0.05 0.11 -0.00 -0.03 0.01 0.02 0.05 0.01

21 6 0.00 0.05 0.11 0.00 -0.03 0.01 0.02 0.07 -0.01

22 6 0.00 0.03 -0.02 0.02 -0.03 0.03 -0.00 0.08 0.03

23 7 0.00 0.03 -0.05 -0.00 -0.03 0.04 -0.02 0.09 0.09

24 6 0.01 0.01 -0.10 0.05 -0.05 -0.00 0.02 0.02 -0.02

25 6 0.00 -0.00 -0.11 0.07 0.07 -0.00 -0.09 -0.08 0.00

26 6 0.04 0.03 -0.08 0.11 0.09 0.01 -0.13 -0.11 -0.00

27 6 0.04 0.04 -0.00 0.11 0.10 0.00 -0.14 -0.12 -0.01

28 6 -0.00 0.00 0.04 0.11 0.11 0.00 -0.14 -0.14 -0.00

29 6 -0.04 -0.04 -0.00 0.10 0.11 -0.00 -0.11 -0.13 0.01

30 6 -0.03 -0.04 -0.08 0.09 0.11 -0.01 -0.11 -0.12 0.01

31 6 0.00 0.00 0.04 -0.11 0.11 0.00 0.01 -0.02 -0.03

32 6 -0.04 0.04 -0.00 -0.11 0.10 0.00 0.03 -0.03 -0.00

33 6 -0.04 0.03 -0.08 -0.11 0.09 0.01 0.04 -0.02 0.04

34 6 -0.00 -0.00 -0.11 -0.07 0.07 -0.00 0.01 -0.00 0.06

35 6 0.03 -0.04 -0.08 -0.09 0.11 -0.01 0.00 0.01 0.05

36 6 0.04 -0.04 -0.00 -0.10 0.11 -0.00 -0.00 0.01 0.00

37 6 0.00 0.00 -0.11 0.07 -0.07 -0.00 0.01 -0.00 -0.06

38 6 -0.03 0.04 -0.08 0.09 -0.11 -0.01 0.00 0.01 -0.05

39 6 -0.04 0.04 -0.00 0.10 -0.11 -0.00 -0.00 0.01 -0.00

40 6 -0.00 -0.00 0.04 0.11 -0.11 0.00 0.01 -0.02 0.03

41 6 0.04 -0.04 -0.00 0.11 -0.10 0.00 0.03 -0.03 0.00

42 6 0.04 -0.03 -0.08 0.11 -0.09 0.01 0.04 -0.02 -0.04

43 6 -0.00 0.00 -0.11 -0.07 -0.07 -0.00 -0.09 -0.08 -0.00

44 6 0.03 0.04 -0.08 -0.09 -0.11 -0.01 -0.11 -0.12 -0.01

45 6 0.04 0.04 -0.00 -0.10 -0.11 -0.00 -0.11 -0.13 -0.01

46 6 0.00 -0.00 0.04 -0.11 -0.11 0.00 -0.14 -0.14 0.00

47 6 -0.04 -0.04 -0.00 -0.11 -0.10 0.00 -0.14 -0.12 0.01

48 6 -0.04 -0.03 -0.08 -0.11 -0.09 0.01 -0.13 -0.11 0.00

49 1 -0.00 -0.06 0.19 0.00 0.04 -0.01 0.04 0.08 0.06

50 1 0.00 -0.06 0.19 -0.00 0.04 -0.01 0.04 0.03 0.02

51 1 0.06 0.00 0.19 0.04 0.00 0.01 0.08 0.05 -0.06

52 1 0.06 -0.00 0.19 0.04 -0.00 0.01 0.02 0.04 -0.01

53 1 -0.06 -0.00 0.19 -0.04 -0.00 0.01 0.08 0.05 0.06

54 1 -0.06 0.00 0.19 -0.04 0.00 0.01 0.02 0.04 0.01

55 1 -0.00 0.06 0.19 0.00 -0.04 -0.01 0.04 0.03 -0.02

56 1 0.00 0.06 0.19 -0.00 -0.04 -0.01 0.04 0.08 -0.06

57 1 0.07 0.07 -0.11 0.12 0.11 -0.01 -0.15 -0.13 0.01

58 1 0.08 0.07 0.03 0.11 0.09 -0.00 -0.13 -0.11 0.00

59 1 -0.01 0.01 0.11 0.11 0.11 0.00 -0.14 -0.14 -0.01

60 1 -0.07 -0.08 0.03 0.09 0.11 0.00 -0.10 -0.12 -0.01

61 1 -0.07 -0.07 -0.11 0.11 0.12 0.01 -0.13 -0.14 -0.00

62 1 0.01 0.01 0.11 -0.11 0.11 0.00 -0.01 -0.03 -0.06

63 1 -0.08 0.07 0.03 -0.11 0.09 -0.00 0.05 -0.04 -0.02

64 1 -0.07 0.07 -0.11 -0.12 0.11 -0.01 0.06 -0.03 0.06

65 1 0.07 -0.07 -0.11 -0.11 0.12 0.01 -0.01 0.03 0.06

66 1 0.07 -0.08 0.03 -0.09 0.11 0.00 -0.02 0.03 -0.02

67 1 -0.07 0.07 -0.11 0.11 -0.12 0.01 -0.01 0.03 -0.06

68 1 -0.07 0.08 0.03 0.09 -0.11 0.00 -0.02 0.03 0.02

69 1 -0.01 -0.01 0.11 0.11 -0.11 0.00 -0.01 -0.03 0.06

70 1 0.08 -0.07 0.03 0.11 -0.09 -0.00 0.05 -0.04 0.02

71 1 0.07 -0.07 -0.11 0.12 -0.11 -0.01 0.06 -0.03 -0.06

72 1 0.07 0.07 -0.11 -0.11 -0.12 0.01 -0.13 -0.14 0.00

73 1 0.07 0.08 0.03 -0.09 -0.11 0.00 -0.10 -0.12 0.01

74 1 0.01 -0.01 0.11 -0.11 -0.11 0.00 -0.14 -0.14 0.01

75 1 -0.08 -0.07 0.03 -0.11 -0.09 -0.00 -0.13 -0.11 -0.00

76 1 -0.07 -0.07 -0.11 -0.12 -0.11 -0.01 -0.15 -0.13 -0.01

77 30 0.00 0.00 0.16 0.00 0.00 0.00 0.15 0.18 -0.00

22 23 24

E E E

Frequencies -- 214.4038 221.3076 221.3076

Red. masses -- 10.0673 6.5273 6.5273

Frc consts -- 0.2727 0.1884 0.1884

IR Inten -- 11.5515 0.1386 0.1386

Atom AN X Y Z X Y Z X Y Z

1 6 0.03 -0.04 0.01 0.00 0.06 -0.00 0.02 -0.02 0.04

2 6 -0.01 -0.02 0.05 -0.01 0.04 0.13 0.02 -0.02 -0.02

3 7 -0.02 -0.07 0.08 0.01 0.05 0.24 0.02 -0.02 -0.08

4 6 -0.01 -0.08 0.02 0.02 0.04 0.12 0.01 -0.00 -0.06

5 6 0.02 -0.07 -0.01 0.01 0.06 -0.03 0.02 -0.01 -0.03

6 6 0.02 -0.02 -0.02 0.01 -0.01 0.01 0.01 -0.00 0.00

7 6 0.08 0.00 0.03 -0.02 -0.02 0.02 -0.04 -0.01 0.13

8 7 0.09 0.02 0.09 -0.02 -0.02 0.08 -0.05 0.01 0.24

9 6 0.04 0.01 0.06 -0.00 -0.01 0.06 -0.04 0.02 0.12

10 6 0.05 -0.02 0.01 -0.01 -0.02 0.03 -0.06 0.01 -0.03

11 6 0.07 -0.02 -0.01 -0.02 -0.02 -0.04 -0.06 0.00 -0.00

12 6 -0.04 0.05 0.00 -0.00 -0.01 0.00 0.01 0.01 -0.01

13 6 0.04 0.01 -0.06 -0.00 -0.01 -0.06 -0.04 0.02 -0.12

14 6 0.05 -0.02 -0.01 -0.01 -0.02 -0.03 -0.06 0.01 0.03

15 6 0.07 -0.02 0.01 -0.02 -0.02 0.04 -0.06 0.00 0.00

16 6 0.08 0.00 -0.03 -0.02 -0.02 -0.02 -0.04 -0.01 -0.13

17 7 0.09 0.02 -0.09 -0.02 -0.02 -0.08 -0.05 0.01 -0.24

18 6 0.02 -0.02 0.02 0.01 -0.01 -0.01 0.01 -0.00 -0.00

19 6 -0.01 -0.08 -0.02 0.02 0.04 -0.12 0.01 -0.00 0.06

20 6 0.02 -0.07 0.01 0.01 0.06 0.03 0.02 -0.01 0.03

21 6 0.03 -0.04 -0.01 0.00 0.06 0.00 0.02 -0.02 -0.04

22 6 -0.01 -0.02 -0.05 -0.01 0.04 -0.13 0.02 -0.02 0.02

23 7 -0.02 -0.07 -0.08 0.01 0.05 -0.24 0.02 -0.02 0.08

24 6 -0.04 0.05 -0.00 -0.00 -0.01 -0.00 0.01 0.01 0.01

25 6 -0.00 -0.01 -0.06 0.07 -0.08 -0.09 0.04 -0.04 -0.04

26 6 0.01 -0.00 -0.05 0.10 -0.08 -0.09 0.06 -0.04 -0.04

27 6 0.01 0.00 -0.00 0.02 -0.00 -0.00 0.02 0.00 -0.00

28 6 -0.02 -0.01 0.03 -0.07 0.06 0.06 -0.03 0.04 0.03

29 6 -0.03 -0.03 0.00 -0.00 -0.03 -0.00 0.00 -0.01 -0.00

30 6 -0.02 -0.04 -0.04 0.08 -0.10 -0.09 0.05 -0.05 -0.05

31 6 -0.14 0.14 -0.00 0.04 0.03 0.03 -0.06 -0.07 -0.06

32 6 -0.13 0.11 0.01 -0.01 -0.00 -0.00 0.03 -0.00 0.00

33 6 -0.12 0.11 0.01 -0.05 -0.05 -0.05 0.10 0.08 0.09

34 6 -0.08 0.09 0.00 -0.04 -0.04 -0.04 0.08 0.07 0.09

35 6 -0.11 0.13 -0.00 -0.04 -0.06 -0.04 0.08 0.10 0.09

36 6 -0.12 0.14 -0.01 0.00 -0.02 -0.00 0.00 0.02 0.00

37 6 -0.08 0.09 -0.00 -0.04 -0.04 0.04 0.08 0.07 -0.09

38 6 -0.11 0.13 0.00 -0.04 -0.06 0.04 0.08 0.10 -0.09

39 6 -0.12 0.14 0.01 0.00 -0.02 0.00 0.00 0.02 -0.00

40 6 -0.14 0.14 0.00 0.04 0.03 -0.03 -0.06 -0.07 0.06

41 6 -0.13 0.11 -0.01 -0.01 -0.00 0.00 0.03 -0.00 -0.00

42 6 -0.12 0.11 -0.01 -0.05 -0.05 0.05 0.10 0.08 -0.09

43 6 -0.00 -0.01 0.06 0.07 -0.08 0.09 0.04 -0.04 0.04

44 6 -0.02 -0.04 0.04 0.08 -0.10 0.09 0.05 -0.05 0.05

45 6 -0.03 -0.03 -0.00 -0.00 -0.03 0.00 0.00 -0.01 0.00

46 6 -0.02 -0.01 -0.03 -0.07 0.06 -0.06 -0.03 0.04 -0.03

47 6 0.01 0.00 0.00 0.02 -0.00 0.00 0.02 0.00 0.00

48 6 0.01 -0.00 0.05 0.10 -0.08 0.09 0.06 -0.04 0.04

49 1 0.04 -0.02 -0.01 0.01 0.07 -0.12 0.02 -0.03 0.11

50 1 0.05 -0.08 -0.06 0.01 0.08 -0.16 0.02 -0.02 -0.01

51 1 0.03 -0.04 -0.02 -0.02 -0.02 0.01 -0.08 0.01 -0.16

52 1 0.08 -0.04 -0.06 -0.03 -0.02 -0.11 -0.07 0.01 -0.12

53 1 0.03 -0.04 0.02 -0.02 -0.02 -0.01 -0.08 0.01 0.16

54 1 0.08 -0.04 0.06 -0.03 -0.02 0.11 -0.07 0.01 0.12

55 1 0.05 -0.08 0.06 0.01 0.08 0.16 0.02 -0.02 0.01

56 1 0.04 -0.02 0.01 0.01 0.07 0.12 0.02 -0.03 -0.11

57 1 0.03 0.01 -0.06 0.14 -0.10 -0.12 0.08 -0.05 -0.06

58 1 0.03 0.02 0.02 0.01 0.03 0.02 0.01 0.02 0.01

59 1 -0.03 0.01 0.06 -0.17 0.16 0.15 -0.08 0.09 0.08

60 1 -0.04 -0.05 0.02 -0.03 -0.02 0.02 -0.02 0.00 0.01

61 1 -0.03 -0.06 -0.06 0.10 -0.14 -0.12 0.06 -0.06 -0.06

62 1 -0.14 0.14 -0.01 0.09 0.08 0.08 -0.16 -0.17 -0.15

63 1 -0.12 0.10 -0.01 0.00 0.02 0.01 0.02 -0.03 -0.02

64 1 -0.14 0.13 -0.00 -0.06 -0.06 -0.06 0.14 0.10 0.12

65 1 -0.13 0.15 0.01 -0.05 -0.08 -0.06 0.10 0.14 0.12

66 1 -0.11 0.13 0.00 0.02 -0.01 0.01 -0.03 0.01 -0.02

67 1 -0.13 0.15 -0.01 -0.05 -0.08 0.06 0.10 0.14 -0.12

68 1 -0.11 0.13 -0.00 0.02 -0.01 -0.01 -0.03 0.01 0.02

69 1 -0.14 0.14 0.01 0.09 0.08 -0.08 -0.16 -0.17 0.15

70 1 -0.12 0.10 0.01 0.00 0.02 -0.01 0.02 -0.03 0.02

71 1 -0.14 0.13 0.00 -0.06 -0.06 0.06 0.14 0.10 -0.12

72 1 -0.03 -0.06 0.06 0.10 -0.14 0.12 0.06 -0.06 0.06

73 1 -0.04 -0.05 -0.02 -0.03 -0.02 -0.02 -0.02 0.00 -0.01

74 1 -0.03 0.01 -0.06 -0.17 0.16 -0.15 -0.08 0.09 -0.08

75 1 0.03 0.02 -0.02 0.01 0.03 -0.02 0.01 0.02 -0.01

76 1 0.03 0.01 0.06 0.14 -0.10 0.12 0.08 -0.05 0.06

77 30 0.18 -0.15 0.00 -0.03 0.08 -0.00 -0.08 -0.03 -0.00

25 26 27

B2 E E

Frequencies -- 222.1289 227.1882 227.1882

Red. masses -- 7.9187 6.2063 6.2063

Frc consts -- 0.2302 0.1887 0.1887

IR Inten -- 1.1739 0.9583 0.9583

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.16 0.04 -0.08 -0.03 0.04 0.01 -0.02 0.02

2 6 0.01 0.14 0.04 -0.04 -0.03 0.02 -0.02 0.00 -0.09

3 7 -0.00 0.14 0.06 -0.02 0.00 -0.03 0.00 0.02 -0.18

4 6 -0.01 0.14 0.04 -0.03 0.03 -0.05 0.03 -0.01 -0.08

5 6 0.00 0.16 0.04 -0.08 0.02 -0.03 0.02 -0.03 0.04

6 6 -0.05 0.05 -0.01 -0.01 0.04 -0.01 0.05 -0.03 0.02

7 6 -0.14 0.01 0.04 0.00 0.02 0.09 0.03 -0.04 0.02

8 7 -0.14 0.00 0.06 0.02 -0.00 0.18 -0.00 -0.02 -0.03

9 6 -0.14 -0.01 0.04 -0.01 -0.03 0.08 -0.03 -0.03 -0.05

10 6 -0.16 0.00 0.04 -0.03 -0.02 -0.04 -0.02 -0.08 -0.03

11 6 -0.16 -0.00 0.04 -0.02 -0.01 -0.02 0.03 -0.08 0.04

12 6 0.05 0.05 -0.01 -0.03 -0.05 0.02 -0.04 -0.01 0.01

13 6 0.14 0.01 0.04 -0.01 -0.03 -0.08 -0.03 -0.03 0.05

14 6 0.16 -0.00 0.04 -0.03 -0.02 0.04 -0.02 -0.08 0.03

15 6 0.16 0.00 0.04 -0.02 -0.01 0.02 0.03 -0.08 -0.04

16 6 0.14 -0.01 0.04 0.00 0.02 -0.09 0.03 -0.04 -0.02

17 7 0.14 0.00 0.06 0.02 -0.00 -0.18 -0.00 -0.02 0.03

18 6 0.05 -0.05 -0.01 -0.01 0.04 0.01 0.05 -0.03 -0.02

19 6 0.01 -0.14 0.04 -0.03 0.03 0.05 0.03 -0.01 0.08

20 6 -0.00 -0.16 0.04 -0.08 0.02 0.03 0.02 -0.03 -0.04

21 6 0.00 -0.16 0.04 -0.08 -0.03 -0.04 0.01 -0.02 -0.02

22 6 -0.01 -0.14 0.04 -0.04 -0.03 -0.02 -0.02 0.00 0.09

23 7 -0.00 -0.14 0.06 -0.02 0.00 0.03 0.00 0.02 0.18

24 6 -0.05 -0.05 -0.01 -0.03 -0.05 -0.02 -0.04 -0.01 -0.01

25 6 0.01 -0.01 -0.08 -0.03 0.09 -0.03 0.10 -0.06 0.04

26 6 0.04 0.00 -0.07 0.01 0.12 -0.01 0.09 -0.09 0.02

27 6 0.02 0.02 -0.00 0.07 0.07 -0.00 0.02 -0.01 0.00

28 6 -0.02 0.02 0.04 0.09 0.01 -0.01 -0.02 0.09 0.02

29 6 -0.02 -0.02 -0.00 0.01 0.04 -0.00 0.07 0.06 0.00

30 6 -0.00 -0.04 -0.07 -0.04 0.09 -0.01 0.14 -0.02 0.01

31 6 0.02 0.02 0.04 0.09 0.02 0.02 -0.01 0.09 0.01

32 6 -0.02 0.02 -0.00 0.06 -0.07 0.00 -0.04 0.01 0.00

33 6 -0.04 0.00 -0.07 -0.02 -0.14 0.01 -0.09 -0.04 0.01

34 6 -0.01 -0.01 -0.08 -0.06 -0.10 0.04 -0.09 -0.03 0.03

35 6 0.00 -0.04 -0.07 -0.09 -0.09 0.02 -0.12 0.01 0.01

36 6 0.02 -0.02 -0.00 -0.01 -0.02 0.00 -0.07 0.07 0.00

37 6 0.01 0.01 -0.08 -0.06 -0.10 -0.04 -0.09 -0.03 -0.03

38 6 -0.00 0.04 -0.07 -0.09 -0.09 -0.02 -0.12 0.01 -0.01

39 6 -0.02 0.02 -0.00 -0.01 -0.02 -0.00 -0.07 0.07 -0.00

40 6 -0.02 -0.02 0.04 0.09 0.02 -0.02 -0.01 0.09 -0.01

41 6 0.02 -0.02 -0.00 0.06 -0.07 -0.00 -0.04 0.01 -0.00

42 6 0.04 -0.00 -0.07 -0.02 -0.14 -0.01 -0.09 -0.04 -0.01

43 6 -0.01 0.01 -0.08 -0.03 0.09 0.03 0.10 -0.06 -0.04

44 6 0.00 0.04 -0.07 -0.04 0.09 0.01 0.14 -0.02 -0.01

45 6 0.02 0.02 -0.00 0.01 0.04 0.00 0.07 0.06 -0.00

46 6 0.02 -0.02 0.04 0.09 0.01 0.01 -0.02 0.09 -0.02

47 6 -0.02 -0.02 -0.00 0.07 0.07 0.00 0.02 -0.01 -0.00

48 6 -0.04 -0.00 -0.07 0.01 0.12 0.01 0.09 -0.09 -0.02

49 1 -0.01 0.15 0.04 -0.10 -0.05 0.09 0.02 -0.02 0.11

50 1 0.01 0.15 0.04 -0.10 0.04 -0.05 0.02 -0.04 0.13

51 1 -0.15 0.01 0.04 -0.04 -0.02 -0.13 -0.04 -0.10 -0.05

52 1 -0.15 -0.01 0.04 -0.02 -0.02 -0.11 0.05 -0.10 0.09

53 1 0.15 -0.01 0.04 -0.04 -0.02 0.13 -0.04 -0.10 0.05

54 1 0.15 0.01 0.04 -0.02 -0.02 0.11 0.05 -0.10 -0.09

55 1 -0.01 -0.15 0.04 -0.10 0.04 0.05 0.02 -0.04 -0.13

56 1 0.01 -0.15 0.04 -0.10 -0.05 -0.09 0.02 -0.02 -0.11

57 1 0.06 0.02 -0.09 0.02 0.17 -0.02 0.10 -0.14 0.01

58 1 0.04 0.05 0.02 0.11 0.06 -0.00 -0.03 -0.03 -0.01

59 1 -0.06 0.06 0.10 0.15 -0.04 -0.02 -0.10 0.17 0.03

60 1 -0.05 -0.04 0.02 -0.00 0.00 0.01 0.07 0.11 -0.00

61 1 -0.02 -0.06 -0.09 -0.08 0.10 -0.01 0.21 -0.02 0.02

62 1 0.06 0.06 0.10 0.17 0.10 0.03 0.04 0.15 0.02

63 1 -0.04 0.05 0.02 0.11 -0.07 -0.00 -0.00 -0.00 -0.01

64 1 -0.06 0.02 -0.09 -0.02 -0.21 0.02 -0.10 -0.08 0.01

65 1 0.02 -0.06 -0.09 -0.14 -0.10 0.01 -0.17 0.02 0.02

66 1 0.05 -0.04 0.02 -0.03 0.03 -0.01 -0.06 0.11 0.00

67 1 -0.02 0.06 -0.09 -0.14 -0.10 -0.01 -0.17 0.02 -0.02

68 1 -0.05 0.04 0.02 -0.03 0.03 0.01 -0.06 0.11 -0.00

69 1 -0.06 -0.06 0.10 0.17 0.10 -0.03 0.04 0.15 -0.02

70 1 0.04 -0.05 0.02 0.11 -0.07 0.00 -0.00 -0.00 0.01

71 1 0.06 -0.02 -0.09 -0.02 -0.21 -0.02 -0.10 -0.08 -0.01

72 1 0.02 0.06 -0.09 -0.08 0.10 0.01 0.21 -0.02 -0.02

73 1 0.05 0.04 0.02 -0.00 0.00 -0.01 0.07 0.11 0.00

74 1 0.06 -0.06 0.10 0.15 -0.04 0.02 -0.10 0.17 -0.03

75 1 -0.04 -0.05 0.02 0.11 0.06 0.00 -0.03 -0.03 0.01

76 1 -0.06 -0.02 -0.09 0.02 0.17 0.02 0.10 -0.14 -0.01

77 30 0.00 -0.00 -0.04 0.09 0.01 -0.00 -0.01 0.09 0.00

28 29 30

A1 B2 B2

Frequencies -- 234.8877 242.1516 271.1972

Red. masses -- 7.6761 5.0841 7.3508

Frc consts -- 0.2495 0.1756 0.3185

IR Inten -- 0.0000 6.4209 36.5718

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.02 -0.06 0.00 0.04 0.00 -0.00 0.05 0.01

2 6 -0.00 0.00 0.14 0.01 0.04 -0.04 -0.00 0.05 -0.09

3 7 0.00 -0.00 0.29 0.00 0.04 -0.05 0.00 0.06 -0.18

4 6 0.00 0.00 0.14 -0.01 0.04 -0.04 0.00 0.05 -0.09

5 6 0.00 0.02 -0.06 -0.00 0.04 0.00 0.00 0.05 0.01

6 6 -0.01 -0.01 -0.00 -0.03 0.03 -0.02 -0.00 0.00 0.00

7 6 0.00 0.00 -0.14 -0.04 0.01 -0.04 -0.05 -0.00 -0.09

8 7 -0.00 0.00 -0.29 -0.04 -0.00 -0.05 -0.06 -0.00 -0.18

9 6 0.00 -0.00 -0.14 -0.04 -0.01 -0.04 -0.05 0.00 -0.09

10 6 0.02 -0.00 0.06 -0.04 -0.00 0.00 -0.05 0.00 0.01

11 6 0.02 0.00 0.06 -0.04 0.00 0.00 -0.05 -0.00 0.01

12 6 0.01 -0.01 -0.00 0.03 0.03 -0.02 0.00 0.00 0.00

13 6 -0.00 0.00 -0.14 0.04 0.01 -0.04 0.05 -0.00 -0.09

14 6 -0.02 0.00 0.06 0.04 0.00 0.00 0.05 -0.00 0.01

15 6 -0.02 -0.00 0.06 0.04 -0.00 0.00 0.05 0.00 0.01

16 6 -0.00 -0.00 -0.14 0.04 -0.01 -0.04 0.05 0.00 -0.09

17 7 0.00 0.00 -0.29 0.04 -0.00 -0.05 0.06 0.00 -0.18

18 6 0.01 0.01 0.00 0.03 -0.03 -0.02 0.00 -0.00 0.00

19 6 -0.00 -0.00 0.14 0.01 -0.04 -0.04 -0.00 -0.05 -0.09

20 6 -0.00 -0.02 -0.06 0.00 -0.04 0.00 -0.00 -0.05 0.01

21 6 0.00 -0.02 -0.06 -0.00 -0.04 0.00 0.00 -0.05 0.01

22 6 0.00 -0.00 0.14 -0.01 -0.04 -0.04 0.00 -0.05 -0.09

23 7 0.00 0.00 0.29 0.00 -0.04 -0.05 0.00 -0.06 -0.18

24 6 -0.01 0.01 -0.00 -0.03 -0.03 -0.02 -0.00 -0.00 0.00

25 6 -0.01 -0.01 0.00 -0.08 0.08 0.02 0.05 -0.05 0.09

26 6 -0.02 -0.01 0.00 -0.09 0.11 0.05 0.02 -0.10 0.05

27 6 -0.03 -0.01 0.01 -0.01 0.03 0.00 -0.03 -0.05 -0.00

28 6 -0.02 -0.02 -0.00 0.07 -0.07 -0.05 -0.04 0.04 -0.01

29 6 -0.01 -0.03 -0.01 -0.03 0.01 0.00 0.05 0.03 -0.00

30 6 -0.01 -0.02 -0.00 -0.11 0.09 0.05 0.10 -0.02 0.05

31 6 0.02 -0.02 -0.00 -0.07 -0.07 -0.05 0.04 0.04 -0.01

32 6 0.03 -0.01 0.01 0.01 0.03 0.00 0.03 -0.05 -0.00

33 6 0.02 -0.01 0.00 0.09 0.11 0.05 -0.02 -0.10 0.05

34 6 0.01 -0.01 0.00 0.08 0.08 0.02 -0.05 -0.05 0.09

35 6 0.01 -0.02 -0.00 0.11 0.09 0.05 -0.10 -0.02 0.05

36 6 0.01 -0.03 -0.01 0.03 0.01 0.00 -0.05 0.03 -0.00

37 6 -0.01 0.01 0.00 -0.08 -0.08 0.02 0.05 0.05 0.09

38 6 -0.01 0.02 -0.00 -0.11 -0.09 0.05 0.10 0.02 0.05

39 6 -0.01 0.03 -0.01 -0.03 -0.01 0.00 0.05 -0.03 -0.00

40 6 -0.02 0.02 -0.00 0.07 0.07 -0.05 -0.04 -0.04 -0.01

41 6 -0.03 0.01 0.01 -0.01 -0.03 0.00 -0.03 0.05 -0.00

42 6 -0.02 0.01 0.00 -0.09 -0.11 0.05 0.02 0.10 0.05

43 6 0.01 0.01 0.00 0.08 -0.08 0.02 -0.05 0.05 0.09

44 6 0.01 0.02 -0.00 0.11 -0.09 0.05 -0.10 0.02 0.05

45 6 0.01 0.03 -0.01 0.03 -0.01 0.00 -0.05 -0.03 -0.00

46 6 0.02 0.02 -0.00 -0.07 0.07 -0.05 0.04 -0.04 -0.01

47 6 0.03 0.01 0.01 0.01 -0.03 0.00 0.03 0.05 -0.00

48 6 0.02 0.01 0.00 0.09 -0.11 0.05 -0.02 0.10 0.05

49 1 0.00 0.05 -0.23 0.00 0.04 0.03 -0.00 0.04 0.08

50 1 -0.00 0.05 -0.23 -0.00 0.04 0.03 0.00 0.04 0.08

51 1 0.05 0.00 0.23 -0.04 -0.00 0.03 -0.04 0.00 0.08

52 1 0.05 -0.00 0.23 -0.04 0.00 0.03 -0.04 -0.00 0.08

53 1 -0.05 -0.00 0.23 0.04 0.00 0.03 0.04 -0.00 0.08

54 1 -0.05 0.00 0.23 0.04 -0.00 0.03 0.04 0.00 0.08

55 1 0.00 -0.05 -0.23 0.00 -0.04 0.03 -0.00 -0.04 0.08

56 1 -0.00 -0.05 -0.23 -0.00 -0.04 0.03 0.00 -0.04 0.08

57 1 -0.03 -0.01 0.00 -0.12 0.15 0.07 0.02 -0.17 0.07

58 1 -0.04 0.00 0.01 0.02 0.01 -0.01 -0.09 -0.08 -0.03

59 1 -0.02 -0.02 -0.00 0.17 -0.17 -0.11 -0.10 0.10 -0.03

60 1 0.00 -0.04 -0.01 -0.01 -0.02 -0.01 0.08 0.09 -0.03

61 1 -0.01 -0.03 -0.00 -0.15 0.12 0.07 0.17 -0.02 0.07

62 1 0.02 -0.02 -0.00 -0.17 -0.17 -0.11 0.10 0.10 -0.03

63 1 0.04 0.00 0.01 -0.02 0.01 -0.01 0.09 -0.08 -0.03

64 1 0.03 -0.01 0.00 0.12 0.15 0.07 -0.02 -0.17 0.07

65 1 0.01 -0.03 -0.00 0.15 0.12 0.07 -0.17 -0.02 0.07

66 1 -0.00 -0.04 -0.01 0.01 -0.02 -0.01 -0.08 0.09 -0.03

67 1 -0.01 0.03 -0.00 -0.15 -0.12 0.07 0.17 0.02 0.07

68 1 0.00 0.04 -0.01 -0.01 0.02 -0.01 0.08 -0.09 -0.03

69 1 -0.02 0.02 -0.00 0.17 0.17 -0.11 -0.10 -0.10 -0.03

70 1 -0.04 -0.00 0.01 0.02 -0.01 -0.01 -0.09 0.08 -0.03

71 1 -0.03 0.01 0.00 -0.12 -0.15 0.07 0.02 0.17 0.07

72 1 0.01 0.03 -0.00 0.15 -0.12 0.07 -0.17 0.02 0.07

73 1 -0.00 0.04 -0.01 0.01 0.02 -0.01 -0.08 -0.09 -0.03

74 1 0.02 0.02 -0.00 -0.17 0.17 -0.11 0.10 -0.10 -0.03

75 1 0.04 -0.00 0.01 -0.02 -0.01 -0.01 0.09 0.08 -0.03

76 1 0.03 0.01 0.00 0.12 -0.15 0.07 -0.02 0.17 0.07

77 30 0.00 -0.00 0.00 0.00 0.00 0.07 -0.00 0.00 0.13

31 32 33

A2 B1 E

Frequencies -- 289.3994 297.4552 309.2117

Red. masses -- 4.4032 4.8754 6.9158

Frc consts -- 0.2173 0.2542 0.3896

IR Inten -- 0.0000 0.0000 0.0071

Atom AN X Y Z X Y Z X Y Z

1 6 0.09 0.03 0.02 -0.01 -0.01 0.15 -0.14 -0.00 -0.04

2 6 0.03 0.04 0.03 -0.00 -0.01 0.14 -0.05 -0.02 -0.07

3 7 0.01 -0.00 0.00 -0.00 -0.00 -0.00 -0.03 0.02 -0.04

4 6 0.03 -0.04 -0.03 -0.00 0.01 -0.14 -0.07 0.08 0.03

5 6 0.09 -0.03 -0.02 -0.01 0.01 -0.15 -0.14 0.07 0.06

6 6 0.03 -0.03 -0.04 0.00 0.00 -0.00 -0.06 0.06 0.04

7 6 0.04 -0.03 -0.03 0.01 -0.00 0.14 -0.09 0.05 -0.02

8 7 -0.00 -0.01 -0.00 0.00 -0.00 0.00 -0.04 0.01 -0.09

9 6 -0.04 -0.03 0.03 -0.01 -0.00 -0.14 -0.04 0.01 -0.06

10 6 -0.03 -0.09 0.02 -0.01 -0.01 -0.15 -0.05 0.06 0.00

11 6 0.03 -0.09 -0.02 0.01 -0.01 0.15 -0.09 0.07 0.04

12 6 0.03 0.03 0.04 0.00 -0.00 0.00 -0.03 -0.01 -0.01

13 6 0.04 0.03 0.03 0.01 0.00 -0.14 -0.04 0.01 0.06

14 6 0.03 0.09 0.02 0.01 0.01 -0.15 -0.05 0.06 -0.00

15 6 -0.03 0.09 -0.02 -0.01 0.01 0.15 -0.09 0.07 -0.04

16 6 -0.04 0.03 -0.03 -0.01 0.00 0.14 -0.09 0.05 0.02

17 7 -0.00 0.01 0.00 0.00 0.00 -0.00 -0.04 0.01 0.09

18 6 -0.03 0.03 -0.04 -0.00 -0.00 -0.00 -0.06 0.06 -0.04

19 6 -0.03 0.04 -0.03 0.00 -0.01 -0.14 -0.07 0.08 -0.03

20 6 -0.09 0.03 -0.02 0.01 -0.01 -0.15 -0.14 0.07 -0.06

21 6 -0.09 -0.03 0.02 0.01 0.01 0.15 -0.14 -0.00 0.04

22 6 -0.03 -0.04 0.03 0.00 0.01 0.14 -0.05 -0.02 0.07

23 7 -0.01 -0.00 0.00 0.00 0.00 0.00 -0.03 0.02 0.04

24 6 -0.03 -0.03 0.04 -0.00 0.00 0.00 -0.03 -0.01 0.01

25 6 -0.04 0.04 0.01 -0.00 -0.00 -0.00 0.03 -0.02 0.01

26 6 -0.08 0.09 0.05 -0.00 -0.01 -0.00 0.08 -0.08 -0.03

27 6 -0.02 0.03 0.01 -0.01 0.00 0.01 0.03 -0.02 -0.01

28 6 0.06 -0.06 -0.05 -0.00 -0.00 -0.00 -0.05 0.08 0.05

29 6 -0.03 0.02 0.01 0.00 -0.01 -0.01 0.04 -0.00 -0.01

30 6 -0.09 0.08 0.05 -0.01 -0.00 0.00 0.10 -0.07 -0.04

31 6 0.06 0.06 0.05 -0.00 0.00 0.00 0.01 -0.06 -0.02

32 6 -0.02 -0.03 -0.01 -0.01 -0.00 -0.01 0.04 -0.01 0.00

33 6 -0.08 -0.09 -0.05 -0.00 0.01 0.00 0.05 0.01 0.01

34 6 -0.04 -0.04 -0.01 -0.00 0.00 -0.00 0.02 0.00 -0.00

35 6 -0.09 -0.08 -0.05 -0.01 0.00 -0.00 0.05 0.00 0.02

36 6 -0.03 -0.02 -0.01 0.00 0.01 0.01 0.03 -0.03 0.00

37 6 0.04 0.04 -0.01 0.00 -0.00 -0.00 0.02 0.00 0.00

38 6 0.09 0.08 -0.05 0.01 -0.00 -0.00 0.05 0.00 -0.02

39 6 0.03 0.02 -0.01 -0.00 -0.01 0.01 0.03 -0.03 -0.00

40 6 -0.06 -0.06 0.05 0.00 -0.00 0.00 0.01 -0.06 0.02

41 6 0.02 0.03 -0.01 0.01 0.00 -0.01 0.04 -0.01 -0.00

42 6 0.08 0.09 -0.05 0.00 -0.01 0.00 0.05 0.01 -0.01

43 6 0.04 -0.04 0.01 0.00 0.00 0.00 0.03 -0.02 -0.01

44 6 0.09 -0.08 0.05 0.01 0.00 0.00 0.10 -0.07 0.04

45 6 0.03 -0.02 0.01 -0.00 0.01 -0.01 0.04 -0.00 0.01

46 6 -0.06 0.06 -0.05 0.00 0.00 -0.00 -0.05 0.08 -0.05

47 6 0.02 -0.03 0.01 0.01 -0.00 0.01 0.03 -0.02 0.01

48 6 0.08 -0.09 0.05 0.00 0.01 -0.00 0.08 -0.08 0.03

49 1 0.12 0.05 0.02 -0.00 -0.03 0.28 -0.19 -0.04 -0.04

50 1 0.12 -0.05 -0.02 -0.00 0.03 -0.28 -0.18 0.09 0.11

51 1 -0.05 -0.12 0.02 -0.03 -0.00 -0.28 -0.02 0.10 0.04

52 1 0.05 -0.12 -0.02 0.03 -0.00 0.28 -0.09 0.07 0.11

53 1 0.05 0.12 0.02 0.03 0.00 -0.28 -0.02 0.10 -0.04

54 1 -0.05 0.12 -0.02 -0.03 0.00 0.28 -0.09 0.07 -0.11

55 1 -0.12 0.05 -0.02 0.00 -0.03 -0.28 -0.18 0.09 -0.11

56 1 -0.12 -0.05 0.02 0.00 0.03 0.28 -0.19 -0.04 0.04

57 1 -0.11 0.13 0.07 0.00 -0.01 -0.01 0.12 -0.13 -0.06

58 1 -0.01 0.02 0.01 -0.02 0.01 0.01 0.02 -0.03 -0.02

59 1 0.16 -0.16 -0.11 -0.00 -0.00 -0.00 -0.15 0.18 0.11

60 1 -0.02 0.01 0.01 0.01 -0.02 -0.01 0.04 0.00 -0.01

61 1 -0.13 0.11 0.07 -0.01 0.00 0.01 0.15 -0.10 -0.06

62 1 0.16 0.16 0.11 -0.00 0.00 0.00 -0.03 -0.09 -0.04

63 1 -0.01 -0.02 -0.01 -0.02 -0.01 -0.01 0.04 0.00 0.01

64 1 -0.11 -0.13 -0.07 0.00 0.01 0.01 0.07 0.02 0.02

65 1 -0.13 -0.11 -0.07 -0.01 -0.00 -0.01 0.08 0.01 0.02

66 1 -0.02 -0.01 -0.01 0.01 0.02 0.01 0.02 -0.03 -0.00

67 1 0.13 0.11 -0.07 0.01 0.00 -0.01 0.08 0.01 -0.02

68 1 0.02 0.01 -0.01 -0.01 -0.02 0.01 0.02 -0.03 0.00

69 1 -0.16 -0.16 0.11 0.00 -0.00 0.00 -0.03 -0.09 0.04

70 1 0.01 0.02 -0.01 0.02 0.01 -0.01 0.04 0.00 -0.01

71 1 0.11 0.13 -0.07 -0.00 -0.01 0.01 0.07 0.02 -0.02

72 1 0.13 -0.11 0.07 0.01 -0.00 0.01 0.15 -0.10 0.06

73 1 0.02 -0.01 0.01 -0.01 0.02 -0.01 0.04 0.00 0.01

74 1 -0.16 0.16 -0.11 0.00 0.00 -0.00 -0.15 0.18 -0.11

75 1 0.01 -0.02 0.01 0.02 -0.01 0.01 0.02 -0.03 0.02

76 1 0.11 -0.13 0.07 -0.00 0.01 -0.01 0.12 -0.13 0.06

77 30 0.00 0.00 -0.00 -0.00 0.00 -0.00 0.15 -0.07 -0.00

34 35 36

E E E

Frequencies -- 309.2117 326.1598 326.1598

Red. masses -- 6.9158 4.7699 4.7699

Frc consts -- 0.3896 0.2990 0.2990

IR Inten -- 0.0071 0.6665 0.6665

Atom AN X Y Z X Y Z X Y Z

1 6 -0.07 -0.09 -0.04 0.02 0.02 -0.16 0.01 0.03 -0.08

2 6 -0.05 -0.09 0.02 0.00 0.02 -0.15 0.00 0.03 -0.06

3 7 -0.01 -0.04 0.09 -0.01 -0.00 0.00 -0.00 0.01 -0.01

4 6 -0.01 -0.04 0.06 0.00 -0.03 0.15 0.00 0.01 0.05

5 6 -0.06 -0.05 -0.00 0.02 -0.03 0.17 0.01 0.01 0.04

6 6 0.01 -0.03 -0.01 0.00 -0.01 0.03 -0.00 0.00 -0.01

7 6 0.02 -0.05 -0.07 0.03 -0.00 0.06 -0.02 0.00 -0.15

8 7 -0.02 -0.03 -0.04 0.01 0.00 0.01 0.00 -0.01 0.00

9 6 -0.08 -0.07 0.03 0.01 -0.00 -0.05 0.03 0.00 0.15

10 6 -0.07 -0.14 0.06 0.01 -0.01 -0.04 0.03 0.02 0.17

11 6 0.00 -0.14 -0.04 0.03 -0.01 0.08 -0.02 0.02 -0.16

12 6 -0.06 -0.06 -0.04 0.00 0.00 -0.01 0.01 0.00 -0.03

13 6 -0.08 -0.07 -0.03 0.01 -0.00 0.05 0.03 0.00 -0.15

14 6 -0.07 -0.14 -0.06 0.01 -0.01 0.04 0.03 0.02 -0.17

15 6 0.00 -0.14 0.04 0.03 -0.01 -0.08 -0.02 0.02 0.16

16 6 0.02 -0.05 0.07 0.03 -0.00 -0.06 -0.02 0.00 0.15

17 7 -0.02 -0.03 0.04 0.01 0.00 -0.01 0.00 -0.01 -0.00

18 6 0.01 -0.03 0.01 0.00 -0.01 -0.03 -0.00 0.00 0.01

19 6 -0.01 -0.04 -0.06 0.00 -0.03 -0.15 0.00 0.01 -0.05

20 6 -0.06 -0.05 0.00 0.02 -0.03 -0.17 0.01 0.01 -0.04

21 6 -0.07 -0.09 0.04 0.02 0.02 0.16 0.01 0.03 0.08

22 6 -0.05 -0.09 -0.02 0.00 0.02 0.15 0.00 0.03 0.06

23 7 -0.01 -0.04 -0.09 -0.01 -0.00 -0.00 -0.00 0.01 0.01

24 6 -0.06 -0.06 0.04 0.00 0.00 0.01 0.01 0.00 0.03

25 6 -0.00 0.02 -0.00 -0.03 0.03 -0.10 0.01 -0.01 0.05

26 6 -0.00 0.05 0.02 0.01 0.06 -0.08 -0.00 -0.02 0.04

27 6 0.03 0.03 0.00 0.04 0.04 -0.01 -0.01 -0.02 -0.00

28 6 0.06 0.01 -0.02 0.01 -0.01 0.03 0.00 0.01 -0.01

29 6 0.01 0.04 0.00 -0.04 -0.04 -0.00 0.02 0.03 0.01

30 6 -0.01 0.05 0.01 -0.06 -0.01 -0.08 0.03 0.01 0.04

31 6 -0.08 -0.05 -0.05 0.01 -0.00 -0.01 0.01 0.01 -0.03

32 6 0.00 0.04 0.01 0.03 -0.02 0.01 0.04 -0.04 0.00

33 6 0.07 0.10 0.04 0.01 -0.03 0.04 0.01 -0.06 0.08

34 6 0.02 0.03 -0.01 -0.01 -0.01 0.05 -0.03 -0.03 0.10

35 6 0.08 0.08 0.03 -0.02 0.00 0.04 -0.06 0.01 0.08

36 6 0.02 0.03 0.01 -0.02 0.01 -0.00 -0.04 0.04 0.01

37 6 0.02 0.03 0.01 -0.01 -0.01 -0.05 -0.03 -0.03 -0.10

38 6 0.08 0.08 -0.03 -0.02 0.00 -0.04 -0.06 0.01 -0.08

39 6 0.02 0.03 -0.01 -0.02 0.01 0.00 -0.04 0.04 -0.01

40 6 -0.08 -0.05 0.05 0.01 -0.00 0.01 0.01 0.01 0.03

41 6 0.00 0.04 -0.01 0.03 -0.02 -0.01 0.04 -0.04 -0.00

42 6 0.07 0.10 -0.04 0.01 -0.03 -0.04 0.01 -0.06 -0.08

43 6 -0.00 0.02 0.00 -0.03 0.03 0.10 0.01 -0.01 -0.05

44 6 -0.01 0.05 -0.01 -0.06 -0.01 0.08 0.03 0.01 -0.04

45 6 0.01 0.04 -0.00 -0.04 -0.04 0.00 0.02 0.03 -0.01

46 6 0.06 0.01 0.02 0.01 -0.01 -0.03 0.00 0.01 0.01

47 6 0.03 0.03 -0.00 0.04 0.04 0.01 -0.01 -0.02 0.00

48 6 -0.00 0.05 -0.02 0.01 0.06 0.08 -0.00 -0.02 -0.04

49 1 -0.07 -0.09 -0.11 0.04 0.04 -0.29 0.01 0.04 -0.16

50 1 -0.10 -0.02 -0.04 0.04 -0.06 0.32 0.01 0.01 0.06

51 1 -0.09 -0.18 0.11 0.01 -0.01 -0.06 0.06 0.04 0.32

52 1 0.04 -0.19 -0.04 0.04 -0.01 0.16 -0.04 0.04 -0.29

53 1 -0.09 -0.18 -0.11 0.01 -0.01 0.06 0.06 0.04 -0.32

54 1 0.04 -0.19 0.04 0.04 -0.01 -0.16 -0.04 0.04 0.29

55 1 -0.10 -0.02 0.04 0.04 -0.06 -0.32 0.01 0.01 -0.06

56 1 -0.07 -0.09 0.11 0.04 0.04 0.29 0.01 0.04 0.16

57 1 -0.01 0.08 0.02 0.03 0.12 -0.10 -0.02 -0.04 0.05

58 1 0.03 0.02 -0.00 0.09 0.07 0.02 -0.03 -0.04 -0.02

59 1 0.09 -0.03 -0.04 0.02 -0.01 0.08 -0.00 0.01 -0.04

60 1 -0.00 0.04 0.01 -0.08 -0.08 0.03 0.03 0.05 -0.01

61 1 -0.02 0.07 0.02 -0.11 -0.03 -0.11 0.06 0.01 0.04

62 1 -0.18 -0.15 -0.11 0.01 0.00 -0.04 0.01 0.02 -0.08

63 1 -0.00 0.04 0.01 0.05 -0.03 -0.01 0.08 -0.08 -0.03

64 1 0.10 0.15 0.06 0.01 -0.06 0.04 0.03 -0.11 0.11

65 1 0.13 0.12 0.06 -0.04 0.02 0.05 -0.12 0.03 0.10

66 1 0.03 0.02 0.02 -0.04 0.03 -0.02 -0.07 0.09 -0.02

67 1 0.13 0.12 -0.06 -0.04 0.02 -0.05 -0.12 0.03 -0.10

68 1 0.03 0.02 -0.02 -0.04 0.03 0.02 -0.07 0.09 0.02

69 1 -0.18 -0.15 0.11 0.01 0.00 0.04 0.01 0.02 0.08

70 1 -0.00 0.04 -0.01 0.05 -0.03 0.01 0.08 -0.08 0.03

71 1 0.10 0.15 -0.06 0.01 -0.06 -0.04 0.03 -0.11 -0.11

72 1 -0.02 0.07 -0.02 -0.11 -0.03 0.11 0.06 0.01 -0.04

73 1 -0.00 0.04 -0.01 -0.08 -0.08 -0.03 0.03 0.05 0.01

74 1 0.09 -0.03 0.04 0.02 -0.01 -0.08 -0.00 0.01 0.04

75 1 0.03 0.02 0.00 0.09 0.07 -0.02 -0.03 -0.04 0.02

76 1 -0.01 0.08 -0.02 0.03 0.12 0.10 -0.02 -0.04 -0.05

77 30 0.07 0.15 0.00 -0.03 0.01 -0.00 -0.01 -0.03 -0.00

37 38 39

A2 A1 B1

Frequencies -- 340.4243 397.7715 410.5553

Red. masses -- 4.7377 8.0186 8.8079

Frc consts -- 0.3235 0.7475 0.8747

IR Inten -- 0.0000 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 -0.02 0.11 -0.01 0.19 0.02 0.10 -0.04 -0.00

2 6 0.00 -0.03 0.11 -0.02 0.15 -0.01 0.13 -0.07 -0.00

3 7 0.01 0.00 0.00 -0.00 0.17 -0.02 0.18 -0.00 -0.00

4 6 0.00 0.03 -0.11 0.02 0.15 -0.01 0.13 0.07 0.00

5 6 -0.03 0.02 -0.11 0.01 0.19 0.02 0.10 0.04 0.00

6 6 -0.00 0.00 -0.05 0.03 0.03 0.00 0.09 0.09 0.00

7 6 -0.03 -0.00 -0.11 0.15 0.02 0.01 0.07 0.13 -0.00

8 7 -0.00 -0.01 0.00 0.17 -0.00 0.02 0.00 0.18 0.00

9 6 0.03 -0.00 0.11 0.15 -0.02 0.01 -0.07 0.13 0.00

10 6 0.02 0.03 0.11 0.19 -0.01 -0.02 -0.04 0.10 0.00

11 6 -0.02 0.03 -0.11 0.19 0.01 -0.02 0.04 0.10 -0.00

12 6 -0.00 -0.00 0.05 -0.03 0.03 0.00 0.09 -0.09 0.00

13 6 -0.03 0.00 0.11 -0.15 0.02 0.01 0.07 -0.13 0.00

14 6 -0.02 -0.03 0.11 -0.19 0.01 -0.02 0.04 -0.10 0.00

15 6 0.02 -0.03 -0.11 -0.19 -0.01 -0.02 -0.04 -0.10 -0.00

16 6 0.03 0.00 -0.11 -0.15 -0.02 0.01 -0.07 -0.13 -0.00

17 7 -0.00 0.01 -0.00 -0.17 0.00 0.02 -0.00 -0.18 0.00

18 6 0.00 -0.00 -0.05 -0.03 -0.03 0.00 -0.09 -0.09 -0.00

19 6 -0.00 -0.03 -0.11 -0.02 -0.15 -0.01 -0.13 -0.07 0.00

20 6 0.03 -0.02 -0.11 -0.01 -0.19 0.02 -0.10 -0.04 0.00

21 6 0.03 0.02 0.11 0.01 -0.19 0.02 -0.10 0.04 -0.00

22 6 -0.00 0.03 0.11 0.02 -0.15 -0.01 -0.13 0.07 -0.00

23 7 -0.01 -0.00 -0.00 0.00 -0.17 -0.02 -0.18 -0.00 -0.00

24 6 0.00 0.00 0.05 0.03 -0.03 -0.00 -0.09 0.09 -0.00

25 6 0.03 -0.03 0.09 0.01 0.01 0.00 0.03 0.03 0.00

26 6 -0.01 -0.05 0.08 -0.03 -0.00 -0.00 -0.06 -0.03 -0.03

27 6 -0.04 -0.04 0.01 -0.02 -0.03 -0.02 -0.08 -0.05 -0.03

28 6 -0.01 0.01 -0.03 -0.04 -0.04 0.00 -0.10 -0.10 0.00

29 6 0.04 0.04 0.01 -0.03 -0.02 0.02 -0.05 -0.08 0.03

30 6 0.05 0.01 0.08 -0.00 -0.03 0.00 -0.03 -0.06 0.03

31 6 -0.01 -0.01 0.03 0.04 -0.04 0.00 -0.10 0.10 0.00

32 6 -0.04 0.04 -0.01 0.02 -0.03 -0.02 -0.08 0.05 0.03

33 6 -0.01 0.05 -0.08 0.03 -0.00 -0.00 -0.06 0.03 0.03

34 6 0.03 0.03 -0.09 -0.01 0.01 0.00 0.03 -0.03 0.00

35 6 0.05 -0.01 -0.08 0.00 -0.03 0.00 -0.03 0.06 -0.03

36 6 0.04 -0.04 -0.01 0.03 -0.02 0.02 -0.05 0.08 -0.03

37 6 -0.03 -0.03 -0.09 0.01 -0.01 0.00 -0.03 0.03 -0.00

38 6 -0.05 0.01 -0.08 -0.00 0.03 0.00 0.03 -0.06 -0.03

39 6 -0.04 0.04 -0.01 -0.03 0.02 0.02 0.05 -0.08 -0.03

40 6 0.01 0.01 0.03 -0.04 0.04 -0.00 0.10 -0.10 -0.00

41 6 0.04 -0.04 -0.01 -0.02 0.03 -0.02 0.08 -0.05 0.03

42 6 0.01 -0.05 -0.08 -0.03 0.00 -0.00 0.06 -0.03 0.03

43 6 -0.03 0.03 0.09 -0.01 -0.01 -0.00 -0.03 -0.03 -0.00

44 6 -0.05 -0.01 0.08 0.00 0.03 0.00 0.03 0.06 0.03

45 6 -0.04 -0.04 0.01 0.03 0.02 0.02 0.05 0.08 0.03

46 6 0.01 -0.01 -0.03 0.04 0.04 0.00 0.10 0.10 -0.00

47 6 0.04 0.04 0.01 0.02 0.03 -0.02 0.08 0.05 -0.03

48 6 0.01 0.05 0.08 0.03 0.00 -0.00 0.06 0.03 -0.03

49 1 -0.04 -0.05 0.21 0.01 0.20 0.04 0.06 -0.08 -0.01

50 1 -0.04 0.05 -0.21 -0.01 0.20 0.04 0.06 0.08 0.01

51 1 0.05 0.04 0.21 0.20 0.01 -0.04 -0.08 0.06 0.01

52 1 -0.05 0.04 -0.21 0.20 -0.01 -0.04 0.08 0.06 -0.01

53 1 -0.05 -0.04 0.21 -0.20 -0.01 -0.04 0.08 -0.06 0.01

54 1 0.05 -0.04 -0.21 -0.20 0.01 -0.04 -0.08 -0.06 -0.01

55 1 0.04 -0.05 -0.21 0.01 -0.20 0.04 -0.06 -0.08 0.01

56 1 0.04 0.05 0.21 -0.01 -0.20 0.04 -0.06 0.08 -0.01

57 1 -0.03 -0.10 0.10 -0.06 -0.02 0.01 -0.09 -0.09 -0.00

58 1 -0.08 -0.07 -0.02 0.01 -0.04 -0.02 -0.04 -0.03 -0.01

59 1 -0.01 0.01 -0.08 -0.04 -0.04 0.00 -0.10 -0.10 0.00

60 1 0.07 0.08 -0.02 -0.04 0.01 0.02 -0.03 -0.04 0.01

61 1 0.10 0.03 0.10 -0.02 -0.06 -0.01 -0.09 -0.09 0.00

62 1 -0.01 -0.01 0.08 0.04 -0.04 0.00 -0.10 0.10 0.00

63 1 -0.08 0.07 0.02 -0.01 -0.04 -0.02 -0.04 0.03 0.01

64 1 -0.03 0.10 -0.10 0.06 -0.02 0.01 -0.09 0.09 0.00

65 1 0.10 -0.03 -0.10 0.02 -0.06 -0.01 -0.09 0.09 -0.00

66 1 0.07 -0.08 0.02 0.04 0.01 0.02 -0.03 0.04 -0.01

67 1 -0.10 0.03 -0.10 -0.02 0.06 -0.01 0.09 -0.09 -0.00

68 1 -0.07 0.08 0.02 -0.04 -0.01 0.02 0.03 -0.04 -0.01

69 1 0.01 0.01 0.08 -0.04 0.04 -0.00 0.10 -0.10 -0.00

70 1 0.08 -0.07 0.02 0.01 0.04 -0.02 0.04 -0.03 0.01

71 1 0.03 -0.10 -0.10 -0.06 0.02 0.01 0.09 -0.09 0.00

72 1 -0.10 -0.03 0.10 0.02 0.06 -0.01 0.09 0.09 0.00

73 1 -0.07 -0.08 -0.02 0.04 -0.01 0.02 0.03 0.04 0.01

74 1 0.01 -0.01 -0.08 0.04 0.04 0.00 0.10 0.10 -0.00

75 1 0.08 0.07 -0.02 -0.01 0.04 -0.02 0.04 0.03 -0.01

76 1 0.03 0.10 0.10 0.06 0.02 0.01 0.09 0.09 -0.00

77 30 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 0.00 0.00

40 41 42

E E B1

Frequencies -- 414.2207 414.2207 414.2978

Red. masses -- 3.1088 3.1088 3.0083

Frc consts -- 0.3143 0.3143 0.3042

IR Inten -- 0.0237 0.0237 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 -0.03 0.01 0.02 -0.02 -0.00 0.03 0.01 -0.01

2 6 -0.00 -0.03 0.01 0.00 -0.01 -0.00 0.00 0.01 -0.01

3 7 0.00 -0.02 -0.00 -0.00 -0.02 -0.00 -0.01 -0.00 -0.00

4 6 -0.00 -0.00 -0.00 -0.00 -0.03 0.00 0.00 -0.01 0.01

5 6 -0.03 -0.01 -0.00 0.02 -0.04 0.00 0.03 -0.01 0.01

6 6 -0.00 0.00 -0.00 -0.01 -0.01 -0.00 -0.00 -0.00 -0.00

7 6 0.01 0.00 -0.00 -0.03 0.00 -0.01 -0.01 0.00 -0.01

8 7 0.02 -0.00 -0.00 -0.02 -0.00 0.00 -0.00 -0.01 0.00

9 6 0.03 -0.00 0.00 -0.00 0.00 0.00 0.01 0.00 0.01

10 6 0.04 0.02 0.00 -0.01 0.03 0.00 0.01 0.03 0.01

11 6 0.02 0.02 -0.00 -0.03 0.03 -0.01 -0.01 0.03 -0.01

12 6 0.01 -0.01 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00

13 6 0.03 -0.00 -0.00 -0.00 0.00 -0.00 -0.01 -0.00 0.01

14 6 0.04 0.02 -0.00 -0.01 0.03 -0.00 -0.01 -0.03 0.01

15 6 0.02 0.02 0.00 -0.03 0.03 0.01 0.01 -0.03 -0.01

16 6 0.01 0.00 0.00 -0.03 0.00 0.01 0.01 -0.00 -0.01

17 7 0.02 -0.00 0.00 -0.02 -0.00 -0.00 -0.00 0.01 -0.00

18 6 -0.00 0.00 0.00 -0.01 -0.01 0.00 0.00 0.00 0.00

19 6 -0.00 -0.00 0.00 -0.00 -0.03 -0.00 -0.00 0.01 0.01

20 6 -0.03 -0.01 0.00 0.02 -0.04 -0.00 -0.03 0.01 0.01

21 6 -0.03 -0.03 -0.01 0.02 -0.02 0.00 -0.03 -0.01 -0.01

22 6 -0.00 -0.03 -0.01 0.00 -0.01 0.00 -0.00 -0.01 -0.01

23 7 0.00 -0.02 0.00 -0.00 -0.02 0.00 0.01 -0.00 0.00

24 6 0.01 -0.01 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00

25 6 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 0.00 0.00

26 6 -0.01 0.01 0.01 0.10 -0.09 -0.06 0.07 -0.07 -0.05

27 6 0.02 -0.02 -0.01 -0.08 0.09 0.07 -0.06 0.07 0.05

28 6 -0.01 0.00 0.00 0.01 0.01 0.00 0.00 0.00 0.00

29 6 -0.01 0.01 0.01 0.09 -0.08 -0.07 0.07 -0.06 -0.05

30 6 0.02 -0.02 -0.01 -0.09 0.09 0.06 -0.07 0.07 0.05

31 6 -0.01 0.01 -0.00 0.00 0.01 0.00 0.00 -0.00 0.00

32 6 0.08 0.09 0.07 0.01 0.01 0.01 -0.06 -0.07 -0.05

33 6 -0.09 -0.09 -0.06 -0.02 -0.02 -0.01 0.07 0.07 0.05

34 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00

35 6 0.09 0.10 0.06 0.01 0.01 0.01 -0.07 -0.07 -0.05

36 6 -0.09 -0.08 -0.07 -0.02 -0.02 -0.01 0.07 0.06 0.05

37 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00

38 6 0.09 0.10 -0.06 0.01 0.01 -0.01 0.07 0.07 -0.05

39 6 -0.09 -0.08 0.07 -0.02 -0.02 0.01 -0.07 -0.06 0.05

40 6 -0.01 0.01 0.00 0.00 0.01 -0.00 -0.00 0.00 -0.00

41 6 0.08 0.09 -0.07 0.01 0.01 -0.01 0.06 0.07 -0.05

42 6 -0.09 -0.09 0.06 -0.02 -0.02 0.01 -0.07 -0.07 0.05

43 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00

44 6 0.02 -0.02 0.01 -0.09 0.09 -0.06 0.07 -0.07 0.05

45 6 -0.01 0.01 -0.01 0.09 -0.08 0.07 -0.07 0.06 -0.05

46 6 -0.01 0.00 -0.00 0.01 0.01 -0.00 -0.00 -0.00 -0.00

47 6 0.02 -0.02 0.01 -0.08 0.09 -0.07 0.06 -0.07 0.05

48 6 -0.01 0.01 -0.01 0.10 -0.09 0.06 -0.07 0.07 -0.05

49 1 -0.05 -0.05 0.00 0.03 -0.01 -0.01 0.04 0.02 -0.01

50 1 -0.05 0.00 -0.01 0.04 -0.05 -0.00 0.04 -0.02 0.01

51 1 0.05 0.04 -0.00 0.00 0.05 0.01 0.02 0.04 0.01

52 1 0.01 0.03 -0.01 -0.05 0.05 -0.00 -0.02 0.04 -0.01

53 1 0.05 0.04 0.00 0.00 0.05 -0.01 -0.02 -0.04 0.01

54 1 0.01 0.03 0.01 -0.05 0.05 0.00 0.02 -0.04 -0.01

55 1 -0.05 0.00 0.01 0.04 -0.05 0.00 -0.04 0.02 0.01

56 1 -0.05 -0.05 -0.00 0.03 -0.01 0.01 -0.04 -0.02 -0.01

57 1 -0.03 0.02 0.02 0.20 -0.19 -0.14 0.14 -0.14 -0.10

58 1 0.04 -0.05 -0.03 -0.19 0.20 0.14 -0.14 0.14 0.10

59 1 -0.01 0.01 0.01 0.00 0.01 0.00 0.00 0.00 0.00

60 1 -0.03 0.03 0.02 0.20 -0.19 -0.14 0.14 -0.14 -0.10

61 1 0.05 -0.05 -0.03 -0.19 0.20 0.14 -0.14 0.14 0.10

62 1 -0.01 0.00 -0.00 0.01 0.01 0.01 0.00 -0.00 0.00

63 1 0.19 0.20 0.14 0.03 0.03 0.02 -0.14 -0.14 -0.10

64 1 -0.20 -0.19 -0.14 -0.05 -0.05 -0.03 0.14 0.14 0.10

65 1 0.19 0.20 0.14 0.02 0.03 0.02 -0.14 -0.14 -0.10

66 1 -0.20 -0.19 -0.14 -0.05 -0.04 -0.03 0.14 0.14 0.10

67 1 0.19 0.20 -0.14 0.02 0.03 -0.02 0.14 0.14 -0.10

68 1 -0.20 -0.19 0.14 -0.05 -0.04 0.03 -0.14 -0.14 0.10

69 1 -0.01 0.00 0.00 0.01 0.01 -0.01 -0.00 0.00 -0.00

70 1 0.19 0.20 -0.14 0.03 0.03 -0.02 0.14 0.14 -0.10

71 1 -0.20 -0.19 0.14 -0.05 -0.05 0.03 -0.14 -0.14 0.10

72 1 0.05 -0.05 0.03 -0.19 0.20 -0.14 0.14 -0.14 0.10

73 1 -0.03 0.03 -0.02 0.20 -0.19 0.14 -0.14 0.14 -0.10

74 1 -0.01 0.01 -0.01 0.00 0.01 -0.00 -0.00 -0.00 -0.00

75 1 0.04 -0.05 0.03 -0.19 0.20 -0.14 0.14 -0.14 0.10

76 1 -0.03 0.02 -0.02 0.20 -0.19 0.14 -0.14 0.14 -0.10

77 30 -0.02 0.01 0.00 0.01 0.02 0.00 0.00 0.00 0.00

43 44 45

A1 E E

Frequencies -- 415.5821 423.0672 423.0672

Red. masses -- 2.9871 6.3064 6.3064

Frc consts -- 0.3040 0.6650 0.6650

IR Inten -- 0.0000 21.3617 21.3617

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.01 -0.01 0.06 -0.15 -0.03 0.14 0.07 -0.01

2 6 0.00 -0.01 0.00 0.04 -0.12 0.01 0.06 0.05 -0.01

3 7 0.00 -0.01 0.01 0.03 -0.13 0.00 0.07 0.05 -0.00

4 6 -0.00 -0.01 0.00 0.01 -0.12 0.01 0.07 0.04 -0.00

5 6 -0.00 -0.01 -0.01 0.05 -0.16 -0.02 0.14 0.05 0.03

6 6 -0.00 -0.00 0.00 0.00 0.02 0.02 0.03 -0.02 -0.04

7 6 -0.01 -0.00 -0.00 -0.05 0.06 -0.01 -0.12 -0.04 -0.01

8 7 -0.01 0.00 -0.01 -0.05 0.07 -0.00 -0.13 -0.03 -0.00

9 6 -0.01 0.00 -0.00 -0.04 0.07 -0.00 -0.12 -0.01 -0.01

10 6 -0.01 0.00 0.01 -0.05 0.14 0.03 -0.16 -0.05 0.02

11 6 -0.01 -0.00 0.01 -0.07 0.14 -0.01 -0.15 -0.06 0.03

12 6 0.00 -0.00 -0.00 0.02 0.03 0.04 0.02 -0.00 0.02

13 6 0.01 -0.00 -0.00 -0.04 0.07 0.00 -0.12 -0.01 0.01

14 6 0.01 -0.00 0.01 -0.05 0.14 -0.03 -0.16 -0.05 -0.02

15 6 0.01 0.00 0.01 -0.07 0.14 0.01 -0.15 -0.06 -0.03

16 6 0.01 0.00 -0.00 -0.05 0.06 0.01 -0.12 -0.04 0.01

17 7 0.01 -0.00 -0.01 -0.05 0.07 0.00 -0.13 -0.03 0.00

18 6 0.00 0.00 -0.00 0.00 0.02 -0.02 0.03 -0.02 0.04

19 6 0.00 0.01 0.00 0.01 -0.12 -0.01 0.07 0.04 0.00

20 6 0.00 0.01 -0.01 0.05 -0.16 0.02 0.14 0.05 -0.03

21 6 -0.00 0.01 -0.01 0.06 -0.15 0.03 0.14 0.07 0.01

22 6 -0.00 0.01 0.00 0.04 -0.12 -0.01 0.06 0.05 0.01

23 7 -0.00 0.01 0.01 0.03 -0.13 -0.00 0.07 0.05 0.00

24 6 -0.00 0.00 0.00 0.02 0.03 -0.04 0.02 -0.00 -0.02

25 6 -0.00 -0.00 0.00 -0.02 0.02 0.01 0.05 -0.04 -0.03

26 6 -0.07 0.07 0.05 -0.03 0.02 0.01 -0.04 0.04 0.03

27 6 0.07 -0.06 -0.05 0.04 -0.05 -0.03 -0.01 0.01 0.01

28 6 0.00 0.00 0.00 -0.03 0.01 0.02 0.04 -0.05 -0.03

29 6 -0.06 0.07 0.05 -0.02 0.01 0.02 -0.04 0.04 0.03

30 6 0.07 -0.07 -0.05 0.04 -0.05 -0.03 -0.01 0.01 0.01

31 6 -0.00 0.00 -0.00 0.05 0.04 0.03 0.01 0.03 0.02

32 6 -0.07 -0.06 -0.05 -0.04 -0.04 -0.03 0.01 0.02 0.02

33 6 0.07 0.07 0.05 -0.01 -0.01 -0.01 -0.05 -0.04 -0.03

34 6 0.00 -0.00 -0.00 0.04 0.05 0.03 0.02 0.02 0.01

35 6 -0.07 -0.07 -0.05 -0.04 -0.04 -0.03 0.02 0.03 0.01

36 6 0.06 0.07 0.05 -0.01 -0.01 -0.01 -0.05 -0.04 -0.03

37 6 -0.00 0.00 0.00 0.04 0.05 -0.03 0.02 0.02 -0.01

38 6 0.07 0.07 -0.05 -0.04 -0.04 0.03 0.02 0.03 -0.01

39 6 -0.06 -0.07 0.05 -0.01 -0.01 0.01 -0.05 -0.04 0.03

40 6 0.00 -0.00 0.00 0.05 0.04 -0.03 0.01 0.03 -0.02

41 6 0.07 0.06 -0.05 -0.04 -0.04 0.03 0.01 0.02 -0.02

42 6 -0.07 -0.07 0.05 -0.01 -0.01 0.01 -0.05 -0.04 0.03

43 6 0.00 0.00 -0.00 -0.02 0.02 -0.01 0.05 -0.04 0.03

44 6 -0.07 0.07 -0.05 0.04 -0.05 0.03 -0.01 0.01 -0.01

45 6 0.06 -0.07 0.05 -0.02 0.01 -0.02 -0.04 0.04 -0.03

46 6 -0.00 -0.00 -0.00 -0.03 0.01 -0.02 0.04 -0.05 0.03

47 6 -0.07 0.06 -0.05 0.04 -0.05 0.03 -0.01 0.01 -0.01

48 6 0.07 -0.07 0.05 -0.03 0.02 -0.01 -0.04 0.04 -0.03

49 1 0.00 -0.01 -0.00 0.06 -0.15 -0.06 0.17 0.10 -0.03

50 1 -0.00 -0.01 -0.00 0.07 -0.18 -0.03 0.17 0.02 0.06

51 1 -0.01 0.00 0.00 -0.02 0.17 0.06 -0.18 -0.07 0.03

52 1 -0.01 -0.00 0.00 -0.10 0.17 -0.03 -0.15 -0.06 0.06

53 1 0.01 -0.00 0.00 -0.02 0.17 -0.06 -0.18 -0.07 -0.03

54 1 0.01 0.00 0.00 -0.10 0.17 0.03 -0.15 -0.06 -0.06

55 1 0.00 0.01 -0.00 0.07 -0.18 0.03 0.17 0.02 -0.06

56 1 -0.00 0.01 -0.00 0.06 -0.15 0.06 0.17 0.10 0.03

57 1 -0.14 0.15 0.10 -0.05 0.04 0.03 -0.10 0.10 0.07

58 1 0.14 -0.14 -0.10 0.09 -0.10 -0.07 -0.04 0.03 0.02

59 1 0.00 0.00 0.00 -0.05 0.03 0.03 0.09 -0.10 -0.07

60 1 -0.14 0.14 0.10 -0.04 0.03 0.03 -0.09 0.09 0.06

61 1 0.15 -0.14 -0.10 0.10 -0.11 -0.08 -0.04 0.03 0.03

62 1 -0.00 0.00 -0.00 0.10 0.09 0.07 0.03 0.05 0.03

63 1 -0.14 -0.14 -0.10 -0.09 -0.09 -0.06 0.03 0.04 0.03

64 1 0.14 0.15 0.10 -0.03 -0.04 -0.03 -0.11 -0.10 -0.08

65 1 -0.15 -0.14 -0.10 -0.10 -0.10 -0.07 0.04 0.05 0.03

66 1 0.14 0.14 0.10 -0.03 -0.04 -0.02 -0.10 -0.09 -0.07

67 1 0.15 0.14 -0.10 -0.10 -0.10 0.07 0.04 0.05 -0.03

68 1 -0.14 -0.14 0.10 -0.03 -0.04 0.02 -0.10 -0.09 0.07

69 1 0.00 -0.00 0.00 0.10 0.09 -0.07 0.03 0.05 -0.03

70 1 0.14 0.14 -0.10 -0.09 -0.09 0.06 0.03 0.04 -0.03

71 1 -0.14 -0.15 0.10 -0.03 -0.04 0.03 -0.11 -0.10 0.08

72 1 -0.15 0.14 -0.10 0.10 -0.11 0.08 -0.04 0.03 -0.03

73 1 0.14 -0.14 0.10 -0.04 0.03 -0.03 -0.09 0.09 -0.06

74 1 -0.00 -0.00 -0.00 -0.05 0.03 -0.03 0.09 -0.10 0.07

75 1 -0.14 0.14 -0.10 0.09 -0.10 0.07 -0.04 0.03 -0.02

76 1 0.14 -0.15 0.10 -0.05 0.04 -0.03 -0.10 0.10 -0.07

77 30 -0.00 -0.00 -0.00 0.03 0.09 -0.00 0.09 -0.03 -0.00

46 47 48

E E B1

Frequencies -- 443.1419 443.1419 447.6985

Red. masses -- 5.5989 5.5989 4.1630

Frc consts -- 0.6478 0.6478 0.4916

IR Inten -- 23.3875 23.3875 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.07 -0.10 -0.02 -0.05 -0.06 -0.01 0.16 0.06 0.01

2 6 0.09 -0.12 -0.02 0.05 -0.07 -0.01 0.01 0.06 0.01

3 7 0.17 -0.00 0.00 0.11 0.01 -0.00 -0.03 0.00 0.00

4 6 0.08 0.12 0.02 0.07 0.08 0.02 0.01 -0.06 -0.01

5 6 -0.07 0.09 0.02 -0.05 0.07 0.01 0.16 -0.06 -0.01

6 6 0.02 0.01 -0.01 0.08 0.08 0.00 -0.02 -0.02 -0.00

7 6 -0.07 -0.05 0.01 0.12 0.09 -0.02 -0.06 0.01 0.01

8 7 0.01 -0.11 0.00 0.00 0.17 0.00 0.00 -0.03 -0.00

9 6 0.08 -0.07 -0.02 -0.12 0.08 0.02 0.06 0.01 -0.01

10 6 0.07 0.05 -0.01 -0.09 -0.07 0.02 0.06 0.16 -0.01

11 6 -0.06 0.05 0.01 0.10 -0.07 -0.02 -0.06 0.16 0.01

12 6 0.08 -0.08 0.00 -0.01 0.02 0.01 -0.02 0.02 -0.00

13 6 0.08 -0.07 0.02 -0.12 0.08 -0.02 -0.06 -0.01 -0.01

14 6 0.07 0.05 0.01 -0.09 -0.07 -0.02 -0.06 -0.16 -0.01

15 6 -0.06 0.05 -0.01 0.10 -0.07 0.02 0.06 -0.16 0.01

16 6 -0.07 -0.05 -0.01 0.12 0.09 0.02 0.06 -0.01 0.01

17 7 0.01 -0.11 -0.00 0.00 0.17 -0.00 -0.00 0.03 -0.00

18 6 0.02 0.01 0.01 0.08 0.08 -0.00 0.02 0.02 0.00

19 6 0.08 0.12 -0.02 0.07 0.08 -0.02 -0.01 0.06 -0.01

20 6 -0.07 0.09 -0.02 -0.05 0.07 -0.01 -0.16 0.06 -0.01

21 6 -0.07 -0.10 0.02 -0.05 -0.06 0.01 -0.16 -0.06 0.01

22 6 0.09 -0.12 0.02 0.05 -0.07 0.01 -0.01 -0.06 0.01

23 7 0.17 -0.00 -0.00 0.11 0.01 0.00 0.03 0.00 0.00

24 6 0.08 -0.08 -0.00 -0.01 0.02 -0.01 0.02 -0.02 0.00

25 6 0.05 -0.04 -0.04 0.02 0.04 0.01 -0.01 -0.01 0.00

26 6 -0.02 0.01 -0.01 -0.02 -0.04 -0.04 -0.01 0.02 0.02

27 6 -0.03 0.02 0.01 -0.06 -0.02 -0.02 0.02 -0.01 -0.00

28 6 0.02 -0.05 -0.02 -0.08 -0.07 0.00 0.02 0.02 0.00

29 6 -0.03 0.00 0.02 -0.01 -0.07 0.01 -0.01 0.02 0.00

30 6 -0.03 0.01 0.01 -0.03 -0.03 0.04 0.02 -0.01 -0.02

31 6 -0.07 0.08 0.00 0.05 0.02 0.02 0.02 -0.02 -0.00

32 6 -0.07 0.01 0.01 -0.00 -0.03 -0.02 0.02 0.01 0.00

33 6 -0.03 0.03 0.04 -0.01 -0.03 -0.01 -0.01 -0.02 -0.02

34 6 0.04 -0.02 0.01 0.04 0.05 0.04 -0.01 0.01 -0.00

35 6 -0.04 0.02 -0.04 -0.01 -0.02 0.01 0.02 0.01 0.02

36 6 -0.02 0.06 -0.02 -0.02 -0.03 -0.01 -0.01 -0.02 -0.00

37 6 0.04 -0.02 -0.01 0.04 0.05 -0.04 0.01 -0.01 -0.00

38 6 -0.04 0.02 0.04 -0.01 -0.02 -0.01 -0.02 -0.01 0.02

39 6 -0.02 0.06 0.02 -0.02 -0.03 0.01 0.01 0.02 -0.00

40 6 -0.07 0.08 -0.00 0.05 0.02 -0.02 -0.02 0.02 -0.00

41 6 -0.07 0.01 -0.01 -0.00 -0.03 0.02 -0.02 -0.01 0.00

42 6 -0.03 0.03 -0.04 -0.01 -0.03 0.01 0.01 0.02 -0.02

43 6 0.05 -0.04 0.04 0.02 0.04 -0.01 0.01 0.01 0.00

44 6 -0.03 0.01 -0.01 -0.03 -0.03 -0.04 -0.02 0.01 -0.02

45 6 -0.03 0.00 -0.02 -0.01 -0.07 -0.01 0.01 -0.02 0.00

46 6 0.02 -0.05 0.02 -0.08 -0.07 -0.00 -0.02 -0.02 0.00

47 6 -0.03 0.02 -0.01 -0.06 -0.02 0.02 -0.02 0.01 -0.00

48 6 -0.02 0.01 0.01 -0.02 -0.04 0.04 0.01 -0.02 0.02

49 1 -0.20 -0.20 -0.02 -0.12 -0.11 -0.03 0.25 0.13 0.01

50 1 -0.19 0.18 0.04 -0.13 0.13 0.01 0.25 -0.13 -0.01

51 1 0.13 0.13 -0.01 -0.18 -0.19 0.04 0.13 0.25 -0.01

52 1 -0.11 0.12 0.03 0.20 -0.20 -0.02 -0.13 0.25 0.01

53 1 0.13 0.13 0.01 -0.18 -0.19 -0.04 -0.13 -0.25 -0.01

54 1 -0.11 0.12 -0.03 0.20 -0.20 0.02 0.13 -0.25 0.01

55 1 -0.19 0.18 -0.04 -0.13 0.13 -0.01 -0.25 0.13 -0.01

56 1 -0.20 -0.20 0.02 -0.12 -0.11 0.03 -0.25 -0.13 0.01

57 1 -0.05 0.04 0.02 -0.02 -0.12 -0.04 -0.03 0.05 0.03

58 1 -0.05 0.07 0.04 -0.04 0.01 0.01 0.03 -0.03 -0.02

59 1 0.05 -0.08 -0.04 -0.09 -0.06 0.01 0.02 0.02 -0.00

60 1 -0.06 0.03 0.04 0.03 -0.06 -0.02 -0.03 0.03 0.02

61 1 -0.08 0.04 0.03 -0.09 -0.04 0.03 0.05 -0.03 -0.03

62 1 -0.06 0.09 0.01 0.08 0.05 0.04 0.02 -0.02 -0.00

63 1 -0.06 -0.03 -0.02 -0.03 -0.06 -0.04 0.03 0.03 0.02

64 1 -0.04 0.09 0.03 -0.04 -0.08 -0.03 -0.03 -0.05 -0.03

65 1 -0.12 0.02 -0.04 -0.04 -0.05 -0.02 0.05 0.03 0.03

66 1 0.01 0.04 0.01 -0.07 -0.05 -0.04 -0.03 -0.03 -0.02

67 1 -0.12 0.02 0.04 -0.04 -0.05 0.02 -0.05 -0.03 0.03

68 1 0.01 0.04 -0.01 -0.07 -0.05 0.04 0.03 0.03 -0.02

69 1 -0.06 0.09 -0.01 0.08 0.05 -0.04 -0.02 0.02 0.00

70 1 -0.06 -0.03 0.02 -0.03 -0.06 0.04 -0.03 -0.03 0.02

71 1 -0.04 0.09 -0.03 -0.04 -0.08 0.03 0.03 0.05 -0.03

72 1 -0.08 0.04 -0.03 -0.09 -0.04 -0.03 -0.05 0.03 -0.03

73 1 -0.06 0.03 -0.04 0.03 -0.06 0.02 0.03 -0.03 0.02

74 1 0.05 -0.08 0.04 -0.09 -0.06 -0.01 -0.02 -0.02 0.00

75 1 -0.05 0.07 -0.04 -0.04 0.01 -0.01 -0.03 0.03 -0.02

76 1 -0.05 0.04 -0.02 -0.02 -0.12 0.04 0.03 -0.05 0.03

77 30 -0.02 0.01 -0.00 -0.01 -0.02 -0.00 0.00 -0.00 -0.00

49 50 51

A2 B2 E

Frequencies -- 458.7534 508.6036 532.6895

Red. masses -- 5.0417 3.9111 4.2720

Frc consts -- 0.6252 0.5961 0.7142

IR Inten -- 0.0000 2.5357 11.6534

Atom AN X Y Z X Y Z X Y Z

1 6 -0.04 -0.08 -0.03 -0.00 0.00 0.01 -0.05 0.04 -0.04

2 6 0.07 -0.10 -0.02 -0.02 0.01 -0.01 -0.02 0.02 0.01

3 7 0.14 0.00 0.00 -0.00 0.01 0.04 -0.05 0.01 -0.04

4 6 0.07 0.10 0.02 0.02 0.01 -0.01 -0.05 -0.01 0.00

5 6 -0.04 0.08 0.03 0.00 0.00 0.01 -0.05 0.01 0.03

6 6 0.02 -0.02 -0.01 0.03 -0.03 -0.08 -0.04 -0.04 0.00

7 6 -0.10 -0.07 0.02 -0.01 -0.02 -0.01 -0.01 -0.05 -0.00

8 7 -0.00 -0.14 -0.00 -0.01 0.00 0.04 0.01 -0.05 0.03

9 6 0.10 -0.07 -0.02 -0.01 0.02 -0.01 0.02 -0.02 -0.01

10 6 0.08 0.04 -0.03 -0.00 0.00 0.01 0.04 -0.05 0.04

11 6 -0.08 0.04 0.03 -0.00 -0.00 0.01 0.01 -0.05 -0.03

12 6 0.02 0.02 0.01 -0.03 -0.03 -0.08 0.02 0.02 0.11

13 6 -0.10 0.07 -0.02 0.01 -0.02 -0.01 0.02 -0.02 0.01

14 6 -0.08 -0.04 -0.03 0.00 -0.00 0.01 0.04 -0.05 -0.04

15 6 0.08 -0.04 0.03 0.00 0.00 0.01 0.01 -0.05 0.03

16 6 0.10 0.07 0.02 0.01 0.02 -0.01 -0.01 -0.05 0.00

17 7 0.00 0.14 -0.00 0.01 -0.00 0.04 0.01 -0.05 -0.03

18 6 -0.02 0.02 -0.01 -0.03 0.03 -0.08 -0.04 -0.04 -0.00

19 6 -0.07 -0.10 0.02 -0.02 -0.01 -0.01 -0.05 -0.01 -0.00

20 6 0.04 -0.08 0.03 -0.00 -0.00 0.01 -0.05 0.01 -0.03

21 6 0.04 0.08 -0.03 0.00 -0.00 0.01 -0.05 0.04 0.04

22 6 -0.07 0.10 -0.02 0.02 -0.01 -0.01 -0.02 0.02 -0.01

23 7 -0.14 0.00 0.00 -0.00 -0.01 0.04 -0.05 0.01 0.04

24 6 -0.02 -0.02 0.01 0.03 0.03 -0.08 0.02 0.02 -0.11

25 6 0.06 -0.06 -0.06 0.11 -0.11 -0.06 -0.03 -0.02 0.00

26 6 -0.01 0.02 0.00 0.00 -0.02 0.02 0.01 -0.00 0.02

27 6 -0.02 0.03 0.02 -0.06 0.04 0.04 0.02 0.00 0.01

28 6 0.05 -0.05 -0.03 0.07 -0.07 -0.06 0.03 0.03 0.00

29 6 -0.03 0.02 0.02 -0.04 0.06 0.04 0.01 0.01 -0.02

30 6 -0.02 0.01 0.00 0.02 -0.00 0.02 -0.00 0.01 -0.02

31 6 0.05 0.05 0.03 -0.07 -0.07 -0.06 0.08 0.09 0.08

32 6 -0.02 -0.03 -0.02 0.06 0.04 0.04 -0.07 -0.04 -0.05

33 6 -0.01 -0.02 -0.00 -0.00 -0.02 0.02 0.02 0.04 -0.03

34 6 0.06 0.06 0.06 -0.11 -0.11 -0.06 0.15 0.15 0.07

35 6 -0.02 -0.01 -0.00 -0.02 -0.00 0.02 0.04 0.02 -0.03

36 6 -0.03 -0.02 -0.02 0.04 0.06 0.04 -0.04 -0.07 -0.05

37 6 -0.06 -0.06 0.06 0.11 0.11 -0.06 0.15 0.15 -0.07

38 6 0.02 0.01 -0.00 0.02 0.00 0.02 0.04 0.02 0.03

39 6 0.03 0.02 -0.02 -0.04 -0.06 0.04 -0.04 -0.07 0.05

40 6 -0.05 -0.05 0.03 0.07 0.07 -0.06 0.08 0.09 -0.08

41 6 0.02 0.03 -0.02 -0.06 -0.04 0.04 -0.07 -0.04 0.05

42 6 0.01 0.02 -0.00 0.00 0.02 0.02 0.02 0.04 0.03

43 6 -0.06 0.06 -0.06 -0.11 0.11 -0.06 -0.03 -0.02 -0.00

44 6 0.02 -0.01 0.00 -0.02 0.00 0.02 -0.00 0.01 0.02

45 6 0.03 -0.02 0.02 0.04 -0.06 0.04 0.01 0.01 0.02

46 6 -0.05 0.05 -0.03 -0.07 0.07 -0.06 0.03 0.03 -0.00

47 6 0.02 -0.03 0.02 0.06 -0.04 0.04 0.02 0.00 -0.01

48 6 0.01 -0.02 0.00 -0.00 0.02 0.02 0.01 -0.00 -0.02

49 1 -0.14 -0.15 -0.05 0.00 0.01 0.01 -0.04 0.04 -0.06

50 1 -0.14 0.15 0.05 -0.00 0.01 0.01 -0.04 0.00 0.05

51 1 0.15 0.14 -0.05 -0.01 -0.00 0.01 0.04 -0.04 0.07

52 1 -0.15 0.14 0.05 -0.01 0.00 0.01 0.00 -0.05 -0.06

53 1 -0.15 -0.14 -0.05 0.01 0.00 0.01 0.04 -0.04 -0.07

54 1 0.15 -0.14 0.05 0.01 -0.00 0.01 0.00 -0.05 0.06

55 1 0.14 -0.15 0.05 0.00 -0.01 0.01 -0.04 0.00 -0.05

56 1 0.14 0.15 -0.05 -0.00 -0.01 0.01 -0.04 0.04 0.06

57 1 -0.06 0.08 0.03 -0.09 0.05 0.09 0.03 0.02 -0.00

58 1 -0.07 0.09 0.06 -0.17 0.13 0.10 0.00 -0.01 0.00

59 1 0.09 -0.09 -0.06 0.11 -0.11 -0.11 0.03 0.03 0.00

60 1 -0.09 0.07 0.06 -0.13 0.17 0.10 -0.00 -0.01 -0.01

61 1 -0.08 0.06 0.03 -0.05 0.09 0.09 0.02 0.03 -0.00

62 1 0.09 0.09 0.06 -0.11 -0.11 -0.11 0.12 0.12 0.13

63 1 -0.07 -0.09 -0.06 0.17 0.13 0.10 -0.24 -0.18 -0.14

64 1 -0.06 -0.08 -0.03 0.09 0.05 0.09 -0.11 -0.05 -0.12

65 1 -0.08 -0.06 -0.03 0.05 0.09 0.09 -0.05 -0.10 -0.12

66 1 -0.09 -0.07 -0.06 0.13 0.17 0.10 -0.18 -0.24 -0.14

67 1 0.08 0.06 -0.03 -0.05 -0.09 0.09 -0.05 -0.10 0.12

68 1 0.09 0.07 -0.06 -0.13 -0.17 0.10 -0.18 -0.24 0.14

69 1 -0.09 -0.09 0.06 0.11 0.11 -0.11 0.12 0.12 -0.13

70 1 0.07 0.09 -0.06 -0.17 -0.13 0.10 -0.24 -0.18 0.14

71 1 0.06 0.08 -0.03 -0.09 -0.05 0.09 -0.11 -0.05 0.12

72 1 0.08 -0.06 0.03 0.05 -0.09 0.09 0.02 0.03 0.00

73 1 0.09 -0.07 0.06 0.13 -0.17 0.10 -0.00 -0.01 0.01

74 1 -0.09 0.09 -0.06 -0.11 0.11 -0.11 0.03 0.03 -0.00

75 1 0.07 -0.09 0.06 0.17 -0.13 0.10 0.00 -0.01 -0.00

76 1 0.06 -0.08 0.03 0.09 -0.05 0.09 0.03 0.02 0.00

77 30 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00

52 53 54

E A2 A2

Frequencies -- 532.6895 554.8587 577.0141

Red. masses -- 4.2720 4.6918 4.2015

Frc consts -- 0.7142 0.8511 0.8242

IR Inten -- 11.6534 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.05 0.01 0.03 0.03 -0.04 0.09 -0.01 0.02 0.09

2 6 0.05 -0.01 0.00 0.05 -0.03 -0.03 -0.03 0.03 -0.04

3 7 0.05 0.01 -0.03 0.08 0.00 -0.00 -0.05 -0.00 0.00

4 6 0.02 0.02 0.01 0.05 0.03 0.03 -0.03 -0.03 0.04

5 6 0.05 0.04 -0.04 0.03 0.04 -0.09 -0.01 -0.02 -0.09

6 6 -0.02 0.02 0.11 0.01 -0.01 0.13 -0.00 0.00 0.13

7 6 -0.02 -0.02 0.01 -0.03 -0.05 0.03 0.03 0.03 0.04

8 7 -0.01 -0.05 -0.04 -0.00 -0.08 -0.00 0.00 0.05 -0.00

9 6 0.01 -0.05 0.00 0.03 -0.05 -0.03 -0.03 0.03 -0.04

10 6 -0.01 -0.05 0.03 0.04 -0.03 0.09 -0.02 0.01 0.09

11 6 -0.04 -0.05 -0.04 -0.04 -0.03 -0.09 0.02 0.01 -0.09

12 6 0.04 -0.04 -0.00 0.01 0.01 -0.13 -0.00 -0.00 -0.13

13 6 0.01 -0.05 -0.00 -0.03 0.05 -0.03 0.03 -0.03 -0.04

14 6 -0.01 -0.05 -0.03 -0.04 0.03 0.09 0.02 -0.01 0.09

15 6 -0.04 -0.05 0.04 0.04 0.03 -0.09 -0.02 -0.01 -0.09

16 6 -0.02 -0.02 -0.01 0.03 0.05 0.03 -0.03 -0.03 0.04

17 7 -0.01 -0.05 0.04 0.00 0.08 -0.00 -0.00 -0.05 -0.00

18 6 -0.02 0.02 -0.11 -0.01 0.01 0.13 0.00 -0.00 0.13

19 6 0.02 0.02 -0.01 -0.05 -0.03 0.03 0.03 0.03 0.04

20 6 0.05 0.04 0.04 -0.03 -0.04 -0.09 0.01 0.02 -0.09

21 6 0.05 0.01 -0.03 -0.03 0.04 0.09 0.01 -0.02 0.09

22 6 0.05 -0.01 -0.00 -0.05 0.03 -0.03 0.03 -0.03 -0.04

23 7 0.05 0.01 0.03 -0.08 0.00 0.00 0.05 -0.00 -0.00

24 6 0.04 -0.04 0.00 -0.01 -0.01 -0.13 0.00 0.00 -0.13

25 6 -0.15 0.15 0.07 -0.08 0.08 0.02 0.06 -0.06 -0.07

26 6 -0.02 0.04 -0.03 -0.02 0.04 -0.03 0.00 -0.02 -0.04

27 6 0.07 -0.04 -0.05 0.04 -0.02 -0.02 -0.03 0.02 0.04

28 6 -0.09 0.08 0.08 -0.04 0.04 0.05 0.05 -0.05 -0.02

29 6 0.04 -0.07 -0.05 0.02 -0.04 -0.02 -0.02 0.03 0.04

30 6 -0.04 0.02 -0.03 -0.04 0.02 -0.03 0.02 -0.00 -0.04

31 6 -0.03 0.03 -0.00 -0.04 -0.04 -0.05 0.05 0.05 0.02

32 6 -0.01 0.01 0.02 0.04 0.02 0.02 -0.03 -0.02 -0.04

33 6 -0.01 -0.00 0.02 -0.02 -0.04 0.03 0.00 0.02 0.04

34 6 0.02 -0.03 -0.00 -0.08 -0.08 -0.02 0.06 0.06 0.07

35 6 0.00 0.01 -0.02 -0.04 -0.02 0.03 0.02 0.00 0.04

36 6 -0.00 0.02 -0.01 0.02 0.04 0.02 -0.02 -0.03 -0.04

37 6 0.02 -0.03 0.00 0.08 0.08 -0.02 -0.06 -0.06 0.07

38 6 0.00 0.01 0.02 0.04 0.02 0.03 -0.02 -0.00 0.04

39 6 -0.00 0.02 0.01 -0.02 -0.04 0.02 0.02 0.03 -0.04

40 6 -0.03 0.03 0.00 0.04 0.04 -0.05 -0.05 -0.05 0.02

41 6 -0.01 0.01 -0.02 -0.04 -0.02 0.02 0.03 0.02 -0.04

42 6 -0.01 -0.00 -0.02 0.02 0.04 0.03 -0.00 -0.02 0.04

43 6 -0.15 0.15 -0.07 0.08 -0.08 0.02 -0.06 0.06 -0.07

44 6 -0.04 0.02 0.03 0.04 -0.02 -0.03 -0.02 0.00 -0.04

45 6 0.04 -0.07 0.05 -0.02 0.04 -0.02 0.02 -0.03 0.04

46 6 -0.09 0.08 -0.08 0.04 -0.04 0.05 -0.05 0.05 -0.02

47 6 0.07 -0.04 0.05 -0.04 0.02 -0.02 0.03 -0.02 0.04

48 6 -0.02 0.04 0.03 0.02 -0.04 -0.03 -0.00 0.02 -0.04

49 1 0.05 0.00 0.06 -0.01 -0.08 0.16 0.02 0.03 0.17

50 1 0.04 0.04 -0.07 -0.01 0.08 -0.16 0.02 -0.03 -0.17

51 1 -0.00 -0.04 0.05 0.08 0.01 0.16 -0.03 -0.02 0.17

52 1 -0.04 -0.04 -0.06 -0.08 0.01 -0.16 0.03 -0.02 -0.17

53 1 -0.00 -0.04 -0.05 -0.08 -0.01 0.16 0.03 0.02 0.17

54 1 -0.04 -0.04 0.06 0.08 -0.01 -0.16 -0.03 0.02 -0.17

55 1 0.04 0.04 0.07 0.01 -0.08 -0.16 -0.02 0.03 -0.17

56 1 0.05 0.00 -0.06 0.01 0.08 0.16 -0.02 -0.03 0.17

57 1 0.10 -0.05 -0.12 0.05 0.00 -0.09 -0.06 0.08 0.00

58 1 0.24 -0.18 -0.14 0.15 -0.09 -0.07 -0.11 0.13 0.12

59 1 -0.12 0.12 0.13 -0.05 0.05 0.07 0.05 -0.05 -0.04

60 1 0.18 -0.24 -0.14 0.09 -0.15 -0.07 -0.13 0.11 0.12

61 1 0.05 -0.11 -0.12 -0.00 -0.05 -0.09 -0.08 0.06 0.00

62 1 -0.03 0.03 -0.00 -0.05 -0.05 -0.07 0.05 0.05 0.04

63 1 0.01 -0.00 0.01 0.15 0.09 0.07 -0.11 -0.13 -0.12

64 1 -0.03 0.02 0.00 0.05 -0.00 0.09 -0.06 -0.08 -0.00

65 1 -0.02 0.03 0.00 -0.00 0.05 0.09 -0.08 -0.06 -0.00

66 1 0.01 0.00 -0.00 0.09 0.15 0.07 -0.13 -0.11 -0.12

67 1 -0.02 0.03 -0.00 0.00 -0.05 0.09 0.08 0.06 -0.00

68 1 0.01 0.00 0.00 -0.09 -0.15 0.07 0.13 0.11 -0.12

69 1 -0.03 0.03 0.00 0.05 0.05 -0.07 -0.05 -0.05 0.04

70 1 0.01 -0.00 -0.01 -0.15 -0.09 0.07 0.11 0.13 -0.12

71 1 -0.03 0.02 -0.00 -0.05 0.00 0.09 0.06 0.08 -0.00

72 1 0.05 -0.11 0.12 0.00 0.05 -0.09 0.08 -0.06 0.00

73 1 0.18 -0.24 0.14 -0.09 0.15 -0.07 0.13 -0.11 0.12

74 1 -0.12 0.12 -0.13 0.05 -0.05 0.07 -0.05 0.05 -0.04

75 1 0.24 -0.18 0.14 -0.15 0.09 -0.07 0.11 -0.13 0.12

76 1 0.10 -0.05 0.12 -0.05 -0.00 -0.09 0.06 -0.08 0.00

77 30 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00 0.00 0.00

55 56 57

E E B2

Frequencies -- 579.5509 579.5509 587.5409

Red. masses -- 5.4289 5.4289 6.8308

Frc consts -- 1.0744 1.0744 1.3893

IR Inten -- 8.4972 8.4972 14.9461

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.00 -0.05 -0.00 -0.01 0.12 -0.00 -0.00 -0.03

2 6 -0.00 -0.01 0.06 -0.01 0.01 -0.05 -0.00 -0.00 0.06

3 7 0.00 0.00 -0.13 -0.01 0.00 -0.03 0.00 0.01 -0.16

4 6 0.01 -0.00 0.03 -0.01 -0.01 0.08 0.00 -0.00 0.06

5 6 0.00 -0.00 0.00 -0.00 0.00 -0.13 0.00 -0.00 -0.03

6 6 0.02 0.01 0.16 0.00 -0.02 0.24 0.01 -0.01 0.25

7 6 0.01 0.01 0.05 0.01 -0.00 0.06 0.00 -0.00 0.06

8 7 0.00 0.01 0.03 -0.00 0.00 -0.13 -0.01 -0.00 -0.16

9 6 -0.01 0.01 -0.08 0.00 0.01 0.03 0.00 0.00 0.06

10 6 0.00 0.00 0.13 0.00 0.00 0.00 0.00 0.00 -0.03

11 6 -0.01 0.00 -0.12 0.00 -0.00 -0.05 0.00 -0.00 -0.03

12 6 -0.02 -0.00 0.24 -0.01 0.02 -0.16 -0.01 -0.01 0.25

13 6 -0.01 0.01 0.08 0.00 0.01 -0.03 -0.00 -0.00 0.06

14 6 0.00 0.00 -0.13 0.00 0.00 -0.00 -0.00 -0.00 -0.03

15 6 -0.01 0.00 0.12 0.00 -0.00 0.05 -0.00 0.00 -0.03

16 6 0.01 0.01 -0.05 0.01 -0.00 -0.06 -0.00 0.00 0.06

17 7 0.00 0.01 -0.03 -0.00 0.00 0.13 0.01 0.00 -0.16

18 6 0.02 0.01 -0.16 0.00 -0.02 -0.24 -0.01 0.01 0.25

19 6 0.01 -0.00 -0.03 -0.01 -0.01 -0.08 -0.00 0.00 0.06

20 6 0.00 -0.00 -0.00 -0.00 0.00 0.13 -0.00 0.00 -0.03

21 6 -0.00 -0.00 0.05 -0.00 -0.01 -0.12 0.00 0.00 -0.03

22 6 -0.00 -0.01 -0.06 -0.01 0.01 0.05 0.00 0.00 0.06

23 7 0.00 0.00 0.13 -0.01 0.00 0.03 -0.00 -0.01 -0.16

24 6 -0.02 -0.00 -0.24 -0.01 0.02 0.16 0.01 0.01 0.25

25 6 0.03 -0.02 -0.05 0.03 -0.04 -0.08 0.03 -0.03 -0.08

26 6 -0.01 -0.00 -0.05 -0.02 -0.00 -0.07 -0.02 -0.00 -0.08

27 6 -0.02 0.01 0.02 -0.02 0.02 0.05 -0.02 0.01 0.04

28 6 0.02 -0.04 -0.00 0.06 -0.05 -0.00 0.05 -0.05 0.01

29 6 -0.01 0.01 0.03 -0.02 0.03 0.04 -0.01 0.02 0.04

30 6 0.00 0.01 -0.04 0.00 0.02 -0.08 0.00 0.02 -0.08

31 6 -0.05 -0.06 -0.00 0.04 0.02 0.00 -0.05 -0.05 0.01

32 6 0.03 0.02 0.04 -0.01 -0.01 -0.03 0.02 0.01 0.04

33 6 0.02 -0.00 -0.08 -0.01 0.00 0.04 0.02 -0.00 -0.08

34 6 -0.04 -0.03 -0.08 0.02 0.03 0.05 -0.03 -0.03 -0.08

35 6 -0.00 0.02 -0.07 0.00 -0.01 0.05 -0.00 0.02 -0.08

36 6 0.02 0.02 0.05 -0.01 -0.02 -0.02 0.01 0.02 0.04

37 6 -0.04 -0.03 0.08 0.02 0.03 -0.05 0.03 0.03 -0.08

38 6 -0.00 0.02 0.07 0.00 -0.01 -0.05 0.00 -0.02 -0.08

39 6 0.02 0.02 -0.05 -0.01 -0.02 0.02 -0.01 -0.02 0.04

40 6 -0.05 -0.06 0.00 0.04 0.02 -0.00 0.05 0.05 0.01

41 6 0.03 0.02 -0.04 -0.01 -0.01 0.03 -0.02 -0.01 0.04

42 6 0.02 -0.00 0.08 -0.01 0.00 -0.04 -0.02 0.00 -0.08

43 6 0.03 -0.02 0.05 0.03 -0.04 0.08 -0.03 0.03 -0.08

44 6 0.00 0.01 0.04 0.00 0.02 0.08 -0.00 -0.02 -0.08

45 6 -0.01 0.01 -0.03 -0.02 0.03 -0.04 0.01 -0.02 0.04

46 6 0.02 -0.04 0.00 0.06 -0.05 0.00 -0.05 0.05 0.01

47 6 -0.02 0.01 -0.02 -0.02 0.02 -0.05 0.02 -0.01 0.04

48 6 -0.01 -0.00 0.05 -0.02 -0.00 0.07 0.02 0.00 -0.08

49 1 -0.00 0.00 -0.10 0.01 -0.01 0.23 -0.00 0.00 -0.06

50 1 -0.00 -0.00 0.01 0.01 0.01 -0.25 0.00 0.00 -0.06

51 1 0.01 -0.01 0.25 0.00 -0.00 0.01 -0.00 0.00 -0.06

52 1 -0.01 -0.01 -0.23 -0.00 -0.00 -0.10 -0.00 -0.00 -0.06

53 1 0.01 -0.01 -0.25 0.00 -0.00 -0.01 0.00 -0.00 -0.06

54 1 -0.01 -0.01 0.23 -0.00 -0.00 0.10 0.00 0.00 -0.06

55 1 -0.00 -0.00 -0.01 0.01 0.01 0.25 -0.00 -0.00 -0.06

56 1 -0.00 0.00 0.10 0.01 -0.01 -0.23 0.00 -0.00 -0.06

57 1 -0.05 0.06 -0.03 -0.07 0.12 -0.04 -0.07 0.11 -0.05

58 1 -0.04 0.10 0.08 -0.07 0.13 0.13 -0.06 0.13 0.13

59 1 0.02 -0.04 -0.01 0.05 -0.04 -0.01 0.03 -0.03 -0.00

60 1 -0.08 0.05 0.08 -0.14 0.07 0.13 -0.13 0.06 0.13

61 1 -0.08 0.04 -0.02 -0.10 0.07 -0.04 -0.11 0.07 -0.05

62 1 -0.04 -0.05 -0.01 0.04 0.02 0.01 -0.03 -0.03 -0.00

63 1 0.07 0.14 0.13 -0.05 -0.08 -0.08 0.06 0.13 0.13

64 1 0.07 0.10 -0.04 -0.04 -0.08 0.02 0.07 0.11 -0.05

65 1 0.12 0.07 -0.04 -0.06 -0.05 0.03 0.11 0.07 -0.05

66 1 0.13 0.07 0.13 -0.10 -0.04 -0.08 0.13 0.06 0.13

67 1 0.12 0.07 0.04 -0.06 -0.05 -0.03 -0.11 -0.07 -0.05

68 1 0.13 0.07 -0.13 -0.10 -0.04 0.08 -0.13 -0.06 0.13

69 1 -0.04 -0.05 0.01 0.04 0.02 -0.01 0.03 0.03 -0.00

70 1 0.07 0.14 -0.13 -0.05 -0.08 0.08 -0.06 -0.13 0.13

71 1 0.07 0.10 0.04 -0.04 -0.08 -0.02 -0.07 -0.11 -0.05

72 1 -0.08 0.04 0.02 -0.10 0.07 0.04 0.11 -0.07 -0.05

73 1 -0.08 0.05 -0.08 -0.14 0.07 -0.13 0.13 -0.06 0.13

74 1 0.02 -0.04 0.01 0.05 -0.04 0.01 -0.03 0.03 -0.00

75 1 -0.04 0.10 -0.08 -0.07 0.13 -0.13 0.06 -0.13 0.13

76 1 -0.05 0.06 0.03 -0.07 0.12 0.04 0.07 -0.11 -0.05

77 30 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.01

58 59 60

A2 E E

Frequencies -- 636.0020 636.4852 636.4852

Red. masses -- 6.3154 6.3351 6.3351

Frc consts -- 1.5051 1.5121 1.5121

IR Inten -- 0.0000 0.1663 0.1663

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.00 0.03 -0.00 0.00 -0.03 0.00 -0.00 -0.00

2 6 -0.00 0.00 -0.03 0.00 -0.00 0.04 0.00 -0.00 0.02

3 7 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.03

4 6 -0.00 -0.00 0.03 0.00 0.00 -0.03 -0.00 -0.00 0.02

5 6 0.00 0.00 -0.03 -0.00 -0.00 0.03 -0.00 -0.00 -0.00

6 6 -0.00 0.00 0.03 0.00 -0.00 -0.04 -0.00 0.00 0.05

7 6 0.00 0.00 0.03 -0.00 -0.00 -0.02 0.00 0.00 0.04

8 7 0.00 0.00 0.00 -0.00 0.00 0.03 0.00 0.00 -0.00

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 0.03 -0.00 0.00 0.00 0.00 -0.00 0.03

11 6 -0.00 -0.00 -0.03 -0.00 -0.00 0.00 -0.00 -0.00 -0.03

12 6 -0.00 -0.00 -0.03 0.00 0.00 0.05 0.00 0.00 0.04

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 0.03 -0.00 0.00 -0.00 0.00 -0.00 -0.03

15 6 0.00 0.00 -0.03 -0.00 -0.00 -0.00 -0.00 -0.00 0.03

16 6 -0.00 -0.00 0.03 -0.00 -0.00 0.02 0.00 0.00 -0.04

17 7 -0.00 -0.00 0.00 -0.00 0.00 -0.03 0.00 0.00 0.00

18 6 0.00 -0.00 0.03 0.00 -0.00 0.04 -0.00 0.00 -0.05

19 6 0.00 0.00 0.03 0.00 0.00 0.03 -0.00 -0.00 -0.02

20 6 -0.00 -0.00 -0.03 -0.00 -0.00 -0.03 -0.00 -0.00 0.00

21 6 -0.00 0.00 0.03 -0.00 0.00 0.03 0.00 -0.00 0.00

22 6 0.00 -0.00 -0.03 0.00 -0.00 -0.04 0.00 -0.00 -0.02

23 7 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.03

24 6 0.00 0.00 -0.03 0.00 0.00 -0.05 0.00 0.00 -0.04

25 6 0.02 -0.02 0.06 -0.02 0.03 -0.06 0.03 -0.02 0.06

26 6 0.12 0.04 0.08 -0.12 -0.04 -0.08 0.12 0.05 0.08

27 6 0.05 0.13 -0.10 -0.05 -0.13 0.10 0.05 0.14 -0.10

28 6 -0.01 0.01 -0.07 0.01 -0.01 0.07 -0.01 0.01 -0.07

29 6 -0.13 -0.05 -0.10 0.13 0.04 0.10 -0.14 -0.05 -0.10

30 6 -0.04 -0.12 0.08 0.04 0.12 -0.08 -0.04 -0.12 0.08

31 6 -0.01 -0.01 0.07 0.01 0.01 -0.07 0.01 0.01 -0.07

32 6 0.05 -0.13 0.10 -0.05 0.14 -0.10 -0.04 0.13 -0.10

33 6 0.12 -0.04 -0.08 -0.12 0.04 0.08 -0.12 0.04 0.08

34 6 0.02 0.02 -0.06 -0.02 -0.03 0.06 -0.03 -0.02 0.06

35 6 -0.04 0.12 -0.08 0.05 -0.12 0.08 0.04 -0.12 0.08

36 6 -0.13 0.05 0.10 0.14 -0.05 -0.10 0.13 -0.05 -0.10

37 6 -0.02 -0.02 -0.06 -0.02 -0.03 -0.06 -0.03 -0.02 -0.06

38 6 0.04 -0.12 -0.08 0.05 -0.12 -0.08 0.04 -0.12 -0.08

39 6 0.13 -0.05 0.10 0.14 -0.05 0.10 0.13 -0.05 0.10

40 6 0.01 0.01 0.07 0.01 0.01 0.07 0.01 0.01 0.07

41 6 -0.05 0.13 0.10 -0.05 0.14 0.10 -0.04 0.13 0.10

42 6 -0.12 0.04 -0.08 -0.12 0.04 -0.08 -0.12 0.04 -0.08

43 6 -0.02 0.02 0.06 -0.02 0.03 0.06 0.03 -0.02 -0.06

44 6 0.04 0.12 0.08 0.04 0.12 0.08 -0.04 -0.12 -0.08

45 6 0.13 0.05 -0.10 0.13 0.04 -0.10 -0.14 -0.05 0.10

46 6 0.01 -0.01 -0.07 0.01 -0.01 -0.07 -0.01 0.01 0.07

47 6 -0.05 -0.13 -0.10 -0.05 -0.13 -0.10 0.05 0.14 0.10

48 6 -0.12 -0.04 0.08 -0.12 -0.04 0.08 0.12 0.05 -0.08

49 1 0.01 -0.00 0.06 -0.01 0.00 -0.07 -0.00 -0.00 -0.03

50 1 0.01 0.00 -0.06 -0.01 -0.00 0.07 0.00 -0.00 -0.03

51 1 0.00 -0.01 0.06 -0.00 -0.00 0.03 0.00 -0.01 0.07

52 1 -0.00 -0.01 -0.06 -0.00 0.00 0.03 -0.00 -0.01 -0.07

53 1 -0.00 0.01 0.06 -0.00 -0.00 -0.03 0.00 -0.01 -0.07

54 1 0.00 0.01 -0.06 -0.00 0.00 -0.03 -0.00 -0.01 0.07

55 1 -0.01 -0.00 -0.06 -0.01 -0.00 -0.07 0.00 -0.00 0.03

56 1 -0.01 0.00 0.06 -0.01 0.00 0.07 -0.00 -0.00 0.03

57 1 0.08 -0.00 0.12 -0.07 -0.00 -0.12 0.07 -0.00 0.12

58 1 -0.04 0.12 -0.12 0.04 -0.12 0.12 -0.04 0.13 -0.12

59 1 0.05 -0.05 0.12 -0.05 0.05 -0.13 0.05 -0.05 0.13

60 1 -0.12 0.04 -0.12 0.12 -0.04 0.12 -0.12 0.04 -0.12

61 1 0.00 -0.08 0.12 -0.00 0.07 -0.12 -0.00 -0.08 0.12

62 1 0.05 0.05 -0.12 -0.05 -0.05 0.13 -0.05 -0.05 0.13

63 1 -0.04 -0.12 0.12 0.04 0.12 -0.12 0.04 0.12 -0.12

64 1 0.08 0.00 -0.12 -0.08 0.00 0.12 -0.07 -0.00 0.12

65 1 0.00 0.08 -0.12 -0.00 -0.07 0.12 0.00 -0.07 0.12

66 1 -0.12 -0.04 0.12 0.13 0.04 -0.12 0.12 0.04 -0.12

67 1 -0.00 -0.08 -0.12 -0.00 -0.07 -0.12 0.00 -0.07 -0.12

68 1 0.12 0.04 0.12 0.13 0.04 0.12 0.12 0.04 0.12

69 1 -0.05 -0.05 -0.12 -0.05 -0.05 -0.13 -0.05 -0.05 -0.13

70 1 0.04 0.12 0.12 0.04 0.12 0.12 0.04 0.12 0.12

71 1 -0.08 -0.00 -0.12 -0.08 0.00 -0.12 -0.07 -0.00 -0.12

72 1 -0.00 0.08 0.12 -0.00 0.07 0.12 -0.00 -0.08 -0.12

73 1 0.12 -0.04 -0.12 0.12 -0.04 -0.12 -0.12 0.04 0.12

74 1 -0.05 0.05 0.12 -0.05 0.05 0.13 0.05 -0.05 -0.13

75 1 0.04 -0.12 -0.12 0.04 -0.12 -0.12 -0.04 0.13 0.12

76 1 -0.08 0.00 0.12 -0.07 -0.00 0.12 0.07 -0.00 -0.12

77 30 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00

61 62 63

B2 A1 E

Frequencies -- 637.3966 653.8423 678.0874

Red. masses -- 6.3995 7.2385 6.2401

Frc consts -- 1.5318 1.8232 1.6905

IR Inten -- 3.6418 0.0000 26.8763

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.00 -0.01 0.00 0.04 0.00 0.02 -0.05 0.02

2 6 0.00 -0.00 0.03 0.04 0.01 0.00 0.05 -0.05 -0.02

3 7 -0.00 -0.00 -0.05 0.00 0.02 -0.01 0.08 0.00 -0.02

4 6 -0.00 -0.00 0.03 -0.04 0.01 0.00 0.02 0.04 0.05

5 6 0.00 -0.00 -0.01 -0.00 0.04 0.00 0.02 0.07 -0.02

6 6 -0.00 0.00 0.06 -0.09 -0.09 0.00 -0.06 -0.08 -0.00

7 6 0.00 0.00 0.03 0.01 -0.04 -0.00 0.02 -0.02 -0.05

8 7 0.00 0.00 -0.05 0.02 -0.00 0.01 0.00 0.04 0.03

9 6 0.00 -0.00 0.03 0.01 0.04 -0.00 -0.03 0.05 -0.01

10 6 0.00 0.00 -0.01 0.04 0.00 -0.00 -0.01 0.01 -0.01

11 6 0.00 -0.00 -0.01 0.04 -0.00 -0.00 0.05 0.01 0.01

12 6 0.00 0.00 0.06 0.09 -0.09 0.00 -0.00 0.05 0.01

13 6 -0.00 0.00 0.03 -0.01 -0.04 -0.00 -0.03 0.05 0.01

14 6 -0.00 -0.00 -0.01 -0.04 -0.00 -0.00 -0.01 0.01 0.01

15 6 -0.00 0.00 -0.01 -0.04 0.00 -0.00 0.05 0.01 -0.01

16 6 -0.00 -0.00 0.03 -0.01 0.04 -0.00 0.02 -0.02 0.05

17 7 -0.00 -0.00 -0.05 -0.02 0.00 0.01 0.00 0.04 -0.03

18 6 0.00 -0.00 0.06 0.09 0.09 0.00 -0.06 -0.08 0.00

19 6 0.00 0.00 0.03 0.04 -0.01 0.00 0.02 0.04 -0.05

20 6 -0.00 0.00 -0.01 0.00 -0.04 0.00 0.02 0.07 0.02

21 6 0.00 0.00 -0.01 -0.00 -0.04 0.00 0.02 -0.05 -0.02

22 6 -0.00 0.00 0.03 -0.04 -0.01 0.00 0.05 -0.05 0.02

23 7 0.00 0.00 -0.05 -0.00 -0.02 -0.01 0.08 0.00 0.02

24 6 -0.00 -0.00 0.06 -0.09 0.09 0.00 -0.00 0.05 -0.01

25 6 0.03 -0.03 0.05 -0.12 -0.12 -0.00 -0.13 -0.13 -0.00

26 6 0.12 0.04 0.07 0.02 -0.06 0.11 0.01 -0.07 0.13

27 6 0.05 0.14 -0.10 0.03 -0.04 0.11 0.04 -0.07 0.12

28 6 -0.01 0.01 -0.07 0.12 0.12 0.00 0.13 0.14 0.01

29 6 -0.14 -0.05 -0.10 -0.04 0.03 -0.11 -0.06 0.02 -0.13

30 6 -0.04 -0.12 0.07 -0.06 0.02 -0.11 -0.08 0.02 -0.12

31 6 0.01 0.01 -0.07 -0.12 0.12 0.00 0.02 -0.07 -0.02

32 6 -0.05 0.14 -0.10 -0.03 -0.04 0.11 0.03 0.04 -0.03

33 6 -0.12 0.04 0.07 -0.02 -0.06 0.11 -0.01 0.00 -0.06

34 6 -0.03 -0.03 0.05 0.12 -0.12 -0.00 -0.05 0.05 0.00

35 6 0.04 -0.12 0.07 0.06 0.02 -0.11 -0.05 -0.03 0.03

36 6 0.14 -0.05 -0.10 0.04 0.03 -0.11 -0.01 0.01 0.06

37 6 0.03 0.03 0.05 -0.12 0.12 -0.00 -0.05 0.05 -0.00

38 6 -0.04 0.12 0.07 -0.06 -0.02 -0.11 -0.05 -0.03 -0.03

39 6 -0.14 0.05 -0.10 -0.04 -0.03 -0.11 -0.01 0.01 -0.06

40 6 -0.01 -0.01 -0.07 0.12 -0.12 0.00 0.02 -0.07 0.02

41 6 0.05 -0.14 -0.10 0.03 0.04 0.11 0.03 0.04 0.03

42 6 0.12 -0.04 0.07 0.02 0.06 0.11 -0.01 0.00 0.06

43 6 -0.03 0.03 0.05 0.12 0.12 -0.00 -0.13 -0.13 0.00

44 6 0.04 0.12 0.07 0.06 -0.02 -0.11 -0.08 0.02 0.12

45 6 0.14 0.05 -0.10 0.04 -0.03 -0.11 -0.06 0.02 0.13

46 6 0.01 -0.01 -0.07 -0.12 -0.12 0.00 0.13 0.14 -0.01

47 6 -0.05 -0.14 -0.10 -0.03 0.04 0.11 0.04 -0.07 -0.12

48 6 -0.12 -0.04 0.07 -0.02 0.06 0.11 0.01 -0.07 -0.13

49 1 -0.00 -0.00 -0.04 -0.02 0.03 -0.00 -0.06 -0.11 0.01

50 1 0.00 -0.00 -0.04 0.02 0.03 -0.00 -0.04 0.12 -0.08

51 1 0.00 0.00 -0.04 0.03 -0.02 0.00 -0.04 -0.04 0.06

52 1 0.00 -0.00 -0.04 0.03 0.02 0.00 0.07 -0.01 0.10

53 1 -0.00 -0.00 -0.04 -0.03 0.02 0.00 -0.04 -0.04 -0.06

54 1 -0.00 0.00 -0.04 -0.03 -0.02 0.00 0.07 -0.01 -0.10

55 1 -0.00 0.00 -0.04 -0.02 -0.03 -0.00 -0.04 0.12 0.08

56 1 0.00 0.00 -0.04 0.02 -0.03 -0.00 -0.06 -0.11 -0.01

57 1 0.07 0.01 0.12 0.09 0.06 0.04 0.09 0.05 0.05

58 1 -0.04 0.13 -0.11 -0.10 -0.12 0.03 -0.11 -0.18 0.02

59 1 0.05 -0.05 0.13 0.12 0.12 -0.00 0.13 0.14 0.00

60 1 -0.13 0.04 -0.11 -0.12 -0.10 -0.03 -0.14 -0.16 -0.05

61 1 -0.01 -0.07 0.12 0.06 0.09 -0.04 0.05 0.09 -0.06

62 1 -0.05 -0.05 0.13 -0.12 0.12 -0.00 0.04 -0.06 -0.01

63 1 0.04 0.13 -0.11 0.10 -0.12 0.03 0.02 0.12 0.04

64 1 -0.07 0.01 0.12 -0.09 0.06 0.04 0.03 -0.02 -0.01

65 1 0.01 -0.07 0.12 -0.06 0.09 -0.04 0.01 -0.03 0.03

66 1 0.13 0.04 -0.11 0.12 -0.10 -0.03 0.01 0.12 0.06

67 1 -0.01 0.07 0.12 0.06 -0.09 -0.04 0.01 -0.03 -0.03

68 1 -0.13 -0.04 -0.11 -0.12 0.10 -0.03 0.01 0.12 -0.06

69 1 0.05 0.05 0.13 0.12 -0.12 -0.00 0.04 -0.06 0.01

70 1 -0.04 -0.13 -0.11 -0.10 0.12 0.03 0.02 0.12 -0.04

71 1 0.07 -0.01 0.12 0.09 -0.06 0.04 0.03 -0.02 0.01

72 1 0.01 0.07 0.12 -0.06 -0.09 -0.04 0.05 0.09 0.06

73 1 0.13 -0.04 -0.11 0.12 0.10 -0.03 -0.14 -0.16 0.05

74 1 -0.05 0.05 0.13 -0.12 -0.12 -0.00 0.13 0.14 -0.00

75 1 0.04 -0.13 -0.11 0.10 0.12 0.03 -0.11 -0.18 -0.02

76 1 -0.07 -0.01 0.12 -0.09 -0.06 0.04 0.09 0.05 -0.05

77 30 -0.00 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

64 65 66

E A1 E

Frequencies -- 678.0874 682.3646 688.3311

Red. masses -- 6.2401 2.8381 3.3091

Frc consts -- 1.6905 0.7786 0.9237

IR Inten -- 26.8763 0.0000 5.0974

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 -0.05 0.01 -0.00 -0.00 -0.00 -0.00 0.00 -0.07

2 6 -0.02 -0.02 -0.05 0.00 0.01 -0.11 0.01 -0.01 0.00

3 7 0.04 -0.00 0.03 0.00 -0.01 0.12 0.01 -0.01 0.10

4 6 0.05 0.03 -0.01 -0.00 0.01 -0.11 0.00 0.02 -0.17

5 6 0.01 0.01 -0.01 0.00 -0.00 -0.00 -0.00 0.00 0.06

6 6 0.05 0.00 -0.01 0.00 0.00 -0.00 -0.00 -0.00 0.00

7 6 -0.05 -0.05 0.02 0.01 -0.00 0.11 0.02 0.00 0.17

8 7 0.00 -0.08 0.02 -0.01 -0.00 -0.12 -0.01 0.01 -0.11

9 6 0.04 -0.02 -0.05 0.01 0.00 0.11 -0.00 0.01 0.03

10 6 0.07 -0.02 0.02 -0.00 -0.00 0.00 0.00 -0.00 0.06

11 6 -0.05 -0.02 -0.02 -0.00 0.00 0.00 0.00 -0.00 -0.05

12 6 -0.08 0.06 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.01

13 6 0.04 -0.02 0.05 -0.01 -0.00 0.11 -0.00 0.01 -0.03

14 6 0.07 -0.02 -0.02 0.00 0.00 0.00 0.00 -0.00 -0.06

15 6 -0.05 -0.02 0.02 0.00 -0.00 0.00 0.00 -0.00 0.05

16 6 -0.05 -0.05 -0.02 -0.01 0.00 0.11 0.02 0.00 -0.17

17 7 0.00 -0.08 -0.02 0.01 0.00 -0.12 -0.01 0.01 0.11

18 6 0.05 0.00 0.01 -0.00 -0.00 0.00 -0.00 -0.00 -0.00

19 6 0.05 0.03 0.01 0.00 -0.01 -0.11 0.00 0.02 0.17

20 6 0.01 0.01 0.01 -0.00 0.00 -0.00 -0.00 0.00 -0.06

21 6 0.01 -0.05 -0.01 0.00 0.00 -0.00 -0.00 0.00 0.07

22 6 -0.02 -0.02 0.05 -0.00 -0.01 -0.11 0.01 -0.01 -0.00

23 7 0.04 -0.00 -0.03 0.00 0.01 0.12 0.01 -0.01 -0.10

24 6 -0.08 0.06 0.00 0.00 -0.00 -0.00 0.00 0.00 0.01

25 6 0.05 0.05 -0.00 -0.00 -0.00 -0.00 -0.02 -0.02 -0.00

26 6 -0.03 0.05 -0.03 0.00 -0.00 0.00 0.00 -0.01 0.02

27 6 0.01 0.01 -0.06 0.00 -0.00 0.00 0.00 -0.01 0.02

28 6 -0.07 -0.02 0.02 0.00 0.00 0.00 0.02 0.02 0.00

29 6 0.04 -0.03 0.03 -0.00 0.00 -0.00 -0.01 0.00 -0.02

30 6 0.00 0.01 0.06 -0.00 0.00 -0.00 -0.01 0.00 -0.02

31 6 0.14 -0.13 0.01 -0.00 0.00 -0.00 0.00 -0.00 -0.00

32 6 0.02 0.06 -0.13 -0.00 -0.00 0.00 0.00 -0.00 0.00

33 6 0.02 0.08 -0.12 -0.00 -0.00 0.00 -0.00 -0.00 0.00

34 6 -0.13 0.13 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00

35 6 -0.07 -0.01 0.13 0.00 0.00 -0.00 -0.01 -0.00 0.00

36 6 -0.07 -0.04 0.12 0.00 0.00 -0.00 -0.00 0.00 0.00

37 6 -0.13 0.13 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

38 6 -0.07 -0.01 -0.13 -0.00 -0.00 -0.00 -0.01 -0.00 -0.00

39 6 -0.07 -0.04 -0.12 -0.00 -0.00 -0.00 -0.00 0.00 -0.00

40 6 0.14 -0.13 -0.01 0.00 -0.00 0.00 0.00 -0.00 0.00

41 6 0.02 0.06 0.13 0.00 0.00 0.00 0.00 -0.00 -0.00

42 6 0.02 0.08 0.12 0.00 0.00 0.00 -0.00 -0.00 -0.00

43 6 0.05 0.05 0.00 0.00 0.00 0.00 -0.02 -0.02 0.00

44 6 0.00 0.01 -0.06 0.00 -0.00 -0.00 -0.01 0.00 0.02

45 6 0.04 -0.03 -0.03 0.00 -0.00 -0.00 -0.01 0.00 0.02

46 6 -0.07 -0.02 -0.02 -0.00 -0.00 -0.00 0.02 0.02 -0.00

47 6 0.01 0.01 0.06 -0.00 0.00 0.00 0.00 -0.01 -0.02

48 6 -0.03 0.05 0.03 -0.00 0.00 0.00 0.00 -0.01 -0.02

49 1 -0.01 -0.07 0.10 -0.01 -0.04 0.32 -0.01 -0.03 0.12

50 1 -0.04 0.04 0.06 0.01 -0.04 0.32 -0.00 -0.04 0.40

51 1 0.12 0.04 0.08 -0.04 -0.01 -0.32 -0.03 -0.01 -0.18

52 1 -0.11 0.06 -0.01 -0.04 0.01 -0.32 -0.04 0.00 -0.42

53 1 0.12 0.04 -0.08 0.04 0.01 -0.32 -0.03 -0.01 0.18

54 1 -0.11 0.06 0.01 0.04 -0.01 -0.32 -0.04 0.00 0.42

55 1 -0.04 0.04 -0.06 -0.01 0.04 0.32 -0.00 -0.04 -0.40

56 1 -0.01 -0.07 -0.10 0.01 0.04 0.32 -0.01 -0.03 -0.12

57 1 -0.03 -0.01 -0.03 0.01 -0.00 -0.01 0.03 -0.00 -0.00

58 1 0.12 -0.01 -0.06 -0.00 -0.00 -0.00 -0.02 -0.03 0.00

59 1 -0.06 -0.04 0.01 0.00 0.00 0.00 0.02 0.02 0.00

60 1 0.12 -0.02 -0.04 -0.00 -0.00 0.00 -0.03 -0.02 -0.00

61 1 -0.02 -0.03 0.01 -0.00 0.01 0.01 -0.00 0.03 0.00

62 1 0.14 -0.13 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.01

63 1 -0.16 0.14 -0.05 0.00 -0.00 -0.00 0.00 -0.00 -0.00

64 1 0.09 -0.05 -0.06 -0.01 -0.00 -0.01 -0.00 -0.01 0.00

65 1 0.05 -0.09 0.05 0.00 0.01 0.01 -0.01 -0.01 0.00

66 1 -0.18 0.11 0.02 0.00 -0.00 0.00 -0.01 0.01 -0.00

67 1 0.05 -0.09 -0.05 -0.00 -0.01 0.01 -0.01 -0.01 -0.00

68 1 -0.18 0.11 -0.02 -0.00 0.00 0.00 -0.01 0.01 0.00

69 1 0.14 -0.13 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.01

70 1 -0.16 0.14 0.05 -0.00 0.00 -0.00 0.00 -0.00 0.00

71 1 0.09 -0.05 0.06 0.01 0.00 -0.01 -0.00 -0.01 -0.00

72 1 -0.02 -0.03 -0.01 0.00 -0.01 0.01 -0.00 0.03 -0.00

73 1 0.12 -0.02 0.04 0.00 0.00 0.00 -0.03 -0.02 0.00

74 1 -0.06 -0.04 -0.01 -0.00 -0.00 -0.00 0.02 0.02 -0.00

75 1 0.12 -0.01 0.06 0.00 0.00 -0.00 -0.02 -0.03 -0.00

76 1 -0.03 -0.01 0.03 -0.01 0.00 -0.01 0.03 -0.00 0.00

77 30 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00

67 68 69

E B1 B1

Frequencies -- 688.3311 691.7080 697.9440

Red. masses -- 3.3091 5.1057 6.1406

Frc consts -- 0.9237 1.4393 1.7624

IR Inten -- 5.0974 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.00 -0.05 -0.02 0.03 -0.11 0.02 -0.04 -0.06

2 6 0.00 -0.02 0.17 -0.01 0.01 0.16 0.03 -0.05 0.08

3 7 0.01 0.01 -0.11 -0.03 0.00 -0.00 0.06 -0.00 -0.00

4 6 0.01 0.00 0.03 -0.01 -0.01 -0.16 0.03 0.05 -0.08

5 6 -0.00 -0.00 0.06 -0.02 -0.03 0.11 0.02 0.04 0.06

6 6 0.00 -0.00 0.01 0.02 0.02 0.00 -0.03 -0.03 -0.00

7 6 -0.01 -0.01 -0.00 -0.01 -0.01 0.16 0.05 0.03 0.08

8 7 -0.01 -0.01 -0.10 0.00 -0.03 0.00 -0.00 0.06 -0.00

9 6 0.02 -0.00 0.17 0.01 -0.01 -0.16 -0.05 0.03 -0.08

10 6 0.00 0.00 -0.06 0.03 -0.02 0.11 -0.04 0.02 0.06

11 6 0.00 0.00 0.07 -0.03 -0.02 -0.11 0.04 0.02 -0.06

12 6 -0.00 0.00 0.00 0.02 -0.02 0.00 -0.03 0.03 -0.00

13 6 0.02 -0.00 -0.17 -0.01 0.01 -0.16 0.05 -0.03 -0.08

14 6 0.00 0.00 0.06 -0.03 0.02 0.11 0.04 -0.02 0.06

15 6 0.00 0.00 -0.07 0.03 0.02 -0.11 -0.04 -0.02 -0.06

16 6 -0.01 -0.01 0.00 0.01 0.01 0.16 -0.05 -0.03 0.08

17 7 -0.01 -0.01 0.10 -0.00 0.03 0.00 0.00 -0.06 -0.00

18 6 0.00 -0.00 -0.01 -0.02 -0.02 -0.00 0.03 0.03 -0.00

19 6 0.01 0.00 -0.03 0.01 0.01 -0.16 -0.03 -0.05 -0.08

20 6 -0.00 -0.00 -0.06 0.02 0.03 0.11 -0.02 -0.04 0.06

21 6 -0.00 -0.00 0.05 0.02 -0.03 -0.11 -0.02 0.04 -0.06

22 6 0.00 -0.02 -0.17 0.01 -0.01 0.16 -0.03 0.05 0.08

23 7 0.01 0.01 0.11 0.03 -0.00 -0.00 -0.06 0.00 0.00

24 6 -0.00 0.00 -0.00 -0.02 0.02 0.00 0.03 -0.03 -0.00

25 6 0.00 0.00 -0.00 0.03 0.03 0.00 -0.09 -0.09 -0.00

26 6 -0.00 0.01 -0.00 -0.00 0.02 -0.04 0.01 -0.06 0.09

27 6 0.00 0.00 -0.00 -0.01 0.02 -0.04 0.02 -0.05 0.10

28 6 -0.00 -0.00 0.00 -0.04 -0.04 -0.00 0.09 0.09 0.00

29 6 -0.00 -0.00 -0.00 0.02 -0.01 0.04 -0.05 0.02 -0.10

30 6 -0.00 0.00 -0.00 0.02 -0.00 0.04 -0.06 0.01 -0.09

31 6 0.02 -0.02 0.00 -0.04 0.04 -0.00 0.09 -0.09 0.00

32 6 0.00 0.01 -0.02 -0.01 -0.02 0.04 0.02 0.05 -0.10

33 6 0.00 0.01 -0.02 -0.00 -0.02 0.04 0.01 0.06 -0.09

34 6 -0.02 0.02 -0.00 0.03 -0.03 -0.00 -0.09 0.09 0.00

35 6 -0.01 -0.00 0.02 0.02 0.00 -0.04 -0.06 -0.01 0.09

36 6 -0.01 -0.00 0.02 0.02 0.01 -0.04 -0.05 -0.02 0.10

37 6 -0.02 0.02 0.00 -0.03 0.03 -0.00 0.09 -0.09 0.00

38 6 -0.01 -0.00 -0.02 -0.02 -0.00 -0.04 0.06 0.01 0.09

39 6 -0.01 -0.00 -0.02 -0.02 -0.01 -0.04 0.05 0.02 0.10

40 6 0.02 -0.02 -0.00 0.04 -0.04 0.00 -0.09 0.09 -0.00

41 6 0.00 0.01 0.02 0.01 0.02 0.04 -0.02 -0.05 -0.10

42 6 0.00 0.01 0.02 0.00 0.02 0.04 -0.01 -0.06 -0.09

43 6 0.00 0.00 0.00 -0.03 -0.03 0.00 0.09 0.09 0.00

44 6 -0.00 0.00 0.00 -0.02 0.00 0.04 0.06 -0.01 -0.09

45 6 -0.00 -0.00 0.00 -0.02 0.01 0.04 0.05 -0.02 -0.10

46 6 -0.00 -0.00 -0.00 0.04 0.04 0.00 -0.09 -0.09 -0.00

47 6 0.00 0.00 0.00 0.01 -0.02 -0.04 -0.02 0.05 0.10

48 6 -0.00 0.01 0.00 0.00 -0.02 -0.04 -0.01 0.06 0.09

49 1 0.00 0.04 -0.42 0.01 0.07 -0.26 -0.02 -0.07 -0.14

50 1 -0.01 0.03 -0.18 0.01 -0.07 0.26 -0.02 0.07 0.14

51 1 -0.04 0.00 -0.40 0.07 0.01 0.26 -0.07 -0.02 0.14

52 1 -0.03 0.01 -0.12 -0.07 0.01 -0.26 0.07 -0.02 -0.14

53 1 -0.04 0.00 0.40 -0.07 -0.01 0.26 0.07 0.02 0.14

54 1 -0.03 0.01 0.12 0.07 -0.01 -0.26 -0.07 0.02 -0.14

55 1 -0.01 0.03 0.18 -0.01 0.07 0.26 0.02 -0.07 0.14

56 1 0.00 0.04 0.42 -0.01 -0.07 -0.26 0.02 0.07 -0.14

57 1 -0.01 0.01 -0.00 -0.02 -0.02 -0.03 0.07 0.02 0.04

58 1 0.01 0.01 0.00 0.04 0.05 -0.01 -0.10 -0.13 0.03

59 1 -0.00 0.00 0.01 -0.04 -0.04 -0.00 0.09 0.09 0.00

60 1 -0.00 -0.00 0.00 0.05 0.04 0.01 -0.13 -0.10 -0.03

61 1 -0.01 0.00 -0.00 -0.02 -0.02 0.03 0.02 0.07 -0.04

62 1 0.02 -0.02 0.00 -0.04 0.04 -0.00 0.09 -0.09 0.00

63 1 -0.02 0.03 -0.00 0.04 -0.05 0.01 -0.10 0.13 -0.03

64 1 0.03 0.00 0.00 -0.02 0.02 0.03 0.07 -0.02 -0.04

65 1 -0.00 -0.03 -0.00 -0.02 0.02 -0.03 0.02 -0.07 0.04

66 1 -0.03 0.02 0.00 0.05 -0.04 -0.01 -0.13 0.10 0.03

67 1 -0.00 -0.03 0.00 0.02 -0.02 -0.03 -0.02 0.07 0.04

68 1 -0.03 0.02 -0.00 -0.05 0.04 -0.01 0.13 -0.10 0.03

69 1 0.02 -0.02 -0.00 0.04 -0.04 0.00 -0.09 0.09 -0.00

70 1 -0.02 0.03 0.00 -0.04 0.05 0.01 0.10 -0.13 -0.03

71 1 0.03 0.00 -0.00 0.02 -0.02 0.03 -0.07 0.02 -0.04

72 1 -0.01 0.00 0.00 0.02 0.02 0.03 -0.02 -0.07 -0.04

73 1 -0.00 -0.00 -0.00 -0.05 -0.04 0.01 0.13 0.10 -0.03

74 1 -0.00 0.00 -0.01 0.04 0.04 0.00 -0.09 -0.09 -0.00

75 1 0.01 0.01 -0.00 -0.04 -0.05 -0.01 0.10 0.13 0.03

76 1 -0.01 0.01 0.00 0.02 0.02 -0.03 -0.07 -0.02 0.04

77 30 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00

70 71 72

B2 E E

Frequencies -- 715.0756 715.4371 715.4371

Red. masses -- 1.6470 1.5913 1.5913

Frc consts -- 0.4962 0.4799 0.4799

IR Inten -- 82.5125 124.0043 124.0044

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 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00

25 6 -0.03 0.03 0.02 -0.01 0.00 0.00 0.04 -0.04 -0.03

26 6 0.02 -0.02 -0.02 0.00 -0.01 0.00 -0.03 0.03 0.02

27 6 -0.04 0.04 0.03 -0.01 0.00 0.01 0.06 -0.06 -0.04

28 6 0.02 -0.02 -0.01 0.01 0.00 -0.00 -0.02 0.02 0.01

29 6 -0.04 0.04 0.03 -0.01 0.01 -0.00 0.06 -0.06 -0.04

30 6 0.02 -0.02 -0.02 -0.00 -0.00 -0.01 -0.03 0.03 0.02

31 6 -0.02 -0.02 -0.01 0.02 0.02 0.01 -0.00 0.01 0.00

32 6 0.04 0.04 0.03 -0.06 -0.06 -0.04 -0.01 -0.01 0.00

33 6 -0.02 -0.02 -0.02 0.03 0.03 0.02 0.00 -0.00 0.01

34 6 0.03 0.03 0.02 -0.04 -0.04 -0.03 -0.00 -0.01 -0.00

35 6 -0.02 -0.02 -0.02 0.03 0.03 0.02 0.01 0.00 -0.00

36 6 0.04 0.04 0.03 -0.06 -0.06 -0.04 -0.00 -0.01 -0.01

37 6 -0.03 -0.03 0.02 -0.04 -0.04 0.03 -0.00 -0.01 0.00

38 6 0.02 0.02 -0.02 0.03 0.03 -0.02 0.01 0.00 0.00

39 6 -0.04 -0.04 0.03 -0.06 -0.06 0.04 -0.00 -0.01 0.01

40 6 0.02 0.02 -0.01 0.02 0.02 -0.01 -0.00 0.01 -0.00

41 6 -0.04 -0.04 0.03 -0.06 -0.06 0.04 -0.01 -0.01 -0.00

42 6 0.02 0.02 -0.02 0.03 0.03 -0.02 0.00 -0.00 -0.01

43 6 0.03 -0.03 0.02 -0.01 0.00 -0.00 0.04 -0.04 0.03

44 6 -0.02 0.02 -0.02 -0.00 -0.00 0.01 -0.03 0.03 -0.02

45 6 0.04 -0.04 0.03 -0.01 0.01 0.00 0.06 -0.06 0.04

46 6 -0.02 0.02 -0.01 0.01 0.00 0.00 -0.02 0.02 -0.01

47 6 0.04 -0.04 0.03 -0.01 0.00 -0.01 0.06 -0.06 0.04

48 6 -0.02 0.02 -0.02 0.00 -0.01 -0.00 -0.03 0.03 -0.02

49 1 -0.00 0.00 -0.02 0.00 -0.01 0.01 -0.00 0.00 0.01

50 1 0.00 0.00 -0.02 0.00 0.00 0.01 -0.00 -0.01 0.01

51 1 -0.00 0.00 -0.02 -0.01 0.00 -0.01 -0.00 0.00 0.01

52 1 -0.00 -0.00 -0.02 0.00 0.00 -0.01 0.01 0.00 0.01

53 1 0.00 -0.00 -0.02 -0.01 0.00 0.01 -0.00 0.00 -0.01

54 1 0.00 0.00 -0.02 0.00 0.00 0.01 0.01 0.00 -0.01

55 1 -0.00 -0.00 -0.02 0.00 0.00 -0.01 -0.00 -0.01 -0.01

56 1 0.00 -0.00 -0.02 0.00 -0.01 -0.01 -0.00 0.00 -0.01

57 1 0.15 -0.15 -0.11 0.02 -0.02 -0.01 -0.21 0.21 0.16

58 1 0.07 -0.07 -0.05 0.00 -0.02 -0.01 -0.11 0.10 0.07

59 1 0.19 -0.19 -0.14 0.03 -0.02 -0.02 -0.27 0.27 0.20

60 1 0.07 -0.07 -0.05 0.00 -0.02 -0.01 -0.10 0.11 0.07

61 1 0.15 -0.15 -0.11 0.02 -0.02 -0.02 -0.21 0.21 0.16

62 1 -0.19 -0.19 -0.14 0.27 0.27 0.20 0.02 0.03 0.02

63 1 -0.07 -0.07 -0.05 0.11 0.10 0.07 0.02 0.00 0.01

64 1 -0.15 -0.15 -0.11 0.21 0.21 0.16 0.02 0.02 0.02

65 1 -0.15 -0.15 -0.11 0.21 0.21 0.16 0.02 0.02 0.01

66 1 -0.07 -0.07 -0.05 0.10 0.11 0.07 0.02 0.00 0.01

67 1 0.15 0.15 -0.11 0.21 0.21 -0.16 0.02 0.02 -0.01

68 1 0.07 0.07 -0.05 0.10 0.11 -0.07 0.02 0.00 -0.01

69 1 0.19 0.19 -0.14 0.27 0.27 -0.20 0.02 0.03 -0.02

70 1 0.07 0.07 -0.05 0.11 0.10 -0.07 0.02 0.00 -0.01

71 1 0.15 0.15 -0.11 0.21 0.21 -0.16 0.02 0.02 -0.02

72 1 -0.15 0.15 -0.11 0.02 -0.02 0.02 -0.21 0.21 -0.16

73 1 -0.07 0.07 -0.05 0.00 -0.02 0.01 -0.10 0.11 -0.07

74 1 -0.19 0.19 -0.14 0.03 -0.02 0.02 -0.27 0.27 -0.20

75 1 -0.07 0.07 -0.05 0.00 -0.02 0.01 -0.11 0.10 -0.07

76 1 -0.15 0.15 -0.11 0.02 -0.02 0.01 -0.21 0.21 -0.16

77 30 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00

73 74 75

A2 B2 E

Frequencies -- 715.6481 731.6341 742.0454

Red. masses -- 1.5490 1.8962 2.8141

Frc consts -- 0.4674 0.5980 0.9130

IR Inten -- 0.0000 122.2768 38.2355

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.00 -0.00 0.00 0.00 -0.03 -0.02 0.00 0.06

2 6 0.00 -0.00 -0.00 0.01 0.00 -0.06 -0.00 0.02 -0.11

3 7 0.00 -0.00 -0.00 0.00 -0.01 0.06 -0.00 0.00 -0.01

4 6 0.00 0.00 0.00 -0.01 0.00 -0.06 0.00 -0.02 0.13

5 6 0.00 0.00 0.00 -0.00 0.00 -0.03 -0.02 -0.00 -0.04

6 6 0.00 -0.00 -0.00 -0.01 0.01 0.07 0.02 -0.02 -0.12

7 6 -0.00 -0.00 0.00 -0.00 0.01 -0.06 0.00 -0.01 0.08

8 7 0.00 -0.00 0.00 0.01 0.00 0.06 -0.02 0.00 -0.05

9 6 0.00 -0.00 -0.00 -0.00 -0.01 -0.06 -0.01 0.01 0.02

10 6 0.00 -0.00 -0.00 -0.00 -0.00 -0.03 0.00 0.01 0.05

11 6 -0.00 -0.00 0.00 -0.00 0.00 -0.03 0.00 0.00 0.02

12 6 0.00 0.00 0.00 0.01 0.01 0.07 0.01 0.02 0.07

13 6 -0.00 0.00 -0.00 0.00 0.01 -0.06 -0.01 0.01 -0.02

14 6 -0.00 0.00 -0.00 0.00 0.00 -0.03 0.00 0.01 -0.05

15 6 0.00 0.00 0.00 0.00 -0.00 -0.03 0.00 0.00 -0.02

16 6 0.00 0.00 0.00 0.00 -0.01 -0.06 0.00 -0.01 -0.08

17 7 -0.00 0.00 0.00 -0.01 -0.00 0.06 -0.02 0.00 0.05

18 6 -0.00 0.00 -0.00 0.01 -0.01 0.07 0.02 -0.02 0.12

19 6 -0.00 -0.00 0.00 0.01 -0.00 -0.06 0.00 -0.02 -0.13

20 6 -0.00 -0.00 0.00 0.00 -0.00 -0.03 -0.02 -0.00 0.04

21 6 -0.00 0.00 -0.00 -0.00 -0.00 -0.03 -0.02 0.00 -0.06

22 6 -0.00 0.00 -0.00 -0.01 -0.00 -0.06 -0.00 0.02 0.11

23 7 -0.00 -0.00 -0.00 -0.00 0.01 0.06 -0.00 0.00 0.01

24 6 -0.00 -0.00 0.00 -0.01 -0.01 0.07 0.01 0.02 -0.07

25 6 -0.03 0.03 0.02 -0.01 0.01 0.01 0.03 -0.03 -0.02

26 6 0.02 -0.02 -0.02 0.01 -0.01 -0.01 -0.02 0.02 0.02

27 6 -0.04 0.04 0.03 -0.00 0.01 0.00 0.00 -0.01 -0.01

28 6 0.01 -0.01 -0.01 0.01 -0.01 -0.01 -0.03 0.02 0.02

29 6 -0.04 0.04 0.03 -0.01 0.00 0.00 0.02 -0.00 0.00

30 6 0.02 -0.02 -0.02 0.01 -0.01 -0.01 -0.01 0.02 0.03

31 6 0.01 0.01 0.01 -0.01 -0.01 -0.01 -0.02 -0.01 -0.01

32 6 -0.04 -0.04 -0.03 0.00 0.01 0.00 0.00 0.00 0.01

33 6 0.02 0.02 0.02 -0.01 -0.01 -0.01 -0.01 -0.02 -0.01

34 6 -0.03 -0.03 -0.02 0.01 0.01 0.01 0.02 0.01 0.01

35 6 0.02 0.02 0.02 -0.01 -0.01 -0.01 -0.01 -0.02 -0.02

36 6 -0.04 -0.04 -0.03 0.01 0.00 0.00 0.02 0.00 -0.01

37 6 0.03 0.03 -0.02 -0.01 -0.01 0.01 0.02 0.01 -0.01

38 6 -0.02 -0.02 0.02 0.01 0.01 -0.01 -0.01 -0.02 0.02

39 6 0.04 0.04 -0.03 -0.01 -0.00 0.00 0.02 0.00 0.01

40 6 -0.01 -0.01 0.01 0.01 0.01 -0.01 -0.02 -0.01 0.01

41 6 0.04 0.04 -0.03 -0.00 -0.01 0.00 0.00 0.00 -0.01

42 6 -0.02 -0.02 0.02 0.01 0.01 -0.01 -0.01 -0.02 0.01

43 6 0.03 -0.03 0.02 0.01 -0.01 0.01 0.03 -0.03 0.02

44 6 -0.02 0.02 -0.02 -0.01 0.01 -0.01 -0.01 0.02 -0.03

45 6 0.04 -0.04 0.03 0.01 -0.00 0.00 0.02 -0.00 -0.00

46 6 -0.01 0.01 -0.01 -0.01 0.01 -0.01 -0.03 0.02 -0.02

47 6 0.04 -0.04 0.03 0.00 -0.01 0.00 0.00 -0.01 0.01

48 6 -0.02 0.02 -0.02 -0.01 0.01 -0.01 -0.02 0.02 -0.02

49 1 -0.00 -0.00 0.00 -0.01 -0.05 0.33 -0.02 0.00 0.08

50 1 -0.00 0.00 -0.00 0.01 -0.05 0.33 -0.03 0.02 -0.24

51 1 0.00 0.00 0.00 0.05 0.01 0.33 -0.05 -0.01 -0.31

52 1 -0.00 0.00 -0.00 0.05 -0.01 0.33 -0.05 0.02 -0.39

53 1 -0.00 -0.00 0.00 -0.05 -0.01 0.33 -0.05 -0.01 0.31

54 1 0.00 -0.00 -0.00 -0.05 0.01 0.33 -0.05 0.02 0.39

55 1 0.00 -0.00 -0.00 -0.01 0.05 0.33 -0.03 0.02 0.24

56 1 0.00 0.00 0.00 0.01 0.05 0.33 -0.02 0.00 -0.08

57 1 0.15 -0.15 -0.11 -0.00 0.01 -0.00 0.01 -0.03 -0.00

58 1 0.08 -0.08 -0.05 -0.04 0.06 0.03 0.10 -0.11 -0.08

59 1 0.19 -0.19 -0.14 -0.02 0.02 0.03 0.05 -0.06 -0.07

60 1 0.08 -0.08 -0.05 -0.06 0.04 0.03 0.13 -0.09 -0.08

61 1 0.15 -0.15 -0.11 -0.01 0.00 -0.00 0.03 -0.02 0.00

62 1 0.19 0.19 0.14 0.02 0.02 0.03 0.03 0.04 0.04

63 1 0.08 0.08 0.05 0.04 0.06 0.03 0.07 0.06 0.05

64 1 0.15 0.15 0.11 0.00 0.01 -0.00 0.00 0.01 0.00

65 1 0.15 0.15 0.11 0.01 0.00 -0.00 0.02 0.02 -0.00

66 1 0.08 0.08 0.05 0.06 0.04 0.03 0.09 0.05 0.05

67 1 -0.15 -0.15 0.11 -0.01 -0.00 -0.00 0.02 0.02 0.00

68 1 -0.08 -0.08 0.05 -0.06 -0.04 0.03 0.09 0.05 -0.05

69 1 -0.19 -0.19 0.14 -0.02 -0.02 0.03 0.03 0.04 -0.04

70 1 -0.08 -0.08 0.05 -0.04 -0.06 0.03 0.07 0.06 -0.05

71 1 -0.15 -0.15 0.11 -0.00 -0.01 -0.00 0.00 0.01 -0.00

72 1 -0.15 0.15 -0.11 0.01 -0.00 -0.00 0.03 -0.02 -0.00

73 1 -0.08 0.08 -0.05 0.06 -0.04 0.03 0.13 -0.09 0.08

74 1 -0.19 0.19 -0.14 0.02 -0.02 0.03 0.05 -0.06 0.07

75 1 -0.08 0.08 -0.05 0.04 -0.06 0.03 0.10 -0.11 0.08

76 1 -0.15 0.15 -0.11 0.00 -0.01 -0.00 0.01 -0.03 0.00

77 30 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00

76 77 78

E A2 B2

Frequencies -- 742.0454 756.5035 763.3827

Red. masses -- 2.8141 4.3534 2.0192

Frc consts -- 0.9130 1.4679 0.6933

IR Inten -- 38.2354 0.0000 1.6332

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.00 -0.02 0.03 -0.01 -0.05 -0.00 0.00 -0.02

2 6 0.01 0.00 -0.08 -0.00 -0.03 0.13 -0.03 0.00 0.00

3 7 -0.00 -0.02 0.05 0.01 -0.00 -0.00 -0.00 0.02 0.00

4 6 -0.01 -0.01 -0.02 -0.00 0.03 -0.13 0.03 0.00 0.00

5 6 -0.01 0.00 -0.05 0.03 0.01 0.05 0.00 0.00 -0.02

6 6 -0.02 0.01 0.07 -0.02 0.02 0.14 0.04 -0.04 0.03

7 6 -0.02 -0.00 -0.11 -0.03 0.00 -0.13 -0.00 -0.03 0.00

8 7 -0.00 -0.00 -0.01 0.00 -0.01 -0.00 -0.02 -0.00 0.00

9 6 0.02 0.00 0.13 0.03 0.00 0.13 -0.00 0.03 0.00

10 6 0.00 -0.02 -0.04 0.01 -0.03 -0.05 -0.00 0.00 -0.02

11 6 -0.00 -0.02 0.06 -0.01 -0.03 0.05 -0.00 -0.00 -0.02

12 6 0.02 0.02 0.12 -0.02 -0.02 -0.14 -0.04 -0.04 0.03

13 6 0.02 0.00 -0.13 -0.03 -0.00 0.13 0.00 -0.03 0.00

14 6 0.00 -0.02 0.04 -0.01 0.03 -0.05 0.00 -0.00 -0.02

15 6 -0.00 -0.02 -0.06 0.01 0.03 0.05 0.00 0.00 -0.02

16 6 -0.02 -0.00 0.11 0.03 -0.00 -0.13 0.00 0.03 0.00

17 7 -0.00 -0.00 0.01 -0.00 0.01 -0.00 0.02 0.00 0.00

18 6 -0.02 0.01 -0.07 0.02 -0.02 0.14 -0.04 0.04 0.03

19 6 -0.01 -0.01 0.02 0.00 -0.03 -0.13 -0.03 -0.00 0.00

20 6 -0.01 0.00 0.05 -0.03 -0.01 0.05 -0.00 -0.00 -0.02

21 6 -0.00 0.00 0.02 -0.03 0.01 -0.05 0.00 -0.00 -0.02

22 6 0.01 0.00 0.08 0.00 0.03 0.13 0.03 -0.00 0.00

23 7 -0.00 -0.02 -0.05 -0.01 -0.00 -0.00 -0.00 -0.02 0.00

24 6 0.02 0.02 -0.12 0.02 0.02 -0.14 0.04 0.04 0.03

25 6 -0.01 0.02 0.01 -0.05 0.05 0.04 0.06 -0.06 -0.04

26 6 0.02 -0.01 -0.02 0.03 -0.02 -0.03 -0.03 0.03 0.02

27 6 -0.00 0.02 -0.01 -0.00 0.02 0.00 0.01 0.00 -0.01

28 6 0.01 -0.02 -0.01 0.04 -0.04 -0.02 -0.04 0.04 0.03

29 6 -0.00 0.00 0.01 -0.02 0.00 0.00 -0.00 -0.01 -0.01

30 6 0.02 -0.01 -0.01 0.02 -0.03 -0.03 -0.03 0.03 0.02

31 6 -0.02 -0.03 -0.02 0.04 0.04 0.02 0.04 0.04 0.03

32 6 0.00 0.02 -0.00 -0.00 -0.02 -0.00 -0.01 0.00 -0.01

33 6 -0.02 -0.01 -0.03 0.03 0.02 0.03 0.03 0.03 0.02

34 6 0.03 0.03 0.02 -0.05 -0.05 -0.04 -0.06 -0.06 -0.04

35 6 -0.02 -0.02 -0.02 0.02 0.03 0.03 0.03 0.03 0.02

36 6 0.01 0.00 0.01 -0.02 -0.00 -0.00 0.00 -0.01 -0.01

37 6 0.03 0.03 -0.02 0.05 0.05 -0.04 0.06 0.06 -0.04

38 6 -0.02 -0.02 0.02 -0.02 -0.03 0.03 -0.03 -0.03 0.02

39 6 0.01 0.00 -0.01 0.02 0.00 -0.00 -0.00 0.01 -0.01

40 6 -0.02 -0.03 0.02 -0.04 -0.04 0.02 -0.04 -0.04 0.03

41 6 0.00 0.02 0.00 0.00 0.02 -0.00 0.01 -0.00 -0.01

42 6 -0.02 -0.01 0.03 -0.03 -0.02 0.03 -0.03 -0.03 0.02

43 6 -0.01 0.02 -0.01 0.05 -0.05 0.04 -0.06 0.06 -0.04

44 6 0.02 -0.01 0.01 -0.02 0.03 -0.03 0.03 -0.03 0.02

45 6 -0.00 0.00 -0.01 0.02 -0.00 0.00 0.00 0.01 -0.01

46 6 0.01 -0.02 0.01 -0.04 0.04 -0.02 0.04 -0.04 0.03

47 6 -0.00 0.02 0.01 0.00 -0.02 0.00 -0.01 -0.00 -0.01

48 6 0.02 -0.01 0.02 -0.03 0.02 -0.03 0.03 -0.03 0.02

49 1 -0.02 -0.05 0.39 0.03 0.01 -0.16 0.02 -0.00 0.14

50 1 0.01 -0.05 0.31 0.03 -0.01 0.16 -0.02 -0.00 0.14

51 1 -0.02 -0.03 -0.24 -0.01 -0.03 -0.16 0.00 -0.02 0.14

52 1 -0.00 -0.02 0.08 0.01 -0.03 0.16 0.00 0.02 0.14

53 1 -0.02 -0.03 0.24 0.01 0.03 -0.16 -0.00 0.02 0.14

54 1 -0.00 -0.02 -0.08 -0.01 0.03 0.16 -0.00 -0.02 0.14

55 1 0.01 -0.05 -0.31 -0.03 0.01 0.16 0.02 0.00 0.14

56 1 -0.02 -0.05 -0.39 -0.03 -0.01 -0.16 -0.02 0.00 0.14

57 1 -0.02 0.02 -0.00 -0.01 0.03 -0.01 0.02 -0.02 -0.02

58 1 -0.05 0.09 0.05 -0.12 0.16 0.10 0.17 -0.16 -0.12

59 1 -0.04 0.03 0.04 -0.09 0.09 0.09 0.14 -0.14 -0.09

60 1 -0.06 0.07 0.05 -0.16 0.12 0.10 0.16 -0.17 -0.12

61 1 -0.01 0.00 0.00 -0.03 0.01 -0.01 0.02 -0.02 -0.02

62 1 0.06 0.05 0.07 -0.09 -0.09 -0.09 -0.14 -0.14 -0.09

63 1 0.09 0.13 0.08 -0.12 -0.16 -0.10 -0.17 -0.16 -0.12

64 1 0.02 0.03 -0.00 -0.01 -0.03 0.01 -0.02 -0.02 -0.02

65 1 0.03 0.01 0.00 -0.03 -0.01 0.01 -0.02 -0.02 -0.02

66 1 0.11 0.10 0.08 -0.16 -0.12 -0.10 -0.16 -0.17 -0.12

67 1 0.03 0.01 -0.00 0.03 0.01 0.01 0.02 0.02 -0.02

68 1 0.11 0.10 -0.08 0.16 0.12 -0.10 0.16 0.17 -0.12

69 1 0.06 0.05 -0.07 0.09 0.09 -0.09 0.14 0.14 -0.09

70 1 0.09 0.13 -0.08 0.12 0.16 -0.10 0.17 0.16 -0.12

71 1 0.02 0.03 0.00 0.01 0.03 0.01 0.02 0.02 -0.02

72 1 -0.01 0.00 -0.00 0.03 -0.01 -0.01 -0.02 0.02 -0.02

73 1 -0.06 0.07 -0.05 0.16 -0.12 0.10 -0.16 0.17 -0.12

74 1 -0.04 0.03 -0.04 0.09 -0.09 0.09 -0.14 0.14 -0.09

75 1 -0.05 0.09 -0.05 0.12 -0.16 0.10 -0.17 0.16 -0.12

76 1 -0.02 0.02 0.00 0.01 -0.03 -0.01 -0.02 0.02 -0.02

77 30 0.00 0.00 0.00 -0.00 0.00 0.00 0.00 0.00 0.00

79 80 81

E E A2

Frequencies -- 771.7720 771.7720 784.6740

Red. masses -- 2.2365 2.2365 3.0331

Frc consts -- 0.7849 0.7849 1.1003

IR Inten -- 109.4944 109.4944 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.04 0.02 -0.01 -0.01 -0.00 -0.03 -0.03 0.02 -0.02

2 6 0.00 0.02 0.04 -0.02 0.00 0.01 0.00 0.01 0.07

3 7 -0.00 0.00 -0.00 0.00 0.02 -0.00 -0.01 -0.00 0.00

4 6 0.00 -0.02 -0.04 0.02 0.00 0.01 0.00 -0.01 -0.07

5 6 -0.04 -0.02 0.01 0.01 -0.00 -0.03 -0.03 -0.02 0.02

6 6 0.03 -0.04 0.05 0.03 -0.03 0.05 0.03 -0.03 0.09

7 6 -0.00 -0.02 0.01 0.02 -0.00 -0.04 0.01 -0.00 -0.07

8 7 -0.02 0.00 -0.00 0.00 0.00 0.00 0.00 0.01 -0.00

9 6 -0.00 0.02 0.01 -0.02 -0.00 0.04 -0.01 -0.00 0.07

10 6 0.00 0.01 -0.03 -0.02 0.04 -0.01 -0.02 0.03 -0.02

11 6 0.00 -0.01 -0.03 0.02 0.04 0.01 0.02 0.03 0.02

12 6 0.03 0.03 -0.05 -0.04 -0.03 0.05 0.03 0.03 -0.09

13 6 -0.00 0.02 -0.01 -0.02 -0.00 -0.04 0.01 0.00 0.07

14 6 0.00 0.01 0.03 -0.02 0.04 0.01 0.02 -0.03 -0.02

15 6 0.00 -0.01 0.03 0.02 0.04 -0.01 -0.02 -0.03 0.02

16 6 -0.00 -0.02 -0.01 0.02 -0.00 0.04 -0.01 0.00 -0.07

17 7 -0.02 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.01 -0.00

18 6 0.03 -0.04 -0.05 0.03 -0.03 -0.05 -0.03 0.03 0.09

19 6 0.00 -0.02 0.04 0.02 0.00 -0.01 -0.00 0.01 -0.07

20 6 -0.04 -0.02 -0.01 0.01 -0.00 0.03 0.03 0.02 0.02

21 6 -0.04 0.02 0.01 -0.01 -0.00 0.03 0.03 -0.02 -0.02

22 6 0.00 0.02 -0.04 -0.02 0.00 -0.01 -0.00 -0.01 0.07

23 7 -0.00 0.00 0.00 0.00 0.02 0.00 0.01 -0.00 0.00

24 6 0.03 0.03 0.05 -0.04 -0.03 -0.05 -0.03 -0.03 -0.09

25 6 0.06 -0.06 -0.04 0.06 -0.06 -0.04 0.07 -0.07 -0.05

26 6 -0.03 0.04 0.01 -0.02 0.03 0.02 -0.03 0.03 0.02

27 6 0.01 0.01 -0.02 0.01 -0.00 -0.00 0.01 0.00 -0.01

28 6 -0.04 0.03 0.03 -0.03 0.04 0.03 -0.04 0.04 0.03

29 6 0.00 -0.01 -0.00 -0.01 -0.01 -0.02 -0.00 -0.01 -0.01

30 6 -0.03 0.02 0.02 -0.04 0.03 0.01 -0.03 0.03 0.02

31 6 -0.04 -0.03 -0.03 0.03 0.04 0.03 -0.04 -0.04 -0.03

32 6 0.01 -0.01 0.02 -0.01 -0.00 -0.00 0.01 -0.00 0.01

33 6 -0.03 -0.04 -0.01 0.02 0.03 0.02 -0.03 -0.03 -0.02

34 6 0.06 0.06 0.04 -0.06 -0.06 -0.04 0.07 0.07 0.05

35 6 -0.03 -0.02 -0.02 0.04 0.03 0.01 -0.03 -0.03 -0.02

36 6 0.00 0.01 0.00 0.01 -0.01 -0.02 -0.00 0.01 0.01

37 6 0.06 0.06 -0.04 -0.06 -0.06 0.04 -0.07 -0.07 0.05

38 6 -0.03 -0.02 0.02 0.04 0.03 -0.01 0.03 0.03 -0.02

39 6 0.00 0.01 -0.00 0.01 -0.01 0.02 0.00 -0.01 0.01

40 6 -0.04 -0.03 0.03 0.03 0.04 -0.03 0.04 0.04 -0.03

41 6 0.01 -0.01 -0.02 -0.01 -0.00 0.00 -0.01 0.00 0.01

42 6 -0.03 -0.04 0.01 0.02 0.03 -0.02 0.03 0.03 -0.02

43 6 0.06 -0.06 0.04 0.06 -0.06 0.04 -0.07 0.07 -0.05

44 6 -0.03 0.02 -0.02 -0.04 0.03 -0.01 0.03 -0.03 0.02

45 6 0.00 -0.01 0.00 -0.01 -0.01 0.02 0.00 0.01 -0.01

46 6 -0.04 0.03 -0.03 -0.03 0.04 -0.03 0.04 -0.04 0.03

47 6 0.01 0.01 0.02 0.01 -0.00 0.00 -0.01 -0.00 -0.01

48 6 -0.03 0.04 -0.01 -0.02 0.03 -0.02 0.03 -0.03 0.02

49 1 -0.03 0.03 -0.05 0.01 -0.02 0.23 -0.02 0.04 -0.07

50 1 -0.03 -0.03 0.05 -0.01 -0.02 0.23 -0.02 -0.04 0.07

51 1 0.02 -0.01 0.23 -0.03 0.03 -0.05 -0.04 0.02 -0.07

52 1 0.02 0.01 0.23 0.03 0.03 0.05 0.04 0.02 0.07

53 1 0.02 -0.01 -0.23 -0.03 0.03 0.05 0.04 -0.02 -0.07

54 1 0.02 0.01 -0.23 0.03 0.03 -0.05 -0.04 -0.02 0.07

55 1 -0.03 -0.03 -0.05 -0.01 -0.02 -0.23 0.02 0.04 0.07

56 1 -0.03 0.03 0.05 0.01 -0.02 -0.23 0.02 -0.04 -0.07

57 1 0.01 -0.01 -0.01 0.01 -0.00 -0.00 -0.00 0.01 -0.00

58 1 0.17 -0.14 -0.12 0.15 -0.15 -0.11 0.17 -0.15 -0.12

59 1 0.13 -0.14 -0.08 0.14 -0.13 -0.08 0.16 -0.16 -0.09

60 1 0.15 -0.15 -0.11 0.13 -0.17 -0.12 0.15 -0.17 -0.12

61 1 0.00 -0.01 -0.00 0.01 -0.01 -0.01 -0.01 0.00 -0.00

62 1 0.13 0.14 0.08 -0.14 -0.13 -0.08 0.16 0.16 0.09

63 1 0.17 0.13 0.12 -0.15 -0.15 -0.11 0.17 0.15 0.12

64 1 0.01 0.01 0.01 -0.01 -0.00 -0.00 -0.00 -0.01 0.00

65 1 0.00 0.01 0.00 -0.01 -0.01 -0.01 -0.01 -0.00 0.00

66 1 0.15 0.15 0.11 -0.14 -0.17 -0.12 0.15 0.17 0.12

67 1 0.00 0.01 -0.00 -0.01 -0.01 0.01 0.01 0.00 0.00

68 1 0.15 0.15 -0.11 -0.14 -0.17 0.12 -0.15 -0.17 0.12

69 1 0.13 0.14 -0.08 -0.14 -0.13 0.08 -0.16 -0.16 0.09

70 1 0.17 0.13 -0.12 -0.15 -0.15 0.11 -0.17 -0.15 0.12

71 1 0.01 0.01 -0.01 -0.01 -0.00 0.00 0.00 0.01 0.00

72 1 0.00 -0.01 0.00 0.01 -0.01 0.01 0.01 -0.00 -0.00

73 1 0.15 -0.15 0.11 0.13 -0.17 0.12 -0.15 0.17 -0.12

74 1 0.13 -0.14 0.08 0.14 -0.13 0.08 -0.16 0.16 -0.09

75 1 0.17 -0.14 0.12 0.15 -0.15 0.11 -0.17 0.15 -0.12

76 1 0.01 -0.01 0.01 0.01 -0.00 0.00 0.00 -0.01 -0.00

77 30 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00

82 83 84

A1 E E

Frequencies -- 797.5961 806.4943 806.4943

Red. masses -- 1.7662 2.4769 2.4769

Frc consts -- 0.6620 0.9492 0.9492

IR Inten -- 0.0000 3.6714 3.6714

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.01 -0.06 0.01 -0.00 -0.01 -0.00 0.01 -0.09

2 6 0.00 -0.00 0.06 0.00 -0.00 -0.01 0.01 -0.01 0.13

3 7 0.00 0.00 -0.03 -0.00 -0.00 -0.01 0.00 -0.00 -0.06

4 6 -0.00 -0.00 0.06 -0.00 -0.00 0.06 -0.01 -0.01 0.11

5 6 0.00 0.01 -0.06 0.01 0.01 -0.02 -0.00 0.01 -0.09

6 6 -0.00 -0.00 -0.00 -0.01 0.01 -0.09 -0.01 0.00 -0.06

7 6 -0.00 -0.00 -0.06 0.01 0.01 0.13 -0.00 -0.00 0.01

8 7 0.00 -0.00 0.03 0.00 0.00 -0.06 -0.00 0.00 0.01

9 6 -0.00 0.00 -0.06 0.01 -0.01 0.11 -0.00 0.00 -0.06

10 6 0.01 -0.00 0.06 -0.01 -0.00 -0.09 0.01 -0.01 0.02

11 6 0.01 0.00 0.06 -0.01 -0.00 -0.09 -0.00 -0.01 0.01

12 6 0.00 -0.00 0.00 -0.00 -0.01 0.06 0.01 0.01 -0.09

13 6 0.00 -0.00 -0.06 0.01 -0.01 -0.11 -0.00 0.00 0.06

14 6 -0.01 0.00 0.06 -0.01 -0.00 0.09 0.01 -0.01 -0.02

15 6 -0.01 -0.00 0.06 -0.01 -0.00 0.09 -0.00 -0.01 -0.01

16 6 0.00 0.00 -0.06 0.01 0.01 -0.13 -0.00 -0.00 -0.01

17 7 -0.00 -0.00 0.03 0.00 0.00 0.06 -0.00 0.00 -0.01

18 6 0.00 0.00 -0.00 -0.01 0.01 0.09 -0.01 0.00 0.06

19 6 0.00 0.00 0.06 -0.00 -0.00 -0.06 -0.01 -0.01 -0.11

20 6 -0.00 -0.01 -0.06 0.01 0.01 0.02 -0.00 0.01 0.09

21 6 0.00 -0.01 -0.06 0.01 -0.00 0.01 -0.00 0.01 0.09

22 6 -0.00 0.00 0.06 0.00 -0.00 0.01 0.01 -0.01 -0.13

23 7 0.00 -0.00 -0.03 -0.00 -0.00 0.01 0.00 -0.00 0.06

24 6 -0.00 0.00 -0.00 -0.00 -0.01 -0.06 0.01 0.01 0.09

25 6 0.00 0.00 0.00 -0.02 0.02 0.01 -0.01 0.01 0.01

26 6 0.00 -0.00 -0.00 0.00 -0.01 0.01 0.01 -0.01 -0.00

27 6 0.00 0.00 -0.00 -0.01 -0.01 0.01 -0.00 -0.00 0.00

28 6 -0.00 -0.00 -0.00 0.01 -0.01 -0.01 0.00 -0.01 -0.01

29 6 0.00 0.00 0.00 0.01 0.00 0.00 0.01 0.00 0.01

30 6 -0.00 0.00 0.00 0.01 -0.01 0.00 0.01 -0.00 0.01

31 6 0.00 -0.00 -0.00 0.01 0.00 0.01 -0.01 -0.01 -0.01

32 6 -0.00 0.00 -0.00 -0.00 0.01 -0.01 0.00 -0.01 0.00

33 6 -0.00 -0.00 -0.00 0.00 0.01 -0.01 -0.01 -0.01 0.00

34 6 -0.00 0.00 0.00 -0.01 -0.01 -0.01 0.02 0.02 0.01

35 6 0.00 0.00 0.00 0.01 0.01 0.00 -0.01 -0.00 0.01

36 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.01 0.01 0.01

37 6 0.00 -0.00 0.00 -0.01 -0.01 0.01 0.02 0.02 -0.01

38 6 -0.00 -0.00 0.00 0.01 0.01 -0.00 -0.01 -0.00 -0.01

39 6 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.01 0.01 -0.01

40 6 -0.00 0.00 -0.00 0.01 0.00 -0.01 -0.01 -0.01 0.01

41 6 0.00 -0.00 -0.00 -0.00 0.01 0.01 0.00 -0.01 -0.00

42 6 0.00 0.00 -0.00 0.00 0.01 0.01 -0.01 -0.01 -0.00

43 6 -0.00 -0.00 0.00 -0.02 0.02 -0.01 -0.01 0.01 -0.01

44 6 0.00 -0.00 0.00 0.01 -0.01 -0.00 0.01 -0.00 -0.01

45 6 -0.00 -0.00 0.00 0.01 0.00 -0.00 0.01 0.00 -0.01

46 6 0.00 0.00 -0.00 0.01 -0.01 0.01 0.00 -0.01 0.01

47 6 -0.00 -0.00 -0.00 -0.01 -0.01 -0.01 -0.00 -0.00 -0.00

48 6 -0.00 0.00 -0.00 0.00 -0.01 -0.01 0.01 -0.01 0.00

49 1 -0.00 -0.04 0.34 0.00 -0.02 0.13 -0.01 -0.05 0.44

50 1 0.00 -0.04 0.34 0.01 0.00 0.04 0.00 -0.05 0.45

51 1 -0.04 -0.00 -0.34 0.05 0.00 0.45 0.00 -0.01 -0.04

52 1 -0.04 0.00 -0.34 0.05 -0.01 0.44 -0.02 -0.00 -0.13

53 1 0.04 0.00 -0.34 0.05 0.00 -0.45 0.00 -0.01 0.04

54 1 0.04 -0.00 -0.34 0.05 -0.01 -0.44 -0.02 -0.00 0.13

55 1 -0.00 0.04 0.34 0.01 0.00 -0.04 0.00 -0.05 -0.45

56 1 0.00 0.04 0.34 0.00 -0.02 -0.13 -0.01 -0.05 -0.44

57 1 -0.01 0.01 0.00 0.01 -0.02 0.00 -0.00 -0.01 0.01

58 1 -0.00 0.01 0.00 -0.04 0.01 0.02 -0.03 0.02 0.02

59 1 -0.00 -0.00 0.00 -0.04 0.04 0.01 -0.03 0.03 0.01

60 1 0.01 -0.00 -0.00 -0.03 0.04 0.03 -0.00 0.03 0.01

61 1 0.01 -0.01 -0.00 0.01 -0.00 0.00 0.02 -0.01 -0.00

62 1 0.00 -0.00 0.00 -0.03 -0.03 -0.01 0.04 0.04 0.01

63 1 0.00 0.01 0.00 -0.03 -0.00 -0.01 0.04 0.03 0.03

64 1 0.01 0.01 0.00 0.01 0.02 0.00 -0.00 -0.01 0.00

65 1 -0.01 -0.01 -0.00 0.01 -0.00 -0.01 -0.02 -0.01 0.00

66 1 -0.01 -0.00 -0.00 -0.02 -0.03 -0.02 0.01 0.04 0.02

67 1 0.01 0.01 -0.00 0.01 -0.00 0.01 -0.02 -0.01 -0.00

68 1 0.01 0.00 -0.00 -0.02 -0.03 0.02 0.01 0.04 -0.02

69 1 -0.00 0.00 0.00 -0.03 -0.03 0.01 0.04 0.04 -0.01

70 1 -0.00 -0.01 0.00 -0.03 -0.00 0.01 0.04 0.03 -0.03

71 1 -0.01 -0.01 0.00 0.01 0.02 -0.00 -0.00 -0.01 -0.00

72 1 -0.01 0.01 -0.00 0.01 -0.00 -0.00 0.02 -0.01 0.00

73 1 -0.01 0.00 -0.00 -0.03 0.04 -0.03 -0.00 0.03 -0.01

74 1 0.00 0.00 0.00 -0.04 0.04 -0.01 -0.03 0.03 -0.01

75 1 0.00 -0.01 0.00 -0.04 0.01 -0.02 -0.03 0.02 -0.02

76 1 0.01 -0.01 0.00 0.01 -0.02 -0.00 -0.00 -0.01 -0.01

77 30 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 0.00

85 86 87

B2 A2 E

Frequencies -- 811.7237 848.9284 856.7038

Red. masses -- 2.8860 5.4222 4.6565

Frc consts -- 1.1204 2.3023 2.0136

IR Inten -- 258.6748 0.0000 17.1145

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.01 -0.06 0.12 -0.07 -0.01 -0.00 -0.01 -0.00

2 6 0.01 -0.01 0.10 -0.07 -0.09 -0.01 -0.08 -0.00 -0.01

3 7 0.00 -0.00 -0.06 -0.06 0.00 0.00 -0.01 0.10 0.01

4 6 -0.01 -0.01 0.10 -0.07 0.09 0.01 0.06 0.02 -0.01

5 6 -0.00 0.01 -0.06 0.12 0.07 0.01 0.03 0.01 0.00

6 6 -0.01 0.01 -0.09 -0.10 0.10 0.00 0.08 -0.11 -0.00

7 6 0.01 0.01 0.10 -0.09 0.07 0.01 0.09 -0.06 -0.01

8 7 0.00 -0.00 -0.06 0.00 0.06 -0.00 0.01 -0.08 -0.00

9 6 0.01 -0.01 0.10 0.09 0.07 -0.01 -0.09 -0.07 0.01

10 6 -0.01 -0.00 -0.06 0.07 -0.12 -0.01 -0.09 0.12 0.01

11 6 -0.01 0.00 -0.06 -0.07 -0.12 0.01 0.09 0.13 -0.01

12 6 0.01 0.01 -0.09 -0.10 -0.10 -0.00 -0.10 -0.12 -0.00

13 6 -0.01 0.01 0.10 -0.09 -0.07 -0.01 -0.09 -0.07 -0.01

14 6 0.01 0.00 -0.06 -0.07 0.12 -0.01 -0.09 0.12 -0.01

15 6 0.01 -0.00 -0.06 0.07 0.12 0.01 0.09 0.13 0.01

16 6 -0.01 -0.01 0.10 0.09 -0.07 0.01 0.09 -0.06 0.01

17 7 -0.00 0.00 -0.06 0.00 -0.06 -0.00 0.01 -0.08 0.00

18 6 0.01 -0.01 -0.09 0.10 -0.10 0.00 0.08 -0.11 0.00

19 6 0.01 0.01 0.10 0.07 -0.09 0.01 0.06 0.02 0.01

20 6 0.00 -0.01 -0.06 -0.12 -0.07 0.01 0.03 0.01 -0.00

21 6 -0.00 -0.01 -0.06 -0.12 0.07 -0.01 -0.00 -0.01 0.00

22 6 -0.01 0.01 0.10 0.07 0.09 -0.01 -0.08 -0.00 0.01

23 7 0.00 0.00 -0.06 0.06 0.00 0.00 -0.01 0.10 -0.01

24 6 -0.01 -0.01 -0.09 0.10 0.10 -0.00 -0.10 -0.12 0.00

25 6 -0.02 0.02 0.01 0.05 -0.05 -0.04 -0.04 0.04 0.04

26 6 0.01 -0.01 0.00 0.00 -0.00 0.01 0.00 0.00 -0.02

27 6 -0.01 -0.01 0.01 -0.01 -0.00 0.01 0.01 0.01 -0.02

28 6 0.01 -0.01 -0.01 -0.03 0.03 0.02 0.02 -0.03 -0.02

29 6 0.01 0.01 0.01 0.00 0.01 0.01 -0.00 0.00 0.01

30 6 0.01 -0.01 0.00 0.00 -0.00 0.01 -0.01 0.01 0.00

31 6 -0.01 -0.01 -0.01 -0.03 -0.03 -0.02 -0.03 -0.04 -0.02

32 6 0.01 -0.01 0.01 -0.01 0.00 -0.01 -0.01 0.01 -0.01

33 6 -0.01 -0.01 0.00 0.00 0.00 -0.01 -0.00 0.00 -0.02

34 6 0.02 0.02 0.01 0.05 0.05 0.04 0.05 0.05 0.04

35 6 -0.01 -0.01 0.00 0.00 0.00 -0.01 0.01 0.01 -0.00

36 6 -0.01 0.01 0.01 0.00 -0.01 -0.01 0.01 -0.00 0.00

37 6 -0.02 -0.02 0.01 -0.05 -0.05 0.04 0.05 0.05 -0.04

38 6 0.01 0.01 0.00 -0.00 -0.00 -0.01 0.01 0.01 0.00

39 6 0.01 -0.01 0.01 -0.00 0.01 -0.01 0.01 -0.00 -0.00

40 6 0.01 0.01 -0.01 0.03 0.03 -0.02 -0.03 -0.04 0.02

41 6 -0.01 0.01 0.01 0.01 -0.00 -0.01 -0.01 0.01 0.01

42 6 0.01 0.01 0.00 -0.00 -0.00 -0.01 -0.00 0.00 0.02

43 6 0.02 -0.02 0.01 -0.05 0.05 -0.04 -0.04 0.04 -0.04

44 6 -0.01 0.01 0.00 -0.00 0.00 0.01 -0.01 0.01 -0.00

45 6 -0.01 -0.01 0.01 -0.00 -0.01 0.01 -0.00 0.00 -0.01

46 6 -0.01 0.01 -0.01 0.03 -0.03 0.02 0.02 -0.03 0.02

47 6 0.01 0.01 0.01 0.01 0.00 0.01 0.01 0.01 0.02

48 6 -0.01 0.01 0.00 -0.00 0.00 0.01 0.00 0.00 0.02

49 1 -0.00 -0.04 0.31 0.15 -0.06 -0.01 0.09 0.06 0.02

50 1 0.00 -0.04 0.31 0.15 0.06 0.01 -0.06 0.08 0.02

51 1 0.04 0.00 0.31 0.06 -0.15 -0.01 -0.09 0.13 0.02

52 1 0.04 -0.00 0.31 -0.06 -0.15 0.01 0.10 0.11 -0.02

53 1 -0.04 -0.00 0.31 -0.06 0.15 -0.01 -0.09 0.13 -0.02

54 1 -0.04 0.00 0.31 0.06 0.15 0.01 0.10 0.11 0.02

55 1 -0.00 0.04 0.31 -0.15 -0.06 0.01 -0.06 0.08 -0.02

56 1 0.00 0.04 0.31 -0.15 0.06 -0.01 0.09 0.06 -0.02

57 1 0.01 -0.02 0.00 -0.07 0.06 0.06 0.03 -0.02 -0.04

58 1 -0.04 0.01 0.02 0.06 -0.09 -0.06 -0.09 0.13 0.08

59 1 -0.04 0.04 0.00 0.13 -0.13 -0.12 -0.13 0.12 0.11

60 1 -0.01 0.04 0.02 0.09 -0.06 -0.06 -0.03 0.02 0.02

61 1 0.02 -0.01 0.00 -0.06 0.07 0.06 0.11 -0.12 -0.09

62 1 0.04 0.04 0.00 0.13 0.13 0.12 0.15 0.15 0.14

63 1 0.04 0.01 0.02 0.06 0.09 0.06 0.09 0.14 0.08

64 1 -0.01 -0.02 0.00 -0.07 -0.06 -0.06 -0.05 -0.04 -0.06

65 1 -0.02 -0.01 0.00 -0.06 -0.07 -0.06 -0.12 -0.12 -0.10

66 1 0.01 0.04 0.02 0.09 0.06 0.06 0.06 0.04 0.04

67 1 0.02 0.01 0.00 0.06 0.07 -0.06 -0.12 -0.12 0.10

68 1 -0.01 -0.04 0.02 -0.09 -0.06 0.06 0.06 0.04 -0.04

69 1 -0.04 -0.04 0.00 -0.13 -0.13 0.12 0.15 0.15 -0.14

70 1 -0.04 -0.01 0.02 -0.06 -0.09 0.06 0.09 0.14 -0.08

71 1 0.01 0.02 0.00 0.07 0.06 -0.06 -0.05 -0.04 0.06

72 1 -0.02 0.01 0.00 0.06 -0.07 0.06 0.11 -0.12 0.09

73 1 0.01 -0.04 0.02 -0.09 0.06 -0.06 -0.03 0.02 -0.02

74 1 0.04 -0.04 0.00 -0.13 0.13 -0.12 -0.13 0.12 -0.11

75 1 0.04 -0.01 0.02 -0.06 0.09 -0.06 -0.09 0.13 -0.08

76 1 -0.01 0.02 0.00 0.07 -0.06 0.06 0.03 -0.02 0.04

77 30 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.01 0.00

88 89 90

E B1 A1

Frequencies -- 856.7038 862.1014 862.1713

Red. masses -- 4.6565 1.2448 1.2467

Frc consts -- 2.0136 0.5451 0.5460

IR Inten -- 17.1145 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.13 -0.09 -0.01 -0.00 0.00 0.00 -0.00 -0.00 -0.00

2 6 -0.06 -0.09 -0.01 0.00 0.00 -0.00 -0.00 0.00 0.00

3 7 -0.08 -0.01 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00

4 6 -0.07 0.09 0.01 0.00 -0.00 0.00 0.00 0.00 0.00

5 6 0.12 0.09 0.01 -0.00 -0.00 -0.00 0.00 -0.00 -0.00

6 6 -0.12 0.10 0.00 0.00 0.00 -0.00 0.00 0.00 0.00

7 6 -0.00 0.08 0.01 -0.00 0.00 -0.00 0.00 0.00 -0.00

8 7 0.10 0.01 -0.01 -0.00 0.00 0.00 0.00 0.00 0.00

9 6 0.02 -0.06 0.01 0.00 0.00 0.00 0.00 -0.00 -0.00

10 6 0.01 -0.03 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00

11 6 -0.01 0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00

12 6 -0.11 -0.08 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

13 6 0.02 -0.06 -0.01 -0.00 -0.00 0.00 -0.00 0.00 -0.00

14 6 0.01 -0.03 0.00 -0.00 0.00 -0.00 0.00 0.00 0.00

15 6 -0.01 0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00

16 6 -0.00 0.08 -0.01 0.00 -0.00 -0.00 -0.00 -0.00 -0.00

17 7 0.10 0.01 0.01 0.00 -0.00 0.00 -0.00 -0.00 0.00

18 6 -0.12 0.10 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

19 6 -0.07 0.09 -0.01 -0.00 0.00 0.00 -0.00 -0.00 0.00

20 6 0.12 0.09 -0.01 0.00 0.00 -0.00 -0.00 0.00 -0.00

21 6 0.13 -0.09 0.01 0.00 -0.00 0.00 0.00 0.00 -0.00

22 6 -0.06 -0.09 0.01 -0.00 -0.00 -0.00 0.00 -0.00 0.00

23 7 -0.08 -0.01 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00

24 6 -0.11 -0.08 0.00 -0.00 0.00 0.00 0.00 -0.00 0.00

25 6 0.05 -0.05 -0.04 0.00 0.00 -0.00 0.00 0.00 0.00

26 6 0.01 -0.01 0.00 -0.02 0.02 0.02 -0.02 0.02 0.02

27 6 -0.00 -0.01 -0.00 -0.02 0.02 0.02 -0.02 0.02 0.02

28 6 -0.04 0.03 0.02 0.00 0.00 0.00 0.00 0.00 -0.00

29 6 0.01 0.01 0.01 0.02 -0.02 -0.02 0.02 -0.02 -0.02

30 6 0.00 0.00 0.02 0.02 -0.02 -0.02 0.02 -0.02 -0.02

31 6 -0.03 -0.02 -0.02 0.00 -0.00 -0.00 -0.00 0.00 -0.00

32 6 0.00 0.00 0.01 -0.02 -0.02 -0.02 0.02 0.02 0.02

33 6 0.01 0.01 0.00 -0.02 -0.02 -0.02 0.02 0.02 0.02

34 6 0.04 0.04 0.04 0.00 -0.00 0.00 -0.00 0.00 0.00

35 6 0.00 -0.00 -0.02 0.02 0.02 0.02 -0.02 -0.02 -0.02

36 6 0.01 -0.01 -0.02 0.02 0.02 0.02 -0.02 -0.02 -0.02

37 6 0.04 0.04 -0.04 -0.00 0.00 0.00 0.00 -0.00 0.00

38 6 0.00 -0.00 0.02 -0.02 -0.02 0.02 0.02 0.02 -0.02

39 6 0.01 -0.01 0.02 -0.02 -0.02 0.02 0.02 0.02 -0.02

40 6 -0.03 -0.02 0.02 -0.00 0.00 -0.00 0.00 -0.00 -0.00

41 6 0.00 0.00 -0.01 0.02 0.02 -0.02 -0.02 -0.02 0.02

42 6 0.01 0.01 -0.00 0.02 0.02 -0.02 -0.02 -0.02 0.02

43 6 0.05 -0.05 0.04 -0.00 -0.00 -0.00 -0.00 -0.00 0.00

44 6 0.00 0.00 -0.02 -0.02 0.02 -0.02 -0.02 0.02 -0.02

45 6 0.01 0.01 -0.01 -0.02 0.02 -0.02 -0.02 0.02 -0.02

46 6 -0.04 0.03 -0.02 -0.00 -0.00 0.00 -0.00 -0.00 -0.00

47 6 -0.00 -0.01 0.00 0.02 -0.02 0.02 0.02 -0.02 0.02

48 6 0.01 -0.01 -0.00 0.02 -0.02 0.02 0.02 -0.02 0.02

49 1 0.11 -0.10 -0.02 0.00 0.01 0.01 0.00 -0.00 0.01

50 1 0.13 0.09 0.02 0.00 -0.01 -0.01 -0.00 -0.00 0.01

51 1 0.08 0.06 -0.02 0.01 0.00 -0.01 -0.00 0.00 -0.01

52 1 0.06 -0.09 -0.02 -0.01 0.00 0.01 -0.00 -0.00 -0.01

53 1 0.08 0.06 0.02 -0.01 -0.00 -0.01 0.00 -0.00 -0.01

54 1 0.06 -0.09 0.02 0.01 -0.00 0.01 0.00 0.00 -0.01

55 1 0.13 0.09 -0.02 -0.00 0.01 -0.01 0.00 0.00 0.01

56 1 0.11 -0.10 0.02 -0.00 -0.01 0.01 -0.00 0.00 0.01

57 1 -0.12 0.12 0.10 0.16 -0.16 -0.11 0.16 -0.16 -0.11

58 1 0.04 -0.06 -0.04 0.15 -0.16 -0.11 0.15 -0.16 -0.11

59 1 0.15 -0.15 -0.14 0.00 0.00 -0.00 0.00 0.00 0.00

60 1 0.14 -0.09 -0.08 -0.16 0.15 0.11 -0.16 0.15 0.11

61 1 -0.04 0.05 0.06 -0.16 0.16 0.11 -0.16 0.16 0.11

62 1 0.12 0.13 0.11 0.00 -0.00 0.00 -0.00 0.00 0.00

63 1 0.02 0.03 0.02 0.15 0.16 0.11 -0.15 -0.16 -0.11

64 1 -0.12 -0.11 -0.09 0.16 0.16 0.11 -0.16 -0.16 -0.11

65 1 -0.02 -0.03 -0.04 -0.16 -0.16 -0.11 0.16 0.16 0.11

66 1 0.13 0.09 0.08 -0.16 -0.15 -0.11 0.16 0.15 0.11

67 1 -0.02 -0.03 0.04 0.16 0.16 -0.11 -0.16 -0.16 0.11

68 1 0.13 0.09 -0.08 0.16 0.15 -0.11 -0.16 -0.15 0.11

69 1 0.12 0.13 -0.11 -0.00 0.00 0.00 0.00 -0.00 0.00

70 1 0.02 0.03 -0.02 -0.15 -0.16 0.11 0.15 0.16 -0.11

71 1 -0.12 -0.11 0.09 -0.16 -0.16 0.11 0.16 0.16 -0.11

72 1 -0.04 0.05 -0.06 0.16 -0.16 0.11 0.16 -0.16 0.11

73 1 0.14 -0.09 0.08 0.16 -0.15 0.11 0.16 -0.15 0.11

74 1 0.15 -0.15 0.14 -0.00 -0.00 -0.00 -0.00 -0.00 0.00

75 1 0.04 -0.06 0.04 -0.15 0.16 -0.11 -0.15 0.16 -0.11

76 1 -0.12 0.12 -0.10 -0.16 0.16 -0.11 -0.16 0.16 -0.11

77 30 -0.01 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00

91 92 93

E E B2

Frequencies -- 862.2530 862.2530 879.2708

Red. masses -- 1.2593 1.2593 3.4974

Frc consts -- 0.5516 0.5516 1.5931

IR Inten -- 0.1323 0.1323 0.0197

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 -0.00 0.00 0.00 -0.00 -0.00 -0.01 -0.01 -0.00

2 6 0.00 -0.00 -0.00 -0.01 -0.00 0.00 -0.09 -0.00 -0.00

3 7 -0.00 -0.01 0.00 -0.00 0.00 -0.00 0.00 0.10 0.01

4 6 -0.01 0.00 -0.00 0.00 0.00 0.00 0.09 -0.00 -0.00

5 6 0.00 0.00 0.00 0.01 0.00 -0.00 0.01 -0.01 -0.00

6 6 -0.01 0.01 0.00 0.00 0.00 0.00 0.10 -0.10 0.00

7 6 -0.00 0.01 -0.00 0.00 0.00 -0.00 0.00 -0.09 -0.00

8 7 0.00 0.00 0.00 0.01 -0.00 0.00 -0.10 0.00 0.01

9 6 0.00 -0.00 -0.00 -0.00 -0.01 -0.00 0.00 0.09 -0.00

10 6 0.00 -0.01 0.00 -0.00 0.00 0.00 0.01 0.01 -0.00

11 6 -0.00 -0.00 0.00 0.00 0.01 0.00 0.01 -0.01 -0.00

12 6 0.00 -0.00 0.00 -0.01 -0.01 -0.00 -0.10 -0.10 0.00

13 6 0.00 -0.00 0.00 -0.00 -0.01 0.00 -0.00 -0.09 -0.00

14 6 0.00 -0.01 -0.00 -0.00 0.00 -0.00 -0.01 -0.01 -0.00

15 6 -0.00 -0.00 -0.00 0.00 0.01 -0.00 -0.01 0.01 -0.00

16 6 -0.00 0.01 0.00 0.00 0.00 0.00 -0.00 0.09 -0.00

17 7 0.00 0.00 -0.00 0.01 -0.00 -0.00 0.10 -0.00 0.01

18 6 -0.01 0.01 -0.00 0.00 0.00 -0.00 -0.10 0.10 0.00

19 6 -0.01 0.00 0.00 0.00 0.00 -0.00 -0.09 0.00 -0.00

20 6 0.00 0.00 -0.00 0.01 0.00 0.00 -0.01 0.01 -0.00

21 6 0.01 -0.00 -0.00 0.00 -0.00 0.00 0.01 0.01 -0.00

22 6 0.00 -0.00 0.00 -0.01 -0.00 -0.00 0.09 0.00 -0.00

23 7 -0.00 -0.01 -0.00 -0.00 0.00 0.00 -0.00 -0.10 0.01

24 6 0.00 -0.00 -0.00 -0.01 -0.01 0.00 0.10 0.10 0.00

25 6 0.01 -0.01 -0.00 0.00 -0.00 -0.00 -0.04 0.04 0.03

26 6 0.00 -0.00 -0.00 -0.03 0.03 0.02 -0.01 0.01 -0.01

27 6 0.00 -0.00 -0.00 -0.03 0.03 0.02 0.01 0.00 -0.01

28 6 -0.00 0.00 0.00 0.00 0.00 0.00 0.03 -0.03 -0.02

29 6 -0.00 0.00 0.00 0.03 -0.03 -0.02 -0.00 -0.01 -0.01

30 6 -0.00 0.00 0.00 0.03 -0.03 -0.02 -0.01 0.01 -0.01

31 6 0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.03 -0.03 -0.02

32 6 -0.03 -0.03 -0.02 -0.00 -0.00 -0.00 -0.01 0.00 -0.01

33 6 -0.03 -0.03 -0.02 -0.00 -0.00 -0.00 0.01 0.01 -0.01

34 6 -0.00 -0.00 -0.00 0.01 0.01 0.00 0.04 0.04 0.03

35 6 0.03 0.03 0.02 0.00 0.00 0.00 0.01 0.01 -0.01

36 6 0.03 0.03 0.02 0.00 0.00 0.00 0.00 -0.01 -0.01

37 6 -0.00 -0.00 0.00 0.01 0.01 -0.00 -0.04 -0.04 0.03

38 6 0.03 0.03 -0.02 0.00 0.00 -0.00 -0.01 -0.01 -0.01

39 6 0.03 0.03 -0.02 0.00 0.00 -0.00 -0.00 0.01 -0.01

40 6 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.03 0.03 -0.02

41 6 -0.03 -0.03 0.02 -0.00 -0.00 0.00 0.01 -0.00 -0.01

42 6 -0.03 -0.03 0.02 -0.00 -0.00 0.00 -0.01 -0.01 -0.01

43 6 0.01 -0.01 0.00 0.00 -0.00 0.00 0.04 -0.04 0.03

44 6 -0.00 0.00 -0.00 0.03 -0.03 0.02 0.01 -0.01 -0.01

45 6 -0.00 0.00 -0.00 0.03 -0.03 0.02 0.00 0.01 -0.01

46 6 -0.00 0.00 -0.00 0.00 0.00 -0.00 -0.03 0.03 -0.02

47 6 0.00 -0.00 0.00 -0.03 0.03 -0.02 -0.01 -0.00 -0.01

48 6 0.00 -0.00 0.00 -0.03 0.03 -0.02 0.01 -0.01 -0.01

49 1 0.00 -0.00 -0.00 0.01 0.00 0.01 0.11 0.08 0.02

50 1 0.01 -0.00 -0.01 0.00 0.00 0.00 -0.11 0.08 0.02

51 1 0.00 -0.00 -0.00 0.00 0.01 -0.01 -0.08 -0.11 0.02

52 1 0.00 -0.01 -0.01 0.00 0.00 -0.00 -0.08 0.11 0.02

53 1 0.00 -0.00 0.00 0.00 0.01 0.01 0.08 0.11 0.02

54 1 0.00 -0.01 0.01 0.00 0.00 0.00 0.08 -0.11 0.02

55 1 0.01 -0.00 0.01 0.00 0.00 -0.00 0.11 -0.08 0.02

56 1 0.00 -0.00 0.00 0.01 0.00 -0.01 -0.11 -0.08 0.02

57 1 -0.03 0.03 0.02 0.22 -0.22 -0.16 0.11 -0.11 -0.10

58 1 -0.01 0.01 0.01 0.21 -0.22 -0.16 -0.05 0.08 0.05

59 1 0.02 -0.02 -0.01 0.00 -0.00 -0.00 -0.16 0.16 0.14

60 1 0.03 -0.02 -0.02 -0.22 0.21 0.16 -0.08 0.05 0.05

61 1 0.01 -0.01 -0.00 -0.22 0.22 0.16 0.11 -0.11 -0.10

62 1 -0.00 -0.00 -0.00 0.02 0.02 0.01 0.16 0.16 0.14

63 1 0.21 0.22 0.16 0.02 0.03 0.02 0.05 0.08 0.05

64 1 0.22 0.22 0.16 0.01 0.01 0.00 -0.11 -0.11 -0.10

65 1 -0.22 -0.22 -0.16 -0.03 -0.03 -0.02 -0.11 -0.11 -0.10

66 1 -0.22 -0.21 -0.16 -0.01 -0.01 -0.01 0.08 0.05 0.05

67 1 -0.22 -0.22 0.16 -0.03 -0.03 0.02 0.11 0.11 -0.10

68 1 -0.22 -0.21 0.16 -0.01 -0.01 0.01 -0.08 -0.05 0.05

69 1 -0.00 -0.00 0.00 0.02 0.02 -0.01 -0.16 -0.16 0.14

70 1 0.21 0.22 -0.16 0.02 0.03 -0.02 -0.05 -0.08 0.05

71 1 0.22 0.22 -0.16 0.01 0.01 -0.00 0.11 0.11 -0.10

72 1 0.01 -0.01 0.00 -0.22 0.22 -0.16 -0.11 0.11 -0.10

73 1 0.03 -0.02 0.02 -0.22 0.21 -0.16 0.08 -0.05 0.05

74 1 0.02 -0.02 0.01 0.00 -0.00 0.00 0.16 -0.16 0.14

75 1 -0.01 0.01 -0.01 0.21 -0.22 0.16 0.05 -0.08 0.05

76 1 -0.03 0.03 -0.02 0.22 -0.22 0.16 -0.11 0.11 -0.10

77 30 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00

94 95 96

B1 E E

Frequencies -- 900.0977 905.0586 905.0586

Red. masses -- 5.2477 4.5776 4.5776

Frc consts -- 2.5050 2.2092 2.2092

IR Inten -- 0.0000 7.0801 7.0800

Atom AN X Y Z X Y Z X Y Z

1 6 -0.08 0.14 0.02 0.05 -0.12 -0.02 -0.01 -0.06 -0.01

2 6 0.04 0.06 -0.00 -0.02 -0.03 0.01 -0.09 0.03 0.01

3 7 0.05 -0.00 0.00 -0.03 0.00 0.00 0.00 0.07 0.00

4 6 0.04 -0.06 0.00 -0.02 0.03 -0.01 0.10 0.02 0.01

5 6 -0.08 -0.14 -0.02 0.05 0.11 0.02 0.00 -0.07 -0.01

6 6 0.09 0.09 -0.00 -0.06 -0.13 0.00 0.14 0.07 0.00

7 6 -0.06 0.04 -0.00 -0.03 -0.09 0.01 -0.03 0.02 -0.01

8 7 -0.00 0.05 -0.00 -0.07 0.00 0.00 0.00 0.03 -0.00

9 6 0.06 0.04 0.00 -0.02 0.10 0.01 0.03 0.02 0.01

10 6 0.14 -0.08 -0.02 0.07 0.00 -0.01 0.11 -0.05 -0.02

11 6 -0.14 -0.08 0.02 0.06 -0.01 -0.01 -0.12 -0.05 0.02

12 6 0.09 -0.09 0.00 -0.07 0.14 -0.00 -0.13 0.06 0.00

13 6 -0.06 -0.04 0.00 -0.02 0.10 -0.01 0.03 0.02 -0.01

14 6 -0.14 0.08 -0.02 0.07 0.00 0.01 0.11 -0.05 0.02

15 6 0.14 0.08 0.02 0.06 -0.01 0.01 -0.12 -0.05 -0.02

16 6 0.06 -0.04 -0.00 -0.03 -0.09 -0.01 -0.03 0.02 0.01

17 7 0.00 -0.05 -0.00 -0.07 0.00 -0.00 0.00 0.03 0.00

18 6 -0.09 -0.09 -0.00 -0.06 -0.13 -0.00 0.14 0.07 -0.00

19 6 -0.04 0.06 0.00 -0.02 0.03 0.01 0.10 0.02 -0.01

20 6 0.08 0.14 -0.02 0.05 0.11 -0.02 0.00 -0.07 0.01

21 6 0.08 -0.14 0.02 0.05 -0.12 0.02 -0.01 -0.06 0.01

22 6 -0.04 -0.06 -0.00 -0.02 -0.03 -0.01 -0.09 0.03 -0.01

23 7 -0.05 -0.00 0.00 -0.03 0.00 -0.00 0.00 0.07 -0.00

24 6 -0.09 0.09 0.00 -0.07 0.14 0.00 -0.13 0.06 -0.00

25 6 0.03 0.03 -0.00 -0.04 -0.02 0.01 0.03 0.04 0.01

26 6 0.00 -0.02 0.03 -0.02 0.04 -0.03 -0.01 -0.02 0.04

27 6 -0.01 -0.05 0.05 0.01 0.06 -0.06 -0.01 -0.06 0.06

28 6 0.02 0.02 0.00 0.00 -0.04 -0.01 0.04 0.00 -0.01

29 6 -0.05 -0.01 -0.05 0.06 0.01 0.05 -0.06 -0.01 -0.06

30 6 -0.02 0.00 -0.03 0.01 0.01 0.04 -0.04 0.02 -0.03

31 6 0.02 -0.02 0.00 -0.00 0.04 0.01 -0.04 -0.00 -0.01

32 6 -0.01 0.05 -0.05 0.01 -0.06 0.06 0.01 -0.06 0.05

33 6 0.00 0.02 -0.03 -0.02 -0.04 0.03 0.01 -0.01 0.04

34 6 0.03 -0.03 -0.00 -0.04 0.03 -0.01 -0.02 0.04 0.01

35 6 -0.02 -0.00 0.03 0.02 -0.01 -0.04 0.04 0.02 -0.03

36 6 -0.05 0.01 0.05 0.06 -0.01 -0.06 0.06 -0.01 -0.06

37 6 -0.03 0.03 0.00 -0.04 0.03 0.01 -0.02 0.04 -0.01

38 6 0.02 0.00 0.03 0.02 -0.01 0.04 0.04 0.02 0.03

39 6 0.05 -0.01 0.05 0.06 -0.01 0.06 0.06 -0.01 0.06

40 6 -0.02 0.02 -0.00 -0.00 0.04 -0.01 -0.04 -0.00 0.01

41 6 0.01 -0.05 -0.05 0.01 -0.06 -0.06 0.01 -0.06 -0.05

42 6 -0.00 -0.02 -0.03 -0.02 -0.04 -0.03 0.01 -0.01 -0.04

43 6 -0.03 -0.03 0.00 -0.04 -0.02 -0.01 0.03 0.04 -0.01

44 6 0.02 -0.00 -0.03 0.01 0.01 -0.04 -0.04 0.02 0.03

45 6 0.05 0.01 -0.05 0.06 0.01 -0.05 -0.06 -0.01 0.06

46 6 -0.02 -0.02 -0.00 0.00 -0.04 0.01 0.04 0.00 0.01

47 6 0.01 0.05 0.05 0.01 0.06 0.06 -0.01 -0.06 -0.06

48 6 -0.00 0.02 0.03 -0.02 0.04 0.03 -0.01 -0.02 -0.04

49 1 0.05 0.24 0.01 -0.08 -0.22 -0.00 0.12 0.03 0.02

50 1 0.05 -0.24 -0.01 -0.09 0.23 0.00 -0.11 0.01 0.02

51 1 0.24 0.05 -0.01 -0.01 -0.11 0.02 0.23 0.09 -0.00

52 1 -0.24 0.05 0.01 -0.03 0.12 0.02 -0.22 0.08 0.00

53 1 -0.24 -0.05 -0.01 -0.01 -0.11 -0.02 0.23 0.09 0.00

54 1 0.24 -0.05 0.01 -0.03 0.12 -0.02 -0.22 0.08 -0.00

55 1 -0.05 0.24 -0.01 -0.09 0.23 -0.00 -0.11 0.01 -0.02

56 1 -0.05 -0.24 0.01 -0.08 -0.22 0.00 0.12 0.03 -0.02

57 1 -0.01 -0.02 0.04 0.09 -0.06 -0.11 0.07 -0.10 -0.01

58 1 -0.09 -0.06 0.04 0.08 0.10 -0.02 -0.12 -0.05 0.06

59 1 0.02 0.02 -0.00 -0.11 0.08 0.08 -0.07 0.10 0.08

60 1 -0.06 -0.09 -0.04 0.04 0.11 0.06 -0.10 -0.09 -0.03

61 1 -0.02 -0.01 -0.04 0.10 -0.08 -0.02 0.05 -0.08 -0.11

62 1 0.02 -0.02 -0.00 -0.10 -0.07 -0.08 0.08 0.11 0.08

63 1 -0.09 0.06 -0.04 0.09 -0.10 0.03 0.11 -0.04 0.06

64 1 -0.01 0.02 -0.04 0.08 0.05 0.11 -0.08 -0.10 -0.02

65 1 -0.02 0.01 0.04 0.10 0.07 0.01 -0.06 -0.09 -0.11

66 1 -0.06 0.09 0.04 0.05 -0.12 -0.06 0.10 -0.08 -0.02

67 1 0.02 -0.01 0.04 0.10 0.07 -0.01 -0.06 -0.09 0.11

68 1 0.06 -0.09 0.04 0.05 -0.12 0.06 0.10 -0.08 0.02

69 1 -0.02 0.02 0.00 -0.10 -0.07 0.08 0.08 0.11 -0.08

70 1 0.09 -0.06 -0.04 0.09 -0.10 -0.03 0.11 -0.04 -0.06

71 1 0.01 -0.02 -0.04 0.08 0.05 -0.11 -0.08 -0.10 0.02

72 1 0.02 0.01 -0.04 0.10 -0.08 0.02 0.05 -0.08 0.11

73 1 0.06 0.09 -0.04 0.04 0.11 -0.06 -0.10 -0.09 0.03

74 1 -0.02 -0.02 0.00 -0.11 0.08 -0.08 -0.07 0.10 -0.08

75 1 0.09 0.06 0.04 0.08 0.10 0.02 -0.12 -0.05 -0.06

76 1 0.01 0.02 0.04 0.09 -0.06 0.11 0.07 -0.10 0.01

77 30 -0.00 0.00 -0.00 0.01 -0.00 0.00 -0.00 -0.01 -0.00

97 98 99

A1 B1 E

Frequencies -- 906.2760 918.3949 919.6683

Red. masses -- 6.8115 1.3329 1.3357

Frc consts -- 3.2962 0.6624 0.6656

IR Inten -- 0.0000 0.0000 0.0174

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.08 -0.01 0.00 0.01 -0.06 -0.00 -0.01 0.08

2 6 -0.09 0.03 0.01 0.00 0.00 0.01 -0.00 0.00 -0.01

3 7 0.00 0.05 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00

4 6 0.09 0.03 0.01 0.00 -0.00 -0.01 0.00 -0.00 0.01

5 6 0.00 -0.08 -0.01 0.00 -0.01 0.06 -0.00 0.01 -0.08

6 6 0.15 0.15 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.01

7 6 0.03 0.09 -0.01 -0.00 0.00 0.01 -0.00 -0.00 0.00

8 7 0.05 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00

9 6 0.03 -0.09 -0.01 0.00 0.00 -0.01 -0.00 0.00 0.00

10 6 -0.08 -0.00 0.01 0.01 0.00 0.06 0.00 0.00 0.00

11 6 -0.08 0.00 0.01 -0.01 0.00 -0.06 0.00 -0.00 -0.00

12 6 -0.15 0.15 0.00 0.00 -0.00 0.00 -0.00 0.00 0.01

13 6 -0.03 0.09 -0.01 -0.00 -0.00 -0.01 -0.00 0.00 -0.00

14 6 0.08 0.00 0.01 -0.01 -0.00 0.06 0.00 0.00 -0.00

15 6 0.08 -0.00 0.01 0.01 -0.00 -0.06 0.00 -0.00 0.00

16 6 -0.03 -0.09 -0.01 0.00 -0.00 0.01 -0.00 -0.00 -0.00

17 7 -0.05 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 0.00

18 6 -0.15 -0.15 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.01

19 6 -0.09 -0.03 0.01 -0.00 0.00 -0.01 0.00 -0.00 -0.01

20 6 -0.00 0.08 -0.01 -0.00 0.01 0.06 -0.00 0.01 0.08

21 6 0.00 0.08 -0.01 -0.00 -0.01 -0.06 -0.00 -0.01 -0.08

22 6 0.09 -0.03 0.01 -0.00 -0.00 0.01 -0.00 0.00 0.01

23 7 -0.00 -0.05 -0.00 0.00 0.00 0.00 0.00 0.00 0.00

24 6 0.15 -0.15 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.01

25 6 0.05 0.05 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00

26 6 0.01 -0.04 0.05 -0.00 -0.00 0.00 0.00 -0.00 0.00

27 6 -0.01 -0.09 0.09 0.00 -0.00 0.00 -0.00 0.00 -0.00

28 6 0.03 0.03 0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00

29 6 -0.09 -0.01 -0.09 -0.00 0.00 -0.00 0.00 0.00 0.00

30 6 -0.04 0.01 -0.05 -0.00 -0.00 -0.00 0.00 -0.00 0.00

31 6 -0.03 0.03 -0.00 0.00 -0.00 0.00 0.00 0.00 0.00

32 6 0.01 -0.09 0.09 0.00 0.00 -0.00 -0.00 -0.00 0.00

33 6 -0.01 -0.04 0.05 -0.00 0.00 -0.00 0.00 -0.00 -0.00

34 6 -0.05 0.05 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00

35 6 0.04 0.01 -0.05 -0.00 0.00 0.00 0.00 0.00 -0.00

36 6 0.09 -0.01 -0.09 -0.00 -0.00 0.00 0.00 -0.00 -0.00

37 6 0.05 -0.05 0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00

38 6 -0.04 -0.01 -0.05 0.00 -0.00 0.00 0.00 0.00 0.00

39 6 -0.09 0.01 -0.09 0.00 0.00 0.00 0.00 -0.00 0.00

40 6 0.03 -0.03 0.00 -0.00 0.00 0.00 0.00 0.00 -0.00

41 6 -0.01 0.09 0.09 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

42 6 0.01 0.04 0.05 0.00 -0.00 -0.00 0.00 -0.00 0.00

43 6 -0.05 -0.05 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00

44 6 0.04 -0.01 -0.05 0.00 0.00 -0.00 0.00 -0.00 -0.00

45 6 0.09 0.01 -0.09 0.00 -0.00 -0.00 0.00 0.00 -0.00

46 6 -0.03 -0.03 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00

47 6 0.01 0.09 0.09 -0.00 0.00 0.00 -0.00 0.00 0.00

48 6 -0.01 0.04 0.05 0.00 0.00 0.00 0.00 -0.00 -0.00

49 1 0.11 -0.01 0.02 0.00 -0.04 0.35 -0.00 0.05 -0.49

50 1 -0.11 -0.01 0.02 0.00 0.04 -0.35 -0.00 -0.05 0.49

51 1 -0.01 0.11 -0.02 -0.04 0.00 -0.35 -0.00 -0.00 -0.02

52 1 -0.01 -0.11 -0.02 0.04 0.00 0.35 0.00 0.00 0.02

53 1 0.01 -0.11 -0.02 0.04 -0.00 -0.35 -0.00 -0.00 0.02

54 1 0.01 0.11 -0.02 -0.04 -0.00 0.35 0.00 0.00 -0.02

55 1 0.11 0.01 0.02 -0.00 -0.04 -0.35 -0.00 -0.05 -0.49

56 1 -0.11 0.01 0.02 -0.00 0.04 0.35 -0.00 0.05 0.49

57 1 -0.01 -0.04 0.07 -0.00 0.00 0.00 0.01 -0.00 -0.00

58 1 -0.15 -0.11 0.06 -0.01 0.00 0.00 0.00 -0.00 -0.00

59 1 0.03 0.03 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00

60 1 -0.11 -0.15 -0.06 0.00 -0.01 -0.00 0.00 0.01 0.00

61 1 -0.04 -0.01 -0.07 0.00 -0.00 -0.00 0.00 -0.00 0.00

62 1 -0.03 0.03 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00

63 1 0.15 -0.11 0.06 -0.01 -0.00 -0.00 0.00 0.00 0.00

64 1 0.01 -0.04 0.07 -0.00 -0.00 -0.00 0.01 0.00 0.00

65 1 0.04 -0.01 -0.07 0.00 0.00 0.00 0.00 0.00 -0.00

66 1 0.11 -0.15 -0.06 0.00 0.01 0.00 0.00 -0.01 -0.00

67 1 -0.04 0.01 -0.07 -0.00 -0.00 0.00 0.00 0.00 0.00

68 1 -0.11 0.15 -0.06 -0.00 -0.01 0.00 0.00 -0.01 0.00

69 1 0.03 -0.03 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00

70 1 -0.15 0.11 0.06 0.01 0.00 -0.00 0.00 0.00 -0.00

71 1 -0.01 0.04 0.07 0.00 0.00 -0.00 0.01 0.00 -0.00

72 1 0.04 0.01 -0.07 -0.00 0.00 -0.00 0.00 -0.00 -0.00

73 1 0.11 0.15 -0.06 -0.00 0.01 -0.00 0.00 0.01 -0.00

74 1 -0.03 -0.03 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00

75 1 0.15 0.11 0.06 0.01 -0.00 0.00 0.00 -0.00 0.00

76 1 0.01 0.04 0.07 0.00 -0.00 0.00 0.01 -0.00 0.00

77 30 -0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00

100 101 102

E A2 A2

Frequencies -- 919.6683 920.6961 938.1103

Red. masses -- 1.3357 1.3359 1.4861

Frc consts -- 0.6656 0.6672 0.7705

IR Inten -- 0.0174 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 0.01 -0.06 -0.01 0.01 0.00

2 6 0.00 -0.00 -0.00 -0.00 -0.00 0.01 0.01 0.01 -0.00

3 7 0.00 -0.00 0.00 -0.00 -0.00 0.00 0.02 -0.00 -0.00

4 6 -0.00 -0.00 -0.00 -0.00 0.00 -0.01 0.01 -0.01 0.00

5 6 -0.00 0.00 -0.00 0.00 -0.01 0.06 -0.01 -0.01 -0.00

6 6 -0.00 -0.00 0.01 0.00 -0.00 0.01 0.00 -0.00 -0.01

7 6 -0.00 -0.00 -0.01 -0.00 0.00 -0.01 0.01 -0.01 0.00

8 7 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.02 0.00

9 6 0.00 0.00 0.01 0.00 0.00 0.01 -0.01 -0.01 -0.00

10 6 -0.01 -0.00 -0.08 -0.01 -0.00 -0.06 -0.01 0.01 0.00

11 6 0.01 -0.00 0.08 0.01 -0.00 0.06 0.01 0.01 -0.00

12 6 0.00 -0.00 0.01 0.00 0.00 -0.01 0.00 0.00 0.01

13 6 0.00 0.00 -0.01 -0.00 -0.00 0.01 0.01 0.01 -0.00

14 6 -0.01 -0.00 0.08 0.01 0.00 -0.06 0.01 -0.01 0.00

15 6 0.01 -0.00 -0.08 -0.01 0.00 0.06 -0.01 -0.01 -0.00

16 6 -0.00 -0.00 0.01 0.00 -0.00 -0.01 -0.01 0.01 0.00

17 7 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 0.02 0.00

18 6 -0.00 -0.00 -0.01 -0.00 0.00 0.01 -0.00 0.00 -0.01

19 6 -0.00 -0.00 0.00 0.00 -0.00 -0.01 -0.01 0.01 0.00

20 6 -0.00 0.00 0.00 -0.00 0.01 0.06 0.01 0.01 -0.00

21 6 0.00 0.00 -0.00 -0.00 -0.01 -0.06 0.01 -0.01 0.00

22 6 0.00 -0.00 0.00 0.00 0.00 0.01 -0.01 -0.01 -0.00

23 7 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.02 -0.00 -0.00

24 6 0.00 -0.00 -0.01 -0.00 -0.00 -0.01 -0.00 -0.00 0.01

25 6 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.03 0.03 0.02

26 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.03 -0.03 -0.02

27 6 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00 0.00

28 6 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.03 0.03 0.02

29 6 0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00

30 6 0.00 0.00 -0.00 -0.00 0.00 -0.00 0.03 -0.03 -0.02

31 6 0.00 0.00 0.00 0.00 0.00 -0.00 -0.03 -0.03 -0.02

32 6 -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 0.03 0.03 0.02

34 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.03 -0.03 -0.02

35 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.03 0.03 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 0.03 0.03 -0.02

38 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.03 -0.03 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 -0.00 -0.00 -0.00 -0.00 0.03 0.03 -0.02

41 6 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 0.00 -0.00

42 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.03 -0.03 0.02

43 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.03 -0.03 0.02

44 6 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.03 0.03 -0.02

45 6 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00

46 6 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.03 -0.03 0.02

47 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00

48 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.03 0.03 -0.02

49 1 -0.00 0.00 -0.02 0.00 -0.04 0.35 -0.01 0.01 0.01

50 1 0.00 -0.00 0.02 0.00 0.04 -0.35 -0.01 -0.01 -0.01

51 1 0.05 -0.00 0.49 0.04 -0.00 0.35 -0.01 0.01 0.01

52 1 -0.05 -0.00 -0.49 -0.04 -0.00 -0.35 0.01 0.01 -0.01

53 1 0.05 -0.00 -0.49 -0.04 0.00 0.35 0.01 -0.01 0.01

54 1 -0.05 -0.00 0.49 0.04 0.00 -0.35 -0.01 -0.01 -0.01

55 1 0.00 -0.00 -0.02 -0.00 -0.04 -0.35 0.01 0.01 -0.01

56 1 -0.00 0.00 0.02 -0.00 0.04 0.35 0.01 -0.01 0.01

57 1 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.18 0.17 0.13

58 1 0.01 0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00

59 1 0.00 -0.00 0.00 0.00 -0.00 0.00 0.18 -0.18 -0.13

60 1 -0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00

61 1 -0.00 0.01 0.00 -0.00 0.00 -0.00 -0.17 0.18 0.13

62 1 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.18 0.18 0.13

63 1 -0.01 0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00

64 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.18 -0.17 -0.13

65 1 0.00 0.01 0.00 -0.00 -0.00 0.00 -0.17 -0.18 -0.13

66 1 0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00

67 1 0.00 0.01 -0.00 0.00 0.00 0.00 0.17 0.18 -0.13

68 1 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00

69 1 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.18 -0.18 0.13

70 1 -0.01 0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00

71 1 0.00 0.00 0.00 0.00 0.00 0.00 0.18 0.17 -0.13

72 1 -0.00 0.01 -0.00 0.00 -0.00 -0.00 0.17 -0.18 0.13

73 1 -0.00 0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00

74 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.18 0.18 -0.13

75 1 0.01 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00

76 1 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.18 -0.17 0.13

77 30 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

103 104 105

E E B2

Frequencies -- 941.2473 941.2473 943.4500

Red. masses -- 1.6012 1.6012 1.6658

Frc consts -- 0.8358 0.8358 0.8736

IR Inten -- 1.7642 1.7642 7.5539

Atom AN X Y Z X Y Z X Y Z

1 6 -0.01 0.00 0.00 -0.00 -0.02 -0.00 -0.00 -0.01 -0.00

2 6 0.01 0.01 -0.00 -0.02 0.01 0.00 -0.02 -0.00 0.00

3 7 0.02 -0.01 -0.00 0.00 0.03 0.00 -0.00 0.04 0.00

4 6 0.00 -0.01 -0.00 0.03 0.00 0.00 0.02 -0.00 0.00

5 6 -0.01 0.01 0.00 0.00 -0.01 -0.00 0.00 -0.01 -0.00

6 6 -0.01 -0.03 -0.01 0.03 -0.01 -0.01 0.02 -0.02 -0.01

7 6 -0.01 -0.02 0.00 0.01 -0.01 0.00 0.00 -0.02 0.00

8 7 -0.03 0.00 0.00 -0.01 -0.02 0.00 -0.04 -0.00 0.00

9 6 -0.00 0.03 0.00 -0.01 -0.00 0.00 0.00 0.02 0.00

10 6 0.01 0.00 -0.00 0.01 0.01 -0.00 0.01 0.00 -0.00

11 6 0.02 -0.00 -0.00 0.00 0.01 -0.00 0.01 -0.00 -0.00

12 6 0.01 0.03 0.01 -0.03 0.01 -0.01 -0.02 -0.02 -0.01

13 6 -0.00 0.03 -0.00 -0.01 -0.00 -0.00 -0.00 -0.02 0.00

14 6 0.01 0.00 0.00 0.01 0.01 0.00 -0.01 -0.00 -0.00

15 6 0.02 -0.00 0.00 0.00 0.01 0.00 -0.01 0.00 -0.00

16 6 -0.01 -0.02 -0.00 0.01 -0.01 -0.00 -0.00 0.02 0.00

17 7 -0.03 0.00 -0.00 -0.01 -0.02 -0.00 0.04 -0.00 0.00

18 6 -0.01 -0.03 0.01 0.03 -0.01 0.01 -0.02 0.02 -0.01

19 6 0.00 -0.01 0.00 0.03 0.00 -0.00 -0.02 0.00 0.00

20 6 -0.01 0.01 -0.00 0.00 -0.01 0.00 -0.00 0.01 -0.00

21 6 -0.01 0.00 -0.00 -0.00 -0.02 0.00 0.00 0.01 -0.00

22 6 0.01 0.01 0.00 -0.02 0.01 -0.00 0.02 0.00 0.00

23 7 0.02 -0.01 0.00 0.00 0.03 -0.00 -0.00 -0.04 0.00

24 6 0.01 0.03 -0.01 -0.03 0.01 0.01 0.02 0.02 -0.01

25 6 -0.03 0.01 0.02 -0.03 0.04 0.03 -0.03 0.03 0.03

26 6 0.02 -0.02 -0.02 0.04 -0.04 -0.03 0.03 -0.03 -0.03

27 6 0.00 0.01 -0.01 -0.00 -0.00 0.01 0.00 0.00 -0.00

28 6 -0.02 0.02 0.02 -0.04 0.04 0.03 -0.03 0.03 0.02

29 6 0.01 0.00 0.01 -0.01 -0.00 -0.01 -0.00 -0.00 -0.00

30 6 0.03 -0.02 -0.01 0.04 -0.04 -0.03 0.03 -0.03 -0.03

31 6 -0.04 -0.04 -0.03 0.02 0.02 0.02 0.03 0.03 0.02

32 6 0.00 -0.01 0.01 0.00 -0.01 0.01 -0.00 0.00 -0.00

33 6 0.04 0.04 0.03 -0.02 -0.03 -0.01 -0.03 -0.03 -0.03

34 6 -0.04 -0.03 -0.03 0.01 0.03 0.02 0.03 0.03 0.03

35 6 0.04 0.04 0.03 -0.02 -0.02 -0.02 -0.03 -0.03 -0.03

36 6 0.00 -0.00 -0.01 0.01 -0.00 -0.01 0.00 -0.00 -0.00

37 6 -0.04 -0.03 0.03 0.01 0.03 -0.02 -0.03 -0.03 0.03

38 6 0.04 0.04 -0.03 -0.02 -0.02 0.02 0.03 0.03 -0.03

39 6 0.00 -0.00 0.01 0.01 -0.00 0.01 -0.00 0.00 -0.00

40 6 -0.04 -0.04 0.03 0.02 0.02 -0.02 -0.03 -0.03 0.02

41 6 0.00 -0.01 -0.01 0.00 -0.01 -0.01 0.00 -0.00 -0.00

42 6 0.04 0.04 -0.03 -0.02 -0.03 0.01 0.03 0.03 -0.03

43 6 -0.03 0.01 -0.02 -0.03 0.04 -0.03 0.03 -0.03 0.03

44 6 0.03 -0.02 0.01 0.04 -0.04 0.03 -0.03 0.03 -0.03

45 6 0.01 0.00 -0.01 -0.01 -0.00 0.01 0.00 0.00 -0.00

46 6 -0.02 0.02 -0.02 -0.04 0.04 -0.03 0.03 -0.03 0.02

47 6 0.00 0.01 0.01 -0.00 -0.00 -0.01 -0.00 -0.00 -0.00

48 6 0.02 -0.02 0.02 0.04 -0.04 0.03 -0.03 0.03 -0.03

49 1 -0.04 -0.02 -0.00 0.03 0.01 0.00 0.04 0.02 0.01

50 1 -0.02 0.01 -0.00 -0.04 0.02 0.00 -0.04 0.02 0.01

51 1 -0.02 -0.04 0.00 0.01 0.02 0.00 -0.02 -0.04 0.01

52 1 -0.01 0.03 0.00 -0.02 0.04 0.00 -0.02 0.04 0.01

53 1 -0.02 -0.04 -0.00 0.01 0.02 -0.00 0.02 0.04 0.01

54 1 -0.01 0.03 -0.00 -0.02 0.04 -0.00 0.02 -0.04 0.01

55 1 -0.02 0.01 0.00 -0.04 0.02 -0.00 0.04 -0.02 0.01

56 1 -0.04 -0.02 0.00 0.03 0.01 -0.00 -0.04 -0.02 0.01

57 1 -0.13 0.13 0.08 -0.21 0.21 0.15 -0.17 0.17 0.12

58 1 0.01 0.02 -0.00 -0.01 0.00 0.01 -0.01 0.01 0.01

59 1 0.13 -0.13 -0.09 0.22 -0.22 -0.16 0.18 -0.18 -0.13

60 1 0.01 0.02 0.01 -0.02 -0.00 0.00 -0.01 0.01 0.01

61 1 -0.12 0.13 0.10 -0.21 0.21 0.15 -0.17 0.17 0.12

62 1 0.22 0.22 0.16 -0.13 -0.13 -0.09 -0.18 -0.18 -0.13

63 1 0.00 -0.02 -0.00 0.02 -0.01 0.01 0.01 0.01 0.01

64 1 -0.21 -0.21 -0.15 0.13 0.12 0.10 0.17 0.17 0.12

65 1 -0.21 -0.21 -0.15 0.13 0.13 0.08 0.17 0.17 0.12

66 1 -0.00 -0.01 -0.01 0.02 -0.01 -0.00 0.01 0.01 0.01

67 1 -0.21 -0.21 0.15 0.13 0.13 -0.08 -0.17 -0.17 0.12

68 1 -0.00 -0.01 0.01 0.02 -0.01 0.00 -0.01 -0.01 0.01

69 1 0.22 0.22 -0.16 -0.13 -0.13 0.09 0.18 0.18 -0.13

70 1 0.00 -0.02 0.00 0.02 -0.01 -0.01 -0.01 -0.01 0.01

71 1 -0.21 -0.21 0.15 0.13 0.12 -0.10 -0.17 -0.17 0.12

72 1 -0.12 0.13 -0.10 -0.21 0.21 -0.15 0.17 -0.17 0.12

73 1 0.01 0.02 -0.01 -0.02 -0.00 -0.00 0.01 -0.01 0.01

74 1 0.13 -0.13 0.09 0.22 -0.22 0.16 -0.18 0.18 -0.13

75 1 0.01 0.02 0.00 -0.01 0.00 -0.01 0.01 -0.01 0.01

76 1 -0.13 0.13 -0.08 -0.21 0.21 -0.15 0.17 -0.17 0.12

77 30 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00

106 107 108

B1 E E

Frequencies -- 980.9188 980.9288 980.9288

Red. masses -- 1.3554 1.3556 1.3556

Frc consts -- 0.7684 0.7685 0.7685

IR Inten -- 0.0000 1.1211 1.1211

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 6 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00

25 6 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

26 6 -0.03 0.03 0.02 -0.03 0.03 0.02 0.02 -0.02 -0.01

27 6 0.03 -0.03 -0.02 0.03 -0.03 -0.03 -0.02 0.02 0.02

28 6 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00

29 6 -0.03 0.03 0.02 -0.03 0.03 0.03 0.02 -0.02 -0.02

30 6 0.03 -0.03 -0.02 0.03 -0.03 -0.02 -0.02 0.02 0.01

31 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00

32 6 0.03 0.03 0.02 0.02 0.02 0.02 0.03 0.03 0.03

33 6 -0.03 -0.03 -0.02 -0.02 -0.02 -0.01 -0.03 -0.03 -0.02

34 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00

35 6 0.03 0.03 0.02 0.02 0.02 0.01 0.03 0.03 0.02

36 6 -0.03 -0.03 -0.02 -0.02 -0.02 -0.02 -0.03 -0.03 -0.03

37 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00

38 6 -0.03 -0.03 0.02 0.02 0.02 -0.01 0.03 0.03 -0.02

39 6 0.03 0.03 -0.02 -0.02 -0.02 0.02 -0.03 -0.03 0.03

40 6 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00

41 6 -0.03 -0.03 0.02 0.02 0.02 -0.02 0.03 0.03 -0.03

42 6 0.03 0.03 -0.02 -0.02 -0.02 0.01 -0.03 -0.03 0.02

43 6 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00

44 6 -0.03 0.03 -0.02 0.03 -0.03 0.02 -0.02 0.02 -0.01

45 6 0.03 -0.03 0.02 -0.03 0.03 -0.03 0.02 -0.02 0.02

46 6 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00

47 6 -0.03 0.03 -0.02 0.03 -0.03 0.03 -0.02 0.02 -0.02

48 6 0.03 -0.03 0.02 -0.03 0.03 -0.02 0.02 -0.02 0.01

49 1 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00

50 1 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

51 1 -0.00 0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

52 1 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00

53 1 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

54 1 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00

55 1 -0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

56 1 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

57 1 0.15 -0.15 -0.11 0.18 -0.18 -0.13 -0.12 0.11 0.09

58 1 -0.15 0.16 0.11 -0.18 0.19 0.13 0.12 -0.12 -0.08

59 1 0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

60 1 0.16 -0.15 -0.11 0.19 -0.18 -0.13 -0.12 0.12 0.09

61 1 -0.15 0.15 0.11 -0.18 0.18 0.13 0.11 -0.12 -0.08

62 1 0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

63 1 -0.15 -0.16 -0.11 -0.12 -0.12 -0.09 -0.18 -0.19 -0.13

64 1 0.15 0.15 0.11 0.12 0.11 0.08 0.18 0.18 0.13

65 1 -0.15 -0.15 -0.11 -0.11 -0.12 -0.09 -0.18 -0.18 -0.13

66 1 0.16 0.15 0.11 0.12 0.12 0.08 0.19 0.18 0.13

67 1 0.15 0.15 -0.11 -0.11 -0.12 0.09 -0.18 -0.18 0.13

68 1 -0.16 -0.15 0.11 0.12 0.12 -0.08 0.19 0.18 -0.13

69 1 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

70 1 0.15 0.16 -0.11 -0.12 -0.12 0.09 -0.18 -0.19 0.13

71 1 -0.15 -0.15 0.11 0.12 0.11 -0.08 0.18 0.18 -0.13

72 1 0.15 -0.15 0.11 -0.18 0.18 -0.13 0.11 -0.12 0.08

73 1 -0.16 0.15 -0.11 0.19 -0.18 0.13 -0.12 0.12 -0.09

74 1 -0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

75 1 0.15 -0.16 0.11 -0.18 0.19 -0.13 0.12 -0.12 0.08

76 1 -0.15 0.15 -0.11 0.18 -0.18 0.13 -0.12 0.11 -0.09

77 30 -0.00 0.00 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00

109 110 111

A1 A2 E

Frequencies -- 980.9734 1002.5222 1002.5604

Red. masses -- 1.3561 1.2843 1.2852

Frc consts -- 0.7689 0.7605 0.7611

IR Inten -- 0.0000 0.0000 0.0266

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 -0.00 0.00 -0.01 -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 -0.01 -0.00 -0.00 -0.01 -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 0.01 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 0.01 -0.00 0.01 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 0.01 -0.00 -0.00 -0.01 -0.00 0.00

11 6 0.00 -0.00 0.00 -0.01 -0.00 0.00 -0.01 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 -0.01 0.00 -0.00 -0.01 -0.00 -0.00

15 6 -0.00 0.00 0.00 0.01 0.00 0.00 -0.01 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 -0.01 -0.00 0.01 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 -0.01 0.00 0.00 0.00 -0.00

21 6 -0.00 -0.00 -0.00 -0.00 0.01 -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 0.01 0.00 0.00 -0.01 -0.00 0.00

24 6 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00

25 6 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

26 6 -0.03 0.03 0.02 -0.01 0.01 0.01 -0.01 0.01 0.01

27 6 0.03 -0.03 -0.02 0.03 -0.03 -0.02 0.03 -0.03 -0.02

28 6 0.00 0.00 -0.00 -0.03 0.03 0.02 -0.03 0.03 0.02

29 6 -0.03 0.03 0.02 0.03 -0.03 -0.02 0.03 -0.03 -0.02

30 6 0.03 -0.03 -0.02 -0.01 0.01 0.01 -0.01 0.01 0.01

31 6 -0.00 0.00 -0.00 -0.03 -0.03 -0.02 -0.03 -0.03 -0.02

32 6 -0.03 -0.03 -0.02 0.03 0.03 0.02 0.02 0.02 0.02

33 6 0.03 0.03 0.02 -0.01 -0.01 -0.01 -0.01 -0.01 -0.01

34 6 0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.00

35 6 -0.03 -0.03 -0.02 -0.01 -0.01 -0.01 -0.01 -0.01 -0.01

36 6 0.03 0.03 0.02 0.03 0.03 0.02 0.02 0.02 0.02

37 6 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

38 6 0.03 0.03 -0.02 0.01 0.01 -0.01 -0.01 -0.01 0.01

39 6 -0.03 -0.03 0.02 -0.03 -0.03 0.02 0.02 0.02 -0.02

40 6 0.00 -0.00 -0.00 0.03 0.03 -0.02 -0.03 -0.03 0.02

41 6 0.03 0.03 -0.02 -0.03 -0.03 0.02 0.02 0.02 -0.02

42 6 -0.03 -0.03 0.02 0.01 0.01 -0.01 -0.01 -0.01 0.01

43 6 0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

44 6 -0.03 0.03 -0.02 0.01 -0.01 0.01 -0.01 0.01 -0.01

45 6 0.03 -0.03 0.02 -0.03 0.03 -0.02 0.03 -0.03 0.02

46 6 -0.00 -0.00 -0.00 0.03 -0.03 0.02 -0.03 0.03 -0.02

47 6 -0.03 0.03 -0.02 -0.03 0.03 -0.02 0.03 -0.03 0.02

48 6 0.03 -0.03 0.02 0.01 -0.01 0.01 -0.01 0.01 -0.01

49 1 -0.00 -0.00 0.00 -0.01 -0.01 -0.00 -0.01 -0.01 -0.00

50 1 0.00 -0.00 0.00 -0.01 0.01 0.00 -0.00 0.01 0.00

51 1 -0.00 -0.00 -0.00 0.01 0.01 -0.00 -0.00 0.00 0.00

52 1 -0.00 0.00 -0.00 -0.01 0.01 0.00 -0.00 -0.00 0.00

53 1 0.00 0.00 -0.00 -0.01 -0.01 -0.00 -0.00 0.00 -0.00

54 1 0.00 -0.00 -0.00 0.01 -0.01 0.00 -0.00 -0.00 -0.00

55 1 -0.00 0.00 0.00 0.01 -0.01 0.00 -0.00 0.01 -0.00

56 1 0.00 0.00 0.00 0.01 0.01 -0.00 -0.01 -0.01 0.00

57 1 0.15 -0.15 -0.11 0.09 -0.09 -0.07 0.10 -0.10 -0.07

58 1 -0.15 0.16 0.11 -0.16 0.16 0.12 -0.17 0.17 0.12

59 1 0.00 0.00 0.00 0.17 -0.17 -0.12 0.18 -0.18 -0.13

60 1 0.16 -0.15 -0.11 -0.16 0.16 0.12 -0.17 0.17 0.12

61 1 -0.15 0.15 0.11 0.09 -0.09 -0.07 0.10 -0.10 -0.07

62 1 -0.00 0.00 0.00 0.17 0.17 0.12 0.16 0.16 0.11

63 1 0.15 0.16 0.11 -0.16 -0.16 -0.12 -0.15 -0.15 -0.11

64 1 -0.15 -0.15 -0.11 0.09 0.09 0.07 0.08 0.08 0.06

65 1 0.15 0.15 0.11 0.09 0.09 0.07 0.08 0.08 0.06

66 1 -0.16 -0.15 -0.11 -0.16 -0.16 -0.12 -0.15 -0.15 -0.11

67 1 -0.15 -0.15 0.11 -0.09 -0.09 0.07 0.08 0.08 -0.06

68 1 0.16 0.15 -0.11 0.16 0.16 -0.12 -0.15 -0.15 0.11

69 1 0.00 -0.00 0.00 -0.17 -0.17 0.12 0.16 0.16 -0.11

70 1 -0.15 -0.16 0.11 0.16 0.16 -0.12 -0.15 -0.15 0.11

71 1 0.15 0.15 -0.11 -0.09 -0.09 0.07 0.08 0.08 -0.06

72 1 0.15 -0.15 0.11 -0.09 0.09 -0.07 0.10 -0.10 0.07

73 1 -0.16 0.15 -0.11 0.16 -0.16 0.12 -0.17 0.17 -0.12

74 1 -0.00 -0.00 0.00 -0.17 0.17 -0.12 0.18 -0.18 0.13

75 1 0.15 -0.16 0.11 0.16 -0.16 0.12 -0.17 0.17 -0.12

76 1 -0.15 0.15 -0.11 -0.09 0.09 -0.07 0.10 -0.10 0.07

77 30 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

112 113 114

E B2 E

Frequencies -- 1002.5604 1002.6527 1019.1215

Red. masses -- 1.2852 1.2838 6.3557

Frc consts -- 0.7611 0.7604 3.8892

IR Inten -- 0.0266 0.4394 2.1348

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.01 -0.00 0.00 0.00 0.00 -0.00 -0.05 -0.00

2 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.02 0.00

3 7 -0.00 0.01 0.00 0.00 -0.01 -0.00 0.00 0.07 0.00

4 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.02 0.00

5 6 0.00 -0.01 -0.00 -0.00 0.00 0.00 0.00 -0.05 -0.01

6 6 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.02 -0.01 0.00

7 6 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.01 0.02 -0.00

8 7 0.00 -0.01 -0.00 0.01 -0.00 -0.00 0.01 0.01 -0.00

9 6 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.01 0.02 -0.00

10 6 -0.00 0.00 0.00 -0.00 -0.00 0.00 0.01 -0.01 -0.00

11 6 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.01 -0.01 0.00

12 6 0.00 0.00 -0.00 0.00 0.00 0.00 0.01 -0.00 0.00

13 6 0.00 0.00 0.00 -0.00 0.00 -0.00 0.01 0.02 0.00

14 6 -0.00 0.00 -0.00 0.00 0.00 0.00 0.01 -0.01 0.00

15 6 0.00 0.00 0.00 0.00 -0.00 0.00 -0.01 -0.01 -0.00

16 6 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.01 0.02 0.00

17 7 0.00 -0.01 0.00 -0.01 0.00 -0.00 0.01 0.01 0.00

18 6 0.00 0.00 0.00 0.00 -0.00 0.00 -0.02 -0.01 -0.00

19 6 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.02 -0.00

20 6 0.00 -0.01 0.00 0.00 -0.00 0.00 0.00 -0.05 0.01

21 6 -0.00 -0.01 0.00 -0.00 -0.00 0.00 -0.00 -0.05 0.00

22 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.02 -0.00

23 7 -0.00 0.01 -0.00 -0.00 0.01 -0.00 0.00 0.07 -0.00

24 6 0.00 0.00 0.00 -0.00 -0.00 0.00 0.01 -0.00 -0.00

25 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.01 -0.01 -0.00

26 6 0.01 -0.01 -0.01 -0.01 0.01 0.01 -0.13 -0.01 -0.16

27 6 -0.02 0.02 0.02 0.03 -0.03 -0.02 0.00 0.00 0.00

28 6 0.03 -0.03 -0.02 -0.03 0.03 0.02 0.15 0.15 0.00

29 6 -0.02 0.02 0.02 0.03 -0.03 -0.02 0.00 -0.00 -0.00

30 6 0.01 -0.01 -0.01 -0.01 0.01 0.01 -0.02 -0.13 0.16

31 6 -0.03 -0.03 -0.02 0.03 0.03 0.02 -0.13 0.13 0.00

32 6 0.03 0.03 0.02 -0.03 -0.03 -0.02 -0.00 -0.00 0.00

33 6 -0.01 -0.01 -0.01 0.01 0.01 0.01 0.11 -0.01 -0.14

34 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.01 -0.01 -0.00

35 6 -0.01 -0.01 -0.01 0.01 0.01 0.01 0.01 -0.11 0.14

36 6 0.03 0.03 0.02 -0.03 -0.03 -0.02 -0.00 -0.00 -0.00

37 6 0.00 0.00 -0.00 0.00 0.00 -0.00 0.01 -0.01 0.00

38 6 -0.01 -0.01 0.01 -0.01 -0.01 0.01 0.01 -0.11 -0.14

39 6 0.03 0.03 -0.02 0.03 0.03 -0.02 -0.00 -0.00 0.00

40 6 -0.03 -0.03 0.02 -0.03 -0.03 0.02 -0.13 0.13 -0.00

41 6 0.03 0.03 -0.02 0.03 0.03 -0.02 -0.00 -0.00 -0.00

42 6 -0.01 -0.01 0.01 -0.01 -0.01 0.01 0.11 -0.01 0.14

43 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.01 -0.01 0.00

44 6 0.01 -0.01 0.01 0.01 -0.01 0.01 -0.02 -0.13 -0.16

45 6 -0.02 0.02 -0.02 -0.03 0.03 -0.02 0.00 -0.00 0.00

46 6 0.03 -0.03 0.02 0.03 -0.03 0.02 0.15 0.15 -0.00

47 6 -0.02 0.02 -0.02 -0.03 0.03 -0.02 0.00 0.00 -0.00

48 6 0.01 -0.01 0.01 0.01 -0.01 0.01 -0.13 -0.01 0.16

49 1 0.00 -0.00 -0.00 -0.01 0.00 0.00 0.03 -0.03 -0.00

50 1 -0.00 -0.00 -0.00 0.01 0.00 0.00 -0.04 -0.03 -0.00

51 1 -0.01 -0.00 0.00 -0.00 0.01 0.00 0.00 -0.01 -0.00

52 1 0.01 -0.01 -0.00 -0.00 -0.01 0.00 -0.01 -0.02 0.01

53 1 -0.01 -0.00 -0.00 0.00 -0.01 0.00 0.00 -0.01 0.00

54 1 0.01 -0.01 0.00 0.00 0.01 0.00 -0.01 -0.02 -0.01

55 1 -0.00 -0.00 0.00 -0.01 -0.00 0.00 -0.04 -0.03 0.00

56 1 0.00 -0.00 0.00 0.01 -0.00 0.00 0.03 -0.03 0.00

57 1 -0.08 0.08 0.06 0.09 -0.09 -0.07 -0.13 -0.00 -0.17

58 1 0.15 -0.15 -0.11 -0.16 0.16 0.12 -0.01 0.01 -0.01

59 1 -0.16 0.16 0.11 0.17 -0.17 -0.12 0.16 0.15 -0.00

60 1 0.15 -0.15 -0.11 -0.16 0.16 0.12 -0.00 0.00 0.01

61 1 -0.08 0.08 0.06 0.09 -0.09 -0.07 0.00 -0.14 0.17

62 1 0.18 0.18 0.13 -0.17 -0.17 -0.12 -0.14 0.13 -0.01

63 1 -0.17 -0.17 -0.12 0.16 0.16 0.12 0.01 0.01 -0.01

64 1 0.10 0.10 0.07 -0.09 -0.09 -0.07 0.11 -0.01 -0.15

65 1 0.10 0.10 0.07 -0.09 -0.09 -0.07 -0.00 -0.12 0.14

66 1 -0.17 -0.17 -0.12 0.16 0.16 0.12 0.00 0.01 0.01

67 1 0.10 0.10 -0.07 0.09 0.09 -0.07 -0.00 -0.12 -0.14

68 1 -0.17 -0.17 0.12 -0.16 -0.16 0.12 0.00 0.01 -0.01

69 1 0.18 0.18 -0.13 0.17 0.17 -0.12 -0.14 0.13 0.01

70 1 -0.17 -0.17 0.12 -0.16 -0.16 0.12 0.01 0.01 0.01

71 1 0.10 0.10 -0.07 0.09 0.09 -0.07 0.11 -0.01 0.15

72 1 -0.08 0.08 -0.06 -0.09 0.09 -0.07 0.00 -0.14 -0.17

73 1 0.15 -0.15 0.11 0.16 -0.16 0.12 -0.00 0.00 -0.01

74 1 -0.16 0.16 -0.11 -0.17 0.17 -0.12 0.16 0.15 0.00

75 1 0.15 -0.15 0.11 0.16 -0.16 0.12 -0.01 0.01 0.01

76 1 -0.08 0.08 -0.06 -0.09 0.09 -0.07 -0.13 -0.00 0.17

77 30 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.01 -0.00

115 116 117

E A1 B1

Frequencies -- 1019.1215 1019.4900 1019.5735

Red. masses -- 6.3557 6.2469 6.2538

Frc consts -- 3.8892 3.8254 3.8303

IR Inten -- 2.1348 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.01 0.01 0.00 -0.00 0.03 0.00 0.00 -0.01 -0.00

2 6 0.02 0.01 -0.00 0.01 -0.01 -0.00 -0.01 -0.00 0.00

3 7 0.01 -0.01 -0.00 0.00 -0.05 -0.00 -0.02 -0.00 -0.00

4 6 0.02 -0.01 -0.00 -0.01 -0.01 -0.00 -0.01 0.00 -0.00

5 6 -0.01 -0.01 -0.00 0.00 0.03 0.00 0.00 0.01 0.00

6 6 -0.00 -0.01 -0.00 0.01 0.01 0.00 0.01 0.01 0.00

7 6 0.02 0.00 -0.00 -0.01 -0.01 0.00 0.00 -0.01 0.00

8 7 0.07 -0.00 -0.00 -0.05 0.00 0.00 -0.00 -0.02 0.00

9 6 0.02 -0.00 -0.00 -0.01 0.01 0.00 -0.00 -0.01 -0.00

10 6 -0.05 -0.00 0.01 0.03 -0.00 -0.00 -0.01 0.00 0.00

11 6 -0.05 0.00 0.00 0.03 0.00 -0.00 0.01 0.00 -0.00

12 6 -0.01 0.02 0.00 -0.01 0.01 -0.00 0.01 -0.01 -0.00

13 6 0.02 -0.00 0.00 0.01 -0.01 0.00 0.00 0.01 -0.00

14 6 -0.05 -0.00 -0.01 -0.03 0.00 -0.00 0.01 -0.00 0.00

15 6 -0.05 0.00 -0.00 -0.03 -0.00 -0.00 -0.01 -0.00 -0.00

16 6 0.02 0.00 0.00 0.01 0.01 0.00 -0.00 0.01 0.00

17 7 0.07 -0.00 0.00 0.05 -0.00 0.00 0.00 0.02 0.00

18 6 -0.00 -0.01 0.00 -0.01 -0.01 0.00 -0.01 -0.01 0.00

19 6 0.02 -0.01 0.00 0.01 0.01 -0.00 0.01 -0.00 -0.00

20 6 -0.01 -0.01 0.00 -0.00 -0.03 0.00 -0.00 -0.01 0.00

21 6 -0.01 0.01 -0.00 0.00 -0.03 0.00 -0.00 0.01 -0.00

22 6 0.02 0.01 0.00 -0.01 0.01 -0.00 0.01 0.00 0.00

23 7 0.01 -0.01 0.00 0.00 0.05 -0.00 0.02 0.00 -0.00

24 6 -0.01 0.02 -0.00 0.01 -0.01 -0.00 -0.01 0.01 -0.00

25 6 -0.01 -0.01 0.00 0.01 0.01 0.00 0.01 0.01 0.00

26 6 -0.11 -0.01 -0.14 0.12 0.01 0.15 0.12 0.01 0.15

27 6 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.01

28 6 0.13 0.13 -0.00 -0.14 -0.14 0.00 -0.14 -0.14 0.00

29 6 -0.00 0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.01

30 6 -0.01 -0.11 0.14 0.01 0.12 -0.15 0.01 0.12 -0.15

31 6 0.15 -0.15 0.00 0.14 -0.14 -0.00 -0.14 0.14 -0.00

32 6 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.01

33 6 -0.13 0.02 0.16 -0.12 0.01 0.15 0.12 -0.01 -0.15

34 6 -0.01 0.01 -0.00 -0.01 0.01 -0.00 0.01 -0.01 -0.00

35 6 -0.01 0.13 -0.16 -0.01 0.12 -0.15 0.01 -0.12 0.15

36 6 0.00 -0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.01

37 6 -0.01 0.01 0.00 0.01 -0.01 -0.00 -0.01 0.01 -0.00

38 6 -0.01 0.13 0.16 0.01 -0.12 -0.15 -0.01 0.12 0.15

39 6 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.01

40 6 0.15 -0.15 -0.00 -0.14 0.14 -0.00 0.14 -0.14 -0.00

41 6 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.01

42 6 -0.13 0.02 -0.16 0.12 -0.01 0.15 -0.12 0.01 -0.15

43 6 -0.01 -0.01 -0.00 -0.01 -0.01 0.00 -0.01 -0.01 0.00

44 6 -0.01 -0.11 -0.14 -0.01 -0.12 -0.15 -0.01 -0.12 -0.15

45 6 -0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.01

46 6 0.13 0.13 0.00 0.14 0.14 0.00 0.14 0.14 0.00

47 6 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.01

48 6 -0.11 -0.01 0.14 -0.12 -0.01 0.15 -0.12 -0.01 0.15

49 1 -0.02 0.01 0.01 -0.05 -0.01 0.00 -0.01 -0.02 -0.01

50 1 -0.01 -0.00 -0.00 0.05 -0.01 0.00 -0.01 0.02 0.01

51 1 -0.03 0.04 0.00 -0.01 -0.05 -0.00 -0.02 -0.01 0.01

52 1 -0.03 -0.03 0.00 -0.01 0.05 -0.00 0.02 -0.01 -0.01

53 1 -0.03 0.04 -0.00 0.01 0.05 -0.00 0.02 0.01 0.01

54 1 -0.03 -0.03 -0.00 0.01 -0.05 -0.00 -0.02 0.01 -0.01

55 1 -0.01 -0.00 0.00 -0.05 0.01 0.00 0.01 -0.02 0.01

56 1 -0.02 0.01 -0.01 0.05 0.01 0.00 0.01 0.02 -0.01

57 1 -0.12 0.00 -0.14 0.13 0.00 0.16 0.13 0.00 0.16

58 1 0.01 -0.00 -0.01 0.00 0.00 0.01 0.00 0.00 0.01

59 1 0.13 0.14 0.01 -0.14 -0.14 0.00 -0.15 -0.15 0.00

60 1 0.01 -0.01 0.01 0.00 0.00 -0.01 0.00 0.00 -0.01

61 1 -0.01 -0.11 0.15 0.00 0.13 -0.16 0.00 0.13 -0.16

62 1 0.15 -0.16 -0.00 0.14 -0.14 0.00 -0.15 0.15 -0.00

63 1 0.00 0.00 0.01 -0.00 0.00 0.01 0.00 -0.00 -0.01

64 1 -0.14 -0.00 0.17 -0.13 0.00 0.16 0.13 -0.00 -0.16

65 1 -0.00 0.13 -0.17 -0.00 0.13 -0.16 0.00 -0.13 0.16

66 1 0.01 0.01 -0.01 -0.00 0.00 -0.01 0.00 -0.00 0.01

67 1 -0.00 0.13 0.17 0.00 -0.13 -0.16 -0.00 0.13 0.16

68 1 0.01 0.01 0.01 0.00 -0.00 -0.01 -0.00 0.00 0.01

69 1 0.15 -0.16 0.00 -0.14 0.14 -0.00 0.15 -0.15 -0.00

70 1 0.00 0.00 -0.01 0.00 -0.00 0.01 -0.00 0.00 -0.01

71 1 -0.14 -0.00 -0.17 0.13 -0.00 0.16 -0.13 0.00 -0.16

72 1 -0.01 -0.11 -0.15 -0.00 -0.13 -0.16 -0.00 -0.13 -0.16

73 1 0.01 -0.01 -0.01 -0.00 -0.00 -0.01 -0.00 -0.00 -0.01

74 1 0.13 0.14 -0.01 0.14 0.14 0.00 0.15 0.15 0.00

75 1 0.01 -0.00 0.01 -0.00 -0.00 0.01 -0.00 -0.00 0.01

76 1 -0.12 0.00 0.14 -0.13 -0.00 0.16 -0.13 -0.00 0.16

77 30 -0.01 0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00

118 119 120

A2 E E

Frequencies -- 1024.4181 1028.7055 1028.7055

Red. masses -- 2.6040 5.9307 5.9307

Frc consts -- 1.6100 3.6978 3.6978

IR Inten -- 0.0000 230.8902 230.8907

Atom AN X Y Z X Y Z X Y Z

1 6 -0.02 0.08 0.01 -0.02 -0.16 -0.01 -0.01 -0.14 -0.01

2 6 -0.02 -0.05 -0.01 0.05 0.11 0.01 -0.02 0.05 0.00

3 7 0.10 -0.00 -0.00 -0.06 0.14 0.01 0.04 0.18 0.01

4 6 -0.02 0.05 0.01 0.03 0.02 0.00 -0.05 0.12 0.01

5 6 -0.02 -0.08 -0.01 0.00 -0.09 -0.01 0.02 -0.19 -0.02

6 6 -0.05 0.05 -0.00 -0.03 -0.05 -0.00 -0.08 0.07 0.00

7 6 -0.05 0.02 0.01 0.05 0.02 -0.00 -0.11 0.05 0.01

8 7 -0.00 -0.10 0.00 0.18 -0.04 -0.01 -0.14 -0.06 0.01

9 6 0.05 0.02 -0.01 0.12 0.05 -0.01 -0.02 0.03 0.00

10 6 -0.08 0.02 0.01 -0.19 -0.02 0.02 0.09 0.00 -0.01

11 6 0.08 0.02 -0.01 -0.14 0.01 0.01 0.16 -0.02 -0.01

12 6 -0.05 -0.05 0.00 0.07 0.08 0.00 0.05 -0.03 0.00

13 6 -0.05 -0.02 -0.01 0.12 0.05 0.01 -0.02 0.03 -0.00

14 6 0.08 -0.02 0.01 -0.19 -0.02 -0.02 0.09 0.00 0.01

15 6 -0.08 -0.02 -0.01 -0.14 0.01 -0.01 0.16 -0.02 0.01

16 6 0.05 -0.02 0.01 0.05 0.02 0.00 -0.11 0.05 -0.01

17 7 0.00 0.10 0.00 0.18 -0.04 0.01 -0.14 -0.06 -0.01

18 6 0.05 -0.05 -0.00 -0.03 -0.05 0.00 -0.08 0.07 -0.00

19 6 0.02 -0.05 0.01 0.03 0.02 -0.00 -0.05 0.12 -0.01

20 6 0.02 0.08 -0.01 0.00 -0.09 0.01 0.02 -0.19 0.02

21 6 0.02 -0.08 0.01 -0.02 -0.16 0.01 -0.01 -0.14 0.01

22 6 0.02 0.05 -0.01 0.05 0.11 -0.01 -0.02 0.05 -0.00

23 7 -0.10 -0.00 0.00 -0.06 0.14 -0.01 0.04 0.18 -0.01

24 6 0.05 0.05 0.00 0.07 0.08 -0.00 0.05 -0.03 -0.00

25 6 0.00 -0.00 -0.01 -0.03 -0.03 0.00 0.00 -0.01 -0.01

26 6 -0.00 0.01 0.01 0.04 -0.00 0.04 0.00 0.01 0.02

27 6 0.00 -0.01 0.00 0.00 0.04 -0.04 -0.00 -0.00 -0.00

28 6 -0.00 0.00 -0.00 -0.03 -0.04 0.00 -0.01 -0.00 -0.00

29 6 0.01 -0.00 0.00 0.03 0.00 0.04 0.01 0.00 0.01

30 6 -0.01 0.00 0.01 0.00 0.04 -0.05 -0.01 0.01 0.00

31 6 -0.00 -0.00 0.00 -0.00 0.01 -0.00 0.04 -0.03 -0.00

32 6 0.00 0.01 -0.00 0.00 -0.01 0.01 -0.00 0.03 -0.04

33 6 -0.00 -0.01 -0.01 0.01 0.01 0.00 -0.04 0.00 0.05

34 6 0.00 0.00 0.01 -0.01 -0.00 -0.01 0.03 -0.03 -0.00

35 6 -0.01 -0.00 -0.01 0.01 -0.00 0.02 0.00 0.04 -0.04

36 6 0.01 0.00 -0.00 -0.00 0.00 -0.00 -0.04 0.00 0.04

37 6 -0.00 -0.00 0.01 -0.01 -0.00 0.01 0.03 -0.03 0.00

38 6 0.01 0.00 -0.01 0.01 -0.00 -0.02 0.00 0.04 0.04

39 6 -0.01 -0.00 -0.00 -0.00 0.00 0.00 -0.04 0.00 -0.04

40 6 0.00 0.00 0.00 -0.00 0.01 0.00 0.04 -0.03 0.00

41 6 -0.00 -0.01 -0.00 0.00 -0.01 -0.01 -0.00 0.03 0.04

42 6 0.00 0.01 -0.01 0.01 0.01 -0.00 -0.04 0.00 -0.05

43 6 -0.00 0.00 -0.01 -0.03 -0.03 -0.00 0.00 -0.01 0.01

44 6 0.01 -0.00 0.01 0.00 0.04 0.05 -0.01 0.01 -0.00

45 6 -0.01 0.00 0.00 0.03 0.00 -0.04 0.01 0.00 -0.01

46 6 0.00 -0.00 -0.00 -0.03 -0.04 -0.00 -0.01 -0.00 0.00

47 6 -0.00 0.01 0.00 0.00 0.04 0.04 -0.00 -0.00 0.00

48 6 0.00 -0.01 0.01 0.04 -0.00 -0.04 0.00 0.01 -0.02

49 1 0.20 0.25 0.04 -0.16 -0.28 -0.03 0.14 -0.03 0.00

50 1 0.20 -0.25 -0.04 -0.18 0.05 0.01 0.11 -0.28 -0.03

51 1 -0.25 -0.20 0.04 -0.28 -0.11 0.03 -0.05 -0.18 0.01

52 1 0.25 -0.20 -0.04 -0.03 -0.14 -0.00 0.28 -0.16 -0.03

53 1 0.25 0.20 0.04 -0.28 -0.11 -0.03 -0.05 -0.18 -0.01

54 1 -0.25 0.20 -0.04 -0.03 -0.14 0.00 0.28 -0.16 0.03

55 1 -0.20 0.25 -0.04 -0.18 0.05 -0.01 0.11 -0.28 0.03

56 1 -0.20 -0.25 0.04 -0.16 -0.28 0.03 0.14 -0.03 -0.00

57 1 0.03 -0.02 -0.02 0.02 -0.01 0.06 0.06 -0.02 -0.02

58 1 -0.02 0.01 0.01 -0.00 0.03 -0.05 -0.04 0.01 0.01

59 1 0.00 -0.00 -0.03 -0.04 -0.03 0.01 0.00 -0.01 -0.04

60 1 -0.01 0.02 0.01 0.03 -0.01 0.05 -0.01 0.04 0.02

61 1 0.02 -0.03 -0.02 -0.02 0.04 -0.05 0.02 -0.05 -0.04

62 1 0.00 0.00 0.03 -0.01 -0.00 -0.04 0.03 -0.04 -0.01

63 1 -0.02 -0.01 -0.01 0.04 0.01 0.02 0.01 0.03 -0.05

64 1 0.03 0.02 0.02 -0.05 -0.02 -0.04 -0.04 -0.02 0.05

65 1 0.02 0.03 0.02 -0.02 -0.06 -0.02 0.01 0.02 -0.06

66 1 -0.01 -0.02 -0.01 0.01 0.04 0.01 -0.03 -0.00 0.05

67 1 -0.02 -0.03 0.02 -0.02 -0.06 0.02 0.01 0.02 0.06

68 1 0.01 0.02 -0.01 0.01 0.04 -0.01 -0.03 -0.00 -0.05

69 1 -0.00 -0.00 0.03 -0.01 -0.00 0.04 0.03 -0.04 0.01

70 1 0.02 0.01 -0.01 0.04 0.01 -0.02 0.01 0.03 0.05

71 1 -0.03 -0.02 0.02 -0.05 -0.02 0.04 -0.04 -0.02 -0.05

72 1 -0.02 0.03 -0.02 -0.02 0.04 0.05 0.02 -0.05 0.04

73 1 0.01 -0.02 0.01 0.03 -0.01 -0.05 -0.01 0.04 -0.02

74 1 -0.00 0.00 -0.03 -0.04 -0.03 -0.01 0.00 -0.01 0.04

75 1 0.02 -0.01 0.01 -0.00 0.03 0.05 -0.04 0.01 -0.01

76 1 -0.03 0.02 -0.02 0.02 -0.01 -0.06 0.06 -0.02 0.02

77 30 -0.00 0.00 0.00 -0.01 -0.01 -0.00 0.01 -0.01 0.00

121 122 123

A1 E E

Frequencies -- 1031.7854 1035.3203 1035.3203

Red. masses -- 6.9348 4.0186 4.0186

Frc consts -- 4.3497 2.5379 2.5379

IR Inten -- 0.0000 124.7734 124.7731

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 -0.13 -0.01 -0.01 0.04 0.00 -0.03 0.07 0.01

2 6 -0.03 0.04 0.00 -0.02 -0.04 -0.00 0.01 -0.02 -0.00

3 7 -0.00 0.21 0.01 0.10 0.06 0.00 0.13 -0.04 -0.00

4 6 0.03 0.04 0.00 0.02 0.00 -0.00 -0.02 0.04 0.00

5 6 -0.01 -0.13 -0.01 -0.03 -0.06 -0.00 -0.02 -0.06 -0.01

6 6 -0.06 -0.06 0.00 -0.06 -0.08 0.00 -0.05 0.03 -0.00

7 6 0.04 0.03 -0.00 0.02 0.01 -0.00 -0.04 0.02 0.00

8 7 0.21 0.00 -0.01 0.04 0.13 -0.00 0.06 -0.10 -0.00

9 6 0.04 -0.03 -0.00 -0.04 -0.02 0.00 0.00 -0.02 0.00

10 6 -0.13 0.01 0.01 0.06 -0.02 -0.01 -0.06 0.03 0.00

11 6 -0.13 -0.01 0.01 -0.07 -0.03 0.01 0.04 0.01 -0.00

12 6 0.06 -0.06 -0.00 -0.03 -0.05 0.00 -0.08 0.06 0.00

13 6 -0.04 0.03 -0.00 -0.04 -0.02 -0.00 0.00 -0.02 -0.00

14 6 0.13 -0.01 0.01 0.06 -0.02 0.01 -0.06 0.03 -0.00

15 6 0.13 0.01 0.01 -0.07 -0.03 -0.01 0.04 0.01 0.00

16 6 -0.04 -0.03 -0.00 0.02 0.01 0.00 -0.04 0.02 -0.00

17 7 -0.21 -0.00 -0.01 0.04 0.13 0.00 0.06 -0.10 0.00

18 6 0.06 0.06 -0.00 -0.06 -0.08 -0.00 -0.05 0.03 0.00

19 6 -0.03 -0.04 0.00 0.02 0.00 0.00 -0.02 0.04 -0.00

20 6 0.01 0.13 -0.01 -0.03 -0.06 0.00 -0.02 -0.06 0.01

21 6 -0.01 0.13 -0.01 -0.01 0.04 -0.00 -0.03 0.07 -0.01

22 6 0.03 -0.04 0.00 -0.02 -0.04 0.00 0.01 -0.02 0.00

23 7 -0.00 -0.21 0.01 0.10 0.06 -0.00 0.13 -0.04 0.00

24 6 -0.06 0.06 0.00 -0.03 -0.05 -0.00 -0.08 0.06 -0.00

25 6 -0.06 -0.06 0.00 -0.08 -0.08 0.00 -0.01 -0.01 -0.01

26 6 0.02 -0.01 0.04 0.01 -0.02 0.04 0.00 0.00 0.01

27 6 0.00 0.06 -0.08 -0.00 0.09 -0.12 -0.00 0.01 -0.02

28 6 -0.02 -0.02 0.00 0.01 0.01 0.00 0.00 0.00 -0.00

29 6 0.06 0.00 0.08 0.08 -0.00 0.12 0.02 0.00 0.02

30 6 -0.01 0.02 -0.04 -0.02 0.01 -0.04 -0.01 0.00 0.00

31 6 0.02 -0.02 -0.00 -0.00 0.00 0.00 0.01 -0.01 0.00

32 6 -0.00 0.06 -0.08 -0.00 0.02 -0.02 -0.00 -0.08 0.12

33 6 -0.02 -0.01 0.04 -0.00 -0.01 -0.00 0.01 0.02 -0.04

34 6 0.06 -0.06 -0.00 0.01 -0.01 0.01 -0.08 0.08 0.00

35 6 0.01 0.02 -0.04 -0.00 0.00 -0.01 -0.02 -0.01 0.04

36 6 -0.06 0.00 0.08 -0.01 -0.00 0.02 0.09 0.00 -0.12

37 6 -0.06 0.06 -0.00 0.01 -0.01 -0.01 -0.08 0.08 -0.00

38 6 -0.01 -0.02 -0.04 -0.00 0.00 0.01 -0.02 -0.01 -0.04

39 6 0.06 -0.00 0.08 -0.01 -0.00 -0.02 0.09 0.00 0.12

40 6 -0.02 0.02 -0.00 -0.00 0.00 -0.00 0.01 -0.01 -0.00

41 6 0.00 -0.06 -0.08 -0.00 0.02 0.02 -0.00 -0.08 -0.12

42 6 0.02 0.01 0.04 -0.00 -0.01 0.00 0.01 0.02 0.04

43 6 0.06 0.06 0.00 -0.08 -0.08 -0.00 -0.01 -0.01 0.01

44 6 0.01 -0.02 -0.04 -0.02 0.01 0.04 -0.01 0.00 -0.00

45 6 -0.06 -0.00 0.08 0.08 -0.00 -0.12 0.02 0.00 -0.02

46 6 0.02 0.02 0.00 0.01 0.01 -0.00 0.00 0.00 0.00

47 6 -0.00 -0.06 -0.08 -0.00 0.09 0.12 -0.00 0.01 0.02

48 6 -0.02 0.01 0.04 0.01 -0.02 -0.04 0.00 0.00 -0.01

49 1 0.20 0.00 0.00 0.22 0.22 0.03 0.06 0.15 0.02

50 1 -0.20 0.00 0.00 0.00 -0.08 -0.01 0.23 -0.26 -0.03

51 1 0.00 0.20 -0.00 0.26 0.23 -0.03 -0.08 -0.00 0.01

52 1 0.00 -0.20 -0.00 -0.15 0.06 0.02 0.22 -0.22 -0.03

53 1 -0.00 -0.20 -0.00 0.26 0.23 0.03 -0.08 -0.00 -0.01

54 1 -0.00 0.20 -0.00 -0.15 0.06 -0.02 0.22 -0.22 0.03

55 1 0.20 -0.00 0.00 0.00 -0.08 0.01 0.23 -0.26 0.03

56 1 -0.20 -0.00 0.00 0.22 0.22 -0.03 0.06 0.15 -0.02

57 1 0.00 -0.04 0.06 -0.04 -0.09 0.08 0.02 -0.02 -0.00

58 1 -0.04 0.04 -0.11 -0.08 0.04 -0.18 -0.03 0.01 -0.02

59 1 -0.01 -0.01 0.00 0.02 0.02 0.00 -0.00 0.01 -0.03

60 1 0.04 -0.04 0.11 0.04 -0.09 0.18 0.01 0.01 0.03

61 1 -0.04 0.00 -0.06 -0.09 -0.03 -0.07 -0.01 -0.03 -0.02

62 1 0.01 -0.01 -0.00 -0.01 -0.00 0.03 0.02 -0.02 0.00

63 1 0.04 0.04 -0.11 -0.01 0.01 -0.03 -0.09 -0.04 0.18

64 1 -0.00 -0.04 0.06 0.03 -0.01 0.02 -0.03 0.09 -0.07

65 1 0.04 0.00 -0.06 0.02 0.02 0.00 -0.09 0.04 0.08

66 1 -0.04 -0.04 0.11 -0.01 -0.03 0.02 0.04 0.08 -0.18

67 1 -0.04 -0.00 -0.06 0.02 0.02 -0.00 -0.09 0.04 -0.08

68 1 0.04 0.04 0.11 -0.01 -0.03 -0.02 0.04 0.08 0.18

69 1 -0.01 0.01 -0.00 -0.01 -0.00 -0.03 0.02 -0.02 -0.00

70 1 -0.04 -0.04 -0.11 -0.01 0.01 0.03 -0.09 -0.04 -0.18

71 1 0.00 0.04 0.06 0.03 -0.01 -0.02 -0.03 0.09 0.07

72 1 0.04 -0.00 -0.06 -0.09 -0.03 0.07 -0.01 -0.03 0.02

73 1 -0.04 0.04 0.11 0.04 -0.09 -0.18 0.01 0.01 -0.03

74 1 0.01 0.01 -0.00 0.02 0.02 -0.00 -0.00 0.01 0.03

75 1 0.04 -0.04 -0.11 -0.08 0.04 0.18 -0.03 0.01 0.02

76 1 -0.00 0.04 0.06 -0.04 -0.09 -0.08 0.02 -0.02 0.00

77 30 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00

124 125 126

B2 B1 A1

Frequencies -- 1037.9813 1041.4033 1054.6554

Red. masses -- 7.2007 3.9833 2.1202

Frc consts -- 4.5709 2.5453 1.3894

IR Inten -- 3.1330 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.01 -0.18 -0.02 0.02 -0.04 -0.00 0.00 -0.02 -0.00

2 6 0.03 0.09 0.01 -0.01 0.00 -0.00 0.00 0.01 0.00

3 7 -0.00 0.18 0.01 -0.09 -0.00 -0.00 -0.00 0.04 0.00

4 6 -0.03 0.09 0.01 -0.01 -0.00 0.00 -0.00 0.01 0.00

5 6 0.01 -0.18 -0.02 0.02 0.04 0.00 -0.00 -0.02 -0.00

6 6 -0.08 0.08 0.00 0.04 0.04 -0.00 -0.02 -0.02 -0.00

7 6 -0.09 0.03 0.01 -0.00 -0.01 -0.00 0.01 -0.00 -0.00

8 7 -0.18 -0.00 0.01 0.00 -0.09 -0.00 0.04 0.00 -0.00

9 6 -0.09 -0.03 0.01 0.00 -0.01 0.00 0.01 0.00 -0.00

10 6 0.18 0.01 -0.02 -0.04 0.02 0.00 -0.02 0.00 0.00

11 6 0.18 -0.01 -0.02 0.04 0.02 -0.00 -0.02 -0.00 0.00

12 6 0.08 0.08 0.00 0.04 -0.04 0.00 0.02 -0.02 -0.00

13 6 0.09 0.03 0.01 -0.00 0.01 0.00 -0.01 -0.00 -0.00

14 6 -0.18 -0.01 -0.02 0.04 -0.02 0.00 0.02 -0.00 0.00

15 6 -0.18 0.01 -0.02 -0.04 -0.02 -0.00 0.02 0.00 0.00

16 6 0.09 -0.03 0.01 0.00 0.01 -0.00 -0.01 0.00 -0.00

17 7 0.18 0.00 0.01 -0.00 0.09 -0.00 -0.04 -0.00 -0.00

18 6 0.08 -0.08 0.00 -0.04 -0.04 -0.00 0.02 0.02 -0.00

19 6 0.03 -0.09 0.01 0.01 0.00 0.00 0.00 -0.01 0.00

20 6 -0.01 0.18 -0.02 -0.02 -0.04 0.00 0.00 0.02 -0.00

21 6 0.01 0.18 -0.02 -0.02 0.04 -0.00 -0.00 0.02 -0.00

22 6 -0.03 -0.09 0.01 0.01 -0.00 -0.00 -0.00 -0.01 0.00

23 7 -0.00 -0.18 0.01 0.09 0.00 -0.00 0.00 -0.04 0.00

24 6 -0.08 -0.08 0.00 -0.04 0.04 -0.00 -0.02 0.02 -0.00

25 6 0.01 -0.01 -0.02 0.06 0.06 0.00 -0.01 -0.01 0.00

26 6 0.00 0.01 0.01 -0.00 0.02 -0.04 0.00 0.03 -0.03

27 6 -0.00 -0.01 0.00 0.01 -0.07 0.12 0.02 -0.03 0.07

28 6 -0.00 0.00 -0.01 -0.03 -0.03 0.00 -0.05 -0.05 0.00

29 6 0.01 0.00 0.00 -0.07 0.01 -0.12 -0.03 0.02 -0.07

30 6 -0.01 -0.00 0.01 0.02 -0.00 0.04 0.03 0.00 0.03

31 6 0.00 0.00 -0.01 -0.03 0.03 -0.00 0.05 -0.05 0.00

32 6 0.00 -0.01 0.00 0.01 0.07 -0.12 -0.02 -0.03 0.07

33 6 -0.00 0.01 0.01 -0.00 -0.02 0.04 -0.00 0.03 -0.03

34 6 -0.01 -0.01 -0.02 0.06 -0.06 0.00 0.01 -0.01 0.00

35 6 0.01 -0.00 0.01 0.02 0.00 -0.04 -0.03 0.00 0.03

36 6 -0.01 0.00 0.00 -0.07 -0.01 0.12 0.03 0.02 -0.07

37 6 0.01 0.01 -0.02 -0.06 0.06 0.00 -0.01 0.01 0.00

38 6 -0.01 0.00 0.01 -0.02 -0.00 -0.04 0.03 -0.00 0.03

39 6 0.01 -0.00 0.00 0.07 0.01 0.12 -0.03 -0.02 -0.07

40 6 -0.00 -0.00 -0.01 0.03 -0.03 0.00 -0.05 0.05 0.00

41 6 -0.00 0.01 0.00 -0.01 -0.07 -0.12 0.02 0.03 0.07

42 6 0.00 -0.01 0.01 0.00 0.02 0.04 0.00 -0.03 -0.03

43 6 -0.01 0.01 -0.02 -0.06 -0.06 0.00 0.01 0.01 0.00

44 6 0.01 0.00 0.01 -0.02 0.00 0.04 -0.03 -0.00 0.03

45 6 -0.01 -0.00 0.00 0.07 -0.01 -0.12 0.03 -0.02 -0.07

46 6 0.00 -0.00 -0.01 0.03 0.03 0.00 0.05 0.05 0.00

47 6 0.00 0.01 0.00 -0.01 0.07 0.12 -0.02 0.03 0.07

48 6 -0.00 -0.01 0.01 0.00 -0.02 -0.04 -0.00 -0.03 -0.03

49 1 -0.03 -0.22 -0.02 -0.04 -0.08 -0.01 0.02 -0.01 -0.00

50 1 0.03 -0.22 -0.02 -0.04 0.08 0.01 -0.02 -0.01 -0.00

51 1 0.22 0.03 -0.02 -0.08 -0.04 0.01 -0.01 0.02 0.00

52 1 0.22 -0.03 -0.02 0.08 -0.04 -0.01 -0.01 -0.02 0.00

53 1 -0.22 -0.03 -0.02 0.08 0.04 0.01 0.01 -0.02 0.00

54 1 -0.22 0.03 -0.02 -0.08 0.04 -0.01 0.01 0.02 0.00

55 1 -0.03 0.22 -0.02 0.04 -0.08 0.01 0.02 0.01 -0.00

56 1 0.03 0.22 -0.02 0.04 0.08 -0.01 -0.02 0.01 -0.00

57 1 0.05 -0.02 -0.03 0.06 0.13 -0.09 0.08 0.16 -0.11

58 1 -0.03 -0.01 0.00 0.13 -0.01 0.19 0.18 0.06 0.16

59 1 -0.01 0.01 -0.05 -0.04 -0.04 0.00 -0.05 -0.05 0.00

60 1 0.01 0.03 0.00 -0.01 0.13 -0.19 0.06 0.18 -0.16

61 1 0.02 -0.05 -0.03 0.13 0.06 0.09 0.16 0.08 0.11

62 1 0.01 0.01 -0.05 -0.04 0.04 0.00 0.05 -0.05 0.00

63 1 0.03 -0.01 0.00 0.13 0.01 -0.19 -0.18 0.06 0.16

64 1 -0.05 -0.02 -0.03 0.06 -0.13 0.09 -0.08 0.16 -0.11

65 1 -0.02 -0.05 -0.03 0.13 -0.06 -0.09 -0.16 0.08 0.11

66 1 -0.01 0.03 0.00 -0.01 -0.13 0.19 -0.06 0.18 -0.16

67 1 0.02 0.05 -0.03 -0.13 0.06 -0.09 0.16 -0.08 0.11

68 1 0.01 -0.03 0.00 0.01 0.13 0.19 0.06 -0.18 -0.16

69 1 -0.01 -0.01 -0.05 0.04 -0.04 -0.00 -0.05 0.05 0.00

70 1 -0.03 0.01 0.00 -0.13 -0.01 -0.19 0.18 -0.06 0.16

71 1 0.05 0.02 -0.03 -0.06 0.13 0.09 0.08 -0.16 -0.11

72 1 -0.02 0.05 -0.03 -0.13 -0.06 0.09 -0.16 -0.08 0.11

73 1 -0.01 -0.03 0.00 0.01 -0.13 -0.19 -0.06 -0.18 -0.16

74 1 0.01 -0.01 -0.05 0.04 0.04 0.00 0.05 0.05 0.00

75 1 0.03 0.01 0.00 -0.13 0.01 0.19 -0.18 -0.06 0.16

76 1 -0.05 0.02 -0.03 -0.06 -0.13 -0.09 -0.08 -0.16 -0.11

77 30 0.00 0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 0.00

127 128 129

E E B1

Frequencies -- 1058.5746 1058.5746 1069.4519

Red. masses -- 2.0948 2.0948 2.4717

Frc consts -- 1.3830 1.3830 1.6656

IR Inten -- 1.8272 1.8272 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 -0.03 -0.00 0.01 -0.01 -0.00 -0.02 0.03 0.00

2 6 0.00 0.01 0.00 -0.00 0.01 0.00 0.01 -0.01 -0.00

3 7 -0.05 0.04 0.00 -0.05 -0.04 -0.00 0.09 0.00 0.00

4 6 -0.00 -0.01 -0.00 0.00 -0.01 -0.00 0.01 0.01 0.00

5 6 0.01 0.01 0.00 0.01 0.03 0.00 -0.02 -0.03 -0.00

6 6 0.01 -0.01 0.00 0.05 0.05 -0.00 -0.05 -0.05 -0.00

7 6 0.01 0.00 -0.00 -0.01 0.00 0.00 0.01 0.01 -0.00

8 7 -0.04 0.05 0.00 -0.04 -0.05 0.00 0.00 0.09 -0.00

9 6 -0.01 -0.00 0.00 0.01 -0.00 -0.00 -0.01 0.01 0.00

10 6 0.03 -0.01 -0.00 -0.01 0.01 0.00 0.03 -0.02 -0.00

11 6 -0.01 -0.01 0.00 0.03 0.01 -0.00 -0.03 -0.02 0.00

12 6 0.05 -0.05 -0.00 0.01 0.01 -0.00 -0.05 0.05 -0.00

13 6 -0.01 -0.00 -0.00 0.01 -0.00 0.00 0.01 -0.01 0.00

14 6 0.03 -0.01 0.00 -0.01 0.01 -0.00 -0.03 0.02 -0.00

15 6 -0.01 -0.01 -0.00 0.03 0.01 0.00 0.03 0.02 0.00

16 6 0.01 0.00 0.00 -0.01 0.00 -0.00 -0.01 -0.01 -0.00

17 7 -0.04 0.05 -0.00 -0.04 -0.05 -0.00 -0.00 -0.09 -0.00

18 6 0.01 -0.01 -0.00 0.05 0.05 0.00 0.05 0.05 0.00

19 6 -0.00 -0.01 0.00 0.00 -0.01 0.00 -0.01 -0.01 0.00

20 6 0.01 0.01 -0.00 0.01 0.03 -0.00 0.02 0.03 -0.00

21 6 0.01 -0.03 0.00 0.01 -0.01 0.00 0.02 -0.03 0.00

22 6 0.00 0.01 -0.00 -0.00 0.01 -0.00 -0.01 0.01 -0.00

23 7 -0.05 0.04 -0.00 -0.05 -0.04 0.00 -0.09 -0.00 0.00

24 6 0.05 -0.05 0.00 0.01 0.01 0.00 0.05 -0.05 -0.00

25 6 0.00 -0.00 0.00 0.03 0.03 -0.00 -0.06 -0.06 0.00

26 6 -0.00 -0.00 -0.00 -0.00 -0.04 0.04 0.00 0.02 -0.03

27 6 0.00 0.00 -0.00 -0.03 0.02 -0.08 0.03 0.01 0.03

28 6 0.00 0.00 0.00 0.06 0.06 -0.00 -0.04 -0.04 0.00

29 6 -0.00 -0.00 -0.00 0.02 -0.03 0.08 0.01 0.03 -0.03

30 6 0.00 0.00 -0.00 -0.04 -0.00 -0.04 0.02 0.00 0.03

31 6 0.06 -0.06 -0.00 -0.00 0.00 -0.00 -0.04 0.04 0.00

32 6 -0.03 -0.02 0.08 0.00 -0.00 0.00 0.03 -0.01 -0.03

33 6 -0.00 0.04 -0.04 -0.00 0.00 0.00 0.00 -0.02 0.03

34 6 0.03 -0.03 -0.00 0.00 0.00 -0.00 -0.06 0.06 0.00

35 6 -0.04 0.00 0.04 0.00 -0.00 0.00 0.02 -0.00 -0.03

36 6 0.02 0.03 -0.08 -0.00 0.00 0.00 0.01 -0.03 0.03

37 6 0.03 -0.03 0.00 0.00 0.00 0.00 0.06 -0.06 -0.00

38 6 -0.04 0.00 -0.04 0.00 -0.00 -0.00 -0.02 0.00 -0.03

39 6 0.02 0.03 0.08 -0.00 0.00 -0.00 -0.01 0.03 0.03

40 6 0.06 -0.06 0.00 -0.00 0.00 0.00 0.04 -0.04 -0.00

41 6 -0.03 -0.02 -0.08 0.00 -0.00 -0.00 -0.03 0.01 -0.03

42 6 -0.00 0.04 0.04 -0.00 0.00 -0.00 -0.00 0.02 0.03

43 6 0.00 -0.00 -0.00 0.03 0.03 0.00 0.06 0.06 -0.00

44 6 0.00 0.00 0.00 -0.04 -0.00 0.04 -0.02 -0.00 0.03

45 6 -0.00 -0.00 0.00 0.02 -0.03 -0.08 -0.01 -0.03 -0.03

46 6 0.00 0.00 -0.00 0.06 0.06 0.00 0.04 0.04 -0.00

47 6 0.00 0.00 0.00 -0.03 0.02 0.08 -0.03 -0.01 0.03

48 6 -0.00 -0.00 0.00 -0.00 -0.04 -0.04 -0.00 -0.02 -0.03

49 1 -0.02 -0.06 -0.01 -0.07 -0.07 -0.01 0.05 0.08 0.01

50 1 -0.07 0.07 0.01 -0.02 0.06 0.01 0.05 -0.08 -0.01

51 1 0.06 0.02 -0.01 -0.07 -0.07 0.01 0.08 0.05 -0.01

52 1 -0.07 0.07 0.01 0.06 -0.02 -0.01 -0.08 0.05 0.01

53 1 0.06 0.02 0.01 -0.07 -0.07 -0.01 -0.08 -0.05 -0.01

54 1 -0.07 0.07 -0.01 0.06 -0.02 0.01 0.08 -0.05 0.01

55 1 -0.07 0.07 -0.01 -0.02 0.06 -0.01 -0.05 0.08 -0.01

56 1 -0.02 -0.06 0.01 -0.07 -0.07 0.01 -0.05 -0.08 0.01

57 1 -0.01 -0.00 0.00 -0.11 -0.22 0.15 0.08 0.16 -0.11

58 1 0.00 0.00 -0.00 -0.26 -0.11 -0.21 0.18 0.10 0.11

59 1 0.00 -0.00 0.01 0.07 0.07 -0.00 -0.05 -0.05 0.00

60 1 -0.00 -0.01 0.00 -0.11 -0.26 0.21 0.10 0.18 -0.11

61 1 0.00 0.00 0.00 -0.22 -0.11 -0.15 0.16 0.08 0.11

62 1 0.07 -0.07 -0.00 0.00 0.00 -0.01 -0.05 0.05 0.00

63 1 -0.26 0.11 0.21 0.01 -0.00 -0.00 0.18 -0.10 -0.11

64 1 -0.11 0.22 -0.15 -0.00 0.00 -0.00 0.08 -0.16 0.11

65 1 -0.22 0.11 0.15 0.00 -0.01 -0.00 0.16 -0.08 -0.11

66 1 -0.11 0.26 -0.21 -0.00 0.00 0.00 0.10 -0.18 0.11

67 1 -0.22 0.11 -0.15 0.00 -0.01 0.00 -0.16 0.08 -0.11

68 1 -0.11 0.26 0.21 -0.00 0.00 -0.00 -0.10 0.18 0.11

69 1 0.07 -0.07 0.00 0.00 0.00 0.01 0.05 -0.05 0.00

70 1 -0.26 0.11 -0.21 0.01 -0.00 0.00 -0.18 0.10 -0.11

71 1 -0.11 0.22 0.15 -0.00 0.00 0.00 -0.08 0.16 0.11

72 1 0.00 0.00 -0.00 -0.22 -0.11 0.15 -0.16 -0.08 0.11

73 1 -0.00 -0.01 -0.00 -0.11 -0.26 -0.21 -0.10 -0.18 -0.11

74 1 0.00 -0.00 -0.01 0.07 0.07 0.00 0.05 0.05 -0.00

75 1 0.00 0.00 0.00 -0.26 -0.11 0.21 -0.18 -0.10 0.11

76 1 -0.01 -0.00 -0.00 -0.11 -0.22 -0.15 -0.08 -0.16 -0.11

77 30 0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 0.00

130 131 132

E E B2

Frequencies -- 1094.7682 1094.7682 1098.3599

Red. masses -- 1.2248 1.2248 1.5253

Frc consts -- 0.8649 0.8649 1.0842

IR Inten -- 56.2012 56.2011 39.5752

Atom AN X Y Z X Y Z X Y Z

1 6 -0.04 0.01 0.00 0.00 -0.02 -0.00 -0.01 0.00 -0.00

2 6 0.02 0.01 0.00 -0.00 0.02 0.00 0.00 0.00 0.00

3 7 0.00 0.02 0.00 -0.00 0.00 0.00 0.00 0.01 0.00

4 6 -0.02 0.01 0.00 -0.01 -0.02 -0.00 -0.00 0.00 0.00

5 6 0.04 0.01 0.00 0.01 0.02 0.00 0.01 0.00 -0.00

6 6 0.01 -0.01 -0.00 0.02 -0.02 -0.00 0.00 -0.00 -0.01

7 6 0.02 0.00 -0.00 -0.01 0.02 0.00 -0.00 0.00 0.00

8 7 0.00 0.00 -0.00 -0.02 0.00 0.00 -0.01 -0.00 0.00

9 6 -0.02 0.01 0.00 -0.01 -0.02 0.00 -0.00 -0.00 0.00

10 6 0.02 -0.01 -0.00 -0.01 0.04 0.00 -0.00 0.01 -0.00

11 6 -0.02 -0.00 0.00 -0.01 -0.04 0.00 -0.00 -0.01 -0.00

12 6 -0.02 -0.02 -0.00 0.01 0.01 0.00 -0.00 -0.00 -0.01

13 6 -0.02 0.01 -0.00 -0.01 -0.02 -0.00 0.00 0.00 0.00

14 6 0.02 -0.01 0.00 -0.01 0.04 -0.00 0.00 -0.01 -0.00

15 6 -0.02 -0.00 -0.00 -0.01 -0.04 -0.00 0.00 0.01 -0.00

16 6 0.02 0.00 0.00 -0.01 0.02 -0.00 0.00 -0.00 0.00

17 7 0.00 0.00 0.00 -0.02 0.00 -0.00 0.01 0.00 0.00

18 6 0.01 -0.01 0.00 0.02 -0.02 0.00 -0.00 0.00 -0.01

19 6 -0.02 0.01 -0.00 -0.01 -0.02 0.00 0.00 -0.00 0.00

20 6 0.04 0.01 -0.00 0.01 0.02 -0.00 -0.01 -0.00 -0.00

21 6 -0.04 0.01 -0.00 0.00 -0.02 0.00 0.01 -0.00 -0.00

22 6 0.02 0.01 -0.00 -0.00 0.02 -0.00 -0.00 -0.00 0.00

23 7 0.00 0.02 -0.00 -0.00 0.00 -0.00 0.00 -0.01 0.00

24 6 -0.02 -0.02 0.00 0.01 0.01 -0.00 0.00 0.00 -0.01

25 6 0.00 0.00 0.01 -0.00 -0.00 0.01 0.01 -0.01 0.03

26 6 -0.01 -0.01 -0.01 -0.01 -0.01 -0.01 -0.04 -0.03 -0.02

27 6 0.00 0.01 -0.01 0.00 0.01 -0.01 0.01 0.03 -0.02

28 6 0.01 -0.00 0.01 0.00 -0.01 0.01 0.01 -0.01 0.04

29 6 -0.01 -0.00 -0.01 -0.01 -0.00 -0.01 -0.03 -0.01 -0.02

30 6 0.01 0.01 -0.01 0.01 0.01 -0.01 0.03 0.04 -0.02

31 6 -0.01 -0.00 0.01 0.00 0.01 -0.01 -0.01 -0.01 0.04

32 6 -0.00 0.01 -0.01 0.00 -0.01 0.01 -0.01 0.03 -0.02

33 6 0.01 -0.01 -0.01 -0.01 0.01 0.01 0.04 -0.03 -0.02

34 6 -0.00 0.00 0.01 -0.00 0.00 -0.01 -0.01 -0.01 0.03

35 6 -0.01 0.01 -0.01 0.01 -0.01 0.01 -0.03 0.04 -0.02

36 6 0.01 -0.00 -0.01 -0.01 0.00 0.01 0.03 -0.01 -0.02

37 6 -0.00 0.00 -0.01 -0.00 0.00 0.01 0.01 0.01 0.03

38 6 -0.01 0.01 0.01 0.01 -0.01 -0.01 0.03 -0.04 -0.02

39 6 0.01 -0.00 0.01 -0.01 0.00 -0.01 -0.03 0.01 -0.02

40 6 -0.01 -0.00 -0.01 0.00 0.01 0.01 0.01 0.01 0.04

41 6 -0.00 0.01 0.01 0.00 -0.01 -0.01 0.01 -0.03 -0.02

42 6 0.01 -0.01 0.01 -0.01 0.01 -0.01 -0.04 0.03 -0.02

43 6 0.00 0.00 -0.01 -0.00 -0.00 -0.01 -0.01 0.01 0.03

44 6 0.01 0.01 0.01 0.01 0.01 0.01 -0.03 -0.04 -0.02

45 6 -0.01 -0.00 0.01 -0.01 -0.00 0.01 0.03 0.01 -0.02

46 6 0.01 -0.00 -0.01 0.00 -0.01 -0.01 -0.01 0.01 0.04

47 6 0.00 0.01 0.01 0.00 0.01 0.01 -0.01 -0.03 -0.02

48 6 -0.01 -0.01 0.01 -0.01 -0.01 0.01 0.04 0.03 -0.02

49 1 -0.39 -0.25 -0.03 -0.08 -0.08 -0.01 -0.11 -0.07 -0.01

50 1 0.40 -0.26 -0.03 -0.02 0.04 0.01 0.11 -0.07 -0.01

51 1 0.04 0.02 -0.01 0.26 0.40 -0.03 0.07 0.11 -0.01

52 1 -0.08 0.08 0.01 0.25 -0.39 -0.03 0.07 -0.11 -0.01

53 1 0.04 0.02 0.01 0.26 0.40 0.03 -0.07 -0.11 -0.01

54 1 -0.08 0.08 -0.01 0.25 -0.39 0.03 -0.07 0.11 -0.01

55 1 0.40 -0.26 0.03 -0.02 0.04 -0.01 -0.11 0.07 -0.01

56 1 -0.39 -0.25 0.03 -0.08 -0.08 0.01 0.11 0.07 -0.01

57 1 -0.04 -0.05 0.02 -0.04 -0.05 0.02 -0.13 -0.17 0.06

58 1 0.02 0.02 0.00 0.04 0.03 0.01 0.10 0.08 0.02

59 1 0.03 -0.02 0.07 0.03 -0.03 0.08 0.09 -0.09 0.24

60 1 -0.03 -0.04 0.01 -0.02 -0.02 0.00 -0.08 -0.10 0.02

61 1 0.04 0.04 0.01 0.05 0.05 0.02 0.17 0.13 0.06

62 1 -0.03 -0.03 0.08 0.02 0.03 -0.07 -0.09 -0.09 0.24

63 1 -0.02 0.02 0.00 0.04 -0.03 -0.01 -0.10 0.08 0.02

64 1 0.05 -0.05 0.02 -0.04 0.04 -0.01 0.13 -0.17 0.06

65 1 -0.05 0.04 0.02 0.05 -0.04 -0.02 -0.17 0.13 0.06

66 1 0.03 -0.04 0.01 -0.02 0.02 -0.00 0.08 -0.10 0.02

67 1 -0.05 0.04 -0.02 0.05 -0.04 0.02 0.17 -0.13 0.06

68 1 0.03 -0.04 -0.01 -0.02 0.02 0.00 -0.08 0.10 0.02

69 1 -0.03 -0.03 -0.08 0.02 0.03 0.07 0.09 0.09 0.24

70 1 -0.02 0.02 -0.00 0.04 -0.03 0.01 0.10 -0.08 0.02

71 1 0.05 -0.05 -0.02 -0.04 0.04 0.01 -0.13 0.17 0.06

72 1 0.04 0.04 -0.01 0.05 0.05 -0.02 -0.17 -0.13 0.06

73 1 -0.03 -0.04 -0.01 -0.02 -0.02 -0.00 0.08 0.10 0.02

74 1 0.03 -0.02 -0.07 0.03 -0.03 -0.08 -0.09 0.09 0.24

75 1 0.02 0.02 -0.00 0.04 0.03 -0.01 -0.10 -0.08 0.02

76 1 -0.04 -0.05 -0.02 -0.04 -0.05 -0.02 0.13 0.17 0.06

77 30 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00

133 134 135

A2 E E

Frequencies -- 1098.7697 1099.3867 1099.3867

Red. masses -- 1.5858 1.5401 1.5401

Frc consts -- 1.1280 1.0967 1.0967

IR Inten -- 0.0000 0.0746 0.0746

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.00 0.02 -0.01 -0.00 -0.00 0.01 0.00

2 6 -0.00 -0.01 -0.00 -0.00 0.00 0.00 -0.00 -0.02 -0.00

3 7 0.00 -0.00 0.00 -0.00 -0.01 -0.00 0.00 -0.00 -0.00

4 6 -0.00 0.01 0.00 0.00 -0.00 0.00 -0.00 0.02 0.00

5 6 0.00 -0.00 -0.00 -0.02 -0.01 -0.00 -0.00 -0.01 -0.00

6 6 -0.00 0.00 -0.01 -0.01 0.01 -0.01 -0.01 0.01 -0.01

7 6 -0.01 0.00 0.00 -0.02 0.00 0.00 -0.00 -0.00 0.00

8 7 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.01 -0.00 -0.00

9 6 0.01 0.00 -0.00 0.02 0.00 -0.00 0.00 0.00 0.00

10 6 -0.00 -0.00 0.00 -0.01 0.00 0.00 0.01 -0.02 -0.00

11 6 0.00 -0.00 -0.00 0.01 0.00 -0.00 0.01 0.02 -0.00

12 6 -0.00 -0.00 0.01 0.01 0.01 -0.01 -0.01 -0.01 0.01

13 6 -0.01 -0.00 -0.00 0.02 0.00 0.00 0.00 0.00 -0.00

14 6 0.00 0.00 0.00 -0.01 0.00 -0.00 0.01 -0.02 0.00

15 6 -0.00 0.00 -0.00 0.01 0.00 0.00 0.01 0.02 0.00

16 6 0.01 -0.00 0.00 -0.02 0.00 -0.00 -0.00 -0.00 -0.00

17 7 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.01 -0.00 0.00

18 6 0.00 -0.00 -0.01 -0.01 0.01 0.01 -0.01 0.01 0.01

19 6 0.00 -0.01 0.00 0.00 -0.00 -0.00 -0.00 0.02 -0.00

20 6 -0.00 0.00 -0.00 -0.02 -0.01 0.00 -0.00 -0.01 0.00

21 6 -0.00 -0.00 0.00 0.02 -0.01 0.00 -0.00 0.01 -0.00

22 6 0.00 0.01 -0.00 -0.00 0.00 -0.00 -0.00 -0.02 0.00

23 7 -0.00 0.00 -0.00 -0.00 -0.01 0.00 0.00 -0.00 0.00

24 6 0.00 0.00 0.01 0.01 0.01 0.01 -0.01 -0.01 -0.01

25 6 0.01 -0.01 0.03 0.01 -0.01 0.02 0.01 -0.01 0.02

26 6 -0.05 -0.03 -0.02 -0.04 -0.03 -0.02 -0.04 -0.03 -0.02

27 6 0.01 0.03 -0.03 0.01 0.03 -0.02 0.01 0.03 -0.03

28 6 0.01 -0.01 0.04 0.01 -0.01 0.04 0.01 -0.01 0.04

29 6 -0.03 -0.01 -0.03 -0.03 -0.01 -0.02 -0.03 -0.01 -0.02

30 6 0.03 0.05 -0.02 0.03 0.04 -0.02 0.03 0.04 -0.02

31 6 0.01 0.01 -0.04 -0.01 -0.01 0.04 0.01 0.01 -0.04

32 6 0.01 -0.03 0.03 -0.01 0.03 -0.02 0.01 -0.03 0.02

33 6 -0.05 0.03 0.02 0.04 -0.03 -0.02 -0.04 0.03 0.02

34 6 0.01 0.01 -0.03 -0.01 -0.01 0.02 0.01 0.01 -0.02

35 6 0.03 -0.05 0.02 -0.03 0.04 -0.02 0.03 -0.04 0.02

36 6 -0.03 0.01 0.03 0.03 -0.01 -0.03 -0.03 0.01 0.02

37 6 -0.01 -0.01 -0.03 -0.01 -0.01 -0.02 0.01 0.01 0.02

38 6 -0.03 0.05 0.02 -0.03 0.04 0.02 0.03 -0.04 -0.02

39 6 0.03 -0.01 0.03 0.03 -0.01 0.03 -0.03 0.01 -0.02

40 6 -0.01 -0.01 -0.04 -0.01 -0.01 -0.04 0.01 0.01 0.04

41 6 -0.01 0.03 0.03 -0.01 0.03 0.02 0.01 -0.03 -0.02

42 6 0.05 -0.03 0.02 0.04 -0.03 0.02 -0.04 0.03 -0.02

43 6 -0.01 0.01 0.03 0.01 -0.01 -0.02 0.01 -0.01 -0.02

44 6 -0.03 -0.05 -0.02 0.03 0.04 0.02 0.03 0.04 0.02

45 6 0.03 0.01 -0.03 -0.03 -0.01 0.02 -0.03 -0.01 0.02

46 6 -0.01 0.01 0.04 0.01 -0.01 -0.04 0.01 -0.01 -0.04

47 6 -0.01 -0.03 -0.03 0.01 0.03 0.02 0.01 0.03 0.03

48 6 0.05 0.03 -0.02 -0.04 -0.03 0.02 -0.04 -0.03 0.02

49 1 0.02 0.02 -0.00 0.14 0.09 0.01 0.05 0.05 0.00

50 1 0.02 -0.02 0.00 -0.14 0.09 0.01 0.04 -0.04 -0.00

51 1 -0.02 -0.02 -0.00 -0.04 -0.04 0.00 -0.09 -0.14 0.01

52 1 0.02 -0.02 0.00 0.05 -0.05 -0.00 -0.09 0.14 0.01

53 1 0.02 0.02 -0.00 -0.04 -0.04 -0.00 -0.09 -0.14 -0.01

54 1 -0.02 0.02 0.00 0.05 -0.05 0.00 -0.09 0.14 -0.01

55 1 -0.02 0.02 0.00 -0.14 0.09 -0.01 0.04 -0.04 0.00

56 1 -0.02 -0.02 -0.00 0.14 0.09 -0.01 0.05 0.05 -0.00

57 1 -0.14 -0.18 0.07 -0.12 -0.17 0.06 -0.13 -0.18 0.07

58 1 0.11 0.09 0.02 0.10 0.08 0.02 0.10 0.08 0.02

59 1 0.09 -0.09 0.26 0.08 -0.08 0.23 0.09 -0.09 0.25

60 1 -0.09 -0.11 0.02 -0.08 -0.09 0.02 -0.09 -0.11 0.03

61 1 0.18 0.14 0.07 0.17 0.12 0.06 0.18 0.13 0.06

62 1 0.09 0.09 -0.26 -0.09 -0.09 0.25 0.08 0.08 -0.23

63 1 0.11 -0.09 -0.02 -0.11 0.09 0.03 0.09 -0.08 -0.02

64 1 -0.14 0.18 -0.07 0.13 -0.18 0.06 -0.12 0.17 -0.06

65 1 0.18 -0.14 -0.07 -0.18 0.13 0.07 0.17 -0.12 -0.06

66 1 -0.09 0.11 -0.02 0.08 -0.10 0.02 -0.08 0.10 -0.02

67 1 -0.18 0.14 -0.07 -0.18 0.13 -0.07 0.17 -0.12 0.06

68 1 0.09 -0.11 -0.02 0.08 -0.10 -0.02 -0.08 0.10 0.02

69 1 -0.09 -0.09 -0.26 -0.09 -0.09 -0.25 0.08 0.08 0.23

70 1 -0.11 0.09 -0.02 -0.11 0.09 -0.03 0.09 -0.08 0.02

71 1 0.14 -0.18 -0.07 0.13 -0.18 -0.06 -0.12 0.17 0.06

72 1 -0.18 -0.14 0.07 0.17 0.12 -0.06 0.18 0.13 -0.06

73 1 0.09 0.11 0.02 -0.08 -0.09 -0.02 -0.09 -0.11 -0.03

74 1 -0.09 0.09 0.26 0.08 -0.08 -0.23 0.09 -0.09 -0.25

75 1 -0.11 -0.09 0.02 0.10 0.08 -0.02 0.10 0.08 -0.02

76 1 0.14 0.18 0.07 -0.12 -0.17 -0.06 -0.13 -0.18 -0.07

77 30 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00

136 137 138

A1 B2 E

Frequencies -- 1103.4882 1107.8969 1172.5500

Red. masses -- 1.1550 1.2405 1.0970

Frc consts -- 0.8287 0.8971 0.8887

IR Inten -- 0.0000 11.1416 0.0333

Atom AN X Y Z X Y Z X Y Z

1 6 0.03 0.01 0.00 0.03 -0.02 -0.00 -0.00 0.00 0.00

2 6 -0.01 -0.01 -0.00 0.00 0.01 0.00 0.00 0.00 0.00

3 7 0.00 -0.03 -0.00 -0.00 -0.02 -0.00 0.00 -0.00 0.00

4 6 0.01 -0.01 -0.00 -0.00 0.01 0.00 -0.00 0.00 0.00

5 6 -0.03 0.01 0.00 -0.03 -0.02 -0.00 0.00 0.00 0.00

6 6 -0.00 -0.00 -0.00 -0.02 0.02 -0.00 0.00 -0.00 -0.00

7 6 -0.01 0.01 0.00 -0.01 0.00 0.00 0.00 0.00 0.00

8 7 -0.03 0.00 0.00 0.02 0.00 -0.00 0.00 -0.00 0.00

9 6 -0.01 -0.01 0.00 -0.01 -0.00 0.00 -0.00 0.00 -0.00

10 6 0.01 0.03 -0.00 0.02 -0.03 -0.00 0.00 -0.00 -0.00

11 6 0.01 -0.03 -0.00 0.02 0.03 -0.00 -0.00 -0.00 0.00

12 6 0.00 -0.00 -0.00 0.02 0.02 -0.00 -0.00 -0.00 -0.00

13 6 0.01 0.01 0.00 0.01 0.00 0.00 -0.00 0.00 0.00

14 6 -0.01 -0.03 -0.00 -0.02 0.03 -0.00 0.00 -0.00 0.00

15 6 -0.01 0.03 -0.00 -0.02 -0.03 -0.00 -0.00 -0.00 -0.00

16 6 0.01 -0.01 0.00 0.01 -0.00 0.00 0.00 0.00 -0.00

17 7 0.03 -0.00 0.00 -0.02 -0.00 -0.00 0.00 -0.00 -0.00

18 6 0.00 0.00 -0.00 0.02 -0.02 -0.00 0.00 -0.00 0.00

19 6 -0.01 0.01 -0.00 0.00 -0.01 0.00 -0.00 0.00 -0.00

20 6 0.03 -0.01 0.00 0.03 0.02 -0.00 0.00 0.00 -0.00

21 6 -0.03 -0.01 0.00 -0.03 0.02 -0.00 -0.00 0.00 -0.00

22 6 0.01 0.01 -0.00 -0.00 -0.01 0.00 0.00 0.00 -0.00

23 7 0.00 0.03 -0.00 -0.00 0.02 -0.00 0.00 -0.00 -0.00

24 6 -0.00 0.00 -0.00 -0.02 -0.02 -0.00 -0.00 -0.00 0.00

25 6 -0.00 -0.00 0.00 0.01 -0.01 -0.00 -0.00 0.00 -0.00

26 6 0.00 0.00 -0.00 -0.01 -0.01 -0.00 0.00 0.00 -0.00

27 6 0.00 0.00 0.00 0.00 0.01 -0.01 -0.02 -0.01 -0.01

28 6 -0.00 -0.00 0.00 0.00 -0.00 0.01 0.01 -0.01 0.03

29 6 0.00 0.00 -0.00 -0.01 -0.00 -0.01 0.01 0.02 -0.01

30 6 0.00 0.00 0.00 0.01 0.01 -0.00 -0.00 -0.00 -0.00

31 6 0.00 -0.00 0.00 -0.00 -0.00 0.01 -0.01 -0.01 0.03

32 6 -0.00 0.00 0.00 -0.00 0.01 -0.01 0.02 -0.01 -0.01

33 6 -0.00 0.00 -0.00 0.01 -0.01 -0.00 -0.00 0.00 -0.00

34 6 0.00 -0.00 0.00 -0.01 -0.01 -0.00 0.00 0.00 -0.00

35 6 -0.00 0.00 0.00 -0.01 0.01 -0.00 0.00 -0.00 -0.00

36 6 -0.00 0.00 -0.00 0.01 -0.00 -0.01 -0.01 0.02 -0.01

37 6 -0.00 0.00 0.00 0.01 0.01 -0.00 0.00 0.00 0.00

38 6 0.00 -0.00 0.00 0.01 -0.01 -0.00 0.00 -0.00 0.00

39 6 0.00 -0.00 -0.00 -0.01 0.00 -0.01 -0.01 0.02 0.01

40 6 -0.00 0.00 0.00 0.00 0.00 0.01 -0.01 -0.01 -0.03

41 6 0.00 -0.00 0.00 0.00 -0.01 -0.01 0.02 -0.01 0.01

42 6 0.00 -0.00 -0.00 -0.01 0.01 -0.00 -0.00 0.00 0.00

43 6 0.00 0.00 -0.00 -0.01 0.01 -0.00 -0.00 0.00 0.00

44 6 -0.00 -0.00 0.00 -0.01 -0.01 -0.00 -0.00 -0.00 0.00

45 6 -0.00 -0.00 -0.00 0.01 0.00 -0.01 0.01 0.02 0.01

46 6 0.00 0.00 0.00 -0.00 0.00 0.01 0.01 -0.01 -0.03

47 6 -0.00 -0.00 0.00 -0.00 -0.01 -0.01 -0.02 -0.01 0.01

48 6 -0.00 -0.00 -0.00 0.01 0.01 -0.00 0.00 0.00 0.00

49 1 0.29 0.20 0.03 0.29 0.17 0.02 0.00 0.00 0.00

50 1 -0.29 0.20 0.03 -0.29 0.17 0.02 -0.00 0.00 0.00

51 1 0.20 0.29 -0.03 -0.17 -0.29 0.02 0.00 0.00 -0.00

52 1 0.20 -0.29 -0.03 -0.17 0.29 0.02 -0.00 0.00 0.00

53 1 -0.20 -0.29 -0.03 0.17 0.29 0.02 0.00 0.00 0.00

54 1 -0.20 0.29 -0.03 0.17 -0.29 0.02 -0.00 0.00 -0.00

55 1 0.29 -0.20 0.03 0.29 -0.17 0.02 -0.00 0.00 -0.00

56 1 -0.29 -0.20 0.03 -0.29 -0.17 0.02 0.00 0.00 -0.00

57 1 0.00 0.01 -0.01 -0.03 -0.06 0.02 0.04 0.07 -0.04

58 1 0.01 0.01 0.01 0.03 0.02 0.01 -0.19 -0.11 -0.11

59 1 -0.00 -0.00 0.00 0.02 -0.02 0.07 0.11 -0.11 0.30

60 1 0.01 0.01 -0.01 -0.02 -0.03 0.01 0.11 0.19 -0.11

61 1 0.01 0.00 0.01 0.06 0.03 0.02 -0.07 -0.04 -0.04

62 1 0.00 -0.00 0.00 -0.02 -0.02 0.07 -0.11 -0.11 0.30

63 1 -0.01 0.01 0.01 -0.03 0.02 0.01 0.19 -0.11 -0.11

64 1 -0.00 0.01 -0.01 0.03 -0.06 0.02 -0.04 0.07 -0.04

65 1 -0.01 0.00 0.01 -0.06 0.03 0.02 0.07 -0.04 -0.04

66 1 -0.01 0.01 -0.01 0.02 -0.03 0.01 -0.11 0.19 -0.11

67 1 0.01 -0.00 0.01 0.06 -0.03 0.02 0.07 -0.04 0.04

68 1 0.01 -0.01 -0.01 -0.02 0.03 0.01 -0.11 0.19 0.11

69 1 -0.00 0.00 0.00 0.02 0.02 0.07 -0.11 -0.11 -0.30

70 1 0.01 -0.01 0.01 0.03 -0.02 0.01 0.19 -0.11 0.11

71 1 0.00 -0.01 -0.01 -0.03 0.06 0.02 -0.04 0.07 0.04

72 1 -0.01 -0.00 0.01 -0.06 -0.03 0.02 -0.07 -0.04 0.04

73 1 -0.01 -0.01 -0.01 0.02 0.03 0.01 0.11 0.19 0.11

74 1 0.00 0.00 0.00 -0.02 0.02 0.07 0.11 -0.11 -0.30

75 1 -0.01 -0.01 0.01 -0.03 -0.02 0.01 -0.19 -0.11 0.11

76 1 -0.00 -0.01 -0.01 0.03 0.06 0.02 0.04 0.07 0.04

77 30 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00

139 140 141

E A2 B2

Frequencies -- 1172.5500 1172.5639 1172.5829

Red. masses -- 1.0970 1.0969 1.0968

Frc consts -- 0.8887 0.8886 0.8885

IR Inten -- 0.0333 0.0000 0.0001

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 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00

25 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

26 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

27 6 0.02 0.01 0.01 -0.02 -0.01 -0.01 -0.02 -0.01 -0.01

28 6 -0.01 0.01 -0.03 0.01 -0.01 0.03 0.01 -0.01 0.03

29 6 -0.01 -0.02 0.01 0.01 0.02 -0.01 0.01 0.02 -0.01

30 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

31 6 -0.01 -0.01 0.03 0.01 0.01 -0.03 -0.01 -0.01 0.03

32 6 0.02 -0.01 -0.01 -0.02 0.01 0.01 0.02 -0.01 -0.01

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 -0.01 0.02 -0.01 0.01 -0.02 0.01 -0.01 0.02 -0.01

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 -0.01 0.02 0.01 -0.01 0.02 0.01 0.01 -0.02 -0.01

40 6 -0.01 -0.01 -0.03 -0.01 -0.01 -0.03 0.01 0.01 0.03

41 6 0.02 -0.01 0.01 0.02 -0.01 0.01 -0.02 0.01 -0.01

42 6 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

43 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

44 6 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

45 6 -0.01 -0.02 -0.01 -0.01 -0.02 -0.01 -0.01 -0.02 -0.01

46 6 -0.01 0.01 0.03 -0.01 0.01 0.03 -0.01 0.01 0.03

47 6 0.02 0.01 -0.01 0.02 0.01 -0.01 0.02 0.01 -0.01

48 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

49 1 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

50 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

51 1 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

52 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

53 1 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

54 1 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

55 1 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

56 1 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

57 1 -0.04 -0.07 0.04 0.04 0.07 -0.04 0.04 0.07 -0.04

58 1 0.19 0.11 0.11 -0.19 -0.11 -0.11 -0.19 -0.11 -0.11

59 1 -0.11 0.11 -0.30 0.11 -0.11 0.30 0.11 -0.11 0.30

60 1 -0.11 -0.19 0.11 0.11 0.19 -0.11 0.11 0.19 -0.11

61 1 0.07 0.04 0.04 -0.07 -0.04 -0.04 -0.07 -0.04 -0.04

62 1 -0.11 -0.11 0.30 0.11 0.11 -0.30 -0.11 -0.11 0.30

63 1 0.19 -0.11 -0.11 -0.19 0.11 0.11 0.19 -0.11 -0.11

64 1 -0.04 0.07 -0.04 0.04 -0.07 0.04 -0.04 0.07 -0.04

65 1 0.07 -0.04 -0.04 -0.07 0.04 0.04 0.07 -0.04 -0.04

66 1 -0.11 0.19 -0.11 0.11 -0.19 0.11 -0.11 0.19 -0.11

67 1 0.07 -0.04 0.04 0.07 -0.04 0.04 -0.07 0.04 -0.04

68 1 -0.11 0.19 0.11 -0.11 0.19 0.11 0.11 -0.19 -0.11

69 1 -0.11 -0.11 -0.30 -0.11 -0.11 -0.30 0.11 0.11 0.30

70 1 0.19 -0.11 0.11 0.19 -0.11 0.11 -0.19 0.11 -0.11

71 1 -0.04 0.07 0.04 -0.04 0.07 0.04 0.04 -0.07 -0.04

72 1 0.07 0.04 -0.04 0.07 0.04 -0.04 0.07 0.04 -0.04

73 1 -0.11 -0.19 -0.11 -0.11 -0.19 -0.11 -0.11 -0.19 -0.11

74 1 -0.11 0.11 0.30 -0.11 0.11 0.30 -0.11 0.11 0.30

75 1 0.19 0.11 -0.11 0.19 0.11 -0.11 0.19 0.11 -0.11

76 1 -0.04 -0.07 -0.04 -0.04 -0.07 -0.04 -0.04 -0.07 -0.04

77 30 0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00

142 143 144

B1 E E

Frequencies -- 1196.2415 1196.6130 1196.6130

Red. masses -- 1.1912 1.1342 1.1342

Frc consts -- 1.0043 0.9568 0.9568

IR Inten -- 0.0000 3.5491 3.5491

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 0.02 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 0.01 -0.02 -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 -0.02 0.01 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 0.02 0.01 -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 -0.02 -0.01 -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 0.02 -0.01 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 -0.01 0.02 -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 -0.01 -0.02 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 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00

25 6 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

26 6 -0.01 -0.02 0.01 0.01 0.02 -0.01 -0.01 -0.02 0.01

27 6 0.02 0.01 0.01 -0.02 -0.01 -0.01 0.02 0.01 0.01

28 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

29 6 0.01 0.02 -0.01 -0.01 -0.02 0.01 0.01 0.02 -0.01

30 6 -0.02 -0.01 -0.01 0.02 0.01 0.01 -0.02 -0.01 -0.01

31 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00

32 6 0.02 -0.01 -0.01 -0.02 0.01 0.01 -0.02 0.01 0.01

33 6 -0.01 0.02 -0.01 0.01 -0.02 0.01 0.01 -0.02 0.01

34 6 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00

35 6 -0.02 0.01 0.01 0.02 -0.01 -0.01 0.02 -0.01 -0.01

36 6 0.01 -0.02 0.01 -0.01 0.02 -0.01 -0.01 0.02 -0.01

37 6 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00

38 6 0.02 -0.01 0.01 0.02 -0.01 0.01 0.02 -0.01 0.01

39 6 -0.01 0.02 0.01 -0.01 0.02 0.01 -0.01 0.02 0.01

40 6 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00

41 6 -0.02 0.01 -0.01 -0.02 0.01 -0.01 -0.02 0.01 -0.01

42 6 0.01 -0.02 -0.01 0.01 -0.02 -0.01 0.01 -0.02 -0.01

43 6 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00

44 6 0.02 0.01 -0.01 0.02 0.01 -0.01 -0.02 -0.01 0.01

45 6 -0.01 -0.02 -0.01 -0.01 -0.02 -0.01 0.01 0.02 0.01

46 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00

47 6 -0.02 -0.01 0.01 -0.02 -0.01 0.01 0.02 0.01 -0.01

48 6 0.01 0.02 0.01 0.01 0.02 0.01 -0.01 -0.02 -0.01

49 1 -0.06 -0.05 -0.01 0.01 0.00 0.00 -0.01 -0.00 -0.00

50 1 -0.06 0.05 0.01 0.01 -0.00 -0.00 0.01 -0.00 -0.00

51 1 -0.05 -0.06 0.01 0.00 0.01 -0.00 -0.00 -0.01 0.00

52 1 0.05 -0.06 -0.01 0.00 -0.01 -0.00 0.00 -0.01 -0.00

53 1 0.05 0.06 0.01 0.00 0.01 0.00 -0.00 -0.01 -0.00

54 1 -0.05 0.06 -0.01 0.00 -0.01 0.00 0.00 -0.01 0.00

55 1 0.06 -0.05 0.01 0.01 -0.00 0.00 0.01 -0.00 0.00

56 1 0.06 0.05 -0.01 0.01 0.00 -0.00 -0.01 -0.00 0.00

57 1 -0.11 -0.19 0.11 0.12 0.20 -0.12 -0.11 -0.19 0.11

58 1 0.19 0.11 0.10 -0.19 -0.11 -0.11 0.18 0.11 0.10

59 1 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00

60 1 0.11 0.19 -0.10 -0.11 -0.19 0.11 0.11 0.18 -0.10

61 1 -0.19 -0.11 -0.11 0.20 0.12 0.12 -0.19 -0.11 -0.11

62 1 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00

63 1 0.19 -0.11 -0.10 -0.18 0.11 0.10 -0.19 0.11 0.11

64 1 -0.11 0.19 -0.11 0.11 -0.19 0.11 0.12 -0.20 0.12

65 1 -0.19 0.11 0.11 0.19 -0.11 -0.11 0.20 -0.12 -0.12

66 1 0.11 -0.19 0.10 -0.11 0.18 -0.10 -0.11 0.19 -0.11

67 1 0.19 -0.11 0.11 0.19 -0.11 0.11 0.20 -0.12 0.12

68 1 -0.11 0.19 0.10 -0.11 0.18 0.10 -0.11 0.19 0.11

69 1 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00

70 1 -0.19 0.11 -0.10 -0.18 0.11 -0.10 -0.19 0.11 -0.11

71 1 0.11 -0.19 -0.11 0.11 -0.19 -0.11 0.12 -0.20 -0.12

72 1 0.19 0.11 -0.11 0.20 0.12 -0.12 -0.19 -0.11 0.11

73 1 -0.11 -0.19 -0.10 -0.11 -0.19 -0.11 0.11 0.18 0.10

74 1 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

75 1 -0.19 -0.11 0.10 -0.19 -0.11 0.11 0.18 0.11 -0.10

76 1 0.11 0.19 0.11 0.12 0.20 0.12 -0.11 -0.19 -0.11

77 30 0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00

145 146 147

A1 B1 E

Frequencies -- 1196.7026 1200.2297 1233.4215

Red. masses -- 1.1334 1.8438 3.1936

Frc consts -- 0.9563 1.5649 2.8625

IR Inten -- 0.0000 0.0000 116.2699

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.00 0.00 0.01 0.00 0.00 -0.02 -0.00 -0.00

2 6 0.00 0.00 0.00 0.03 0.09 0.01 0.08 -0.10 -0.01

3 7 0.00 0.00 -0.00 0.02 0.00 0.00 -0.10 -0.01 0.00

4 6 -0.00 0.00 0.00 0.03 -0.09 -0.01 -0.01 0.15 0.01

5 6 -0.00 -0.00 0.00 0.01 -0.00 -0.00 -0.03 -0.03 -0.00

6 6 -0.00 -0.00 -0.00 0.01 0.01 -0.00 -0.02 -0.04 -0.00

7 6 0.00 -0.00 -0.00 -0.09 0.03 0.01 0.11 -0.06 -0.01

8 7 0.00 0.00 0.00 0.00 0.02 -0.00 -0.01 -0.06 -0.00

9 6 0.00 0.00 -0.00 0.09 0.03 -0.01 -0.04 0.10 0.00

10 6 -0.00 0.00 -0.00 0.00 0.01 -0.00 -0.02 -0.00 0.00

11 6 -0.00 -0.00 -0.00 -0.00 0.01 0.00 -0.03 -0.03 0.00

12 6 0.00 -0.00 -0.00 0.01 -0.01 0.00 0.03 0.04 0.00

13 6 -0.00 -0.00 -0.00 -0.09 -0.03 -0.01 -0.04 0.10 -0.00

14 6 0.00 -0.00 -0.00 -0.00 -0.01 -0.00 -0.02 -0.00 -0.00

15 6 0.00 0.00 -0.00 0.00 -0.01 0.00 -0.03 -0.03 -0.00

16 6 -0.00 0.00 -0.00 0.09 -0.03 0.01 0.11 -0.06 0.01

17 7 -0.00 -0.00 0.00 -0.00 -0.02 -0.00 -0.01 -0.06 0.00

18 6 0.00 0.00 -0.00 -0.01 -0.01 -0.00 -0.02 -0.04 0.00

19 6 0.00 -0.00 0.00 -0.03 0.09 -0.01 -0.01 0.15 -0.01

20 6 0.00 0.00 0.00 -0.01 0.00 -0.00 -0.03 -0.03 0.00

21 6 -0.00 0.00 0.00 -0.01 -0.00 0.00 -0.02 -0.00 0.00

22 6 -0.00 -0.00 0.00 -0.03 -0.09 0.01 0.08 -0.10 0.01

23 7 0.00 -0.00 -0.00 -0.02 -0.00 0.00 -0.10 -0.01 -0.00

24 6 -0.00 0.00 -0.00 -0.01 0.01 0.00 0.03 0.04 -0.00

25 6 -0.00 -0.00 0.00 -0.02 -0.02 0.00 0.04 0.04 0.01

26 6 0.01 0.02 -0.01 0.00 0.01 -0.01 0.01 0.01 -0.00

27 6 -0.02 -0.01 -0.01 -0.00 0.00 -0.01 -0.01 -0.01 0.01

28 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

29 6 -0.01 -0.02 0.01 0.00 -0.00 0.01 -0.01 -0.00 -0.01

30 6 0.02 0.01 0.01 0.01 0.00 0.01 0.00 0.00 -0.00

31 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00

32 6 0.02 -0.01 -0.01 -0.00 -0.00 0.01 -0.01 0.01 -0.00

33 6 -0.01 0.02 -0.01 0.00 -0.01 0.01 0.00 -0.01 0.01

34 6 0.00 -0.00 0.00 -0.02 0.02 -0.00 0.01 -0.02 -0.03

35 6 -0.02 0.01 0.01 0.01 -0.00 -0.01 -0.00 0.00 0.01

36 6 0.01 -0.02 0.01 0.00 0.00 -0.01 -0.00 -0.00 0.01

37 6 -0.00 0.00 -0.00 0.02 -0.02 -0.00 0.01 -0.02 0.03

38 6 0.02 -0.01 0.01 -0.01 0.00 -0.01 -0.00 0.00 -0.01

39 6 -0.01 0.02 0.01 -0.00 -0.00 -0.01 -0.00 -0.00 -0.01

40 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00 0.00

41 6 -0.02 0.01 -0.01 0.00 0.00 0.01 -0.01 0.01 0.00

42 6 0.01 -0.02 -0.01 -0.00 0.01 0.01 0.00 -0.01 -0.01

43 6 0.00 0.00 0.00 0.02 0.02 0.00 0.04 0.04 -0.01

44 6 -0.02 -0.01 0.01 -0.01 -0.00 0.01 0.00 0.00 0.00

45 6 0.01 0.02 0.01 -0.00 0.00 0.01 -0.01 -0.00 0.01

46 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 -0.00

47 6 0.02 0.01 -0.01 0.00 -0.00 -0.01 -0.01 -0.01 -0.01

48 6 -0.01 -0.02 -0.01 -0.00 -0.01 -0.01 0.01 0.01 0.00

49 1 0.01 0.00 0.00 -0.24 -0.19 -0.02 0.34 0.26 0.03

50 1 -0.01 0.00 0.00 -0.24 0.19 0.02 0.17 -0.19 -0.02

51 1 0.00 0.01 -0.00 -0.19 -0.24 0.02 0.20 0.29 -0.02

52 1 0.00 -0.01 -0.00 0.19 -0.24 -0.02 -0.07 0.01 0.00

53 1 -0.00 -0.01 -0.00 0.19 0.24 0.02 0.20 0.29 0.02

54 1 -0.00 0.01 -0.00 -0.19 0.24 -0.02 -0.07 0.01 -0.00

55 1 0.01 -0.00 0.00 0.24 -0.19 0.02 0.17 -0.19 0.02

56 1 -0.01 -0.00 0.00 0.24 0.19 -0.02 0.34 0.26 -0.03

57 1 0.11 0.20 -0.11 0.06 0.11 -0.06 -0.03 -0.05 0.04

58 1 -0.19 -0.11 -0.11 -0.05 -0.03 -0.04 -0.03 -0.03 -0.00

59 1 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00

60 1 -0.11 -0.19 0.11 -0.03 -0.05 0.04 -0.03 -0.03 0.00

61 1 0.20 0.11 0.11 0.11 0.06 0.06 -0.08 -0.04 -0.05

62 1 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.01 -0.01 0.02

63 1 0.19 -0.11 -0.11 -0.05 0.03 0.04 -0.00 0.00 -0.00

64 1 -0.11 0.20 -0.11 0.06 -0.11 0.06 0.00 -0.03 0.01

65 1 -0.20 0.11 0.11 0.11 -0.06 -0.06 -0.07 0.02 0.03

66 1 0.11 -0.19 0.11 -0.03 0.05 -0.04 -0.01 0.01 -0.00

67 1 0.20 -0.11 0.11 -0.11 0.06 -0.06 -0.07 0.02 -0.03

68 1 -0.11 0.19 0.11 0.03 -0.05 -0.04 -0.01 0.01 0.00

69 1 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.01 -0.01 -0.02

70 1 -0.19 0.11 -0.11 0.05 -0.03 0.04 -0.00 0.00 0.00

71 1 0.11 -0.20 -0.11 -0.06 0.11 0.06 0.00 -0.03 -0.01

72 1 -0.20 -0.11 0.11 -0.11 -0.06 0.06 -0.08 -0.04 0.05

73 1 0.11 0.19 0.11 0.03 0.05 0.04 -0.03 -0.03 -0.00

74 1 0.00 0.00 0.00 0.00 0.00 -0.00 0.00 0.00 0.00

75 1 0.19 0.11 -0.11 0.05 0.03 -0.04 -0.03 -0.03 0.00

76 1 -0.11 -0.20 -0.11 -0.06 -0.11 -0.06 -0.03 -0.05 -0.04

77 30 -0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 -0.00

148 149 150

E E E

Frequencies -- 1233.4215 1260.1301 1260.1301

Red. masses -- 3.1936 5.4144 5.4144

Frc consts -- 2.8625 5.0656 5.0656

IR Inten -- 116.2697 2.2736 2.2736

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 0.03 0.00 0.04 0.00 0.00 0.01 -0.05 -0.01

2 6 -0.06 -0.11 -0.01 0.05 -0.09 -0.01 -0.11 0.03 0.00

3 7 -0.06 0.01 -0.00 -0.01 0.14 0.01 0.13 0.02 0.00

4 6 0.10 0.04 0.00 -0.03 -0.08 -0.01 -0.12 -0.04 -0.01

5 6 -0.00 0.02 0.00 -0.05 -0.01 0.00 -0.00 0.05 0.01

6 6 0.04 -0.03 -0.00 -0.10 -0.02 0.00 -0.05 -0.11 -0.00

7 6 -0.10 -0.08 0.01 -0.03 -0.11 0.00 -0.09 -0.05 0.01

8 7 -0.01 0.10 -0.00 -0.02 0.13 0.00 0.14 0.01 -0.01

9 6 0.15 0.01 -0.01 0.04 -0.12 -0.01 -0.08 0.03 0.01

10 6 -0.03 0.03 0.00 -0.05 -0.00 0.01 -0.01 0.05 -0.00

11 6 -0.00 0.02 0.00 0.05 0.01 -0.01 0.00 -0.04 -0.00

12 6 -0.04 0.02 -0.00 0.11 -0.05 0.00 -0.02 0.10 0.00

13 6 0.15 0.01 0.01 0.04 -0.12 0.01 -0.08 0.03 -0.01

14 6 -0.03 0.03 -0.00 -0.05 -0.00 -0.01 -0.01 0.05 0.00

15 6 -0.00 0.02 -0.00 0.05 0.01 0.01 0.00 -0.04 0.00

16 6 -0.10 -0.08 -0.01 -0.03 -0.11 -0.00 -0.09 -0.05 -0.01

17 7 -0.01 0.10 0.00 -0.02 0.13 -0.00 0.14 0.01 0.01

18 6 0.04 -0.03 0.00 -0.10 -0.02 -0.00 -0.05 -0.11 0.00

19 6 0.10 0.04 -0.00 -0.03 -0.08 0.01 -0.12 -0.04 0.01

20 6 -0.00 0.02 -0.00 -0.05 -0.01 -0.00 -0.00 0.05 -0.01

21 6 -0.03 0.03 -0.00 0.04 0.00 -0.00 0.01 -0.05 0.01

22 6 -0.06 -0.11 0.01 0.05 -0.09 0.01 -0.11 0.03 -0.00

23 7 -0.06 0.01 0.00 -0.01 0.14 -0.01 0.13 0.02 -0.00

24 6 -0.04 0.02 0.00 0.11 -0.05 -0.00 -0.02 0.10 -0.00

25 6 -0.02 -0.01 0.03 0.11 0.11 -0.02 0.13 0.13 0.02

26 6 0.00 0.00 -0.01 0.01 0.02 0.00 0.02 0.03 -0.01

27 6 -0.00 0.00 -0.01 -0.01 -0.03 0.03 -0.02 -0.05 0.03

28 6 0.00 -0.00 0.00 0.00 0.01 -0.00 0.01 0.01 0.00

29 6 0.01 0.01 0.00 -0.04 -0.02 -0.03 -0.04 -0.01 -0.04

30 6 -0.01 -0.00 -0.01 0.03 0.02 0.01 0.02 0.02 0.00

31 6 0.00 -0.00 0.00 -0.01 0.01 -0.00 0.01 -0.00 -0.00

32 6 -0.00 0.01 -0.01 0.01 -0.04 0.04 -0.02 0.04 -0.03

33 6 0.00 -0.00 -0.00 -0.02 0.02 -0.00 0.02 -0.03 0.01

34 6 0.04 -0.04 0.01 -0.13 0.13 -0.02 0.11 -0.11 -0.02

35 6 0.01 -0.01 -0.00 -0.03 0.02 0.01 0.02 -0.01 0.00

36 6 -0.01 0.01 0.01 0.05 -0.02 -0.03 -0.03 0.01 0.03

37 6 0.04 -0.04 -0.01 -0.13 0.13 0.02 0.11 -0.11 0.02

38 6 0.01 -0.01 0.00 -0.03 0.02 -0.01 0.02 -0.01 -0.00

39 6 -0.01 0.01 -0.01 0.05 -0.02 0.03 -0.03 0.01 -0.03

40 6 0.00 -0.00 -0.00 -0.01 0.01 0.00 0.01 -0.00 0.00

41 6 -0.00 0.01 0.01 0.01 -0.04 -0.04 -0.02 0.04 0.03

42 6 0.00 -0.00 0.00 -0.02 0.02 0.00 0.02 -0.03 -0.01

43 6 -0.02 -0.01 -0.03 0.11 0.11 0.02 0.13 0.13 -0.02

44 6 -0.01 -0.00 0.01 0.03 0.02 -0.01 0.02 0.02 -0.00

45 6 0.01 0.01 -0.00 -0.04 -0.02 0.03 -0.04 -0.01 0.04

46 6 0.00 -0.00 -0.00 0.00 0.01 0.00 0.01 0.01 -0.00

47 6 -0.00 0.00 0.01 -0.01 -0.03 -0.03 -0.02 -0.05 -0.03

48 6 0.00 0.00 0.01 0.01 0.02 -0.00 0.02 0.03 0.01

49 1 0.01 0.07 0.00 -0.03 -0.06 -0.01 0.11 0.03 0.00

50 1 0.29 -0.20 -0.02 0.01 -0.05 -0.01 0.12 -0.04 -0.00

51 1 -0.19 -0.17 0.02 0.04 0.12 -0.00 -0.05 -0.01 0.01

52 1 0.26 -0.34 -0.03 -0.03 0.11 0.00 -0.06 0.03 0.01

53 1 -0.19 -0.17 -0.02 0.04 0.12 0.00 -0.05 -0.01 -0.01

54 1 0.26 -0.34 0.03 -0.03 0.11 -0.00 -0.06 0.03 -0.01

55 1 0.29 -0.20 0.02 0.01 -0.05 0.01 0.12 -0.04 0.00

56 1 0.01 0.07 -0.00 -0.03 -0.06 0.01 0.11 0.03 -0.00

57 1 0.02 0.07 -0.03 -0.08 -0.17 0.10 -0.08 -0.15 0.09

58 1 0.01 0.01 0.00 -0.12 -0.10 -0.03 -0.12 -0.10 -0.02

59 1 -0.01 0.01 -0.02 0.01 -0.00 0.02 0.00 0.01 -0.01

60 1 0.00 0.00 0.00 -0.08 -0.09 0.01 -0.12 -0.14 0.03

61 1 -0.03 -0.00 -0.01 -0.11 -0.06 -0.07 -0.20 -0.09 -0.12

62 1 0.00 -0.00 -0.00 -0.01 0.00 0.01 -0.00 -0.01 0.02

63 1 -0.03 0.03 0.00 0.14 -0.12 -0.03 -0.09 0.08 0.01

64 1 -0.04 0.08 -0.05 0.09 -0.20 0.12 -0.06 0.11 -0.07

65 1 -0.05 0.03 0.04 0.15 -0.08 -0.09 -0.17 0.08 0.10

66 1 -0.03 0.03 -0.00 0.10 -0.12 0.02 -0.10 0.12 -0.03

67 1 -0.05 0.03 -0.04 0.15 -0.08 0.09 -0.17 0.08 -0.10

68 1 -0.03 0.03 0.00 0.10 -0.12 -0.02 -0.10 0.12 0.03

69 1 0.00 -0.00 0.00 -0.01 0.00 -0.01 -0.00 -0.01 -0.02

70 1 -0.03 0.03 -0.00 0.14 -0.12 0.03 -0.09 0.08 -0.01

71 1 -0.04 0.08 0.05 0.09 -0.20 -0.12 -0.06 0.11 0.07

72 1 -0.03 -0.00 0.01 -0.11 -0.06 0.07 -0.20 -0.09 0.12

73 1 0.00 0.00 -0.00 -0.08 -0.09 -0.01 -0.12 -0.14 -0.03

74 1 -0.01 0.01 0.02 0.01 -0.00 -0.02 0.00 0.01 0.01

75 1 0.01 0.01 -0.00 -0.12 -0.10 0.03 -0.12 -0.10 0.02

76 1 0.02 0.07 0.03 -0.08 -0.17 -0.10 -0.08 -0.15 -0.09

77 30 0.00 -0.00 -0.00 0.00 -0.01 -0.00 -0.01 -0.00 0.00

151 152 153

A1 A2 B1

Frequencies -- 1263.0982 1271.7966 1297.1002

Red. masses -- 4.5224 6.0348 5.5975

Frc consts -- 4.2510 5.7510 5.5487

IR Inten -- 0.0000 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.02 -0.00 0.00 0.03 -0.03 -0.00 -0.00 -0.02 -0.00

2 6 0.06 -0.04 -0.01 -0.11 0.13 0.01 -0.06 0.06 0.01

3 7 -0.00 0.07 0.00 0.19 0.00 0.00 0.15 -0.00 0.00

4 6 -0.06 -0.04 -0.01 -0.11 -0.13 -0.01 -0.06 -0.06 -0.01

5 6 -0.02 -0.00 0.00 0.03 0.03 0.00 -0.00 0.02 0.00

6 6 -0.09 -0.09 0.00 -0.04 0.04 0.01 -0.11 -0.11 0.00

7 6 -0.04 -0.06 0.01 0.13 0.11 -0.01 -0.06 -0.06 0.01

8 7 0.07 0.00 -0.00 0.00 -0.19 -0.00 -0.00 0.15 -0.00

9 6 -0.04 0.06 0.01 -0.13 0.11 0.01 0.06 -0.06 -0.01

10 6 -0.00 0.02 -0.00 0.03 -0.03 -0.00 -0.02 -0.00 0.00

11 6 -0.00 -0.02 -0.00 -0.03 -0.03 0.00 0.02 -0.00 -0.00

12 6 0.09 -0.09 0.00 -0.04 -0.04 -0.01 -0.11 0.11 -0.00

13 6 0.04 -0.06 0.01 0.13 -0.11 0.01 -0.06 0.06 -0.01

14 6 0.00 -0.02 -0.00 -0.03 0.03 -0.00 0.02 0.00 0.00

15 6 0.00 0.02 -0.00 0.03 0.03 0.00 -0.02 0.00 -0.00

16 6 0.04 0.06 0.01 -0.13 -0.11 -0.01 0.06 0.06 0.01

17 7 -0.07 -0.00 -0.00 -0.00 0.19 -0.00 0.00 -0.15 -0.00

18 6 0.09 0.09 -0.00 0.04 -0.04 0.01 0.11 0.11 0.00

19 6 0.06 0.04 -0.01 0.11 0.13 -0.01 0.06 0.06 -0.01

20 6 0.02 0.00 0.00 -0.03 -0.03 0.00 0.00 -0.02 0.00

21 6 -0.02 0.00 0.00 -0.03 0.03 -0.00 0.00 0.02 -0.00

22 6 -0.06 0.04 -0.01 0.11 -0.13 0.01 0.06 -0.06 0.01

23 7 -0.00 -0.07 0.00 -0.19 -0.00 -0.00 -0.15 0.00 0.00

24 6 -0.09 0.09 0.00 0.04 0.04 -0.01 0.11 -0.11 -0.00

25 6 0.14 0.14 -0.00 -0.00 0.00 -0.06 0.12 0.12 -0.00

26 6 0.02 0.03 -0.01 -0.01 -0.02 0.02 0.02 0.03 -0.01

27 6 -0.02 -0.04 0.04 0.02 0.01 0.01 -0.01 -0.04 0.04

28 6 0.01 0.01 -0.00 -0.01 0.01 -0.02 0.00 0.00 -0.00

29 6 -0.04 -0.02 -0.04 -0.01 -0.02 0.01 -0.04 -0.01 -0.04

30 6 0.03 0.02 0.01 0.02 0.01 0.02 0.03 0.02 0.01

31 6 -0.01 0.01 -0.00 -0.01 -0.01 0.02 0.00 -0.00 0.00

32 6 0.02 -0.04 0.04 0.02 -0.01 -0.01 -0.01 0.04 -0.04

33 6 -0.02 0.03 -0.01 -0.01 0.02 -0.02 0.02 -0.03 0.01

34 6 -0.14 0.14 -0.00 -0.00 -0.00 0.06 0.12 -0.12 0.00

35 6 -0.03 0.02 0.01 0.02 -0.01 -0.02 0.03 -0.02 -0.01

36 6 0.04 -0.02 -0.04 -0.01 0.02 -0.01 -0.04 0.01 0.04

37 6 0.14 -0.14 -0.00 0.00 0.00 0.06 -0.12 0.12 0.00

38 6 0.03 -0.02 0.01 -0.02 0.01 -0.02 -0.03 0.02 -0.01

39 6 -0.04 0.02 -0.04 0.01 -0.02 -0.01 0.04 -0.01 0.04

40 6 0.01 -0.01 -0.00 0.01 0.01 0.02 -0.00 0.00 0.00

41 6 -0.02 0.04 0.04 -0.02 0.01 -0.01 0.01 -0.04 -0.04

42 6 0.02 -0.03 -0.01 0.01 -0.02 -0.02 -0.02 0.03 0.01

43 6 -0.14 -0.14 0.00 0.00 -0.00 -0.06 -0.12 -0.12 -0.00

44 6 -0.03 -0.02 0.01 -0.02 -0.01 0.02 -0.03 -0.02 0.01

45 6 0.04 0.02 -0.04 0.01 0.02 0.01 0.04 0.01 -0.04

46 6 -0.01 -0.01 0.00 0.01 -0.01 -0.02 -0.00 -0.00 -0.00

47 6 0.02 0.04 0.04 -0.02 -0.01 0.01 0.01 0.04 0.04

48 6 -0.02 -0.03 -0.01 0.01 0.02 0.02 -0.02 -0.03 -0.01

49 1 0.06 0.03 0.00 -0.16 -0.18 -0.02 0.01 -0.02 -0.00

50 1 -0.06 0.03 0.00 -0.16 0.18 0.02 0.01 0.02 0.00

51 1 0.03 0.06 -0.00 0.18 0.16 -0.02 -0.02 0.01 0.00

52 1 0.03 -0.06 -0.00 -0.18 0.16 0.02 0.02 0.01 -0.00

53 1 -0.03 -0.06 -0.00 -0.18 -0.16 -0.02 0.02 -0.01 0.00

54 1 -0.03 0.06 -0.00 0.18 -0.16 0.02 -0.02 -0.01 -0.00

55 1 0.06 -0.03 0.00 0.16 -0.18 0.02 -0.01 -0.02 0.00

56 1 -0.06 -0.03 0.00 0.16 0.18 -0.02 -0.01 0.02 -0.00

57 1 -0.08 -0.18 0.11 -0.03 -0.08 0.04 -0.09 -0.17 0.10

58 1 -0.13 -0.11 -0.02 -0.04 -0.03 -0.02 -0.13 -0.11 -0.02

59 1 0.00 0.00 -0.00 0.01 -0.01 0.03 0.00 0.00 0.00

60 1 -0.11 -0.13 0.02 0.03 0.04 -0.02 -0.11 -0.13 0.02

61 1 -0.18 -0.08 -0.11 0.08 0.03 0.04 -0.17 -0.09 -0.10

62 1 -0.00 0.00 -0.00 0.01 0.01 -0.03 0.00 -0.00 -0.00

63 1 0.13 -0.11 -0.02 -0.04 0.03 0.02 -0.13 0.11 0.02

64 1 0.08 -0.18 0.11 -0.03 0.08 -0.04 -0.09 0.17 -0.10

65 1 0.18 -0.08 -0.11 0.08 -0.03 -0.04 -0.17 0.09 0.10

66 1 0.11 -0.13 0.02 0.03 -0.04 0.02 -0.11 0.13 -0.02

67 1 -0.18 0.08 -0.11 -0.08 0.03 -0.04 0.17 -0.09 0.10

68 1 -0.11 0.13 0.02 -0.03 0.04 0.02 0.11 -0.13 -0.02

69 1 0.00 -0.00 0.00 -0.01 -0.01 -0.03 -0.00 0.00 -0.00

70 1 -0.13 0.11 -0.02 0.04 -0.03 0.02 0.13 -0.11 0.02

71 1 -0.08 0.18 0.11 0.03 -0.08 -0.04 0.09 -0.17 -0.10

72 1 0.18 0.08 -0.11 -0.08 -0.03 0.04 0.17 0.09 -0.10

73 1 0.11 0.13 0.02 -0.03 -0.04 -0.02 0.11 0.13 0.02

74 1 -0.00 -0.00 -0.00 -0.01 0.01 0.03 -0.00 -0.00 0.00

75 1 0.13 0.11 -0.02 0.04 0.03 -0.02 0.13 0.11 -0.02

76 1 0.08 0.18 0.11 0.03 0.08 0.04 0.09 0.17 0.10

77 30 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00

154 155 156

B2 E E

Frequencies -- 1304.8978 1312.5688 1312.5688

Red. masses -- 5.9878 4.5417 4.5417

Frc consts -- 6.0072 4.6101 4.6101

IR Inten -- 1.5286 0.1369 0.1369

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 -0.03 -0.00 -0.00 -0.03 -0.00 -0.01 0.00 -0.00

2 6 -0.05 0.12 0.01 -0.03 0.00 -0.00 0.04 0.01 0.00

3 7 -0.00 -0.13 -0.01 -0.01 -0.00 0.00 0.00 -0.01 0.00

4 6 0.05 0.12 0.01 -0.04 0.00 0.00 -0.02 0.01 0.00

5 6 0.03 -0.03 -0.00 -0.00 0.02 0.00 0.01 -0.01 -0.00

6 6 0.01 -0.01 -0.02 0.05 0.01 -0.02 -0.03 -0.06 -0.01

7 6 -0.12 -0.05 0.01 -0.01 0.04 0.00 0.00 0.03 0.00

8 7 0.13 -0.00 -0.01 0.01 0.00 0.00 -0.00 0.01 -0.00

9 6 -0.12 0.05 0.01 -0.01 -0.02 0.00 0.00 0.04 -0.00

10 6 0.03 0.03 -0.00 0.01 0.01 -0.00 0.02 0.00 -0.00

11 6 0.03 -0.03 -0.00 -0.00 -0.01 -0.00 -0.03 0.00 0.00

12 6 -0.01 -0.01 -0.02 0.06 -0.03 0.01 0.01 -0.05 -0.02

13 6 0.12 -0.05 0.01 -0.01 -0.02 -0.00 0.00 0.04 0.00

14 6 -0.03 -0.03 -0.00 0.01 0.01 0.00 0.02 0.00 0.00

15 6 -0.03 0.03 -0.00 -0.00 -0.01 0.00 -0.03 0.00 -0.00

16 6 0.12 0.05 0.01 -0.01 0.04 -0.00 0.00 0.03 -0.00

17 7 -0.13 0.00 -0.01 0.01 0.00 -0.00 -0.00 0.01 0.00

18 6 -0.01 0.01 -0.02 0.05 0.01 0.02 -0.03 -0.06 0.01

19 6 -0.05 -0.12 0.01 -0.04 0.00 -0.00 -0.02 0.01 -0.00

20 6 -0.03 0.03 -0.00 -0.00 0.02 -0.00 0.01 -0.01 0.00

21 6 0.03 0.03 -0.00 -0.00 -0.03 0.00 -0.01 0.00 0.00

22 6 0.05 -0.12 0.01 -0.03 0.00 0.00 0.04 0.01 -0.00

23 7 0.00 0.13 -0.01 -0.01 -0.00 -0.00 0.00 -0.01 -0.00

24 6 0.01 0.01 -0.02 0.06 -0.03 -0.01 0.01 -0.05 0.02

25 6 0.04 -0.04 0.15 0.05 -0.09 0.18 0.08 -0.01 0.12

26 6 0.02 0.05 -0.05 0.03 0.07 -0.06 0.03 0.06 -0.05

27 6 -0.06 -0.03 -0.04 -0.08 -0.04 -0.07 -0.06 -0.04 -0.03

28 6 0.02 -0.02 0.06 0.03 -0.03 0.08 0.02 -0.02 0.06

29 6 0.03 0.06 -0.04 0.05 0.09 -0.05 0.02 0.06 -0.05

30 6 -0.05 -0.02 -0.05 -0.08 -0.03 -0.06 -0.04 -0.01 -0.04

31 6 -0.02 -0.02 0.06 0.02 0.02 -0.06 -0.03 -0.03 0.08

32 6 0.06 -0.03 -0.04 -0.06 0.02 0.05 0.09 -0.05 -0.05

33 6 -0.02 0.05 -0.05 0.01 -0.04 0.04 -0.03 0.08 -0.06

34 6 -0.04 -0.04 0.15 0.01 0.08 -0.12 -0.09 -0.05 0.18

35 6 0.05 -0.02 -0.05 -0.06 0.03 0.05 0.07 -0.03 -0.06

36 6 -0.03 0.06 -0.04 0.04 -0.06 0.03 -0.04 0.08 -0.07

37 6 0.04 0.04 0.15 0.01 0.08 0.12 -0.09 -0.05 -0.18

38 6 -0.05 0.02 -0.05 -0.06 0.03 -0.05 0.07 -0.03 0.06

39 6 0.03 -0.06 -0.04 0.04 -0.06 -0.03 -0.04 0.08 0.07

40 6 0.02 0.02 0.06 0.02 0.02 0.06 -0.03 -0.03 -0.08

41 6 -0.06 0.03 -0.04 -0.06 0.02 -0.05 0.09 -0.05 0.05

42 6 0.02 -0.05 -0.05 0.01 -0.04 -0.04 -0.03 0.08 0.06

43 6 -0.04 0.04 0.15 0.05 -0.09 -0.18 0.08 -0.01 -0.12

44 6 0.05 0.02 -0.05 -0.08 -0.03 0.06 -0.04 -0.01 0.04

45 6 -0.03 -0.06 -0.04 0.05 0.09 0.05 0.02 0.06 0.05

46 6 -0.02 0.02 0.06 0.03 -0.03 -0.08 0.02 -0.02 -0.06

47 6 0.06 0.03 -0.04 -0.08 -0.04 0.07 -0.06 -0.04 0.03

48 6 -0.02 -0.05 -0.05 0.03 0.07 0.06 0.03 0.06 0.05

49 1 -0.00 -0.01 0.00 0.09 0.04 0.00 0.04 0.04 0.01

50 1 0.00 -0.01 0.00 0.07 -0.02 0.00 -0.07 0.05 0.01

51 1 0.01 0.00 0.00 -0.05 -0.07 0.01 -0.02 -0.07 -0.00

52 1 0.01 -0.00 0.00 -0.04 0.04 0.01 0.04 -0.09 -0.00

53 1 -0.01 -0.00 0.00 -0.05 -0.07 -0.01 -0.02 -0.07 0.00

54 1 -0.01 0.00 0.00 -0.04 0.04 -0.01 0.04 -0.09 0.00

55 1 -0.00 0.01 0.00 0.07 -0.02 -0.00 -0.07 0.05 -0.01

56 1 0.00 0.01 0.00 0.09 0.04 -0.00 0.04 0.04 -0.01

57 1 0.07 0.16 -0.10 0.09 0.20 -0.13 0.03 0.07 -0.05

58 1 0.13 0.09 0.07 0.20 0.13 0.09 0.09 0.05 0.05

59 1 -0.02 0.02 -0.05 -0.02 0.03 -0.07 -0.02 0.02 -0.05

60 1 -0.09 -0.13 0.07 -0.09 -0.15 0.08 -0.11 -0.16 0.07

61 1 -0.16 -0.07 -0.10 -0.13 -0.06 -0.09 -0.16 -0.08 -0.11

62 1 0.02 0.02 -0.05 -0.02 -0.02 0.05 0.03 0.02 -0.07

63 1 -0.13 0.09 0.07 0.16 -0.11 -0.07 -0.15 0.09 0.08

64 1 -0.07 0.16 -0.10 0.08 -0.16 0.11 -0.06 0.13 -0.09

65 1 0.16 -0.07 -0.10 -0.07 0.03 0.05 0.20 -0.09 -0.13

66 1 0.09 -0.13 0.07 -0.05 0.09 -0.05 0.13 -0.20 0.09

67 1 -0.16 0.07 -0.10 -0.07 0.03 -0.05 0.20 -0.09 0.13

68 1 -0.09 0.13 0.07 -0.05 0.09 0.05 0.13 -0.20 -0.09

69 1 -0.02 -0.02 -0.05 -0.02 -0.02 -0.05 0.03 0.02 0.07

70 1 0.13 -0.09 0.07 0.16 -0.11 0.07 -0.15 0.09 -0.08

71 1 0.07 -0.16 -0.10 0.08 -0.16 -0.11 -0.06 0.13 0.09

72 1 0.16 0.07 -0.10 -0.13 -0.06 0.09 -0.16 -0.08 0.11

73 1 0.09 0.13 0.07 -0.09 -0.15 -0.08 -0.11 -0.16 -0.07

74 1 0.02 -0.02 -0.05 -0.02 0.03 0.07 -0.02 0.02 0.05

75 1 -0.13 -0.09 0.07 0.20 0.13 -0.09 0.09 0.05 -0.05

76 1 -0.07 -0.16 -0.10 0.09 0.20 0.13 0.03 0.07 0.05

77 30 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00

157 158 159

A2 E E

Frequencies -- 1316.3228 1318.9675 1318.9675

Red. masses -- 5.0765 3.6368 3.6368

Frc consts -- 5.1825 3.7277 3.7277

IR Inten -- 0.0000 0.6555 0.6555

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.02 -0.00 -0.02 0.06 0.01 0.02 0.10 0.01

2 6 -0.04 0.03 -0.00 0.05 -0.10 -0.01 0.11 0.00 0.00

3 7 0.04 -0.00 -0.00 -0.01 0.08 0.01 -0.07 -0.01 -0.00

4 6 -0.04 -0.03 0.00 -0.01 -0.10 -0.01 0.12 0.03 0.00

5 6 0.00 0.02 0.00 0.02 0.02 0.00 0.02 -0.11 -0.01

6 6 0.00 -0.00 -0.02 -0.01 -0.09 0.00 -0.09 0.02 -0.00

7 6 0.03 0.04 0.00 -0.00 0.11 0.00 -0.10 -0.05 0.01

8 7 -0.00 -0.04 -0.00 0.01 -0.07 -0.00 0.08 0.01 -0.01

9 6 -0.03 0.04 -0.00 -0.03 0.12 0.00 -0.10 0.01 0.01

10 6 0.02 -0.00 -0.00 0.11 0.02 -0.01 0.02 -0.02 -0.00

11 6 -0.02 -0.00 0.00 -0.10 0.02 0.01 0.06 0.02 -0.01

12 6 0.00 0.00 0.02 -0.02 -0.09 0.00 -0.09 0.01 0.00

13 6 0.03 -0.04 -0.00 -0.03 0.12 -0.00 -0.10 0.01 -0.01

14 6 -0.02 0.00 -0.00 0.11 0.02 0.01 0.02 -0.02 0.00

15 6 0.02 0.00 0.00 -0.10 0.02 -0.01 0.06 0.02 0.01

16 6 -0.03 -0.04 0.00 -0.00 0.11 -0.00 -0.10 -0.05 -0.01

17 7 0.00 0.04 -0.00 0.01 -0.07 0.00 0.08 0.01 0.01

18 6 -0.00 0.00 -0.02 -0.01 -0.09 -0.00 -0.09 0.02 0.00

19 6 0.04 0.03 0.00 -0.01 -0.10 0.01 0.12 0.03 -0.00

20 6 -0.00 -0.02 0.00 0.02 0.02 -0.00 0.02 -0.11 0.01

21 6 -0.00 0.02 -0.00 -0.02 0.06 -0.01 0.02 0.10 -0.01

22 6 0.04 -0.03 -0.00 0.05 -0.10 0.01 0.11 0.00 -0.00

23 7 -0.04 -0.00 0.00 -0.01 0.08 -0.01 -0.07 -0.01 0.00

24 6 -0.00 -0.00 0.02 -0.02 -0.09 -0.00 -0.09 0.01 -0.00

25 6 0.07 -0.07 0.16 0.02 0.04 -0.02 0.04 0.01 0.03

26 6 0.03 0.07 -0.06 -0.00 -0.00 0.01 0.01 0.02 -0.01

27 6 -0.08 -0.04 -0.06 0.01 0.00 0.02 -0.02 -0.02 -0.01

28 6 0.03 -0.03 0.08 -0.01 0.00 -0.01 0.01 -0.01 0.02

29 6 0.04 0.08 -0.06 -0.01 -0.02 0.00 0.00 0.02 -0.02

30 6 -0.07 -0.03 -0.06 0.02 0.01 0.01 -0.01 -0.00 -0.01

31 6 0.03 0.03 -0.08 0.01 0.01 -0.02 0.00 0.01 -0.01

32 6 -0.08 0.04 0.06 -0.02 0.00 0.02 -0.02 0.01 0.00

33 6 0.03 -0.07 0.06 0.00 -0.01 0.01 0.01 -0.02 0.01

34 6 0.07 0.07 -0.16 -0.01 0.04 -0.03 0.04 -0.02 -0.02

35 6 -0.07 0.03 0.06 -0.02 0.01 0.01 -0.00 0.00 0.01

36 6 0.04 -0.08 0.06 0.02 -0.02 0.01 0.00 -0.01 0.02

37 6 -0.07 -0.07 -0.16 -0.01 0.04 0.03 0.04 -0.02 0.02

38 6 0.07 -0.03 0.06 -0.02 0.01 -0.01 -0.00 0.00 -0.01

39 6 -0.04 0.08 0.06 0.02 -0.02 -0.01 0.00 -0.01 -0.02

40 6 -0.03 -0.03 -0.08 0.01 0.01 0.02 0.00 0.01 0.01

41 6 0.08 -0.04 0.06 -0.02 0.00 -0.02 -0.02 0.01 -0.00

42 6 -0.03 0.07 0.06 0.00 -0.01 -0.01 0.01 -0.02 -0.01

43 6 -0.07 0.07 0.16 0.02 0.04 0.02 0.04 0.01 -0.03

44 6 0.07 0.03 -0.06 0.02 0.01 -0.01 -0.01 -0.00 0.01

45 6 -0.04 -0.08 -0.06 -0.01 -0.02 -0.00 0.00 0.02 0.02

46 6 -0.03 0.03 0.08 -0.01 0.00 0.01 0.01 -0.01 -0.02

47 6 0.08 0.04 -0.06 0.01 0.00 -0.02 -0.02 -0.02 0.01

48 6 -0.03 -0.07 -0.06 -0.00 -0.00 -0.01 0.01 0.02 0.01

49 1 0.01 -0.01 -0.00 -0.02 0.06 0.01 -0.37 -0.19 -0.02

50 1 0.01 0.01 0.00 -0.10 0.12 0.01 -0.36 0.16 0.02

51 1 0.01 -0.01 -0.00 -0.16 -0.36 0.02 0.12 0.10 -0.01

52 1 -0.01 -0.01 0.00 0.19 -0.37 -0.02 0.06 0.02 -0.01

53 1 -0.01 0.01 -0.00 -0.16 -0.36 -0.02 0.12 0.10 0.01

54 1 0.01 0.01 0.00 0.19 -0.37 0.02 0.06 0.02 0.01

55 1 -0.01 -0.01 0.00 -0.10 0.12 -0.01 -0.36 0.16 -0.02

56 1 -0.01 0.01 -0.00 -0.02 0.06 -0.01 -0.37 -0.19 0.02

57 1 0.07 0.14 -0.10 -0.02 -0.05 0.03 -0.00 -0.01 0.00

58 1 0.16 0.10 0.08 -0.05 -0.04 -0.02 0.01 0.00 0.01

59 1 -0.02 0.02 -0.06 0.00 -0.00 0.01 -0.01 0.00 -0.01

60 1 -0.10 -0.16 0.08 -0.01 -0.01 -0.00 -0.04 -0.05 0.02

61 1 -0.14 -0.07 -0.10 -0.03 -0.01 -0.01 -0.04 -0.02 -0.03

62 1 -0.02 -0.02 0.06 -0.00 -0.01 0.01 -0.00 -0.00 0.01

63 1 0.16 -0.10 -0.08 0.05 -0.04 -0.02 -0.01 0.01 -0.00

64 1 0.07 -0.14 0.10 0.02 -0.04 0.03 -0.01 0.03 -0.01

65 1 -0.14 0.07 0.10 0.01 -0.00 -0.00 -0.05 0.02 0.03

66 1 -0.10 0.16 -0.08 -0.00 0.01 -0.01 -0.04 0.05 -0.02

67 1 0.14 -0.07 0.10 0.01 -0.00 0.00 -0.05 0.02 -0.03

68 1 0.10 -0.16 -0.08 -0.00 0.01 0.01 -0.04 0.05 0.02

69 1 0.02 0.02 0.06 -0.00 -0.01 -0.01 -0.00 -0.00 -0.01

70 1 -0.16 0.10 -0.08 0.05 -0.04 0.02 -0.01 0.01 0.00

71 1 -0.07 0.14 0.10 0.02 -0.04 -0.03 -0.01 0.03 0.01

72 1 0.14 0.07 -0.10 -0.03 -0.01 0.01 -0.04 -0.02 0.03

73 1 0.10 0.16 0.08 -0.01 -0.01 0.00 -0.04 -0.05 -0.02

74 1 0.02 -0.02 -0.06 0.00 -0.00 -0.01 -0.01 0.00 0.01

75 1 -0.16 -0.10 0.08 -0.05 -0.04 0.02 0.01 0.00 -0.01

76 1 -0.07 -0.14 -0.10 -0.02 -0.05 -0.03 -0.00 -0.01 -0.00

77 30 -0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00

160 161 162

B2 A2 E

Frequencies -- 1325.6357 1351.5561 1352.2555

Red. masses -- 8.4381 1.7491 1.9567

Frc consts -- 8.7366 1.8824 2.1081

IR Inten -- 0.0759 0.0000 8.3357

Atom AN X Y Z X Y Z X Y Z

1 6 0.04 0.03 0.00 -0.01 -0.04 -0.00 -0.01 -0.00 -0.00

2 6 0.08 -0.14 -0.01 -0.02 0.01 0.00 -0.00 0.03 0.00

3 7 -0.00 0.15 0.01 0.01 -0.00 0.00 0.02 -0.02 -0.00

4 6 -0.08 -0.14 -0.01 -0.02 -0.01 -0.00 -0.00 0.02 0.00

5 6 -0.04 0.03 0.00 -0.01 0.04 0.00 0.01 -0.01 -0.00

6 6 -0.03 0.03 -0.01 0.03 -0.03 -0.01 -0.04 -0.02 0.00

7 6 0.14 0.08 -0.01 0.01 0.02 -0.00 0.04 -0.00 -0.00

8 7 -0.15 0.00 0.01 0.00 -0.01 0.00 -0.04 0.01 0.00

9 6 0.14 -0.08 -0.01 -0.01 0.02 0.00 0.05 0.00 -0.00

10 6 -0.03 -0.04 0.00 0.04 0.01 -0.00 -0.01 -0.01 0.00

11 6 -0.03 0.04 0.00 -0.04 0.01 0.00 -0.02 0.01 0.00

12 6 0.03 0.03 -0.01 0.03 0.03 0.01 -0.03 -0.01 -0.01

13 6 -0.14 0.08 -0.01 0.01 -0.02 0.00 0.05 0.00 0.00

14 6 0.03 0.04 0.00 -0.04 -0.01 -0.00 -0.01 -0.01 -0.00

15 6 0.03 -0.04 0.00 0.04 -0.01 0.00 -0.02 0.01 -0.00

16 6 -0.14 -0.08 -0.01 -0.01 -0.02 -0.00 0.04 -0.00 0.00

17 7 0.15 -0.00 0.01 -0.00 0.01 0.00 -0.04 0.01 -0.00

18 6 0.03 -0.03 -0.01 -0.03 0.03 -0.01 -0.04 -0.02 -0.00

19 6 0.08 0.14 -0.01 0.02 0.01 -0.00 -0.00 0.02 -0.00

20 6 0.04 -0.03 0.00 0.01 -0.04 0.00 0.01 -0.01 0.00

21 6 -0.04 -0.03 0.00 0.01 0.04 -0.00 -0.01 -0.00 0.00

22 6 -0.08 0.14 -0.01 0.02 -0.01 0.00 -0.00 0.03 -0.00

23 7 -0.00 -0.15 0.01 -0.01 0.00 -0.00 0.02 -0.02 0.00

24 6 -0.03 -0.03 -0.01 -0.03 -0.03 0.01 -0.03 -0.01 0.01

25 6 0.07 -0.07 0.13 0.00 -0.00 0.02 0.02 0.02 -0.01

26 6 0.04 0.08 -0.05 -0.03 -0.04 0.02 0.02 0.03 -0.01

27 6 -0.09 -0.04 -0.05 0.02 0.01 0.00 -0.01 -0.01 0.00

28 6 0.03 -0.03 0.09 -0.02 0.02 -0.05 0.01 -0.01 0.02

29 6 0.04 0.09 -0.05 -0.01 -0.02 0.00 0.00 0.01 -0.01

30 6 -0.08 -0.04 -0.05 0.04 0.03 0.02 -0.01 -0.01 -0.00

31 6 -0.03 -0.03 0.09 -0.02 -0.02 0.05 0.03 0.03 -0.08

32 6 0.09 -0.04 -0.05 0.02 -0.01 -0.00 -0.03 0.02 0.01

33 6 -0.04 0.08 -0.05 -0.03 0.04 -0.02 0.05 -0.07 0.03

34 6 -0.07 -0.07 0.13 0.00 0.00 -0.02 0.00 -0.01 0.02

35 6 0.08 -0.04 -0.05 0.04 -0.03 -0.02 -0.07 0.05 0.03

36 6 -0.04 0.09 -0.05 -0.01 0.02 -0.00 0.02 -0.03 0.01

37 6 0.07 0.07 0.13 -0.00 -0.00 -0.02 0.00 -0.01 -0.02

38 6 -0.08 0.04 -0.05 -0.04 0.03 -0.02 -0.07 0.05 -0.03

39 6 0.04 -0.09 -0.05 0.01 -0.02 -0.00 0.02 -0.03 -0.01

40 6 0.03 0.03 0.09 0.02 0.02 0.05 0.03 0.03 0.08

41 6 -0.09 0.04 -0.05 -0.02 0.01 -0.00 -0.03 0.02 -0.01

42 6 0.04 -0.08 -0.05 0.03 -0.04 -0.02 0.05 -0.07 -0.03

43 6 -0.07 0.07 0.13 -0.00 0.00 0.02 0.02 0.02 0.01

44 6 0.08 0.04 -0.05 -0.04 -0.03 0.02 -0.01 -0.01 0.00

45 6 -0.04 -0.09 -0.05 0.01 0.02 0.00 0.00 0.01 0.01

46 6 -0.03 0.03 0.09 0.02 -0.02 -0.05 0.01 -0.01 -0.02

47 6 0.09 0.04 -0.05 -0.02 -0.01 0.00 -0.01 -0.01 -0.00

48 6 -0.04 -0.08 -0.05 0.03 0.04 0.02 0.02 0.03 0.01

49 1 0.03 0.03 0.01 0.15 0.08 0.01 -0.02 -0.01 0.00

50 1 -0.03 0.03 0.01 0.15 -0.08 -0.01 -0.03 0.02 0.00

51 1 -0.03 -0.03 0.01 -0.08 -0.15 0.01 -0.00 0.00 -0.00

52 1 -0.03 0.03 0.01 0.08 -0.15 -0.01 0.01 -0.03 -0.00

53 1 0.03 0.03 0.01 0.08 0.15 0.01 -0.00 0.00 0.00

54 1 0.03 -0.03 0.01 -0.08 0.15 -0.01 0.01 -0.03 0.00

55 1 0.03 -0.03 0.01 -0.15 0.08 -0.01 -0.03 0.02 -0.00

56 1 -0.03 -0.03 0.01 -0.15 -0.08 0.01 -0.02 -0.01 -0.00

57 1 0.04 0.05 -0.05 0.11 0.20 -0.12 -0.06 -0.12 0.07

58 1 0.14 0.08 0.07 0.09 0.06 0.04 -0.06 -0.04 -0.02

59 1 -0.03 0.03 -0.07 0.04 -0.04 0.12 -0.02 0.02 -0.06

60 1 -0.08 -0.14 0.07 -0.06 -0.09 0.04 0.01 0.02 -0.01

61 1 -0.05 -0.04 -0.05 -0.20 -0.11 -0.12 0.06 0.03 0.04

62 1 0.03 0.03 -0.07 0.04 0.04 -0.12 -0.07 -0.07 0.19

63 1 -0.14 0.08 0.07 0.09 -0.06 -0.04 -0.14 0.09 0.07

64 1 -0.04 0.05 -0.05 0.11 -0.20 0.12 -0.17 0.32 -0.19

65 1 0.05 -0.04 -0.05 -0.20 0.11 0.12 0.30 -0.16 -0.18

66 1 0.08 -0.14 0.07 -0.06 0.09 -0.04 0.08 -0.13 0.06

67 1 -0.05 0.04 -0.05 0.20 -0.11 0.12 0.30 -0.16 0.18

68 1 -0.08 0.14 0.07 0.06 -0.09 -0.04 0.08 -0.13 -0.06

69 1 -0.03 -0.03 -0.07 -0.04 -0.04 -0.12 -0.07 -0.07 -0.19

70 1 0.14 -0.08 0.07 -0.09 0.06 -0.04 -0.14 0.09 -0.07

71 1 0.04 -0.05 -0.05 -0.11 0.20 0.12 -0.17 0.32 0.19

72 1 0.05 0.04 -0.05 0.20 0.11 -0.12 0.06 0.03 -0.04

73 1 0.08 0.14 0.07 0.06 0.09 0.04 0.01 0.02 0.01

74 1 0.03 -0.03 -0.07 -0.04 0.04 0.12 -0.02 0.02 0.06

75 1 -0.14 -0.08 0.07 -0.09 -0.06 0.04 -0.06 -0.04 0.02

76 1 -0.04 -0.05 -0.05 -0.11 -0.20 -0.12 -0.06 -0.12 -0.07

77 30 0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00 0.00

163 164 165

E B2 A2

Frequencies -- 1352.2555 1354.8354 1360.3089

Red. masses -- 1.9567 1.4829 1.7617

Frc consts -- 2.1081 1.6037 1.9207

IR Inten -- 8.3357 0.6827 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 0.02 0.00 0.01 0.00 -0.00 -0.03 -0.06 -0.01

2 6 -0.00 -0.04 -0.00 0.01 -0.01 -0.00 -0.02 0.01 0.00

3 7 0.01 0.04 0.00 0.00 0.01 0.00 0.01 -0.00 -0.00

4 6 0.00 -0.05 -0.00 -0.01 -0.01 -0.00 -0.02 -0.01 -0.00

5 6 -0.01 0.01 0.00 -0.01 0.00 -0.00 -0.03 0.06 0.01

6 6 -0.01 0.03 0.01 -0.00 0.00 -0.01 0.04 -0.04 0.00

7 6 0.03 0.00 -0.00 0.01 0.01 -0.00 0.01 0.02 -0.00

8 7 -0.02 -0.02 0.00 -0.01 -0.00 0.00 -0.00 -0.01 -0.00

9 6 0.02 0.00 -0.00 0.01 -0.01 -0.00 -0.01 0.02 0.00

10 6 -0.01 -0.01 0.00 -0.00 -0.01 -0.00 0.06 0.03 -0.01

11 6 -0.00 0.01 0.00 -0.00 0.01 -0.00 -0.06 0.03 0.01

12 6 -0.02 0.04 0.00 0.00 0.00 -0.01 0.04 0.04 -0.00

13 6 0.02 0.00 0.00 -0.01 0.01 -0.00 0.01 -0.02 0.00

14 6 -0.01 -0.01 -0.00 0.00 0.01 -0.00 -0.06 -0.03 -0.01

15 6 -0.00 0.01 -0.00 0.00 -0.01 -0.00 0.06 -0.03 0.01

16 6 0.03 0.00 0.00 -0.01 -0.01 -0.00 -0.01 -0.02 -0.00

17 7 -0.02 -0.02 -0.00 0.01 0.00 0.00 0.00 0.01 -0.00

18 6 -0.01 0.03 -0.01 0.00 -0.00 -0.01 -0.04 0.04 0.00

19 6 0.00 -0.05 0.00 0.01 0.01 -0.00 0.02 0.01 -0.00

20 6 -0.01 0.01 -0.00 0.01 -0.00 -0.00 0.03 -0.06 0.01

21 6 0.01 0.02 -0.00 -0.01 -0.00 -0.00 0.03 0.06 -0.01

22 6 -0.00 -0.04 0.00 -0.01 0.01 -0.00 0.02 -0.01 0.00

23 7 0.01 0.04 -0.00 0.00 -0.01 0.00 -0.01 -0.00 0.00

24 6 -0.02 0.04 -0.00 -0.00 -0.00 -0.01 -0.04 -0.04 -0.00

25 6 -0.01 -0.00 -0.02 0.01 -0.01 0.02 -0.01 0.01 -0.02

26 6 0.05 0.07 -0.03 -0.03 -0.04 0.02 0.02 0.02 -0.01

27 6 -0.03 -0.02 -0.01 0.01 0.01 -0.00 0.00 -0.00 0.00

28 6 0.03 -0.03 0.08 -0.02 0.02 -0.05 0.01 -0.01 0.03

29 6 0.02 0.03 -0.01 -0.01 -0.01 -0.00 0.00 -0.00 0.00

30 6 -0.07 -0.05 -0.03 0.04 0.03 0.02 -0.02 -0.02 -0.01

31 6 -0.01 -0.01 0.02 0.02 0.02 -0.05 0.01 0.01 -0.03

32 6 0.01 -0.00 -0.01 -0.01 0.01 -0.00 0.00 0.00 -0.00

33 6 -0.01 0.01 -0.00 0.03 -0.04 0.02 0.02 -0.02 0.01

34 6 0.02 -0.02 -0.01 -0.01 -0.01 0.02 -0.01 -0.01 0.02

35 6 0.03 -0.02 -0.01 -0.04 0.03 0.02 -0.02 0.02 0.01

36 6 -0.01 0.01 0.00 0.01 -0.01 -0.00 0.00 0.00 -0.00

37 6 0.02 -0.02 0.01 0.01 0.01 0.02 0.01 0.01 0.02

38 6 0.03 -0.02 0.01 0.04 -0.03 0.02 0.02 -0.02 0.01

39 6 -0.01 0.01 -0.00 -0.01 0.01 -0.00 -0.00 -0.00 -0.00

40 6 -0.01 -0.01 -0.02 -0.02 -0.02 -0.05 -0.01 -0.01 -0.03

41 6 0.01 -0.00 0.01 0.01 -0.01 -0.00 -0.00 -0.00 -0.00

42 6 -0.01 0.01 0.00 -0.03 0.04 0.02 -0.02 0.02 0.01

43 6 -0.01 -0.00 0.02 -0.01 0.01 0.02 0.01 -0.01 -0.02

44 6 -0.07 -0.05 0.03 -0.04 -0.03 0.02 0.02 0.02 -0.01

45 6 0.02 0.03 0.01 0.01 0.01 -0.00 -0.00 0.00 0.00

46 6 0.03 -0.03 -0.08 0.02 -0.02 -0.05 -0.01 0.01 0.03

47 6 -0.03 -0.02 0.01 -0.01 -0.01 -0.00 -0.00 0.00 0.00

48 6 0.05 0.07 0.03 0.03 0.04 0.02 -0.02 -0.02 -0.01

49 1 -0.03 -0.01 -0.00 0.00 -0.00 0.00 0.23 0.12 0.01

50 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.23 -0.12 -0.01

51 1 0.02 0.03 -0.00 0.00 -0.00 0.00 -0.12 -0.23 0.01

52 1 -0.01 0.02 -0.00 0.00 0.00 0.00 0.12 -0.23 -0.01

53 1 0.02 0.03 0.00 -0.00 0.00 0.00 0.12 0.23 0.01

54 1 -0.01 0.02 0.00 -0.00 -0.00 0.00 -0.12 0.23 -0.01

55 1 0.00 0.00 0.00 0.00 0.00 0.00 -0.23 0.12 -0.01

56 1 -0.03 -0.01 0.00 -0.00 0.00 0.00 -0.23 -0.12 0.01

57 1 -0.16 -0.30 0.18 0.12 0.23 -0.14 -0.08 -0.14 0.09

58 1 -0.13 -0.08 -0.06 0.12 0.07 0.06 -0.09 -0.05 -0.04

59 1 -0.07 0.07 -0.19 0.05 -0.05 0.14 -0.04 0.04 -0.10

60 1 0.09 0.14 -0.07 -0.07 -0.12 0.06 0.05 0.09 -0.04

61 1 0.32 0.17 0.19 -0.23 -0.12 -0.14 0.14 0.08 0.09

62 1 0.02 0.02 -0.06 -0.05 -0.05 0.14 -0.04 -0.04 0.10

63 1 0.02 -0.01 -0.01 -0.12 0.07 0.06 -0.09 0.05 0.04

64 1 0.03 -0.06 0.04 -0.12 0.23 -0.14 -0.08 0.14 -0.09

65 1 -0.12 0.06 0.07 0.23 -0.12 -0.14 0.14 -0.08 -0.09

66 1 -0.04 0.06 -0.02 0.07 -0.12 0.06 0.05 -0.09 0.04

67 1 -0.12 0.06 -0.07 -0.23 0.12 -0.14 -0.14 0.08 -0.09

68 1 -0.04 0.06 0.02 -0.07 0.12 0.06 -0.05 0.09 0.04

69 1 0.02 0.02 0.06 0.05 0.05 0.14 0.04 0.04 0.10

70 1 0.02 -0.01 0.01 0.12 -0.07 0.06 0.09 -0.05 0.04

71 1 0.03 -0.06 -0.04 0.12 -0.23 -0.14 0.08 -0.14 -0.09

72 1 0.32 0.17 -0.19 0.23 0.12 -0.14 -0.14 -0.08 0.09

73 1 0.09 0.14 0.07 0.07 0.12 0.06 -0.05 -0.09 -0.04

74 1 -0.07 0.07 0.19 -0.05 0.05 0.14 0.04 -0.04 -0.10

75 1 -0.13 -0.08 0.06 -0.12 -0.07 0.06 0.09 0.05 -0.04

76 1 -0.16 -0.30 -0.18 -0.12 -0.23 -0.14 0.08 0.14 0.09

77 30 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

166 167 168

E E A1

Frequencies -- 1363.0213 1363.0213 1370.0653

Red. masses -- 3.4402 3.4402 10.6004

Frc consts -- 3.7657 3.7657 11.7234

IR Inten -- 69.5385 69.5387 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.02 0.00 -0.05 -0.04 -0.00 0.01 -0.10 -0.01

2 6 -0.00 0.04 0.00 -0.01 0.13 0.01 0.08 0.27 0.02

3 7 0.06 -0.02 -0.00 -0.01 -0.13 -0.01 0.00 -0.17 -0.01

4 6 -0.00 0.01 -0.00 0.01 0.14 0.01 -0.08 0.27 0.02

5 6 0.02 -0.04 -0.00 0.05 -0.03 -0.00 -0.01 -0.10 -0.01

6 6 -0.11 -0.03 -0.00 0.01 -0.10 0.01 -0.05 -0.05 -0.00

7 6 0.13 0.01 -0.01 -0.04 -0.00 0.00 0.27 -0.08 -0.02

8 7 -0.13 0.01 0.01 0.02 0.06 -0.00 -0.17 0.00 0.01

9 6 0.14 -0.01 -0.01 -0.01 -0.00 -0.00 0.27 0.08 -0.02

10 6 -0.03 -0.05 0.00 0.04 0.02 -0.00 -0.10 0.01 0.01

11 6 -0.04 0.05 0.00 -0.02 0.00 0.00 -0.10 -0.01 0.01

12 6 -0.10 -0.01 0.01 0.03 -0.11 0.00 0.05 -0.05 0.00

13 6 0.14 -0.01 0.01 -0.01 -0.00 0.00 -0.27 -0.08 -0.02

14 6 -0.03 -0.05 -0.00 0.04 0.02 0.00 0.10 -0.01 0.01

15 6 -0.04 0.05 -0.00 -0.02 0.00 -0.00 0.10 0.01 0.01

16 6 0.13 0.01 0.01 -0.04 -0.00 -0.00 -0.27 0.08 -0.02

17 7 -0.13 0.01 -0.01 0.02 0.06 0.00 0.17 -0.00 0.01

18 6 -0.11 -0.03 0.00 0.01 -0.10 -0.01 0.05 0.05 0.00

19 6 -0.00 0.01 0.00 0.01 0.14 -0.01 0.08 -0.27 0.02

20 6 0.02 -0.04 0.00 0.05 -0.03 0.00 0.01 0.10 -0.01

21 6 0.00 0.02 -0.00 -0.05 -0.04 0.00 -0.01 0.10 -0.01

22 6 -0.00 0.04 -0.00 -0.01 0.13 -0.01 -0.08 -0.27 0.02

23 7 0.06 -0.02 0.00 -0.01 -0.13 0.01 0.00 0.17 -0.01

24 6 -0.10 -0.01 -0.01 0.03 -0.11 -0.00 -0.05 0.05 -0.00

25 6 0.06 0.02 0.02 -0.00 0.05 -0.04 0.03 0.03 0.00

26 6 -0.00 0.00 -0.00 0.03 0.03 -0.01 0.01 0.01 -0.01

27 6 -0.01 -0.01 0.00 0.01 -0.00 0.02 -0.00 -0.01 0.01

28 6 -0.01 0.00 -0.02 0.01 -0.01 0.02 -0.00 -0.00 0.00

29 6 -0.01 0.01 -0.02 -0.01 -0.02 0.00 -0.01 -0.00 -0.01

30 6 0.03 0.02 0.01 -0.01 -0.01 -0.00 0.01 0.01 0.01

31 6 -0.01 -0.01 0.02 -0.00 -0.01 0.02 0.00 -0.00 0.00

32 6 -0.02 0.01 0.00 -0.01 -0.01 0.02 0.00 -0.01 0.01

33 6 -0.01 0.01 -0.00 -0.02 0.03 -0.01 -0.01 0.01 -0.01

34 6 0.05 0.00 -0.04 -0.02 0.06 -0.02 -0.03 0.03 -0.00

35 6 0.03 -0.03 -0.01 -0.00 -0.00 0.00 -0.01 0.01 0.01

36 6 -0.00 -0.01 0.02 0.01 -0.01 -0.00 0.01 -0.00 -0.01

37 6 0.05 0.00 0.04 -0.02 0.06 0.02 0.03 -0.03 0.00

38 6 0.03 -0.03 0.01 -0.00 -0.00 -0.00 0.01 -0.01 0.01

39 6 -0.00 -0.01 -0.02 0.01 -0.01 0.00 -0.01 0.00 -0.01

40 6 -0.01 -0.01 -0.02 -0.00 -0.01 -0.02 -0.00 0.00 -0.00

41 6 -0.02 0.01 -0.00 -0.01 -0.01 -0.02 -0.00 0.01 0.01

42 6 -0.01 0.01 0.00 -0.02 0.03 0.01 0.01 -0.01 -0.01

43 6 0.06 0.02 -0.02 -0.00 0.05 0.04 -0.03 -0.03 -0.00

44 6 0.03 0.02 -0.01 -0.01 -0.01 0.00 -0.01 -0.01 0.01

45 6 -0.01 0.01 0.02 -0.01 -0.02 -0.00 0.01 0.00 -0.01

46 6 -0.01 0.00 0.02 0.01 -0.01 -0.02 0.00 0.00 0.00

47 6 -0.01 -0.01 -0.00 0.01 -0.00 -0.02 0.00 0.01 0.01

48 6 -0.00 0.00 0.00 0.03 0.03 0.01 -0.01 -0.01 -0.01

49 1 -0.12 -0.07 -0.01 0.06 0.04 0.01 0.07 -0.07 -0.01

50 1 -0.13 0.08 0.01 -0.01 0.02 0.00 -0.07 -0.07 -0.01

51 1 0.02 0.01 -0.00 -0.08 -0.13 0.01 -0.07 0.07 0.01

52 1 0.04 -0.06 -0.01 0.07 -0.12 -0.01 -0.07 -0.07 0.01

53 1 0.02 0.01 0.00 -0.08 -0.13 -0.01 0.07 -0.07 0.01

54 1 0.04 -0.06 0.01 0.07 -0.12 0.01 0.07 0.07 0.01

55 1 -0.13 0.08 -0.01 -0.01 0.02 -0.00 0.07 0.07 -0.01

56 1 -0.12 -0.07 0.01 0.06 0.04 -0.01 -0.07 0.07 -0.01

57 1 0.04 0.06 -0.05 -0.14 -0.23 0.15 -0.03 -0.06 0.04

58 1 0.05 0.02 0.04 -0.17 -0.11 -0.08 -0.04 -0.03 -0.01

59 1 0.03 -0.04 0.09 -0.05 0.05 -0.13 -0.00 -0.00 0.00

60 1 -0.10 -0.14 0.06 0.06 0.11 -0.06 -0.03 -0.04 0.01

61 1 -0.20 -0.11 -0.12 0.14 0.09 0.10 -0.06 -0.03 -0.04

62 1 0.05 0.05 -0.13 0.04 0.03 -0.09 0.00 -0.00 -0.00

63 1 0.11 -0.06 -0.06 0.14 -0.10 -0.06 0.04 -0.03 -0.01

64 1 0.09 -0.14 0.10 0.11 -0.20 0.12 0.03 -0.06 0.04

65 1 -0.23 0.14 0.15 -0.06 0.04 0.05 0.06 -0.03 -0.04

66 1 -0.11 0.17 -0.08 -0.02 0.05 -0.04 0.03 -0.04 0.01

67 1 -0.23 0.14 -0.15 -0.06 0.04 -0.05 -0.06 0.03 -0.04

68 1 -0.11 0.17 0.08 -0.02 0.05 0.04 -0.03 0.04 0.01

69 1 0.05 0.05 0.13 0.04 0.03 0.09 -0.00 0.00 0.00

70 1 0.11 -0.06 0.06 0.14 -0.10 0.06 -0.04 0.03 -0.01

71 1 0.09 -0.14 -0.10 0.11 -0.20 -0.12 -0.03 0.06 0.04

72 1 -0.20 -0.11 0.12 0.14 0.09 -0.10 0.06 0.03 -0.04

73 1 -0.10 -0.14 -0.06 0.06 0.11 0.06 0.03 0.04 0.01

74 1 0.03 -0.04 -0.09 -0.05 0.05 0.13 0.00 0.00 -0.00

75 1 0.05 0.02 -0.04 -0.17 -0.11 0.08 0.04 0.03 -0.01

76 1 0.04 0.06 0.05 -0.14 -0.23 -0.15 0.03 0.06 0.04

77 30 0.00 0.00 0.00 -0.00 0.00 0.00 0.00 0.00 0.00

169 170 171

B1 E E

Frequencies -- 1383.8417 1453.0929 1453.0929

Red. masses -- 3.9138 3.7936 3.7936

Frc consts -- 4.4159 4.7194 4.7194

IR Inten -- 0.0000 0.8733 0.8732

Atom AN X Y Z X Y Z X Y Z

1 6 0.02 0.10 0.01 -0.05 0.07 0.01 0.11 0.10 0.01

2 6 0.07 -0.08 -0.00 -0.08 -0.09 -0.01 -0.10 -0.07 -0.01

3 7 -0.05 -0.00 -0.00 0.02 0.00 0.00 0.03 -0.00 -0.00

4 6 0.07 0.08 0.00 -0.04 0.02 0.00 -0.12 0.11 0.01

5 6 0.02 -0.10 -0.01 0.12 -0.04 -0.00 0.01 -0.11 -0.01

6 6 -0.08 -0.08 0.00 0.03 -0.06 -0.00 0.05 0.03 -0.00

7 6 0.08 0.07 -0.00 -0.07 0.10 0.01 0.09 -0.08 -0.01

8 7 0.00 -0.05 -0.00 -0.00 -0.03 0.00 -0.00 0.02 0.00

9 6 -0.08 0.07 0.00 0.11 0.12 -0.01 -0.02 -0.04 0.00

10 6 0.10 0.02 -0.01 -0.11 -0.01 0.01 0.04 0.12 -0.00

11 6 -0.10 0.02 0.01 0.10 -0.11 -0.01 -0.07 -0.05 0.01

12 6 -0.08 0.08 -0.00 0.03 -0.05 -0.00 0.06 0.03 0.00

13 6 0.08 -0.07 0.00 0.11 0.12 0.01 -0.02 -0.04 -0.00

14 6 -0.10 -0.02 -0.01 -0.11 -0.01 -0.01 0.04 0.12 0.00

15 6 0.10 -0.02 0.01 0.10 -0.11 0.01 -0.07 -0.05 -0.01

16 6 -0.08 -0.07 -0.00 -0.07 0.10 -0.01 0.09 -0.08 0.01

17 7 -0.00 0.05 -0.00 -0.00 -0.03 -0.00 -0.00 0.02 -0.00

18 6 0.08 0.08 0.00 0.03 -0.06 0.00 0.05 0.03 0.00

19 6 -0.07 -0.08 0.00 -0.04 0.02 -0.00 -0.12 0.11 -0.01

20 6 -0.02 0.10 -0.01 0.12 -0.04 0.00 0.01 -0.11 0.01

21 6 -0.02 -0.10 0.01 -0.05 0.07 -0.01 0.11 0.10 -0.01

22 6 -0.07 0.08 -0.00 -0.08 -0.09 0.01 -0.10 -0.07 0.01

23 7 0.05 -0.00 0.00 0.02 0.00 -0.00 0.03 -0.00 0.00

24 6 0.08 -0.08 -0.00 0.03 -0.05 0.00 0.06 0.03 -0.00

25 6 0.03 0.03 -0.00 0.00 0.00 0.01 -0.01 -0.01 0.00

26 6 0.01 0.01 -0.01 -0.01 -0.00 -0.01 -0.00 -0.01 0.00

27 6 -0.00 -0.01 0.01 0.01 0.01 0.00 -0.00 0.00 -0.00

28 6 -0.00 -0.00 -0.00 0.00 -0.00 0.01 0.00 0.00 0.00

29 6 -0.01 -0.00 -0.01 -0.01 -0.01 0.00 -0.00 -0.01 0.01

30 6 0.01 0.01 0.01 0.01 0.01 -0.00 -0.00 -0.00 -0.00

31 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 0.00 -0.01

32 6 -0.00 0.01 -0.01 -0.01 0.00 0.01 0.01 -0.01 -0.00

33 6 0.01 -0.01 0.01 -0.00 0.00 -0.00 -0.01 0.01 0.00

34 6 0.03 -0.03 -0.00 -0.01 0.01 0.00 -0.00 0.00 -0.01

35 6 0.01 -0.01 -0.01 -0.01 0.00 0.00 0.00 -0.01 0.01

36 6 -0.01 0.00 0.01 0.00 0.00 -0.00 -0.01 0.01 -0.00

37 6 -0.03 0.03 0.00 -0.01 0.01 -0.00 -0.00 0.00 0.01

38 6 -0.01 0.01 -0.01 -0.01 0.00 -0.00 0.00 -0.01 -0.01

39 6 0.01 -0.00 0.01 0.00 0.00 0.00 -0.01 0.01 0.00

40 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.01

41 6 0.00 -0.01 -0.01 -0.01 0.00 -0.01 0.01 -0.01 0.00

42 6 -0.01 0.01 0.01 -0.00 0.00 0.00 -0.01 0.01 -0.00

43 6 -0.03 -0.03 0.00 0.00 0.00 -0.01 -0.01 -0.01 -0.00

44 6 -0.01 -0.01 0.01 0.01 0.01 0.00 -0.00 -0.00 0.00

45 6 0.01 0.00 -0.01 -0.01 -0.01 -0.00 -0.00 -0.01 -0.01

46 6 0.00 0.00 0.00 0.00 -0.00 -0.01 0.00 0.00 -0.00

47 6 0.00 0.01 0.01 0.01 0.01 -0.00 -0.00 0.00 0.00

48 6 -0.01 -0.01 -0.01 -0.01 -0.00 0.01 -0.00 -0.01 -0.00

49 1 -0.27 -0.11 -0.02 -0.15 0.02 0.00 -0.33 -0.23 -0.03

50 1 -0.27 0.11 0.02 -0.20 0.20 0.02 -0.30 0.10 0.01

51 1 -0.11 -0.27 0.02 0.10 0.30 -0.01 -0.20 -0.20 0.02

52 1 0.11 -0.27 -0.02 -0.23 0.33 0.03 -0.02 -0.15 0.00

53 1 0.11 0.27 0.02 0.10 0.30 0.01 -0.20 -0.20 -0.02

54 1 -0.11 0.27 -0.02 -0.23 0.33 -0.03 -0.02 -0.15 -0.00

55 1 0.27 -0.11 0.02 -0.20 0.20 -0.02 -0.30 0.10 -0.01

56 1 0.27 0.11 -0.02 -0.15 0.02 -0.00 -0.33 -0.23 0.03

57 1 -0.02 -0.05 0.03 -0.01 -0.00 -0.00 0.01 0.02 -0.01

58 1 -0.04 -0.03 -0.01 -0.04 -0.02 -0.03 0.01 0.01 0.00

59 1 -0.00 -0.00 0.00 -0.02 0.02 -0.05 -0.00 0.01 -0.02

60 1 -0.03 -0.04 0.01 0.01 0.03 -0.02 0.02 0.03 -0.02

61 1 -0.05 -0.02 -0.03 -0.01 0.00 -0.01 0.02 0.01 0.01

62 1 -0.00 0.00 0.00 0.01 0.00 -0.02 -0.02 -0.02 0.05

63 1 -0.04 0.03 0.01 0.03 -0.02 -0.02 -0.03 0.01 0.02

64 1 -0.02 0.05 -0.03 0.01 -0.02 0.01 -0.00 -0.01 0.01

65 1 -0.05 0.02 0.03 0.02 -0.01 -0.01 0.00 -0.01 0.00

66 1 -0.03 0.04 -0.01 0.01 -0.01 0.00 0.02 -0.04 0.03

67 1 0.05 -0.02 0.03 0.02 -0.01 0.01 0.00 -0.01 -0.00

68 1 0.03 -0.04 -0.01 0.01 -0.01 -0.00 0.02 -0.04 -0.03

69 1 0.00 -0.00 0.00 0.01 0.00 0.02 -0.02 -0.02 -0.05

70 1 0.04 -0.03 0.01 0.03 -0.02 0.02 -0.03 0.01 -0.02

71 1 0.02 -0.05 -0.03 0.01 -0.02 -0.01 -0.00 -0.01 -0.01

72 1 0.05 0.02 -0.03 -0.01 0.00 0.01 0.02 0.01 -0.01

73 1 0.03 0.04 0.01 0.01 0.03 0.02 0.02 0.03 0.02

74 1 0.00 0.00 -0.00 -0.02 0.02 0.05 -0.00 0.01 0.02

75 1 0.04 0.03 -0.01 -0.04 -0.02 0.03 0.01 0.01 -0.00

76 1 0.02 0.05 0.03 -0.01 -0.00 0.00 0.01 0.02 0.01

77 30 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00

172 173 174

A2 B2 E

Frequencies -- 1471.9659 1473.2523 1473.2836

Red. masses -- 2.2190 2.1875 2.2431

Frc consts -- 2.8328 2.7974 2.8687

IR Inten -- 0.0000 31.2182 31.4672

Atom AN X Y Z X Y Z X Y Z

1 6 -0.01 -0.01 -0.00 -0.01 0.00 0.00 -0.03 0.00 0.00

2 6 0.02 0.01 0.00 -0.01 0.00 -0.00 -0.03 0.00 -0.00

3 7 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.01 -0.00

4 6 0.02 -0.01 -0.00 0.01 0.00 -0.00 0.03 0.00 -0.00

5 6 -0.01 0.01 0.00 0.01 0.00 0.00 0.03 0.00 0.00

6 6 -0.02 0.02 0.01 -0.00 0.00 0.01 -0.02 -0.01 0.01

7 6 0.01 -0.02 -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 -0.01 -0.02 0.00 -0.00 0.01 -0.00 0.00 0.00 0.00

10 6 0.01 0.01 -0.00 -0.00 0.01 0.00 -0.00 -0.00 -0.00

11 6 -0.01 0.01 0.00 -0.00 -0.01 0.00 0.00 0.00 0.00

12 6 -0.02 -0.02 -0.01 0.00 0.00 0.01 0.01 -0.01 0.01

13 6 0.01 0.02 0.00 0.00 -0.01 -0.00 0.00 0.00 -0.00

14 6 -0.01 -0.01 -0.00 0.00 -0.01 0.00 -0.00 -0.00 0.00

15 6 0.01 -0.01 0.00 0.00 0.01 0.00 0.00 0.00 -0.00

16 6 -0.01 0.02 -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 0.02 -0.02 0.01 0.00 -0.00 0.01 -0.02 -0.01 -0.01

19 6 -0.02 0.01 -0.00 -0.01 -0.00 -0.00 0.03 0.00 0.00

20 6 0.01 -0.01 0.00 -0.01 -0.00 0.00 0.03 0.00 -0.00

21 6 0.01 0.01 -0.00 0.01 -0.00 0.00 -0.03 0.00 -0.00

22 6 -0.02 -0.01 0.00 0.01 -0.00 -0.00 -0.03 0.00 0.00

23 7 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.01 0.00

24 6 0.02 0.02 -0.01 -0.00 -0.00 0.01 0.01 -0.01 -0.01

25 6 -0.02 0.02 -0.06 -0.03 0.03 -0.07 -0.02 0.03 -0.06

26 6 0.04 0.02 0.03 0.04 0.02 0.03 0.04 0.02 0.02

27 6 -0.06 -0.05 -0.00 -0.06 -0.05 -0.00 -0.05 -0.05 -0.00

28 6 -0.02 0.02 -0.05 -0.02 0.02 -0.05 -0.02 0.02 -0.05

29 6 0.05 0.06 -0.00 0.05 0.06 -0.00 0.05 0.05 -0.00

30 6 -0.02 -0.04 0.03 -0.02 -0.04 0.03 -0.02 -0.04 0.03

31 6 -0.02 -0.02 0.05 0.02 0.02 -0.05 0.02 0.02 -0.05

32 6 -0.06 0.05 0.00 0.06 -0.05 -0.00 0.06 -0.06 -0.00

33 6 0.04 -0.02 -0.03 -0.04 0.02 0.03 -0.04 0.02 0.03

34 6 -0.02 -0.02 0.06 0.03 0.03 -0.07 0.03 0.03 -0.07

35 6 -0.02 0.04 -0.03 0.02 -0.04 0.03 0.02 -0.04 0.03

36 6 0.05 -0.06 0.00 -0.05 0.06 -0.00 -0.06 0.06 -0.01

37 6 0.02 0.02 0.06 -0.03 -0.03 -0.07 0.03 0.03 0.07

38 6 0.02 -0.04 -0.03 -0.02 0.04 0.03 0.02 -0.04 -0.03

39 6 -0.05 0.06 0.00 0.05 -0.06 -0.00 -0.06 0.06 0.01

40 6 0.02 0.02 0.05 -0.02 -0.02 -0.05 0.02 0.02 0.05

41 6 0.06 -0.05 0.00 -0.06 0.05 -0.00 0.06 -0.06 0.00

42 6 -0.04 0.02 -0.03 0.04 -0.02 0.03 -0.04 0.02 -0.03

43 6 0.02 -0.02 -0.06 0.03 -0.03 -0.07 -0.02 0.03 0.06

44 6 0.02 0.04 0.03 0.02 0.04 0.03 -0.02 -0.04 -0.03

45 6 -0.05 -0.06 -0.00 -0.05 -0.06 -0.00 0.05 0.05 0.00

46 6 0.02 -0.02 -0.05 0.02 -0.02 -0.05 -0.02 0.02 0.05

47 6 0.06 0.05 -0.00 0.06 0.05 -0.00 -0.05 -0.05 0.00

48 6 -0.04 -0.02 0.03 -0.04 -0.02 0.03 0.04 0.02 -0.02

49 1 0.04 0.02 0.00 -0.01 0.01 -0.00 -0.01 0.02 0.00

50 1 0.04 -0.02 -0.00 0.01 0.01 -0.00 0.01 0.02 0.00

51 1 -0.02 -0.04 0.00 -0.01 0.01 -0.00 0.01 0.00 0.00

52 1 0.02 -0.04 -0.00 -0.01 -0.01 -0.00 -0.00 0.00 -0.00

53 1 0.02 0.04 0.00 0.01 -0.01 -0.00 0.01 0.00 -0.00

54 1 -0.02 0.04 -0.00 0.01 0.01 -0.00 -0.00 0.00 0.00

55 1 -0.04 0.02 -0.00 -0.01 -0.01 -0.00 0.01 0.02 -0.00

56 1 -0.04 -0.02 0.00 0.01 -0.01 -0.00 -0.01 0.02 -0.00

57 1 0.00 -0.06 0.08 -0.00 -0.06 0.08 -0.01 -0.07 0.08

58 1 0.17 0.07 0.13 0.17 0.07 0.13 0.15 0.06 0.12

59 1 0.10 -0.10 0.28 0.10 -0.10 0.28 0.09 -0.09 0.26

60 1 -0.07 -0.17 0.13 -0.07 -0.17 0.13 -0.07 -0.16 0.12

61 1 0.06 -0.00 0.08 0.06 0.00 0.08 0.05 -0.00 0.07

62 1 0.10 0.10 -0.28 -0.10 -0.10 0.28 -0.11 -0.11 0.30

63 1 0.17 -0.07 -0.13 -0.17 0.07 0.13 -0.17 0.08 0.14

64 1 0.00 0.06 -0.08 0.00 -0.06 0.08 0.01 -0.07 0.09

65 1 0.06 0.00 -0.08 -0.06 0.00 0.08 -0.06 -0.00 0.08

66 1 -0.07 0.17 -0.13 0.07 -0.17 0.13 0.09 -0.19 0.14

67 1 -0.06 -0.00 -0.08 0.06 -0.00 0.08 -0.06 -0.00 -0.08

68 1 0.07 -0.17 -0.13 -0.07 0.17 0.13 0.09 -0.19 -0.14

69 1 -0.10 -0.10 -0.28 0.10 0.10 0.28 -0.11 -0.11 -0.30

70 1 -0.17 0.07 -0.13 0.17 -0.07 0.13 -0.17 0.08 -0.14

71 1 -0.00 -0.06 -0.08 -0.00 0.06 0.08 0.01 -0.07 -0.09

72 1 -0.06 0.00 0.08 -0.06 -0.00 0.08 0.05 -0.00 -0.07

73 1 0.07 0.17 0.13 0.07 0.17 0.13 -0.07 -0.16 -0.12

74 1 -0.10 0.10 0.28 -0.10 0.10 0.28 0.09 -0.09 -0.26

75 1 -0.17 -0.07 0.13 -0.17 -0.07 0.13 0.15 0.06 -0.12

76 1 -0.00 0.06 0.08 0.00 0.06 0.08 -0.01 -0.07 -0.08

77 30 -0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00

175 176 177

E A1 B1

Frequencies -- 1473.2836 1476.2188 1482.7581

Red. masses -- 2.2431 7.8517 4.9057

Frc consts -- 2.8687 10.0813 6.3546

IR Inten -- 31.4673 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.00 -0.00 0.19 0.00 0.00 -0.06 -0.07 -0.01

2 6 -0.01 -0.00 0.00 0.17 -0.01 0.00 0.15 0.05 0.01

3 7 0.00 -0.00 -0.00 -0.00 0.07 0.00 -0.08 -0.00 -0.00

4 6 -0.00 0.00 -0.00 -0.17 -0.01 0.00 0.15 -0.05 -0.01

5 6 0.00 -0.00 0.00 -0.19 0.00 0.00 -0.06 0.07 0.01

6 6 0.01 0.01 0.01 0.10 0.10 0.00 -0.07 -0.07 -0.00

7 6 -0.00 -0.03 -0.00 -0.01 -0.17 -0.00 -0.05 0.15 0.01

8 7 0.01 -0.00 -0.00 0.07 -0.00 -0.00 0.00 -0.08 0.00

9 6 -0.00 0.03 -0.00 -0.01 0.17 -0.00 0.05 0.15 -0.01

10 6 -0.00 0.03 0.00 0.00 0.19 -0.00 -0.07 -0.06 0.01

11 6 -0.00 -0.03 0.00 0.00 -0.19 -0.00 0.07 -0.06 -0.01

12 6 0.01 -0.02 -0.01 -0.10 0.10 0.00 -0.07 0.07 -0.00

13 6 -0.00 0.03 0.00 0.01 -0.17 -0.00 -0.05 -0.15 -0.01

14 6 -0.00 0.03 -0.00 -0.00 -0.19 -0.00 0.07 0.06 0.01

15 6 -0.00 -0.03 -0.00 -0.00 0.19 -0.00 -0.07 0.06 -0.01

16 6 -0.00 -0.03 0.00 0.01 0.17 -0.00 0.05 -0.15 0.01

17 7 0.01 -0.00 0.00 -0.07 -0.00 -0.00 -0.00 0.08 0.00

18 6 0.01 0.01 -0.01 -0.10 -0.10 0.00 0.07 0.07 0.00

19 6 -0.00 0.00 0.00 0.17 0.01 0.00 -0.15 0.05 -0.01

20 6 0.00 -0.00 -0.00 0.19 -0.00 0.00 0.06 -0.07 0.01

21 6 -0.00 0.00 0.00 -0.19 -0.00 0.00 0.06 0.07 -0.01

22 6 -0.01 -0.00 -0.00 -0.17 0.01 0.00 -0.15 -0.05 0.01

23 7 0.00 -0.00 0.00 0.00 -0.07 0.00 0.08 -0.00 -0.00

24 6 0.01 -0.02 0.01 0.10 -0.10 0.00 0.07 -0.07 0.00

25 6 -0.03 0.03 -0.07 -0.02 -0.02 -0.00 0.01 0.01 0.00

26 6 0.04 0.02 0.03 -0.01 -0.02 0.02 0.00 0.01 -0.01

27 6 -0.06 -0.06 -0.01 -0.01 0.00 -0.02 0.01 0.00 0.01

28 6 -0.02 0.02 -0.05 0.01 0.01 -0.00 -0.01 -0.01 0.00

29 6 0.06 0.06 -0.00 0.00 -0.01 0.02 0.00 0.01 -0.01

30 6 -0.02 -0.04 0.03 -0.02 -0.01 -0.02 0.01 0.00 0.01

31 6 -0.02 -0.02 0.05 -0.01 0.01 -0.00 -0.01 0.01 0.00

32 6 -0.05 0.05 0.00 0.01 0.00 -0.02 0.01 -0.00 -0.01

33 6 0.04 -0.02 -0.03 0.01 -0.02 0.02 0.00 -0.01 0.01

34 6 -0.03 -0.02 0.06 0.02 -0.02 -0.00 0.01 -0.01 0.00

35 6 -0.02 0.04 -0.02 0.02 -0.01 -0.02 0.01 -0.00 -0.01

36 6 0.05 -0.05 0.00 -0.00 -0.01 0.02 0.00 -0.01 0.01

37 6 -0.03 -0.02 -0.06 -0.02 0.02 -0.00 -0.01 0.01 -0.00

38 6 -0.02 0.04 0.02 -0.02 0.01 -0.02 -0.01 0.00 -0.01

39 6 0.05 -0.05 -0.00 0.00 0.01 0.02 -0.00 0.01 0.01

40 6 -0.02 -0.02 -0.05 0.01 -0.01 -0.00 0.01 -0.01 -0.00

41 6 -0.05 0.05 -0.00 -0.01 -0.00 -0.02 -0.01 0.00 -0.01

42 6 0.04 -0.02 0.03 -0.01 0.02 0.02 -0.00 0.01 0.01

43 6 -0.03 0.03 0.07 0.02 0.02 -0.00 -0.01 -0.01 -0.00

44 6 -0.02 -0.04 -0.03 0.02 0.01 -0.02 -0.01 -0.00 0.01

45 6 0.06 0.06 0.00 -0.00 0.01 0.02 -0.00 -0.01 -0.01

46 6 -0.02 0.02 0.05 -0.01 -0.01 -0.00 0.01 0.01 -0.00

47 6 -0.06 -0.06 0.01 0.01 -0.00 -0.02 -0.01 -0.00 0.01

48 6 0.04 0.02 -0.03 0.01 0.02 0.02 -0.00 -0.01 -0.01

49 1 -0.00 -0.00 0.00 0.02 -0.16 -0.02 0.24 0.14 0.02

50 1 -0.00 0.01 -0.00 -0.02 -0.16 -0.02 0.24 -0.14 -0.02

51 1 -0.02 0.01 0.00 -0.16 0.02 0.02 0.14 0.24 -0.02

52 1 -0.02 -0.01 0.00 -0.16 -0.02 0.02 -0.14 0.24 0.02

53 1 -0.02 0.01 -0.00 0.16 -0.02 0.02 -0.14 -0.24 -0.02

54 1 -0.02 -0.01 -0.00 0.16 0.02 0.02 0.14 -0.24 0.02

55 1 -0.00 0.01 0.00 0.02 0.16 -0.02 -0.24 0.14 -0.02

56 1 -0.00 -0.00 -0.00 -0.02 0.16 -0.02 -0.24 -0.14 0.02

57 1 0.00 -0.06 0.08 0.05 0.09 -0.04 -0.02 -0.04 0.02

58 1 0.19 0.09 0.14 0.08 0.06 0.03 -0.04 -0.03 -0.02

59 1 0.11 -0.11 0.30 0.01 0.01 0.00 -0.01 -0.01 -0.00

60 1 -0.08 -0.17 0.14 0.06 0.08 -0.03 -0.03 -0.04 0.02

61 1 0.07 0.01 0.09 0.09 0.05 0.04 -0.04 -0.02 -0.02

62 1 0.09 0.09 -0.26 -0.01 0.01 0.00 -0.01 0.01 -0.00

63 1 0.16 -0.07 -0.12 -0.08 0.06 0.03 -0.04 0.03 0.02

64 1 0.00 0.05 -0.07 -0.05 0.09 -0.04 -0.02 0.04 -0.02

65 1 0.07 -0.01 -0.08 -0.09 0.05 0.04 -0.04 0.02 0.02

66 1 -0.06 0.15 -0.12 -0.06 0.08 -0.03 -0.03 0.04 -0.02

67 1 0.07 -0.01 0.08 0.09 -0.05 0.04 0.04 -0.02 0.02

68 1 -0.06 0.15 0.12 0.06 -0.08 -0.03 0.03 -0.04 -0.02

69 1 0.09 0.09 0.26 0.01 -0.01 0.00 0.01 -0.01 0.00

70 1 0.16 -0.07 0.12 0.08 -0.06 0.03 0.04 -0.03 0.02

71 1 0.00 0.05 0.07 0.05 -0.09 -0.04 0.02 -0.04 -0.02

72 1 0.07 0.01 -0.09 -0.09 -0.05 0.04 0.04 0.02 -0.02

73 1 -0.08 -0.17 -0.14 -0.06 -0.08 -0.03 0.03 0.04 0.02

74 1 0.11 -0.11 -0.30 -0.01 -0.01 0.00 0.01 0.01 0.00

75 1 0.19 0.09 -0.14 -0.08 -0.06 0.03 0.04 0.03 -0.02

76 1 0.00 -0.06 -0.08 -0.05 -0.09 -0.04 0.02 0.04 0.02

77 30 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00

178 179 180

E E A2

Frequencies -- 1515.3402 1515.3402 1517.8570

Red. masses -- 6.4424 6.4424 7.0729

Frc consts -- 8.7160 8.7160 9.6008

IR Inten -- 150.3997 150.3998 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.08 0.02 0.00 -0.04 -0.03 -0.00 0.04 0.07 0.01

2 6 -0.21 -0.06 -0.00 -0.10 0.07 0.00 -0.14 -0.11 -0.01

3 7 -0.02 -0.02 -0.00 0.05 -0.01 -0.00 0.02 0.00 -0.00

4 6 0.22 0.01 -0.00 0.09 -0.09 -0.00 -0.14 0.11 0.01

5 6 0.09 -0.01 -0.00 0.03 0.04 0.00 0.04 -0.07 -0.01

6 6 -0.13 -0.01 -0.00 -0.13 0.19 -0.00 0.17 -0.17 0.00

7 6 0.07 0.10 -0.00 0.06 -0.21 -0.00 -0.11 0.14 0.01

8 7 -0.01 -0.05 0.00 0.02 -0.02 -0.00 -0.00 -0.02 -0.00

9 6 -0.09 -0.09 0.00 -0.01 0.22 -0.00 0.11 0.14 -0.01

10 6 0.04 -0.03 -0.00 0.01 0.09 -0.00 -0.07 -0.04 0.01

11 6 -0.03 0.04 0.00 -0.02 -0.08 0.00 0.07 -0.04 -0.01

12 6 0.19 0.13 -0.00 0.01 -0.13 0.00 0.17 0.17 -0.00

13 6 -0.09 -0.09 -0.00 -0.01 0.22 0.00 -0.11 -0.14 -0.01

14 6 0.04 -0.03 0.00 0.01 0.09 0.00 0.07 0.04 0.01

15 6 -0.03 0.04 -0.00 -0.02 -0.08 -0.00 -0.07 0.04 -0.01

16 6 0.07 0.10 0.00 0.06 -0.21 0.00 0.11 -0.14 0.01

17 7 -0.01 -0.05 -0.00 0.02 -0.02 0.00 0.00 0.02 -0.00

18 6 -0.13 -0.01 0.00 -0.13 0.19 0.00 -0.17 0.17 0.00

19 6 0.22 0.01 0.00 0.09 -0.09 0.00 0.14 -0.11 0.01

20 6 0.09 -0.01 0.00 0.03 0.04 -0.00 -0.04 0.07 -0.01

21 6 -0.08 0.02 -0.00 -0.04 -0.03 0.00 -0.04 -0.07 0.01

22 6 -0.21 -0.06 0.00 -0.10 0.07 -0.00 0.14 0.11 -0.01

23 7 -0.02 -0.02 0.00 0.05 -0.01 0.00 -0.02 0.00 0.00

24 6 0.19 0.13 0.00 0.01 -0.13 -0.00 -0.17 -0.17 -0.00

25 6 -0.01 -0.03 0.01 0.03 -0.01 0.02 -0.03 0.03 -0.02

26 6 0.00 0.04 -0.04 -0.03 -0.03 0.01 0.02 0.01 0.00

27 6 0.05 0.02 0.04 -0.00 0.01 -0.02 -0.01 -0.02 0.01

28 6 -0.02 -0.03 0.01 0.02 -0.00 0.03 -0.01 0.01 -0.03

29 6 0.00 0.04 -0.04 -0.02 -0.03 0.01 0.02 0.01 0.01

30 6 0.05 0.02 0.04 -0.00 0.02 -0.02 -0.01 -0.02 0.00

31 6 -0.00 -0.02 0.03 0.03 -0.02 -0.01 -0.01 -0.01 0.03

32 6 -0.03 0.02 0.01 -0.04 0.00 0.04 -0.01 0.02 -0.01

33 6 0.02 0.00 -0.02 -0.02 0.05 -0.04 0.02 -0.01 -0.00

34 6 -0.01 -0.03 0.02 0.03 -0.01 -0.01 -0.03 -0.03 0.02

35 6 -0.03 0.03 0.01 -0.04 0.00 0.04 -0.01 0.02 -0.00

36 6 0.01 0.00 -0.02 -0.02 0.05 -0.04 0.02 -0.01 -0.01

37 6 -0.01 -0.03 -0.02 0.03 -0.01 0.01 0.03 0.03 0.02

38 6 -0.03 0.03 -0.01 -0.04 0.00 -0.04 0.01 -0.02 -0.00

39 6 0.01 0.00 0.02 -0.02 0.05 0.04 -0.02 0.01 -0.01

40 6 -0.00 -0.02 -0.03 0.03 -0.02 0.01 0.01 0.01 0.03

41 6 -0.03 0.02 -0.01 -0.04 0.00 -0.04 0.01 -0.02 -0.01

42 6 0.02 0.00 0.02 -0.02 0.05 0.04 -0.02 0.01 -0.00

43 6 -0.01 -0.03 -0.01 0.03 -0.01 -0.02 0.03 -0.03 -0.02

44 6 0.05 0.02 -0.04 -0.00 0.02 0.02 0.01 0.02 0.00

45 6 0.00 0.04 0.04 -0.02 -0.03 -0.01 -0.02 -0.01 0.01

46 6 -0.02 -0.03 -0.01 0.02 -0.00 -0.03 0.01 -0.01 -0.03

47 6 0.05 0.02 -0.04 -0.00 0.01 0.02 0.01 0.02 0.01

48 6 0.00 0.04 0.04 -0.03 -0.03 -0.01 -0.02 -0.01 0.00

49 1 -0.10 0.03 -0.00 0.02 0.02 0.00 -0.17 -0.09 -0.01

50 1 0.06 0.03 0.00 0.09 0.01 -0.00 -0.17 0.09 0.01

51 1 0.01 -0.09 0.00 -0.03 0.06 0.00 0.09 0.17 -0.01

52 1 0.02 -0.02 -0.00 -0.03 -0.10 -0.00 -0.09 0.17 0.01

53 1 0.01 -0.09 -0.00 -0.03 0.06 -0.00 -0.09 -0.17 -0.01

54 1 0.02 -0.02 0.00 -0.03 -0.10 0.00 0.09 -0.17 0.01

55 1 0.06 0.03 -0.00 0.09 0.01 0.00 0.17 -0.09 0.01

56 1 -0.10 0.03 0.00 0.02 0.02 -0.00 0.17 0.09 -0.01

57 1 -0.10 -0.15 0.05 0.06 0.10 -0.08 -0.03 -0.04 0.06

58 1 -0.17 -0.11 -0.09 0.02 0.03 -0.02 0.04 0.01 0.05

59 1 -0.05 -0.02 -0.04 -0.02 0.05 -0.11 0.04 -0.04 0.12

60 1 -0.10 -0.14 0.05 0.06 0.10 -0.07 -0.01 -0.04 0.05

61 1 -0.17 -0.11 -0.09 0.02 0.02 -0.02 0.04 0.03 0.06

62 1 0.05 0.02 -0.11 0.02 -0.05 0.04 0.04 0.04 -0.12

63 1 0.10 -0.06 -0.07 0.14 -0.10 -0.05 0.04 -0.01 -0.05

64 1 0.02 -0.02 -0.02 0.11 -0.17 0.09 -0.03 0.04 -0.06

65 1 0.10 -0.06 -0.08 0.15 -0.10 -0.05 0.04 -0.03 -0.06

66 1 0.03 -0.02 -0.02 0.11 -0.17 0.09 -0.01 0.04 -0.05

67 1 0.10 -0.06 0.08 0.15 -0.10 0.05 -0.04 0.03 -0.06

68 1 0.03 -0.02 0.02 0.11 -0.17 -0.09 0.01 -0.04 -0.05

69 1 0.05 0.02 0.11 0.02 -0.05 -0.04 -0.04 -0.04 -0.12

70 1 0.10 -0.06 0.07 0.14 -0.10 0.05 -0.04 0.01 -0.05

71 1 0.02 -0.02 0.02 0.11 -0.17 -0.09 0.03 -0.04 -0.06

72 1 -0.17 -0.11 0.09 0.02 0.02 0.02 -0.04 -0.03 0.06

73 1 -0.10 -0.14 -0.05 0.06 0.10 0.07 0.01 0.04 0.05

74 1 -0.05 -0.02 0.04 -0.02 0.05 0.11 -0.04 0.04 0.12

75 1 -0.17 -0.11 0.09 0.02 0.03 0.02 -0.04 -0.01 0.05

76 1 -0.10 -0.15 -0.05 0.06 0.10 0.08 0.03 0.04 0.06

77 30 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00

181 182 183

B2 A1 B1

Frequencies -- 1525.5571 1527.9408 1528.1657

Red. masses -- 5.3142 2.3240 2.3075

Frc consts -- 7.2869 3.1967 3.1749

IR Inten -- 1.4327 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.21 0.01 0.00 0.02 0.00 0.00 0.00 0.00 0.00

2 6 -0.07 0.02 0.00 -0.00 -0.00 0.00 -0.01 -0.00 -0.00

3 7 0.00 -0.01 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

4 6 0.07 0.02 0.00 0.00 -0.00 0.00 -0.01 0.00 0.00

5 6 -0.21 0.01 0.00 -0.02 0.00 0.00 0.00 -0.00 -0.00

6 6 -0.01 0.01 -0.00 0.02 0.02 -0.00 0.02 0.02 0.00

7 6 -0.02 -0.07 0.00 -0.00 0.00 -0.00 0.00 -0.01 -0.00

8 7 0.01 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

9 6 -0.02 0.07 0.00 -0.00 -0.00 -0.00 -0.00 -0.01 0.00

10 6 -0.01 -0.21 0.00 0.00 0.02 -0.00 0.00 0.00 -0.00

11 6 -0.01 0.21 0.00 0.00 -0.02 -0.00 -0.00 0.00 0.00

12 6 0.01 0.01 -0.00 -0.02 0.02 -0.00 0.02 -0.02 -0.00

13 6 0.02 -0.07 0.00 0.00 0.00 -0.00 0.00 0.01 0.00

14 6 0.01 0.21 0.00 -0.00 -0.02 -0.00 -0.00 -0.00 -0.00

15 6 0.01 -0.21 0.00 -0.00 0.02 -0.00 0.00 -0.00 0.00

16 6 0.02 0.07 0.00 0.00 -0.00 -0.00 -0.00 0.01 -0.00

17 7 -0.01 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

18 6 0.01 -0.01 -0.00 -0.02 -0.02 -0.00 -0.02 -0.02 0.00

19 6 -0.07 -0.02 0.00 -0.00 0.00 0.00 0.01 -0.00 0.00

20 6 0.21 -0.01 0.00 0.02 -0.00 0.00 -0.00 0.00 -0.00

21 6 -0.21 -0.01 0.00 -0.02 -0.00 0.00 -0.00 -0.00 0.00

22 6 0.07 -0.02 0.00 0.00 0.00 0.00 0.01 0.00 -0.00

23 7 0.00 0.01 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00

24 6 -0.01 -0.01 -0.00 0.02 -0.02 -0.00 -0.02 0.02 -0.00

25 6 -0.00 0.00 -0.00 -0.05 -0.05 -0.00 -0.06 -0.06 -0.00

26 6 0.00 0.00 -0.00 0.01 0.04 -0.04 0.01 0.04 -0.04

27 6 -0.00 -0.00 0.00 0.06 0.02 0.05 0.06 0.02 0.05

28 6 -0.00 0.00 -0.00 -0.04 -0.04 -0.00 -0.04 -0.04 -0.00

29 6 0.00 0.00 0.00 0.02 0.06 -0.05 0.02 0.06 -0.05

30 6 -0.00 -0.00 -0.00 0.04 0.01 0.04 0.04 0.01 0.04

31 6 0.00 0.00 -0.00 0.04 -0.04 -0.00 -0.04 0.04 0.00

32 6 0.00 -0.00 0.00 -0.06 0.02 0.05 0.06 -0.02 -0.05

33 6 -0.00 0.00 -0.00 -0.01 0.04 -0.04 0.01 -0.04 0.04

34 6 0.00 0.00 -0.00 0.05 -0.05 -0.00 -0.06 0.06 0.00

35 6 0.00 -0.00 -0.00 -0.04 0.01 0.04 0.04 -0.01 -0.04

36 6 -0.00 0.00 0.00 -0.02 0.06 -0.05 0.02 -0.06 0.05

37 6 -0.00 -0.00 -0.00 -0.05 0.05 -0.00 0.06 -0.06 0.00

38 6 -0.00 0.00 -0.00 0.04 -0.01 0.04 -0.04 0.01 -0.04

39 6 0.00 -0.00 0.00 0.02 -0.06 -0.05 -0.02 0.06 0.05

40 6 -0.00 -0.00 -0.00 -0.04 0.04 -0.00 0.04 -0.04 0.00

41 6 -0.00 0.00 0.00 0.06 -0.02 0.05 -0.06 0.02 -0.05

42 6 0.00 -0.00 -0.00 0.01 -0.04 -0.04 -0.01 0.04 0.04

43 6 0.00 -0.00 -0.00 0.05 0.05 -0.00 0.06 0.06 -0.00

44 6 0.00 0.00 -0.00 -0.04 -0.01 0.04 -0.04 -0.01 0.04

45 6 -0.00 -0.00 0.00 -0.02 -0.06 -0.05 -0.02 -0.06 -0.05

46 6 0.00 -0.00 -0.00 0.04 0.04 -0.00 0.04 0.04 -0.00

47 6 0.00 0.00 0.00 -0.06 -0.02 0.05 -0.06 -0.02 0.05

48 6 -0.00 -0.00 -0.00 -0.01 -0.04 -0.04 -0.01 -0.04 -0.04

49 1 -0.11 -0.25 -0.03 -0.01 -0.03 -0.00 -0.01 -0.01 0.00

50 1 0.11 -0.25 -0.03 0.01 -0.03 -0.00 -0.01 0.01 -0.00

51 1 0.25 0.11 -0.03 -0.03 -0.01 0.00 -0.01 -0.01 -0.00

52 1 0.25 -0.11 -0.03 -0.03 0.01 0.00 0.01 -0.01 0.00

53 1 -0.25 -0.11 -0.03 0.03 0.01 0.00 0.01 0.01 -0.00

54 1 -0.25 0.11 -0.03 0.03 -0.01 0.00 -0.01 0.01 0.00

55 1 -0.11 0.25 -0.03 -0.01 0.03 -0.00 0.01 -0.01 -0.00

56 1 0.11 0.25 -0.03 0.01 0.03 -0.00 0.01 0.01 0.00

57 1 -0.00 -0.01 0.01 -0.12 -0.17 0.08 -0.12 -0.18 0.08

58 1 0.01 0.00 0.01 -0.18 -0.12 -0.09 -0.19 -0.12 -0.09

59 1 0.01 -0.01 0.01 -0.04 -0.04 0.00 -0.04 -0.04 0.00

60 1 -0.00 -0.01 0.01 -0.12 -0.18 0.09 -0.12 -0.19 0.09

61 1 0.01 0.00 0.01 -0.17 -0.12 -0.08 -0.18 -0.12 -0.08

62 1 -0.01 -0.01 0.01 0.04 -0.04 0.00 -0.04 0.04 -0.00

63 1 -0.01 0.00 0.01 0.18 -0.12 -0.09 -0.19 0.12 0.09

64 1 0.00 -0.01 0.01 0.12 -0.17 0.08 -0.12 0.18 -0.08

65 1 -0.01 0.00 0.01 0.17 -0.12 -0.08 -0.18 0.12 0.08

66 1 0.00 -0.01 0.01 0.12 -0.18 0.09 -0.12 0.19 -0.09

67 1 0.01 -0.00 0.01 -0.17 0.12 -0.08 0.18 -0.12 0.08

68 1 -0.00 0.01 0.01 -0.12 0.18 0.09 0.12 -0.19 -0.09

69 1 0.01 0.01 0.01 -0.04 0.04 0.00 0.04 -0.04 -0.00

70 1 0.01 -0.00 0.01 -0.18 0.12 -0.09 0.19 -0.12 0.09

71 1 -0.00 0.01 0.01 -0.12 0.17 0.08 0.12 -0.18 -0.08

72 1 -0.01 -0.00 0.01 0.17 0.12 -0.08 0.18 0.12 -0.08

73 1 0.00 0.01 0.01 0.12 0.18 0.09 0.12 0.19 0.09

74 1 -0.01 0.01 0.01 0.04 0.04 0.00 0.04 0.04 0.00

75 1 -0.01 -0.00 0.01 0.18 0.12 -0.09 0.19 0.12 -0.09

76 1 0.00 0.01 0.01 0.12 0.17 0.08 0.12 0.18 0.08

77 30 0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

184 185 186

E E E

Frequencies -- 1528.9089 1528.9089 1553.6346

Red. masses -- 2.5868 2.5868 5.9616

Frc consts -- 3.5627 3.5627 8.4783

IR Inten -- 0.4186 0.4186 57.6429

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.01 -0.00 -0.05 -0.00 -0.00 -0.25 -0.02 -0.00

2 6 0.01 0.02 0.00 -0.04 -0.01 -0.00 0.10 -0.04 -0.00

3 7 0.00 -0.00 -0.00 -0.00 -0.01 -0.00 0.01 0.03 0.00

4 6 0.01 -0.02 -0.00 0.04 -0.01 -0.00 -0.15 -0.03 -0.00

5 6 -0.00 0.01 0.00 0.05 -0.00 -0.00 0.26 -0.03 -0.00

6 6 0.00 0.06 0.00 -0.06 -0.00 0.00 0.05 0.09 0.00

7 6 0.01 -0.04 -0.00 0.02 -0.01 -0.00 0.01 -0.13 -0.00

8 7 0.01 -0.00 -0.00 -0.00 -0.00 0.00 0.01 0.04 -0.00

9 6 0.01 0.04 -0.00 -0.02 -0.01 0.00 -0.02 -0.07 0.00

10 6 0.00 0.05 -0.00 0.01 0.00 -0.00 0.01 -0.04 -0.00

11 6 0.00 -0.05 -0.00 -0.01 0.00 0.00 -0.03 0.08 0.00

12 6 0.00 -0.06 -0.00 0.06 -0.00 0.00 -0.02 0.08 0.00

13 6 0.01 0.04 0.00 -0.02 -0.01 -0.00 -0.02 -0.07 -0.00

14 6 0.00 0.05 0.00 0.01 0.00 0.00 0.01 -0.04 0.00

15 6 0.00 -0.05 0.00 -0.01 0.00 -0.00 -0.03 0.08 -0.00

16 6 0.01 -0.04 0.00 0.02 -0.01 0.00 0.01 -0.13 0.00

17 7 0.01 -0.00 0.00 -0.00 -0.00 -0.00 0.01 0.04 0.00

18 6 0.00 0.06 -0.00 -0.06 -0.00 -0.00 0.05 0.09 -0.00

19 6 0.01 -0.02 0.00 0.04 -0.01 0.00 -0.15 -0.03 0.00

20 6 -0.00 0.01 -0.00 0.05 -0.00 0.00 0.26 -0.03 0.00

21 6 -0.00 -0.01 0.00 -0.05 -0.00 0.00 -0.25 -0.02 0.00

22 6 0.01 0.02 -0.00 -0.04 -0.01 0.00 0.10 -0.04 0.00

23 7 0.00 -0.00 0.00 -0.00 -0.01 0.00 0.01 0.03 -0.00

24 6 0.00 -0.06 0.00 0.06 -0.00 -0.00 -0.02 0.08 -0.00

25 6 -0.05 -0.06 0.00 0.06 0.05 0.00 -0.03 -0.03 0.00

26 6 0.01 0.04 -0.04 -0.01 -0.04 0.04 -0.00 0.00 -0.01

27 6 0.06 0.03 0.04 -0.06 -0.02 -0.05 0.01 0.01 0.01

28 6 -0.04 -0.04 0.00 0.04 0.04 0.00 -0.01 -0.01 0.01

29 6 0.02 0.06 -0.05 -0.03 -0.06 0.04 0.00 0.01 -0.01

30 6 0.04 0.01 0.04 -0.04 -0.01 -0.04 0.01 0.00 0.01

31 6 -0.04 0.04 -0.00 -0.04 0.04 0.00 0.00 -0.01 0.01

32 6 0.06 -0.03 -0.04 0.06 -0.02 -0.05 -0.01 0.01 0.00

33 6 0.01 -0.04 0.04 0.01 -0.04 0.04 0.00 -0.00 -0.00

34 6 -0.05 0.06 -0.00 -0.06 0.05 0.00 0.01 -0.02 0.00

35 6 0.04 -0.01 -0.04 0.04 -0.01 -0.04 -0.01 0.01 0.01

36 6 0.02 -0.06 0.05 0.03 -0.06 0.04 0.00 0.01 -0.01

37 6 -0.05 0.06 0.00 -0.06 0.05 -0.00 0.01 -0.02 -0.00

38 6 0.04 -0.01 0.04 0.04 -0.01 0.04 -0.01 0.01 -0.01

39 6 0.02 -0.06 -0.05 0.03 -0.06 -0.04 0.00 0.01 0.01

40 6 -0.04 0.04 0.00 -0.04 0.04 -0.00 0.00 -0.01 -0.01

41 6 0.06 -0.03 0.04 0.06 -0.02 0.05 -0.01 0.01 -0.00

42 6 0.01 -0.04 -0.04 0.01 -0.04 -0.04 0.00 -0.00 0.00

43 6 -0.05 -0.06 -0.00 0.06 0.05 -0.00 -0.03 -0.03 -0.00

44 6 0.04 0.01 -0.04 -0.04 -0.01 0.04 0.01 0.00 -0.01

45 6 0.02 0.06 0.05 -0.03 -0.06 -0.04 0.00 0.01 0.01

46 6 -0.04 -0.04 -0.00 0.04 0.04 -0.00 -0.01 -0.01 -0.01

47 6 0.06 0.03 -0.04 -0.06 -0.02 0.05 0.01 0.01 -0.01

48 6 0.01 0.04 0.04 -0.01 -0.04 -0.04 -0.00 0.00 0.01

49 1 0.02 0.01 0.00 -0.00 0.05 0.00 0.12 0.30 0.03

50 1 0.02 -0.01 -0.00 0.00 0.05 0.01 -0.15 0.32 0.03

51 1 -0.05 0.00 0.01 -0.01 -0.02 0.00 0.02 -0.04 -0.00

52 1 -0.05 -0.00 0.00 0.01 -0.02 -0.00 0.12 -0.10 -0.01

53 1 -0.05 0.00 -0.01 -0.01 -0.02 -0.00 0.02 -0.04 0.00

54 1 -0.05 -0.00 -0.00 0.01 -0.02 0.00 0.12 -0.10 0.01

55 1 0.02 -0.01 0.00 0.00 0.05 -0.01 -0.15 0.32 -0.03

56 1 0.02 0.01 -0.00 -0.00 0.05 -0.00 0.12 0.30 -0.03

57 1 -0.12 -0.16 0.07 0.12 0.18 -0.08 -0.02 -0.03 0.01

58 1 -0.19 -0.12 -0.09 0.18 0.12 0.08 -0.04 -0.02 -0.02

59 1 -0.05 -0.04 -0.01 0.04 0.05 -0.01 -0.02 -0.00 -0.02

60 1 -0.12 -0.18 0.08 0.12 0.19 -0.09 -0.02 -0.03 0.01

61 1 -0.18 -0.12 -0.08 0.17 0.12 0.07 -0.04 -0.03 -0.02

62 1 -0.05 0.04 0.01 -0.04 0.05 -0.01 0.02 0.00 -0.03

63 1 -0.19 0.12 0.09 -0.18 0.12 0.08 0.03 -0.01 -0.02

64 1 -0.12 0.17 -0.07 -0.12 0.18 -0.08 0.01 -0.01 -0.00

65 1 -0.18 0.12 0.08 -0.16 0.12 0.07 0.03 -0.03 -0.02

66 1 -0.12 0.18 -0.08 -0.12 0.19 -0.09 0.02 -0.02 0.00

67 1 -0.18 0.12 -0.08 -0.16 0.12 -0.07 0.03 -0.03 0.02

68 1 -0.12 0.18 0.08 -0.12 0.19 0.09 0.02 -0.02 -0.00

69 1 -0.05 0.04 -0.01 -0.04 0.05 0.01 0.02 0.00 0.03

70 1 -0.19 0.12 -0.09 -0.18 0.12 -0.08 0.03 -0.01 0.02

71 1 -0.12 0.17 0.07 -0.12 0.18 0.08 0.01 -0.01 0.00

72 1 -0.18 -0.12 0.08 0.17 0.12 -0.07 -0.04 -0.03 0.02

73 1 -0.12 -0.18 -0.08 0.12 0.19 0.09 -0.02 -0.03 -0.01

74 1 -0.05 -0.04 0.01 0.04 0.05 0.01 -0.02 -0.00 0.02

75 1 -0.19 -0.12 0.09 0.18 0.12 -0.08 -0.04 -0.02 0.02

76 1 -0.12 -0.16 -0.07 0.12 0.18 0.08 -0.02 -0.03 -0.01

77 30 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

187 188 189

E B2 A1

Frequencies -- 1553.6346 1575.5021 1576.6880

Red. masses -- 5.9616 10.4762 6.4725

Frc consts -- 8.4783 15.3211 9.4801

IR Inten -- 57.6428 0.0938 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.08 -0.03 -0.00 0.08 -0.02 -0.00 0.17 0.02 0.00

2 6 0.13 0.01 0.00 0.22 0.08 0.01 -0.16 0.02 -0.00

3 7 -0.04 0.01 0.00 -0.00 -0.01 0.00 -0.00 -0.04 -0.00

4 6 0.07 -0.02 -0.00 -0.22 0.08 0.01 0.16 0.02 -0.00

5 6 0.04 0.01 0.00 -0.08 -0.02 -0.00 -0.17 0.02 0.00

6 6 -0.08 -0.02 0.00 0.21 -0.21 -0.00 -0.08 -0.08 0.00

7 6 0.04 0.10 -0.00 -0.08 0.22 0.01 0.02 0.16 0.00

8 7 -0.03 0.01 0.00 0.01 0.00 0.00 -0.04 -0.00 0.00

9 6 0.03 -0.15 -0.00 -0.08 -0.22 0.01 0.02 -0.16 0.00

10 6 0.03 0.26 -0.00 0.02 -0.08 -0.00 0.02 0.17 -0.00

11 6 0.02 -0.25 -0.00 0.02 0.08 -0.00 0.02 -0.17 -0.00

12 6 -0.09 0.05 -0.00 -0.21 -0.21 -0.00 0.08 -0.08 0.00

13 6 0.03 -0.15 0.00 0.08 0.22 0.01 -0.02 0.16 0.00

14 6 0.03 0.26 0.00 -0.02 0.08 -0.00 -0.02 -0.17 -0.00

15 6 0.02 -0.25 0.00 -0.02 -0.08 -0.00 -0.02 0.17 -0.00

16 6 0.04 0.10 0.00 0.08 -0.22 0.01 -0.02 -0.16 0.00

17 7 -0.03 0.01 -0.00 -0.01 -0.00 0.00 0.04 0.00 0.00

18 6 -0.08 -0.02 -0.00 -0.21 0.21 -0.00 0.08 0.08 0.00

19 6 0.07 -0.02 0.00 0.22 -0.08 0.01 -0.16 -0.02 -0.00

20 6 0.04 0.01 -0.00 0.08 0.02 -0.00 0.17 -0.02 0.00

21 6 -0.08 -0.03 0.00 -0.08 0.02 -0.00 -0.17 -0.02 0.00

22 6 0.13 0.01 -0.00 -0.22 -0.08 0.01 0.16 -0.02 -0.00

23 7 -0.04 0.01 -0.00 -0.00 0.01 0.00 -0.00 0.04 -0.00

24 6 -0.09 0.05 0.00 0.21 0.21 -0.00 -0.08 0.08 0.00

25 6 0.02 0.01 0.00 -0.01 0.01 0.01 0.02 0.02 -0.00

26 6 -0.01 -0.01 0.01 0.02 0.02 -0.01 -0.00 -0.00 0.01

27 6 -0.01 0.00 -0.01 0.01 -0.01 0.02 -0.01 -0.00 -0.00

28 6 0.01 0.00 0.01 -0.02 0.02 -0.05 0.00 0.00 0.00

29 6 -0.01 -0.01 0.00 0.01 -0.01 0.02 -0.00 -0.01 0.00

30 6 0.00 0.00 -0.00 -0.02 -0.02 -0.01 -0.00 -0.00 -0.01

31 6 0.01 -0.01 -0.01 0.02 0.02 -0.05 -0.00 0.00 0.00

32 6 -0.01 0.00 0.01 -0.01 -0.01 0.02 0.01 -0.00 -0.00

33 6 -0.00 0.01 -0.01 -0.02 0.02 -0.01 0.00 -0.00 0.01

34 6 0.03 -0.03 -0.00 0.01 0.01 0.01 -0.02 0.02 -0.00

35 6 -0.00 -0.00 0.01 0.02 -0.02 -0.01 0.00 -0.00 -0.01

36 6 -0.01 0.01 -0.01 -0.01 -0.01 0.02 0.00 -0.01 0.00

37 6 0.03 -0.03 0.00 -0.01 -0.01 0.01 0.02 -0.02 -0.00

38 6 -0.00 -0.00 -0.01 -0.02 0.02 -0.01 -0.00 0.00 -0.01

39 6 -0.01 0.01 0.01 0.01 0.01 0.02 -0.00 0.01 0.00

40 6 0.01 -0.01 0.01 -0.02 -0.02 -0.05 0.00 -0.00 0.00

41 6 -0.01 0.00 -0.01 0.01 0.01 0.02 -0.01 0.00 -0.00

42 6 -0.00 0.01 0.01 0.02 -0.02 -0.01 -0.00 0.00 0.01

43 6 0.02 0.01 -0.00 0.01 -0.01 0.01 -0.02 -0.02 -0.00

44 6 0.00 0.00 0.00 0.02 0.02 -0.01 0.00 0.00 -0.01

45 6 -0.01 -0.01 -0.00 -0.01 0.01 0.02 0.00 0.01 0.00

46 6 0.01 0.00 -0.01 0.02 -0.02 -0.05 -0.00 -0.00 0.00

47 6 -0.01 0.00 0.01 -0.01 0.01 0.02 0.01 0.00 -0.00

48 6 -0.01 -0.01 -0.01 -0.02 -0.02 -0.01 0.00 0.00 0.01

49 1 0.10 0.12 0.01 0.07 -0.04 -0.00 -0.12 -0.22 -0.02

50 1 0.04 0.02 0.00 -0.07 -0.04 -0.00 0.12 -0.22 -0.02

51 1 -0.32 -0.15 0.03 0.04 -0.07 -0.00 -0.22 -0.12 0.02

52 1 -0.30 0.12 0.03 0.04 0.07 -0.00 -0.22 0.12 0.02

53 1 -0.32 -0.15 -0.03 -0.04 0.07 -0.00 0.22 0.12 0.02

54 1 -0.30 0.12 -0.03 -0.04 -0.07 -0.00 0.22 -0.12 0.02

55 1 0.04 0.02 -0.00 0.07 0.04 -0.00 -0.12 0.22 -0.02

56 1 0.10 0.12 -0.01 -0.07 0.04 -0.00 0.12 0.22 -0.02

57 1 0.03 0.03 -0.02 -0.04 -0.04 0.04 0.01 0.02 -0.01

58 1 0.02 0.02 0.00 0.00 -0.01 0.02 0.02 0.01 0.01

59 1 -0.00 0.02 -0.03 0.03 -0.03 0.09 0.01 0.01 -0.00

60 1 0.01 0.03 -0.02 0.01 -0.00 0.02 0.01 0.02 -0.01

61 1 0.01 0.01 -0.00 0.04 0.04 0.04 0.02 0.01 0.01

62 1 0.00 -0.02 0.02 -0.03 -0.03 0.09 -0.01 0.01 -0.00

63 1 0.03 -0.02 -0.01 -0.00 -0.01 0.02 -0.02 0.01 0.01

64 1 0.03 -0.04 0.02 0.04 -0.04 0.04 -0.01 0.02 -0.01

65 1 0.03 -0.02 -0.01 -0.04 0.04 0.04 -0.02 0.01 0.01

66 1 0.02 -0.04 0.02 -0.01 -0.00 0.02 -0.01 0.02 -0.01

67 1 0.03 -0.02 0.01 0.04 -0.04 0.04 0.02 -0.01 0.01

68 1 0.02 -0.04 -0.02 0.01 0.00 0.02 0.01 -0.02 -0.01

69 1 0.00 -0.02 -0.02 0.03 0.03 0.09 0.01 -0.01 -0.00

70 1 0.03 -0.02 0.01 0.00 0.01 0.02 0.02 -0.01 0.01

71 1 0.03 -0.04 -0.02 -0.04 0.04 0.04 0.01 -0.02 -0.01

72 1 0.01 0.01 0.00 -0.04 -0.04 0.04 -0.02 -0.01 0.01

73 1 0.01 0.03 0.02 -0.01 0.00 0.02 -0.01 -0.02 -0.01

74 1 -0.00 0.02 0.03 -0.03 0.03 0.09 -0.01 -0.01 -0.00

75 1 0.02 0.02 -0.00 -0.00 0.01 0.02 -0.02 -0.01 0.01

76 1 0.03 0.03 0.02 0.04 0.04 0.04 -0.01 -0.02 -0.01

77 30 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 0.00

190 191 192

E E A2

Frequencies -- 1618.2256 1618.2256 1618.4110

Red. masses -- 5.4670 5.4670 5.4836

Frc consts -- 8.4348 8.4348 8.4624

IR Inten -- 1.2541 1.2541 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.00 0.00 0.01 0.00 0.00 0.00 0.00 -0.00

2 6 0.00 0.01 -0.00 0.00 0.01 -0.00 -0.01 -0.01 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 -0.01 0.00 -0.00 0.01 -0.00 -0.01 0.01 -0.00

5 6 -0.00 0.00 -0.00 -0.01 0.00 0.00 0.00 -0.00 0.00

6 6 -0.01 0.01 -0.01 0.01 -0.01 0.01 0.01 -0.01 0.01

7 6 0.01 -0.00 0.00 -0.01 0.00 -0.00 -0.01 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 0.01 0.00 0.00 0.01 0.00 0.00 0.01 0.01 0.00

10 6 0.00 0.01 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

11 6 0.00 -0.01 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

12 6 -0.01 -0.01 0.01 -0.01 -0.01 0.01 0.01 0.01 -0.01

13 6 0.01 0.00 -0.00 0.01 0.00 -0.00 -0.01 -0.01 0.00

14 6 0.00 0.01 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

15 6 0.00 -0.01 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

16 6 0.01 -0.00 -0.00 -0.01 0.00 0.00 0.01 -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 -0.01 0.01 0.01 0.01 -0.01 -0.01 -0.01 0.01 0.01

19 6 0.00 -0.01 -0.00 -0.00 0.01 0.00 0.01 -0.01 -0.00

20 6 -0.00 0.00 0.00 -0.01 0.00 -0.00 -0.00 0.00 0.00

21 6 -0.00 -0.00 -0.00 0.01 0.00 -0.00 -0.00 -0.00 -0.00

22 6 0.00 0.01 0.00 0.00 0.01 0.00 0.01 0.01 0.00

23 7 0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

24 6 -0.01 -0.01 -0.01 -0.01 -0.01 -0.01 -0.01 -0.01 -0.01

25 6 0.05 -0.05 0.12 -0.05 0.05 -0.12 -0.05 0.05 -0.12

26 6 0.01 0.07 -0.08 -0.01 -0.07 0.08 -0.01 -0.07 0.08

27 6 0.06 -0.01 0.09 -0.06 0.01 -0.09 -0.06 0.01 -0.09

28 6 -0.06 0.06 -0.17 0.06 -0.06 0.17 0.06 -0.06 0.17

29 6 0.01 -0.06 0.09 -0.01 0.06 -0.09 -0.01 0.06 -0.09

30 6 -0.07 -0.01 -0.08 0.07 0.01 0.08 0.07 0.01 0.08

31 6 -0.06 -0.06 0.17 -0.06 -0.06 0.17 0.06 0.06 -0.17

32 6 0.06 0.01 -0.09 0.06 0.01 -0.09 -0.06 -0.01 0.09

33 6 0.01 -0.07 0.08 0.01 -0.07 0.08 -0.01 0.07 -0.08

34 6 0.05 0.05 -0.12 0.05 0.05 -0.12 -0.05 -0.05 0.12

35 6 -0.07 0.01 0.08 -0.07 0.01 0.08 0.07 -0.01 -0.08

36 6 0.01 0.06 -0.09 0.01 0.06 -0.09 -0.01 -0.06 0.09

37 6 0.05 0.05 0.12 0.05 0.05 0.12 0.05 0.05 0.12

38 6 -0.07 0.01 -0.08 -0.07 0.01 -0.08 -0.07 0.01 -0.08

39 6 0.01 0.06 0.09 0.01 0.06 0.09 0.01 0.06 0.09

40 6 -0.06 -0.06 -0.17 -0.06 -0.06 -0.17 -0.06 -0.06 -0.17

41 6 0.06 0.01 0.09 0.06 0.01 0.09 0.06 0.01 0.09

42 6 0.01 -0.07 -0.08 0.01 -0.07 -0.08 0.01 -0.07 -0.08

43 6 0.05 -0.05 -0.12 -0.05 0.05 0.12 0.05 -0.05 -0.12

44 6 -0.07 -0.01 0.08 0.07 0.01 -0.08 -0.07 -0.01 0.08

45 6 0.01 -0.06 -0.09 -0.01 0.06 0.09 0.01 -0.06 -0.09

46 6 -0.06 0.06 0.17 0.06 -0.06 -0.17 -0.06 0.06 0.17

47 6 0.06 -0.01 -0.09 -0.06 0.01 0.09 0.06 -0.01 -0.09

48 6 0.01 0.07 0.08 -0.01 -0.07 -0.08 0.01 0.07 0.08

49 1 -0.00 -0.00 -0.00 -0.00 -0.01 -0.00 -0.00 0.00 0.00

50 1 -0.00 0.00 0.00 0.00 -0.01 -0.00 -0.00 -0.00 -0.00

51 1 -0.01 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00

52 1 -0.01 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00

53 1 -0.01 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00

54 1 -0.01 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00

55 1 -0.00 0.00 -0.00 0.00 -0.01 0.00 0.00 0.00 -0.00

56 1 -0.00 -0.00 0.00 -0.00 -0.01 0.00 0.00 -0.00 0.00

57 1 -0.10 -0.12 0.02 0.10 0.12 -0.02 0.10 0.12 -0.02

58 1 -0.07 -0.09 0.03 0.07 0.09 -0.03 0.07 0.09 -0.03

59 1 0.08 -0.08 0.23 -0.09 0.08 -0.23 -0.08 0.08 -0.23

60 1 0.09 0.07 0.03 -0.09 -0.07 -0.03 -0.09 -0.07 -0.03

61 1 0.12 0.10 0.02 -0.12 -0.10 -0.02 -0.12 -0.10 -0.02

62 1 0.08 0.09 -0.23 0.08 0.08 -0.23 -0.08 -0.08 0.23

63 1 -0.07 0.09 -0.03 -0.07 0.09 -0.03 0.07 -0.09 0.03

64 1 -0.10 0.12 -0.02 -0.10 0.12 -0.02 0.10 -0.12 0.02

65 1 0.12 -0.10 -0.02 0.12 -0.10 -0.02 -0.12 0.10 0.02

66 1 0.09 -0.07 -0.03 0.09 -0.07 -0.03 -0.09 0.07 0.03

67 1 0.12 -0.10 0.02 0.12 -0.10 0.02 0.12 -0.10 0.02

68 1 0.09 -0.07 0.03 0.09 -0.07 0.03 0.09 -0.07 0.03

69 1 0.08 0.09 0.23 0.08 0.08 0.23 0.08 0.08 0.23

70 1 -0.07 0.09 0.03 -0.07 0.09 0.03 -0.07 0.09 0.03

71 1 -0.10 0.12 0.02 -0.10 0.12 0.02 -0.10 0.12 0.02

72 1 0.12 0.10 -0.02 -0.12 -0.10 0.02 0.12 0.10 -0.02

73 1 0.09 0.07 -0.03 -0.09 -0.07 0.03 0.09 0.07 -0.03

74 1 0.08 -0.08 -0.23 -0.09 0.08 0.23 0.08 -0.08 -0.23

75 1 -0.07 -0.09 -0.03 0.07 0.09 0.03 -0.07 -0.09 -0.03

76 1 -0.10 -0.12 -0.02 0.10 0.12 0.02 -0.10 -0.12 -0.02

77 30 0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00

193 194 195

B2 B1 E

Frequencies -- 1618.8221 1643.2028 1643.2434

Red. masses -- 5.5518 5.6688 5.6695

Frc consts -- 8.5721 9.0183 9.0198

IR Inten -- 7.4300 0.0000 28.7060

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

2 6 0.02 0.01 -0.00 0.01 0.00 -0.00 0.00 0.00 -0.00

3 7 0.00 -0.00 -0.00 -0.01 -0.00 -0.00 -0.00 -0.00 -0.00

4 6 -0.02 0.01 -0.00 0.01 -0.00 0.00 -0.00 0.00 -0.00

5 6 -0.01 -0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

6 6 0.03 -0.03 0.01 0.01 0.01 -0.00 -0.01 -0.01 0.00

7 6 -0.01 0.02 -0.00 -0.00 0.01 -0.00 0.00 -0.01 0.00

8 7 0.00 -0.00 -0.00 0.00 -0.01 0.00 0.00 0.01 -0.00

9 6 -0.01 -0.02 -0.00 0.00 0.01 0.00 -0.00 -0.01 -0.00

10 6 0.00 -0.01 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

11 6 0.00 0.01 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

12 6 -0.03 -0.03 0.01 0.01 -0.01 0.00 0.01 -0.01 0.00

13 6 0.01 0.02 -0.00 -0.00 -0.01 0.00 -0.00 -0.01 0.00

14 6 -0.00 0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00

15 6 -0.00 -0.01 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

16 6 0.01 -0.02 -0.00 0.00 -0.01 -0.00 0.00 -0.01 -0.00

17 7 -0.00 0.00 -0.00 -0.00 0.01 0.00 0.00 0.01 0.00

18 6 -0.03 0.03 0.01 -0.01 -0.01 -0.00 -0.01 -0.01 -0.00

19 6 0.02 -0.01 -0.00 -0.01 0.00 0.00 -0.00 0.00 0.00

20 6 0.01 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

21 6 -0.01 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

22 6 -0.02 -0.01 -0.00 -0.01 -0.00 -0.00 0.00 0.00 0.00

23 7 0.00 0.00 -0.00 0.01 -0.00 0.00 -0.00 -0.00 0.00

24 6 0.03 0.03 0.01 -0.01 0.01 0.00 0.01 -0.01 -0.00

25 6 -0.05 0.05 -0.12 -0.08 -0.08 0.00 0.07 0.07 0.00

26 6 -0.01 -0.07 0.08 0.09 0.12 -0.04 -0.09 -0.11 0.04

27 6 -0.06 0.01 -0.09 -0.11 -0.09 -0.03 0.11 0.08 0.03

28 6 0.06 -0.06 0.17 0.05 0.05 -0.00 -0.05 -0.05 -0.00

29 6 -0.01 0.06 -0.09 -0.09 -0.11 0.03 0.08 0.11 -0.03

30 6 0.07 0.01 0.08 0.12 0.09 0.04 -0.11 -0.09 -0.04

31 6 -0.06 -0.06 0.17 0.05 -0.05 0.00 0.05 -0.05 -0.00

32 6 0.06 0.01 -0.09 -0.11 0.09 0.03 -0.11 0.09 0.03

33 6 0.01 -0.07 0.08 0.09 -0.12 0.04 0.09 -0.12 0.04

34 6 0.05 0.05 -0.12 -0.08 0.08 -0.00 -0.08 0.08 0.00

35 6 -0.07 0.01 0.08 0.12 -0.09 -0.04 0.12 -0.09 -0.04

36 6 0.01 0.06 -0.09 -0.09 0.11 -0.03 -0.09 0.11 -0.03

37 6 -0.05 -0.05 -0.12 0.08 -0.08 -0.00 -0.08 0.08 -0.00

38 6 0.07 -0.01 0.08 -0.12 0.09 -0.04 0.12 -0.09 0.04

39 6 -0.01 -0.06 -0.09 0.09 -0.11 -0.03 -0.09 0.11 0.03

40 6 0.06 0.06 0.17 -0.05 0.05 0.00 0.05 -0.05 0.00

41 6 -0.06 -0.01 -0.09 0.11 -0.09 0.03 -0.11 0.09 -0.03

42 6 -0.01 0.07 0.08 -0.09 0.12 0.04 0.09 -0.12 -0.04

43 6 0.05 -0.05 -0.12 0.08 0.08 0.00 0.07 0.07 -0.00

44 6 -0.07 -0.01 0.08 -0.12 -0.09 0.04 -0.11 -0.09 0.04

45 6 0.01 -0.06 -0.09 0.09 0.11 0.03 0.08 0.11 0.03

46 6 -0.06 0.06 0.17 -0.05 -0.05 -0.00 -0.05 -0.05 0.00

47 6 0.06 -0.01 -0.09 0.11 0.09 -0.03 0.11 0.08 -0.03

48 6 0.01 0.07 0.08 -0.09 -0.12 -0.04 -0.09 -0.11 -0.04

49 1 0.00 -0.01 -0.00 0.00 0.00 0.00 0.00 0.00 0.00

50 1 -0.00 -0.01 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

51 1 0.01 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

52 1 0.01 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

53 1 -0.01 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

54 1 -0.01 -0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

55 1 0.00 0.01 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

56 1 -0.00 0.01 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

57 1 0.10 0.12 -0.02 -0.06 -0.15 0.12 0.06 0.14 -0.11

58 1 0.07 0.09 -0.03 0.13 0.05 0.11 -0.12 -0.05 -0.10

59 1 -0.08 0.08 -0.23 0.06 0.06 0.00 -0.06 -0.06 0.00

60 1 -0.09 -0.07 -0.03 0.05 0.13 -0.11 -0.05 -0.12 0.10

61 1 -0.12 -0.10 -0.02 -0.15 -0.06 -0.12 0.14 0.06 0.11

62 1 0.08 0.08 -0.23 0.06 -0.06 -0.00 0.06 -0.06 0.00

63 1 -0.07 0.09 -0.03 0.13 -0.05 -0.11 0.13 -0.05 -0.11

64 1 -0.10 0.12 -0.02 -0.06 0.15 -0.12 -0.06 0.15 -0.12

65 1 0.12 -0.10 -0.02 -0.15 0.06 0.12 -0.15 0.06 0.12

66 1 0.09 -0.07 -0.03 0.05 -0.13 0.11 0.05 -0.13 0.11

67 1 -0.12 0.10 -0.02 0.15 -0.06 0.12 -0.15 0.06 -0.12

68 1 -0.09 0.07 -0.03 -0.05 0.13 0.11 0.05 -0.13 -0.11

69 1 -0.08 -0.08 -0.23 -0.06 0.06 -0.00 0.06 -0.06 -0.00

70 1 0.07 -0.09 -0.03 -0.13 0.05 -0.11 0.13 -0.05 0.11

71 1 0.10 -0.12 -0.02 0.06 -0.15 -0.12 -0.06 0.15 0.12

72 1 0.12 0.10 -0.02 0.15 0.06 -0.12 0.14 0.06 -0.11

73 1 0.09 0.07 -0.03 -0.05 -0.13 -0.11 -0.05 -0.12 -0.10

74 1 0.08 -0.08 -0.23 -0.06 -0.06 0.00 -0.06 -0.06 -0.00

75 1 -0.07 -0.09 -0.03 -0.13 -0.05 0.11 -0.12 -0.05 0.10

76 1 -0.10 -0.12 -0.02 0.06 0.15 0.12 0.06 0.14 0.11

77 30 0.00 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

196 197 198

E A1 B1

Frequencies -- 1643.2434 1643.5052 3170.8551

Red. masses -- 5.6695 5.6642 1.0862

Frc consts -- 9.0198 9.0143 6.4347

IR Inten -- 28.7060 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 -0.00

2 6 0.01 0.00 -0.00 -0.01 -0.00 0.00 -0.00 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 -0.00 -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 0.01 0.01 0.00 0.01 0.01 -0.00 0.00 0.00 0.00

7 6 -0.00 0.00 -0.00 -0.00 0.01 -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 -0.01 -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 0.01 -0.01 -0.00 -0.01 0.01 -0.00 0.00 -0.00 -0.00

13 6 -0.00 -0.00 0.00 0.00 0.01 -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 -0.01 -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 0.01 0.01 -0.00 -0.01 -0.01 -0.00 -0.00 -0.00 0.00

19 6 0.01 -0.00 -0.00 -0.01 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 0.01 0.00 0.00 0.01 0.00 0.00 0.00 -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 6 0.01 -0.01 0.00 0.01 -0.01 -0.00 -0.00 0.00 -0.00

25 6 -0.08 -0.08 0.00 -0.08 -0.08 0.00 0.00 0.00 0.00

26 6 0.09 0.12 -0.04 0.09 0.12 -0.04 0.01 0.00 0.01

27 6 -0.11 -0.09 -0.03 -0.11 -0.09 -0.03 0.00 0.01 -0.02

28 6 0.05 0.05 -0.00 0.05 0.05 -0.00 -0.02 -0.02 -0.00

29 6 -0.09 -0.11 0.03 -0.09 -0.11 0.03 0.01 0.00 0.02

30 6 0.12 0.09 0.04 0.12 0.09 0.04 0.00 0.01 -0.01

31 6 0.05 -0.05 0.00 -0.05 0.05 -0.00 -0.02 0.02 0.00

32 6 -0.11 0.08 0.03 0.11 -0.09 -0.03 0.00 -0.01 0.02

33 6 0.09 -0.11 0.04 -0.09 0.12 -0.04 0.01 -0.00 -0.01

34 6 -0.07 0.07 -0.00 0.08 -0.08 0.00 0.00 -0.00 -0.00

35 6 0.11 -0.09 -0.04 -0.12 0.09 0.04 0.00 -0.01 0.01

36 6 -0.08 0.11 -0.03 0.09 -0.11 0.03 0.01 -0.00 -0.02

37 6 -0.07 0.07 0.00 -0.08 0.08 0.00 -0.00 0.00 -0.00

38 6 0.11 -0.09 0.04 0.12 -0.09 0.04 -0.00 0.01 0.01

39 6 -0.08 0.11 0.03 -0.09 0.11 0.03 -0.01 0.00 -0.02

40 6 0.05 -0.05 -0.00 0.05 -0.05 -0.00 0.02 -0.02 0.00

41 6 -0.11 0.08 -0.03 -0.11 0.09 -0.03 -0.00 0.01 0.02

42 6 0.09 -0.11 -0.04 0.09 -0.12 -0.04 -0.01 0.00 -0.01

43 6 -0.08 -0.08 -0.00 0.08 0.08 0.00 -0.00 -0.00 0.00

44 6 0.12 0.09 -0.04 -0.12 -0.09 0.04 -0.00 -0.01 -0.01

45 6 -0.09 -0.11 -0.03 0.09 0.11 0.03 -0.01 -0.00 0.02

46 6 0.05 0.05 0.00 -0.05 -0.05 -0.00 0.02 0.02 -0.00

47 6 -0.11 -0.09 0.03 0.11 0.09 -0.03 -0.00 -0.01 -0.02

48 6 0.09 0.12 0.04 -0.09 -0.12 -0.04 -0.01 -0.00 0.01

49 1 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00

50 1 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00

51 1 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00

52 1 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00

53 1 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00

54 1 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 0.00 0.00

55 1 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00

56 1 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00

57 1 -0.06 -0.15 0.12 -0.06 -0.15 0.12 -0.08 -0.01 -0.09

58 1 0.13 0.05 0.11 0.13 0.05 0.11 -0.02 -0.16 0.20

59 1 0.06 0.06 0.00 0.06 0.06 0.00 0.21 0.21 0.00

60 1 0.05 0.13 -0.11 0.05 0.13 -0.11 -0.16 -0.02 -0.20

61 1 -0.15 -0.06 -0.12 -0.15 -0.06 -0.12 -0.01 -0.08 0.09

62 1 0.06 -0.06 -0.00 -0.06 0.06 0.00 0.21 -0.21 -0.00

63 1 0.12 -0.05 -0.10 -0.13 0.05 0.11 -0.02 0.16 -0.20

64 1 -0.06 0.14 -0.11 0.06 -0.15 0.12 -0.08 0.01 0.09

65 1 -0.14 0.06 0.11 0.15 -0.06 -0.12 -0.01 0.08 -0.09

66 1 0.05 -0.12 0.10 -0.05 0.13 -0.11 -0.16 0.02 0.20

67 1 -0.14 0.06 -0.11 -0.15 0.06 -0.12 0.01 -0.08 -0.09

68 1 0.05 -0.12 -0.10 0.05 -0.13 -0.11 0.16 -0.02 0.20

69 1 0.06 -0.06 0.00 0.06 -0.06 0.00 -0.21 0.21 -0.00

70 1 0.12 -0.05 0.10 0.13 -0.05 0.11 0.02 -0.16 -0.20

71 1 -0.06 0.14 0.11 -0.06 0.15 0.12 0.08 -0.01 0.09

72 1 -0.15 -0.06 0.12 0.15 0.06 -0.12 0.01 0.08 0.09

73 1 0.05 0.13 0.11 -0.05 -0.13 -0.11 0.16 0.02 -0.20

74 1 0.06 0.06 -0.00 -0.06 -0.06 0.00 -0.21 -0.21 0.00

75 1 0.13 0.05 -0.11 -0.13 -0.05 0.11 0.02 0.16 0.20

76 1 -0.06 -0.15 -0.12 0.06 0.15 0.12 0.08 0.01 -0.09

77 30 0.00 0.00 0.00 -0.00 0.00 0.00 0.00 0.00 -0.00

199 200 201

E E A1

Frequencies -- 3170.8553 3170.8553 3170.8610

Red. masses -- 1.0862 1.0862 1.0862

Frc consts -- 6.4347 6.4347 6.4347

IR Inten -- 5.4484 5.4485 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 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00

25 6 0.00 0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.00

26 6 0.01 0.00 0.01 0.01 0.00 0.01 0.01 0.00 0.01

27 6 0.00 0.01 -0.02 0.00 0.01 -0.02 0.00 0.01 -0.02

28 6 -0.02 -0.02 -0.00 -0.02 -0.02 0.00 -0.02 -0.02 -0.00

29 6 0.01 0.00 0.02 0.01 0.00 0.02 0.01 0.00 0.02

30 6 0.00 0.01 -0.01 0.00 0.01 -0.01 0.00 0.01 -0.01

31 6 0.02 -0.02 -0.00 -0.02 0.02 -0.00 0.02 -0.02 -0.00

32 6 -0.00 0.01 -0.02 0.00 -0.01 0.02 -0.00 0.01 -0.02

33 6 -0.01 0.00 0.01 0.01 -0.00 -0.01 -0.01 0.00 0.01

34 6 -0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

35 6 -0.00 0.01 -0.01 0.00 -0.01 0.01 -0.00 0.01 -0.01

36 6 -0.01 0.00 0.02 0.01 -0.00 -0.02 -0.01 0.00 0.02

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 0.01 0.00 -0.01 -0.01 0.00 -0.01 -0.01

39 6 -0.01 0.00 -0.02 0.01 -0.00 0.02 0.01 -0.00 0.02

40 6 0.02 -0.02 0.00 -0.02 0.02 0.00 -0.02 0.02 -0.00

41 6 -0.00 0.01 0.02 0.00 -0.01 -0.02 0.00 -0.01 -0.02

42 6 -0.01 0.00 -0.01 0.01 -0.00 0.01 0.01 -0.00 0.01

43 6 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

44 6 0.00 0.01 0.01 0.00 0.01 0.01 -0.00 -0.01 -0.01

45 6 0.01 0.00 -0.02 0.01 0.00 -0.02 -0.01 -0.00 0.02

46 6 -0.02 -0.02 0.00 -0.02 -0.02 -0.00 0.02 0.02 -0.00

47 6 0.00 0.01 0.02 0.00 0.01 0.02 -0.00 -0.01 -0.02

48 6 0.01 0.00 -0.01 0.01 0.00 -0.01 -0.01 -0.00 0.01

49 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

50 1 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

51 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

52 1 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

53 1 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

54 1 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

55 1 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

56 1 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

57 1 -0.08 -0.01 -0.09 -0.08 -0.01 -0.09 -0.08 -0.01 -0.09

58 1 -0.02 -0.16 0.20 -0.02 -0.16 0.20 -0.02 -0.16 0.20

59 1 0.21 0.21 -0.00 0.21 0.21 0.00 0.21 0.21 0.00

60 1 -0.16 -0.02 -0.20 -0.16 -0.02 -0.20 -0.16 -0.02 -0.20

61 1 -0.01 -0.08 0.09 -0.01 -0.08 0.09 -0.01 -0.08 0.09

62 1 -0.21 0.21 -0.00 0.21 -0.21 -0.00 -0.21 0.21 0.00

63 1 0.02 -0.16 0.20 -0.02 0.16 -0.20 0.02 -0.16 0.20

64 1 0.08 -0.01 -0.09 -0.08 0.01 0.09 0.08 -0.01 -0.09

65 1 0.01 -0.08 0.09 -0.01 0.08 -0.09 0.01 -0.08 0.09

66 1 0.16 -0.02 -0.20 -0.16 0.02 0.20 0.16 -0.02 -0.20

67 1 0.01 -0.08 -0.09 -0.01 0.08 0.09 -0.01 0.08 0.09

68 1 0.16 -0.02 0.20 -0.16 0.02 -0.20 -0.16 0.02 -0.20

69 1 -0.21 0.21 0.00 0.21 -0.21 0.00 0.21 -0.21 0.00

70 1 0.02 -0.16 -0.20 -0.02 0.16 0.20 -0.02 0.16 0.20

71 1 0.08 -0.01 0.09 -0.08 0.01 -0.09 -0.08 0.01 -0.09

72 1 -0.01 -0.08 -0.09 -0.01 -0.08 -0.09 0.01 0.08 0.09

73 1 -0.16 -0.02 0.20 -0.16 -0.02 0.20 0.16 0.02 -0.20

74 1 0.21 0.21 0.00 0.21 0.21 -0.00 -0.21 -0.21 0.00

75 1 -0.02 -0.16 -0.20 -0.02 -0.16 -0.20 0.02 0.16 0.20

76 1 -0.08 -0.01 0.09 -0.08 -0.01 0.09 0.08 0.01 -0.09

77 30 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 0.00

202 203 204

A2 E E

Frequencies -- 3177.4863 3177.4889 3177.4889

Red. masses -- 1.0881 1.0881 1.0881

Frc consts -- 6.4727 6.4727 6.4727

IR Inten -- 0.0000 1.8494 1.8494

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 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

25 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

26 6 0.01 0.00 0.01 -0.01 -0.00 -0.01 0.01 0.00 0.01

27 6 0.00 0.01 -0.02 -0.00 -0.01 0.02 0.00 0.01 -0.02

28 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

29 6 -0.01 -0.00 -0.02 0.01 0.00 0.02 -0.01 -0.00 -0.02

30 6 -0.00 -0.01 0.01 0.00 0.01 -0.01 -0.00 -0.01 0.01

31 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

32 6 0.00 -0.01 0.02 -0.00 0.01 -0.02 -0.00 0.01 -0.02

33 6 0.01 -0.00 -0.01 -0.01 0.00 0.01 -0.01 0.00 0.01

34 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

35 6 -0.00 0.01 -0.01 0.00 -0.01 0.01 0.00 -0.01 0.01

36 6 -0.01 0.00 0.02 0.01 -0.00 -0.02 0.01 -0.00 -0.02

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 -0.01 0.00 -0.01 -0.01 0.00 -0.01 -0.01

39 6 0.01 -0.00 0.02 0.01 -0.00 0.02 0.01 -0.00 0.02

40 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

41 6 -0.00 0.01 0.02 -0.00 0.01 0.02 -0.00 0.01 0.02

42 6 -0.01 0.00 -0.01 -0.01 0.00 -0.01 -0.01 0.00 -0.01

43 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

44 6 0.00 0.01 0.01 0.00 0.01 0.01 -0.00 -0.01 -0.01

45 6 0.01 0.00 -0.02 0.01 0.00 -0.02 -0.01 -0.00 0.02

46 6 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

47 6 -0.00 -0.01 -0.02 -0.00 -0.01 -0.02 0.00 0.01 0.02

48 6 -0.01 -0.00 0.01 -0.01 -0.00 0.01 0.01 0.00 -0.01

49 1 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

50 1 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

51 1 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

52 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

53 1 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

54 1 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

55 1 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

56 1 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

57 1 -0.14 -0.02 -0.17 0.14 0.02 0.17 -0.14 -0.02 -0.17

58 1 -0.02 -0.17 0.21 0.02 0.17 -0.21 -0.02 -0.18 0.22

59 1 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

60 1 0.17 0.02 0.21 -0.17 -0.02 -0.21 0.18 0.02 0.22

61 1 0.02 0.14 -0.17 -0.02 -0.14 0.17 0.02 0.14 -0.17

62 1 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

63 1 -0.02 0.17 -0.21 0.02 -0.18 0.22 0.02 -0.17 0.21

64 1 -0.14 0.02 0.17 0.14 -0.02 -0.17 0.14 -0.02 -0.17

65 1 0.02 -0.14 0.17 -0.02 0.14 -0.17 -0.02 0.14 -0.17

66 1 0.17 -0.02 -0.21 -0.18 0.02 0.22 -0.17 0.02 0.21

67 1 -0.02 0.14 0.17 -0.02 0.14 0.17 -0.02 0.14 0.17

68 1 -0.17 0.02 -0.21 -0.18 0.02 -0.22 -0.17 0.02 -0.21

69 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

70 1 0.02 -0.17 -0.21 0.02 -0.18 -0.22 0.02 -0.17 -0.21

71 1 0.14 -0.02 0.17 0.14 -0.02 0.17 0.14 -0.02 0.17

72 1 -0.02 -0.14 -0.17 -0.02 -0.14 -0.17 0.02 0.14 0.17

73 1 -0.17 -0.02 0.21 -0.17 -0.02 0.21 0.18 0.02 -0.22

74 1 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

75 1 0.02 0.17 0.21 0.02 0.17 0.21 -0.02 -0.18 -0.22

76 1 0.14 0.02 -0.17 0.14 0.02 -0.17 -0.14 -0.02 0.17

77 30 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00

205 206 207

B2 E E

Frequencies -- 3177.4930 3185.9439 3185.9439

Red. masses -- 1.0881 1.0916 1.0916

Frc consts -- 6.4728 6.5283 6.5283

IR Inten -- 9.0976 65.2340 65.2340

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 6 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

25 6 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00

26 6 0.01 0.00 0.01 -0.01 -0.00 -0.02 0.01 0.00 0.02

27 6 0.00 0.01 -0.02 0.00 -0.00 0.00 -0.00 0.00 -0.00

28 6 0.00 -0.00 0.00 -0.02 -0.02 -0.00 0.02 0.02 -0.00

29 6 -0.01 -0.00 -0.02 -0.00 0.00 -0.00 0.00 -0.00 0.00

30 6 -0.00 -0.01 0.01 -0.00 -0.01 0.02 0.00 0.01 -0.02

31 6 -0.00 -0.00 0.00 0.02 -0.02 -0.00 0.02 -0.02 0.00

32 6 -0.00 0.01 -0.02 -0.00 -0.00 0.00 -0.00 -0.00 0.00

33 6 -0.01 0.00 0.01 0.01 -0.00 -0.02 0.01 -0.00 -0.02

34 6 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00

35 6 0.00 -0.01 0.01 0.00 -0.01 0.02 0.00 -0.01 0.02

36 6 0.01 -0.00 -0.02 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 0.01 0.00 -0.01 -0.02 0.00 -0.01 -0.02

39 6 -0.01 0.00 -0.02 0.00 0.00 0.00 0.00 0.00 0.00

40 6 0.00 0.00 0.00 0.02 -0.02 0.00 0.02 -0.02 -0.00

41 6 0.00 -0.01 -0.02 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

42 6 0.01 -0.00 0.01 0.01 -0.00 0.02 0.01 -0.00 0.02

43 6 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

44 6 0.00 0.01 0.01 -0.00 -0.01 -0.02 0.00 0.01 0.02

45 6 0.01 0.00 -0.02 -0.00 0.00 0.00 0.00 -0.00 -0.00

46 6 -0.00 0.00 0.00 -0.02 -0.02 0.00 0.02 0.02 0.00

47 6 -0.00 -0.01 -0.02 0.00 -0.00 -0.00 -0.00 0.00 0.00

48 6 -0.01 -0.00 0.01 -0.01 -0.00 0.02 0.01 0.00 -0.02

49 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

50 1 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

51 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

52 1 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

53 1 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

54 1 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

55 1 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

56 1 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

57 1 -0.14 -0.02 -0.17 0.17 0.02 0.21 -0.17 -0.02 -0.21

58 1 -0.02 -0.17 0.21 0.00 0.03 -0.04 -0.00 -0.03 0.04

59 1 -0.00 0.00 -0.00 0.22 0.22 0.00 -0.22 -0.22 0.00

60 1 0.17 0.02 0.21 0.03 0.00 0.04 -0.03 -0.00 -0.04

61 1 0.02 0.14 -0.17 0.02 0.17 -0.21 -0.02 -0.17 0.21

62 1 0.00 0.00 -0.00 -0.22 0.22 0.00 -0.22 0.22 -0.00

63 1 0.02 -0.17 0.21 -0.00 0.03 -0.04 -0.00 0.03 -0.04

64 1 0.14 -0.02 -0.17 -0.17 0.02 0.21 -0.17 0.02 0.21

65 1 -0.02 0.14 -0.17 -0.02 0.17 -0.21 -0.02 0.17 -0.21

66 1 -0.17 0.02 0.21 -0.03 0.00 0.04 -0.03 0.00 0.04

67 1 0.02 -0.14 -0.17 -0.02 0.17 0.21 -0.02 0.17 0.21

68 1 0.17 -0.02 0.21 -0.03 0.00 -0.04 -0.03 0.00 -0.04

69 1 -0.00 -0.00 -0.00 -0.22 0.22 -0.00 -0.22 0.22 0.00

70 1 -0.02 0.17 0.21 -0.00 0.03 0.04 -0.00 0.03 0.04

71 1 -0.14 0.02 -0.17 -0.17 0.02 -0.21 -0.17 0.02 -0.21

72 1 -0.02 -0.14 -0.17 0.02 0.17 0.21 -0.02 -0.17 -0.21

73 1 -0.17 -0.02 0.21 0.03 0.00 -0.04 -0.03 -0.00 0.04

74 1 0.00 -0.00 -0.00 0.22 0.22 -0.00 -0.22 -0.22 -0.00

75 1 0.02 0.17 0.21 0.00 0.03 0.04 -0.00 -0.03 -0.04

76 1 0.14 0.02 -0.17 0.17 0.02 -0.21 -0.17 -0.02 0.21

77 30 0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00 0.00

208 209 210

B1 A1 A2

Frequencies -- 3185.9529 3185.9581 3192.0855

Red. masses -- 1.0916 1.0916 1.0945

Frc consts -- 6.5284 6.5284 6.5708

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 0.00 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 6 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 0.00

25 6 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00

26 6 -0.01 -0.00 -0.02 -0.01 -0.00 -0.02 -0.02 -0.00 -0.02

27 6 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 0.01 -0.01

28 6 -0.02 -0.02 0.00 -0.02 -0.02 0.00 0.00 -0.00 0.00

29 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.01 -0.00 -0.01

30 6 -0.00 -0.01 0.02 -0.00 -0.01 0.02 0.00 0.02 -0.02

31 6 -0.02 0.02 -0.00 0.02 -0.02 0.00 0.00 0.00 -0.00

32 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.01 0.01

33 6 -0.01 0.00 0.02 0.01 -0.00 -0.02 -0.02 0.00 0.02

34 6 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00

35 6 -0.00 0.01 -0.02 0.00 -0.01 0.02 0.00 -0.02 0.02

36 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.01 0.00 0.01

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 -0.02 -0.00 0.01 0.02 -0.00 0.02 0.02

39 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.01 -0.00 0.01

40 6 0.02 -0.02 -0.00 -0.02 0.02 0.00 -0.00 -0.00 -0.00

41 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.01 0.01

42 6 0.01 -0.00 0.02 -0.01 0.00 -0.02 0.02 -0.00 0.02

43 6 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00

44 6 0.00 0.01 0.02 0.00 0.01 0.02 -0.00 -0.02 -0.02

45 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.01 0.00 -0.01

46 6 0.02 0.02 0.00 0.02 0.02 0.00 -0.00 0.00 0.00

47 6 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.01 -0.01

48 6 0.01 0.00 -0.02 0.01 0.00 -0.02 0.02 0.00 -0.02

49 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

50 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

51 1 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

52 1 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

53 1 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

54 1 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

55 1 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

56 1 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

57 1 0.17 0.02 0.21 0.17 0.02 0.21 0.18 0.02 0.21

58 1 0.00 0.03 -0.04 0.00 0.03 -0.04 -0.02 -0.14 0.17

59 1 0.22 0.22 -0.00 0.22 0.22 -0.00 -0.00 0.00 -0.00

60 1 0.03 0.00 0.04 0.03 0.00 0.04 0.14 0.02 0.17

61 1 0.02 0.17 -0.21 0.02 0.17 -0.21 -0.02 -0.18 0.21

62 1 0.22 -0.22 0.00 -0.22 0.22 -0.00 -0.00 -0.00 0.00

63 1 0.00 -0.03 0.04 -0.00 0.03 -0.04 -0.02 0.14 -0.17

64 1 0.17 -0.02 -0.21 -0.17 0.02 0.21 0.18 -0.02 -0.21

65 1 0.02 -0.17 0.21 -0.02 0.17 -0.21 -0.02 0.18 -0.21

66 1 0.03 -0.00 -0.04 -0.03 0.00 0.04 0.14 -0.02 -0.17

67 1 -0.02 0.17 0.21 0.02 -0.17 -0.21 0.02 -0.18 -0.21

68 1 -0.03 0.00 -0.04 0.03 -0.00 0.04 -0.14 0.02 -0.17

69 1 -0.22 0.22 0.00 0.22 -0.22 -0.00 0.00 0.00 0.00

70 1 -0.00 0.03 0.04 0.00 -0.03 -0.04 0.02 -0.14 -0.17

71 1 -0.17 0.02 -0.21 0.17 -0.02 0.21 -0.18 0.02 -0.21

72 1 -0.02 -0.17 -0.21 -0.02 -0.17 -0.21 0.02 0.18 0.21

73 1 -0.03 -0.00 0.04 -0.03 -0.00 0.04 -0.14 -0.02 0.17

74 1 -0.22 -0.22 -0.00 -0.22 -0.22 -0.00 0.00 -0.00 -0.00

75 1 -0.00 -0.03 -0.04 -0.00 -0.03 -0.04 0.02 0.14 0.17

76 1 -0.17 -0.02 0.21 -0.17 -0.02 0.21 -0.18 -0.02 0.21

77 30 0.00 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

211 212 213

E E B2

Frequencies -- 3192.0947 3192.0947 3192.1144

Red. masses -- 1.0945 1.0945 1.0945

Frc consts -- 6.5709 6.5709 6.5709

IR Inten -- 19.5862 19.5860 174.9912

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 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

25 6 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

26 6 -0.01 -0.00 -0.02 -0.02 -0.00 -0.02 -0.02 -0.00 -0.02

27 6 0.00 0.01 -0.01 0.00 0.01 -0.02 0.00 0.01 -0.01

28 6 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

29 6 -0.01 -0.00 -0.01 -0.01 -0.00 -0.02 -0.01 -0.00 -0.01

30 6 0.00 0.01 -0.02 0.00 0.02 -0.02 0.00 0.02 -0.02

31 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

32 6 -0.00 0.01 -0.02 0.00 -0.01 0.01 -0.00 0.01 -0.01

33 6 0.02 -0.00 -0.02 -0.01 0.00 0.02 0.02 -0.00 -0.02

34 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

35 6 -0.00 0.02 -0.02 0.00 -0.01 0.02 -0.00 0.02 -0.02

36 6 0.01 -0.00 -0.02 -0.01 0.00 0.01 0.01 -0.00 -0.01

37 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.00

38 6 -0.00 0.02 0.02 0.00 -0.01 -0.02 0.00 -0.02 -0.02

39 6 0.01 -0.00 0.02 -0.01 0.00 -0.01 -0.01 0.00 -0.01

40 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.00

41 6 -0.00 0.01 0.02 0.00 -0.01 -0.01 0.00 -0.01 -0.01

42 6 0.02 -0.00 0.02 -0.01 0.00 -0.02 -0.02 0.00 -0.02

43 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

44 6 0.00 0.01 0.02 0.00 0.02 0.02 -0.00 -0.02 -0.02

45 6 -0.01 -0.00 0.01 -0.01 -0.00 0.02 0.01 0.00 -0.01

46 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

47 6 0.00 0.01 0.01 0.00 0.01 0.02 -0.00 -0.01 -0.01

48 6 -0.01 -0.00 0.02 -0.02 -0.00 0.02 0.02 0.00 -0.02

49 1 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

50 1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

51 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

52 1 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

53 1 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

54 1 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

55 1 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

56 1 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

57 1 0.15 0.02 0.19 0.19 0.02 0.24 0.18 0.02 0.21

58 1 -0.01 -0.12 0.15 -0.02 -0.15 0.19 -0.02 -0.14 0.17

59 1 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

60 1 0.12 0.01 0.15 0.15 0.02 0.19 0.14 0.02 0.17

61 1 -0.02 -0.15 0.19 -0.02 -0.19 0.24 -0.02 -0.18 0.21

62 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

63 1 0.02 -0.15 0.19 -0.01 0.12 -0.15 0.02 -0.14 0.17

64 1 -0.19 0.02 0.24 0.15 -0.02 -0.19 -0.18 0.02 0.21

65 1 0.02 -0.19 0.24 -0.02 0.15 -0.19 0.02 -0.18 0.21

66 1 -0.15 0.02 0.19 0.12 -0.01 -0.15 -0.14 0.02 0.17

67 1 0.02 -0.19 -0.24 -0.02 0.15 0.19 -0.02 0.18 0.21

68 1 -0.15 0.02 -0.19 0.12 -0.01 0.15 0.14 -0.02 0.17

69 1 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

70 1 0.02 -0.15 -0.19 -0.01 0.12 0.15 -0.02 0.14 0.17

71 1 -0.19 0.02 -0.24 0.15 -0.02 0.19 0.18 -0.02 0.21

72 1 -0.02 -0.15 -0.19 -0.02 -0.19 -0.24 0.02 0.18 0.21

73 1 0.12 0.01 -0.15 0.15 0.02 -0.19 -0.14 -0.02 0.17

74 1 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

75 1 -0.01 -0.12 -0.15 -0.02 -0.15 -0.19 0.02 0.14 0.17

76 1 0.15 0.02 -0.19 0.19 0.02 -0.24 -0.18 -0.02 0.21

77 30 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00

214 215 216

E E B1

Frequencies -- 3199.1524 3199.1524 3199.1632

Red. masses -- 1.0980 1.0980 1.0980

Frc consts -- 6.6210 6.6210 6.6210

IR Inten -- 62.2629 62.2627 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 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 0.00

25 6 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

26 6 0.01 0.00 0.01 -0.01 -0.00 -0.01 -0.01 -0.00 -0.01

27 6 -0.00 -0.01 0.02 0.00 0.01 -0.02 0.00 0.01 -0.02

28 6 -0.02 -0.02 -0.00 0.02 0.02 -0.00 0.02 0.02 -0.00

29 6 -0.01 -0.00 -0.02 0.01 0.00 0.02 0.01 0.00 0.02

30 6 0.00 0.01 -0.01 -0.00 -0.01 0.01 -0.00 -0.01 0.01

31 6 -0.02 0.02 0.00 -0.02 0.02 -0.00 0.02 -0.02 0.00

32 6 -0.00 0.01 -0.02 -0.00 0.01 -0.02 0.00 -0.01 0.02

33 6 0.01 -0.00 -0.01 0.01 -0.00 -0.01 -0.01 0.00 0.01

34 6 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

35 6 0.00 -0.01 0.01 0.00 -0.01 0.01 -0.00 0.01 -0.01

36 6 -0.01 0.00 0.02 -0.01 0.00 0.02 0.01 -0.00 -0.02

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 -0.01 0.00 -0.01 -0.01 0.00 -0.01 -0.01

39 6 -0.01 0.00 -0.02 -0.01 0.00 -0.02 -0.01 0.00 -0.02

40 6 -0.02 0.02 -0.00 -0.02 0.02 0.00 -0.02 0.02 0.00

41 6 -0.00 0.01 0.02 -0.00 0.01 0.02 -0.00 0.01 0.02

42 6 0.01 -0.00 0.01 0.01 -0.00 0.01 0.01 -0.00 0.01

43 6 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

44 6 0.00 0.01 0.01 -0.00 -0.01 -0.01 0.00 0.01 0.01

45 6 -0.01 -0.00 0.02 0.01 0.00 -0.02 -0.01 -0.00 0.02

46 6 -0.02 -0.02 0.00 0.02 0.02 0.00 -0.02 -0.02 -0.00

47 6 -0.00 -0.01 -0.02 0.00 0.01 0.02 -0.00 -0.01 -0.02

48 6 0.01 0.00 -0.01 -0.01 -0.00 0.01 0.01 0.00 -0.01

49 1 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

50 1 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.00

51 1 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

52 1 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

53 1 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

54 1 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

55 1 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

56 1 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

57 1 -0.12 -0.01 -0.14 0.12 0.01 0.14 0.12 0.01 0.14

58 1 0.02 0.15 -0.18 -0.02 -0.15 0.18 -0.02 -0.15 0.18

59 1 0.18 0.18 -0.00 -0.18 -0.18 -0.00 -0.18 -0.18 0.00

60 1 0.15 0.02 0.18 -0.15 -0.02 -0.18 -0.15 -0.02 -0.18

61 1 -0.01 -0.12 0.14 0.01 0.12 -0.14 0.01 0.12 -0.14

62 1 0.18 -0.18 0.00 0.18 -0.18 -0.00 -0.18 0.18 -0.00

63 1 0.02 -0.15 0.18 0.02 -0.15 0.18 -0.02 0.15 -0.18

64 1 -0.12 0.01 0.14 -0.12 0.01 0.14 0.12 -0.01 -0.14

65 1 -0.01 0.12 -0.14 -0.01 0.12 -0.14 0.01 -0.12 0.14

66 1 0.15 -0.02 -0.18 0.15 -0.02 -0.18 -0.15 0.02 0.18

67 1 -0.01 0.12 0.14 -0.01 0.12 0.14 -0.01 0.12 0.14

68 1 0.15 -0.02 0.18 0.15 -0.02 0.18 0.15 -0.02 0.18

69 1 0.18 -0.18 -0.00 0.18 -0.18 0.00 0.18 -0.18 -0.00

70 1 0.02 -0.15 -0.18 0.02 -0.15 -0.18 0.02 -0.15 -0.18

71 1 -0.12 0.01 -0.14 -0.12 0.01 -0.14 -0.12 0.01 -0.14

72 1 -0.01 -0.12 -0.14 0.01 0.12 0.14 -0.01 -0.12 -0.14

73 1 0.15 0.02 -0.18 -0.15 -0.02 0.18 0.15 0.02 -0.18

74 1 0.18 0.18 0.00 -0.18 -0.18 0.00 0.18 0.18 0.00

75 1 0.02 0.15 0.18 -0.02 -0.15 -0.18 0.02 0.15 0.18

76 1 -0.12 -0.01 0.14 0.12 0.01 -0.14 -0.12 -0.01 0.14

77 30 -0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

217 218 219

A1 A2 E

Frequencies -- 3199.2303 3245.4292 3245.6078

Red. masses -- 1.0980 1.0900 1.0901

Frc consts -- 6.6213 6.7646 6.7659

IR Inten -- 0.0000 0.0000 9.6006

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.00 0.00 0.02 -0.02 -0.00 0.02 -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 0.02 0.02 0.00 0.02 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 -0.00 0.00 -0.00 0.02 -0.02 -0.00 -0.00 0.00 0.00

11 6 -0.00 -0.00 -0.00 -0.02 -0.02 0.00 0.00 0.00 -0.00

12 6 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00

13 6 -0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00

14 6 0.00 -0.00 -0.00 -0.02 0.02 -0.00 -0.00 0.00 -0.00

15 6 0.00 0.00 -0.00 0.02 0.02 0.00 0.00 0.00 0.00

16 6 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

17 7 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00

18 6 0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 0.00 -0.00

19 6 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

20 6 0.00 0.00 0.00 -0.02 -0.02 0.00 0.02 0.04 -0.00

21 6 -0.00 0.00 0.00 -0.02 0.02 -0.00 0.02 -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 6 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00

25 6 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

26 6 -0.01 -0.00 -0.01 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

27 6 0.00 0.01 -0.02 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

28 6 0.02 0.02 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00

29 6 0.01 0.00 0.02 0.00 0.00 -0.00 -0.00 0.00 -0.00

30 6 -0.00 -0.01 0.01 0.00 0.00 -0.00 -0.00 0.00 -0.00

31 6 -0.02 0.02 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

32 6 -0.00 0.01 -0.02 -0.00 0.00 0.00 -0.00 0.00 0.00

33 6 0.01 -0.00 -0.01 -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 -0.01 0.01 0.00 -0.00 0.00 -0.00 -0.00 0.00

36 6 -0.01 0.00 0.02 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 0.01 -0.00 0.00 0.00 -0.00 -0.00 -0.00

39 6 0.01 -0.00 0.02 -0.00 0.00 0.00 -0.00 -0.00 -0.00

40 6 0.02 -0.02 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

41 6 0.00 -0.01 -0.02 0.00 -0.00 0.00 -0.00 0.00 -0.00

42 6 -0.01 0.00 -0.01 0.00 -0.00 0.00 -0.00 0.00 -0.00

43 6 0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

44 6 0.00 0.01 0.01 -0.00 -0.00 -0.00 -0.00 0.00 0.00

45 6 -0.01 -0.00 0.02 -0.00 -0.00 -0.00 -0.00 0.00 0.00

46 6 -0.02 -0.02 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00

47 6 -0.00 -0.01 -0.02 0.00 0.00 -0.00 -0.00 -0.00 0.00

48 6 0.01 0.00 -0.01 0.00 0.00 -0.00 -0.00 -0.00 0.00

49 1 -0.00 0.00 0.00 -0.21 0.28 0.03 -0.30 0.40 0.04

50 1 0.00 0.00 0.00 -0.21 -0.28 -0.03 -0.30 -0.39 -0.04

51 1 0.00 -0.00 -0.00 -0.28 0.21 0.03 0.02 -0.02 -0.00

52 1 0.00 0.00 -0.00 0.28 0.21 -0.03 -0.01 -0.01 0.00

53 1 -0.00 0.00 -0.00 0.28 -0.21 0.03 0.02 -0.02 0.00

54 1 -0.00 -0.00 -0.00 -0.28 -0.21 -0.03 -0.01 -0.01 -0.00

55 1 -0.00 -0.00 0.00 0.21 0.28 -0.03 -0.30 -0.39 0.04

56 1 0.00 -0.00 0.00 0.21 -0.28 0.03 -0.30 0.40 -0.04

57 1 0.12 0.01 0.14 0.00 0.00 0.00 0.00 0.00 0.00

58 1 -0.02 -0.15 0.18 -0.00 -0.00 0.00 -0.00 0.00 -0.00

59 1 -0.18 -0.18 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00

60 1 -0.15 -0.02 -0.18 0.00 0.00 0.00 0.00 0.00 0.00

61 1 0.01 0.12 -0.14 -0.00 -0.00 0.00 -0.00 -0.00 0.00

62 1 0.18 -0.18 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00

63 1 0.02 -0.15 0.18 -0.00 0.00 -0.00 -0.00 -0.00 0.00

64 1 -0.12 0.01 0.14 0.00 -0.00 -0.00 0.00 -0.00 -0.00

65 1 -0.01 0.12 -0.14 -0.00 0.00 -0.00 -0.00 0.00 -0.00

66 1 0.15 -0.02 -0.18 0.00 -0.00 -0.00 0.00 -0.00 -0.00

67 1 0.01 -0.12 -0.14 0.00 -0.00 -0.00 -0.00 0.00 0.00

68 1 -0.15 0.02 -0.18 -0.00 0.00 -0.00 0.00 -0.00 0.00

69 1 -0.18 0.18 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00

70 1 -0.02 0.15 0.18 0.00 -0.00 -0.00 -0.00 -0.00 -0.00

71 1 0.12 -0.01 0.14 -0.00 0.00 -0.00 0.00 -0.00 0.00

72 1 -0.01 -0.12 -0.14 0.00 0.00 0.00 -0.00 -0.00 -0.00

73 1 0.15 0.02 -0.18 -0.00 -0.00 0.00 0.00 0.00 -0.00

74 1 0.18 0.18 -0.00 0.00 -0.00 0.00 0.00 0.00 -0.00

75 1 0.02 0.15 0.18 0.00 0.00 0.00 -0.00 0.00 0.00

76 1 -0.12 -0.01 0.14 -0.00 -0.00 0.00 0.00 0.00 -0.00

77 30 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00

220 221 222

E B1 B2

Frequencies -- 3245.6078 3245.7727 3261.9880

Red. masses -- 1.0901 1.0902 1.1034

Frc consts -- 6.7659 6.7670 6.9173

IR Inten -- 9.6006 0.0000 0.5376

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.00 -0.00 0.02 -0.02 -0.00 0.02 -0.02 -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 0.02 0.02 0.00 -0.02 -0.02 -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 -0.02 0.02 0.00 0.02 -0.02 -0.00

11 6 -0.04 -0.02 0.00 0.02 0.02 -0.00 0.02 0.02 -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 0.02 -0.02 0.00 -0.02 0.02 -0.00

15 6 -0.04 -0.02 -0.00 -0.02 -0.02 -0.00 -0.02 -0.02 -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 -0.02 -0.02 0.00 0.02 0.02 -0.00

21 6 0.00 -0.00 0.00 -0.02 0.02 -0.00 -0.02 0.02 -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 6 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00

25 6 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00 0.00

26 6 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

27 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 0.00 0.00

28 6 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00

29 6 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00

30 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

31 6 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00

32 6 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 6 0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

43 6 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00

44 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

45 6 0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00 0.00

46 6 0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00

47 6 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00

48 6 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

49 1 -0.01 0.01 0.00 -0.21 0.28 0.03 -0.21 0.28 0.03

50 1 -0.02 -0.02 -0.00 -0.21 -0.28 -0.03 0.21 0.28 0.03

51 1 -0.39 0.30 0.04 0.28 -0.21 -0.03 -0.28 0.21 0.03

52 1 0.40 0.30 -0.04 -0.28 -0.21 0.03 -0.28 -0.21 0.03

53 1 -0.39 0.30 -0.04 -0.28 0.21 -0.03 0.28 -0.21 0.03

54 1 0.40 0.30 0.04 0.28 0.21 0.03 0.28 0.21 0.03

55 1 -0.02 -0.02 0.00 0.21 0.28 -0.03 -0.21 -0.28 0.03

56 1 -0.01 0.01 -0.00 0.21 -0.28 0.03 0.21 -0.28 0.03

57 1 0.00 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

58 1 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

59 1 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00

60 1 -0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

61 1 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

62 1 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00

63 1 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

64 1 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

65 1 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

66 1 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

67 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

68 1 0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

69 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.00

70 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

71 1 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

72 1 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

73 1 -0.00 0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

74 1 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00

75 1 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

76 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

77 30 -0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00

223 224 225

E E A1

Frequencies -- 3262.1615 3262.1615 3262.4963

Red. masses -- 1.1034 1.1034 1.1034

Frc consts -- 6.9182 6.9182 6.9193

IR Inten -- 46.3912 46.3914 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.03 -0.03 -0.00 0.02 -0.02 -0.00 0.02 -0.02 -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 -0.03 -0.00 -0.02 -0.02 -0.00 -0.02 -0.02 -0.00

6 6 0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00

7 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

8 7 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

9 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

10 6 0.02 -0.02 -0.00 -0.03 0.03 0.00 -0.02 0.02 0.00

11 6 0.02 0.02 -0.00 -0.03 -0.03 0.00 -0.02 -0.02 0.00

12 6 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00

13 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

14 6 0.02 -0.02 0.00 -0.03 0.03 -0.00 0.02 -0.02 0.00

15 6 0.02 0.02 0.00 -0.03 -0.03 -0.00 0.02 0.02 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 -0.03 0.00 -0.02 -0.02 0.00 0.02 0.02 -0.00

21 6 0.03 -0.03 0.00 0.02 -0.02 0.00 -0.02 0.02 -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 6 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00

25 6 -0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00

26 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

27 6 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

28 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00

29 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00

30 6 0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

31 6 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00

32 6 -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 6 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00

43 6 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

44 6 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

45 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00

46 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00 0.00

47 6 0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

48 6 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

49 1 -0.25 0.33 0.04 -0.16 0.21 0.02 -0.21 0.28 0.03

50 1 0.25 0.33 0.04 0.17 0.22 0.02 0.21 0.28 0.03

51 1 -0.22 0.17 0.02 0.33 -0.25 -0.04 0.28 -0.21 -0.03

52 1 -0.21 -0.16 0.02 0.33 0.25 -0.04 0.28 0.21 -0.03

53 1 -0.22 0.17 -0.02 0.33 -0.25 0.04 -0.28 0.21 -0.03

54 1 -0.21 -0.16 -0.02 0.33 0.25 0.04 -0.28 -0.21 -0.03

55 1 0.25 0.33 -0.04 0.17 0.22 -0.02 -0.21 -0.28 0.03

56 1 -0.25 0.33 -0.04 -0.16 0.21 -0.02 0.21 -0.28 0.03

57 1 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

58 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

59 1 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

60 1 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 0.00

61 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

62 1 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

63 1 -0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

64 1 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

65 1 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

66 1 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

67 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

68 1 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

69 1 0.00 -0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

70 1 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

71 1 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

72 1 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

73 1 -0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00

74 1 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

75 1 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

76 1 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

77 30 -0.00 0.00 0.00 0.00 0.00 0.00 0.00 -0.00 -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 6 and mass 12.00000

Atom 25 has atomic number 6 and mass 12.00000

Atom 26 has atomic number 6 and mass 12.00000

Atom 27 has atomic number 6 and mass 12.00000

Atom 28 has atomic number 6 and mass 12.00000

Atom 29 has atomic number 6 and mass 12.00000

Atom 30 has atomic number 6 and mass 12.00000

Atom 31 has atomic number 6 and mass 12.00000

Atom 32 has atomic number 6 and mass 12.00000

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 6 and mass 12.00000

Atom 43 has atomic number 6 and mass 12.00000

Atom 44 has atomic number 6 and mass 12.00000

Atom 45 has atomic number 6 and mass 12.00000

Atom 46 has atomic number 6 and mass 12.00000

Atom 47 has atomic number 6 and mass 12.00000

Atom 48 has atomic number 6 and mass 12.00000

Atom 49 has atomic number 1 and mass 1.00783

Atom 50 has atomic number 1 and mass 1.00783

Atom 51 has atomic number 1 and mass 1.00783

Atom 52 has atomic number 1 and mass 1.00783

Atom 53 has atomic number 1 and mass 1.00783

Atom 54 has atomic number 1 and mass 1.00783

Atom 55 has atomic number 1 and mass 1.00783

Atom 56 has atomic number 1 and mass 1.00783

Atom 57 has atomic number 1 and mass 1.00783

Atom 58 has atomic number 1 and mass 1.00783

Atom 59 has atomic number 1 and mass 1.00783

Atom 60 has atomic number 1 and mass 1.00783

Atom 61 has atomic number 1 and mass 1.00783

Atom 62 has atomic number 1 and mass 1.00783

Atom 63 has atomic number 1 and mass 1.00783

Atom 64 has atomic number 1 and mass 1.00783

Atom 65 has atomic number 1 and mass 1.00783

Atom 66 has atomic number 1 and mass 1.00783

Atom 67 has atomic number 1 and mass 1.00783

Atom 68 has atomic number 1 and mass 1.00783

Atom 69 has atomic number 1 and mass 1.00783

Atom 70 has atomic number 1 and mass 1.00783

Atom 71 has atomic number 1 and mass 1.00783

Atom 72 has atomic number 1 and mass 1.00783

Atom 73 has atomic number 1 and mass 1.00783

Atom 74 has atomic number 1 and mass 1.00783

Atom 75 has atomic number 1 and mass 1.00783

Atom 76 has atomic number 1 and mass 1.00783

Atom 77 has atomic number 30 and mass 63.92915

Molecular mass: 676.16054 amu.

Principal axes and moments of inertia in atomic units:

1 2 3

Eigenvalues -- \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

X 0.88012 0.47476 0.00000

Y -0.47476 0.88012 0.00000

Z -0.00000 -0.00000 1.00000

This molecule is an oblate symmetric top.

Rotational symmetry number 4.

Warning -- assumption of classical behavior for rotation

may cause significant error

Rotational temperatures (Kelvin) 0.00279 0.00279 0.00144

Rotational constants (GHZ): 0.05821 0.05821 0.03008

Zero-point vibrational energy 1561491.5 (Joules/Mol)

373.20543 (Kcal/Mol)

Warning -- explicit consideration of 57 degrees of freedom as

vibrations may cause significant error

Vibrational temperatures: 12.17 29.07 56.72 63.26 63.26

(Kelvin) 63.36 72.07 72.07 82.22 93.66

93.66 114.19 123.05 136.48 147.20

170.54 203.67 203.67 286.73 289.69

308.48 308.48 318.41 318.41 319.59

326.87 326.87 337.95 348.40 390.19

416.38 427.97 444.89 444.89 469.27

469.27 489.79 572.30 590.70 595.97

595.97 596.08 597.93 608.70 608.70

637.58 637.58 644.14 660.04 731.77

766.42 766.42 798.32 830.19 833.84

833.84 845.34 915.06 915.76 915.76

917.07 940.73 975.62 975.62 981.77

990.35 990.35 995.21 1004.18 1028.83

1029.35 1029.35 1029.66 1052.66 1067.64

1067.64 1088.44 1098.34 1110.41 1110.41

1128.97 1147.56 1160.36 1160.36 1167.89

1221.42 1232.60 1232.60 1240.37 1240.47

1240.59 1240.59 1265.07 1295.04 1302.18

1302.18 1303.93 1321.36 1323.20 1323.20

1324.67 1349.73 1354.24 1354.24 1357.41

1411.32 1411.34 1411.34 1411.40 1442.40

1442.46 1442.46 1442.59 1466.29 1466.29

1466.82 1466.94 1473.91 1480.08 1480.08

1484.51 1489.59 1489.59 1493.42 1498.35

1517.41 1523.05 1523.05 1538.70 1575.13

1575.13 1580.29 1580.88 1581.77 1581.77

1587.67 1594.01 1687.04 1687.04 1687.06

1687.08 1721.12 1721.66 1721.66 1721.79

1726.86 1774.62 1774.62 1813.04 1813.04

1817.31 1829.83 1866.24 1877.45 1888.49

1888.49 1893.89 1897.70 1897.70 1907.29

1944.59 1945.59 1945.59 1949.30 1957.18

1961.08 1961.08 1971.22 1991.04 2090.67

2090.67 2117.83 2119.68 2119.72 2119.72

2123.95 2133.36 2180.23 2180.23 2183.86

2194.93 2198.36 2198.69 2199.76 2199.76

2235.33 2235.33 2266.79 2268.50 2328.26

2328.26 2328.53 2329.12 2364.20 2364.26

2364.26 2364.63 4562.15 4562.15 4562.15

4562.16 4571.69 4571.69 4571.69 4571.70

4583.86 4583.86 4583.87 4583.88 4592.69

4592.71 4592.71 4592.73 4602.86 4602.86

4602.88 4602.97 4669.44 4669.70 4669.70

4669.94 4693.27 4693.52 4693.52 4694.00

Zero-point correction= 0.594741 (Hartree/Particle)

Thermal correction to Energy= 0.631574

Thermal correction to Enthalpy= 0.632518

Thermal correction to Gibbs Free Energy= 0.525323

Sum of electronic and zero-point Energies= -1978.309613

Sum of electronic and thermal Energies= -1978.272779

Sum of electronic and thermal Enthalpies= -1978.271835

Sum of electronic and thermal Free Energies= -1978.379031

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 396.319 150.606 225.612

Electronic 0.000 0.000 0.000

Translational 0.889 2.981 45.415

Rotational 0.889 2.981 36.531

Vibrational 394.541 144.644 143.666

Vibration 1 0.593 1.987 8.343

Vibration 2 0.593 1.986 6.614

Vibration 3 0.594 1.981 5.288

Vibration 4 0.595 1.980 5.072

Vibration 5 0.595 1.980 5.072

Vibration 6 0.595 1.980 5.069

Vibration 7 0.595 1.978 4.814

Vibration 8 0.595 1.978 4.814

Vibration 9 0.596 1.975 4.553

Vibration 10 0.597 1.971 4.296

Vibration 11 0.597 1.971 4.296

Vibration 12 0.600 1.963 3.907

Vibration 13 0.601 1.959 3.760

Vibration 14 0.603 1.953 3.557

Vibration 15 0.604 1.947 3.410

Vibration 16 0.609 1.934 3.124

Vibration 17 0.615 1.912 2.783

Vibration 18 0.615 1.912 2.783

Vibration 19 0.637 1.841 2.140

Vibration 20 0.638 1.838 2.121

Vibration 21 0.644 1.819 2.006

Vibration 22 0.644 1.819 2.006

Vibration 23 0.648 1.809 1.948

Vibration 24 0.648 1.809 1.948

Vibration 25 0.648 1.807 1.942

Vibration 26 0.651 1.800 1.901

Vibration 27 0.651 1.800 1.901

Vibration 28 0.655 1.787 1.841

Vibration 29 0.658 1.776 1.787

Vibration 30 0.675 1.726 1.589

Vibration 31 0.686 1.693 1.477

Vibration 32 0.691 1.678 1.431

Vibration 33 0.699 1.656 1.367

Vibration 34 0.699 1.656 1.367

Vibration 35 0.710 1.623 1.279

Vibration 36 0.710 1.623 1.279

Vibration 37 0.720 1.595 1.210

Vibration 38 0.764 1.475 0.971

Vibration 39 0.775 1.447 0.925

Vibration 40 0.778 1.439 0.912

Vibration 41 0.778 1.439 0.912

Vibration 42 0.778 1.439 0.912

Vibration 43 0.779 1.436 0.907

Vibration 44 0.785 1.420 0.882

Vibration 45 0.785 1.420 0.882

Vibration 46 0.803 1.376 0.817

Vibration 47 0.803 1.376 0.817

Vibration 48 0.807 1.366 0.803

Vibration 49 0.817 1.342 0.770

Vibration 50 0.864 1.231 0.637

Vibration 51 0.888 1.178 0.581

Vibration 52 0.888 1.178 0.581

Vibration 53 0.910 1.129 0.534

Vibration 54 0.933 1.081 0.491

Vibration 55 0.936 1.076 0.486

Vibration 56 0.936 1.076 0.486

Vibration 57 0.945 1.058 0.472

Q Log10(Q) Ln(Q)

Total Bot 0.233821-241 -241.631117 -556.376208

Total V=0 0.851205D+32 31.930034 73.521620

Vib (Bot) 0.157438-257 -257.802891 -593.613095

Vib (Bot) 1 0.244896D+02 1.388982 3.198250

Vib (Bot) 2 0.102537D+02 1.010880 2.327636

Vib (Bot) 3 0.524896D+01 0.720073 1.658030

Vib (Bot) 4 0.470425D+01 0.672491 1.548467

Vib (Bot) 5 0.470425D+01 0.672491 1.548467

Vib (Bot) 6 0.469693D+01 0.671814 1.546908

Vib (Bot) 7 0.412676D+01 0.615609 1.417492

Vib (Bot) 8 0.412676D+01 0.615609 1.417492

Vib (Bot) 9 0.361493D+01 0.558100 1.285073

Vib (Bot) 10 0.317017D+01 0.501083 1.153786

Vib (Bot) 11 0.317017D+01 0.501083 1.153786

Vib (Bot) 12 0.259515D+01 0.414162 0.953644

Vib (Bot) 13 0.240583D+01 0.381264 0.877893

Vib (Bot) 14 0.216558D+01 0.335573 0.772686

Vib (Bot) 15 0.200510D+01 0.302137 0.695696

Vib (Bot) 16 0.172470D+01 0.236714 0.545055

Vib (Bot) 17 0.143578D+01 0.157089 0.361711

Vib (Bot) 18 0.143578D+01 0.157089 0.361711

Vib (Bot) 19 0.100080D+01 0.000347 0.000799

Vib (Bot) 20 0.989799D+00 -0.004453 -0.010253

Vib (Bot) 21 0.924716D+00 -0.033992 -0.078269

Vib (Bot) 22 0.924716D+00 -0.033992 -0.078269

Vib (Bot) 23 0.893305D+00 -0.049000 -0.112827

Vib (Bot) 24 0.893305D+00 -0.049000 -0.112827

Vib (Bot) 25 0.889693D+00 -0.050760 -0.116879

Vib (Bot) 26 0.868000D+00 -0.061480 -0.141563

Vib (Bot) 27 0.868000D+00 -0.061480 -0.141563

Vib (Bot) 28 0.836713D+00 -0.077424 -0.178275

Vib (Bot) 29 0.808947D+00 -0.092080 -0.212021

Vib (Bot) 30 0.712188D+00 -0.147405 -0.339413

Vib (Bot) 31 0.661010D+00 -0.179792 -0.413986

Vib (Bot) 32 0.640259D+00 -0.193645 -0.445883

Vib (Bot) 33 0.611812D+00 -0.213382 -0.491331

Vib (Bot) 34 0.611812D+00 -0.213382 -0.491331

Vib (Bot) 35 0.574214D+00 -0.240926 -0.554753

Vib (Bot) 36 0.574214D+00 -0.240926 -0.554753

Vib (Bot) 37 0.545306D+00 -0.263360 -0.606409

Vib (Bot) 38 0.448817D+00 -0.347931 -0.801140

Vib (Bot) 39 0.430755D+00 -0.365770 -0.842216

Vib (Bot) 40 0.425768D+00 -0.370827 -0.853861

Vib (Bot) 41 0.425768D+00 -0.370827 -0.853861

Vib (Bot) 42 0.425664D+00 -0.370933 -0.854105

Vib (Bot) 43 0.423937D+00 -0.372699 -0.858171

Vib (Bot) 44 0.414064D+00 -0.382932 -0.881734

Vib (Bot) 45 0.414064D+00 -0.382932 -0.881734

Vib (Bot) 46 0.389126D+00 -0.409910 -0.943852

Vib (Bot) 47 0.389126D+00 -0.409910 -0.943852

Vib (Bot) 48 0.383756D+00 -0.415944 -0.957747

Vib (Bot) 49 0.371143D+00 -0.430458 -0.991167

Vib (Bot) 50 0.320670D+00 -0.493941 -1.137342

Vib (Bot) 51 0.299477D+00 -0.523637 -1.205719

Vib (Bot) 52 0.299477D+00 -0.523637 -1.205719

Vib (Bot) 53 0.281513D+00 -0.550502 -1.267578

Vib (Bot) 54 0.264877D+00 -0.576956 -1.328491

Vib (Bot) 55 0.263050D+00 -0.579962 -1.335412

Vib (Bot) 56 0.263050D+00 -0.579962 -1.335412

Vib (Bot) 57 0.257394D+00 -0.589401 -1.357145

Vib (V=0) 0.573138D+16 15.758260 36.284734

Vib (V=0) 1 0.249947D+02 1.397849 3.218666

Vib (V=0) 2 0.107659D+02 1.032049 2.376380

Vib (V=0) 3 0.577272D+01 0.761380 1.753143

Vib (V=0) 4 0.523075D+01 0.718564 1.654555

Vib (V=0) 5 0.523075D+01 0.718564 1.654554

Vib (V=0) 6 0.522346D+01 0.717959 1.653161

Vib (V=0) 7 0.465694D+01 0.668100 1.538358

Vib (V=0) 8 0.465694D+01 0.668100 1.538358

Vib (V=0) 9 0.414935D+01 0.617980 1.422951

Vib (V=0) 10 0.370936D+01 0.569299 1.310859

Vib (V=0) 11 0.370936D+01 0.569299 1.310859

Vib (V=0) 12 0.314288D+01 0.497327 1.145139

Vib (V=0) 13 0.295723D+01 0.470886 1.084254

Vib (V=0) 14 0.272255D+01 0.434975 1.001568

Vib (V=0) 15 0.256651D+01 0.409342 0.942545

Vib (V=0) 16 0.229572D+01 0.360918 0.831045

Vib (V=0) 17 0.202035D+01 0.305427 0.703273

Vib (V=0) 18 0.202035D+01 0.305427 0.703273

Vib (V=0) 19 0.161875D+01 0.209180 0.481654

Vib (V=0) 20 0.160892D+01 0.206534 0.475563

Vib (V=0) 21 0.155124D+01 0.190678 0.439053

Vib (V=0) 22 0.155124D+01 0.190678 0.439053

Vib (V=0) 23 0.152372D+01 0.182904 0.421152

Vib (V=0) 24 0.152372D+01 0.182904 0.421152

Vib (V=0) 25 0.152057D+01 0.182005 0.419082

Vib (V=0) 26 0.150171D+01 0.176586 0.406605

Vib (V=0) 27 0.150171D+01 0.176586 0.406605

Vib (V=0) 28 0.147472D+01 0.168711 0.388471

Vib (V=0) 29 0.145100D+01 0.161667 0.372251

Vib (V=0) 30 0.137018D+01 0.136777 0.314941

Vib (V=0) 31 0.132882D+01 0.123465 0.284288

Vib (V=0) 32 0.131236D+01 0.118053 0.271828

Vib (V=0) 33 0.129014D+01 0.110635 0.254747

Vib (V=0) 34 0.129014D+01 0.110635 0.254747

Vib (V=0) 35 0.126139D+01 0.100851 0.232218

Vib (V=0) 36 0.126139D+01 0.100851 0.232218

Vib (V=0) 37 0.123984D+01 0.093364 0.214980

Vib (V=0) 38 0.117189D+01 0.068887 0.158618

Vib (V=0) 39 0.115996D+01 0.064444 0.148387

Vib (V=0) 40 0.115672D+01 0.063227 0.145587

Vib (V=0) 41 0.115672D+01 0.063227 0.145587

Vib (V=0) 42 0.115665D+01 0.063202 0.145528

Vib (V=0) 43 0.115553D+01 0.062782 0.144561

Vib (V=0) 44 0.114919D+01 0.060392 0.139058

Vib (V=0) 45 0.114919D+01 0.060392 0.139058

Vib (V=0) 46 0.113358D+01 0.054451 0.125378

Vib (V=0) 47 0.113358D+01 0.054451 0.125378

Vib (V=0) 48 0.113029D+01 0.053191 0.122477

Vib (V=0) 49 0.112269D+01 0.050261 0.115731

Vib (V=0) 50 0.109399D+01 0.039015 0.089836

Vib (V=0) 51 0.108283D+01 0.034559 0.079574

Vib (V=0) 52 0.108283D+01 0.034559 0.079574

Vib (V=0) 53 0.107380D+01 0.030924 0.071206

Vib (V=0) 54 0.106583D+01 0.027687 0.063751

Vib (V=0) 55 0.106497D+01 0.027339 0.062950

Vib (V=0) 56 0.106497D+01 0.027339 0.062950

Vib (V=0) 57 0.106236D+01 0.026273 0.060495

Electronic 0.100000D+01 0.000000 0.000000

Translational 0.691083D+09 8.839530 20.353770

Rotational 0.214904D+08 7.332244 16.883117

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000008440 -0.000009592 -0.000003289

2 6 -0.000023890 0.000035090 0.000010372

3 7 0.000000000 -0.000028903 -0.000005114

4 6 0.000023890 0.000035090 0.000010372

5 6 0.000008440 -0.000009592 -0.000003289

6 6 -0.000041625 -0.000041625 0.000000000

7 6 0.000035090 0.000023890 -0.000010372

8 7 -0.000028903 0.000000000 0.000005114

9 6 0.000035090 -0.000023890 -0.000010372

10 6 -0.000009592 -0.000008440 0.000003289

11 6 -0.000009592 0.000008440 0.000003289

12 6 0.000041625 -0.000041625 0.000000000

13 6 -0.000035090 0.000023890 -0.000010372

14 6 0.000009592 0.000008440 0.000003289

15 6 0.000009592 -0.000008440 0.000003289

16 6 -0.000035090 -0.000023890 -0.000010372

17 7 0.000028903 -0.000000000 0.000005114

18 6 0.000041625 0.000041625 0.000000000

19 6 -0.000023890 -0.000035090 0.000010372

20 6 -0.000008440 0.000009592 -0.000003289

21 6 0.000008440 0.000009592 -0.000003289

22 6 0.000023890 -0.000035090 0.000010372

23 7 -0.000000000 0.000028903 -0.000005114

24 6 -0.000041625 0.000041625 -0.000000000

25 6 0.000043896 0.000043896 0.000000000

26 6 -0.000018112 -0.000024401 0.000000559

27 6 0.000010048 0.000011572 0.000001364

28 6 -0.000005595 -0.000005595 -0.000000000

29 6 0.000011572 0.000010048 -0.000001364

30 6 -0.000024401 -0.000018112 -0.000000559

31 6 0.000005595 -0.000005595 -0.000000000

32 6 -0.000010048 0.000011572 0.000001364

33 6 0.000018112 -0.000024401 0.000000559

34 6 -0.000043896 0.000043896 -0.000000000

35 6 0.000024401 -0.000018112 -0.000000559

36 6 -0.000011572 0.000010048 -0.000001364

37 6 0.000043896 -0.000043896 -0.000000000

38 6 -0.000024401 0.000018112 -0.000000559

39 6 0.000011572 -0.000010048 -0.000001364

40 6 -0.000005595 0.000005595 0.000000000

41 6 0.000010048 -0.000011572 0.000001364

42 6 -0.000018112 0.000024401 0.000000559

43 6 -0.000043896 -0.000043896 -0.000000000

44 6 0.000024401 0.000018112 -0.000000559

45 6 -0.000011572 -0.000010048 -0.000001364

46 6 0.000005595 0.000005595 -0.000000000

47 6 -0.000010048 -0.000011572 0.000001364

48 6 0.000018112 0.000024401 0.000000559

49 1 -0.000005999 -0.000003130 -0.000001804

50 1 0.000005999 -0.000003130 -0.000001804

51 1 -0.000003130 -0.000005999 0.000001804

52 1 -0.000003130 0.000005999 0.000001804

53 1 0.000003130 0.000005999 0.000001804

54 1 0.000003130 -0.000005999 0.000001804

55 1 -0.000005999 0.000003130 -0.000001804

56 1 0.000005999 0.000003130 -0.000001804

57 1 -0.000001735 0.000002604 0.000001962

58 1 0.000000905 0.000000025 0.000000637

59 1 0.000001286 0.000001286 -0.000000000

60 1 0.000000025 0.000000905 -0.000000637

61 1 0.000002604 -0.000001735 -0.000001962

62 1 -0.000001286 0.000001286 -0.000000000

63 1 -0.000000905 0.000000025 0.000000637

64 1 0.000001735 0.000002604 0.000001962

65 1 -0.000002604 -0.000001735 -0.000001962

66 1 -0.000000025 0.000000905 -0.000000637

67 1 0.000002604 0.000001735 -0.000001962

68 1 0.000000025 -0.000000905 -0.000000637

69 1 0.000001286 -0.000001286 0.000000000

70 1 0.000000905 -0.000000025 0.000000637

71 1 -0.000001735 -0.000002604 0.000001962

72 1 -0.000002604 0.000001735 -0.000001962

73 1 -0.000000025 -0.000000905 -0.000000637

74 1 -0.000001286 -0.000001286 -0.000000000

75 1 -0.000000905 -0.000000025 0.000000637

76 1 0.000001735 -0.000002604 0.000001962

77 30 0.000000000 0.000000000 0.000000000

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

Cartesian Forces: Max 0.000043896 RMS 0.000016042

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

Leave Link 716 at Tue Aug 13 22:09:00 2019, MaxMem= 671088640 cpu: 1.4

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000028981 RMS 0.000005793

Search for a local minimum.

Step number 1 out of a maximum of 2

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

Second derivative matrix not updated -- analytic derivatives used.

ITU= 0

Eigenvalues --- 0.00283 0.00414 0.00568 0.00568 0.00592

Eigenvalues --- 0.00931 0.00997 0.00997 0.01031 0.01061

Eigenvalues --- 0.01197 0.01216 0.01216 0.01329 0.01407

Eigenvalues --- 0.01407 0.01412 0.01469 0.01505 0.01564

Eigenvalues --- 0.01564 0.01594 0.01594 0.01607 0.01630

Eigenvalues --- 0.01653 0.01737 0.01737 0.01737 0.01738

Eigenvalues --- 0.01761 0.01793 0.01794 0.01794 0.01908

Eigenvalues --- 0.01946 0.01946 0.01994 0.02163 0.02179

Eigenvalues --- 0.02179 0.02236 0.02307 0.02400 0.02400

Eigenvalues --- 0.02402 0.02487 0.02487 0.02492 0.02514

Eigenvalues --- 0.02534 0.02593 0.02593 0.02596 0.02609

Eigenvalues --- 0.02770 0.02770 0.02774 0.02785 0.02853

Eigenvalues --- 0.02897 0.02897 0.02903 0.02923 0.02988

Eigenvalues --- 0.02988 0.03224 0.03224 0.03494 0.03651

Eigenvalues --- 0.04190 0.04315 0.04315 0.04345 0.06443

Eigenvalues --- 0.06443 0.09732 0.09772 0.09772 0.09832

Eigenvalues --- 0.09864 0.10189 0.10492 0.10535 0.10535

Eigenvalues --- 0.10659 0.10659 0.10660 0.10660 0.10852

Eigenvalues --- 0.11315 0.11315 0.11316 0.11319 0.11828

Eigenvalues --- 0.11830 0.11836 0.11836 0.12251 0.12251

Eigenvalues --- 0.12251 0.12252 0.12684 0.12684 0.12684

Eigenvalues --- 0.12685 0.13117 0.13509 0.13509 0.15890

Eigenvalues --- 0.16421 0.16421 0.16733 0.16833 0.16930

Eigenvalues --- 0.17643 0.17643 0.19129 0.19274 0.19282

Eigenvalues --- 0.19282 0.19339 0.19364 0.19367 0.19367

Eigenvalues --- 0.19440 0.19561 0.19561 0.19563 0.19564

Eigenvalues --- 0.19887 0.19887 0.20042 0.20213 0.20802

Eigenvalues --- 0.20802 0.21795 0.23783 0.24085 0.24085

Eigenvalues --- 0.24875 0.25973 0.25973 0.26230 0.28072

Eigenvalues --- 0.28213 0.28213 0.28232 0.28923 0.29605

Eigenvalues --- 0.29926 0.30623 0.30623 0.31139 0.31916

Eigenvalues --- 0.31916 0.32896 0.34755 0.34755 0.34902

Eigenvalues --- 0.35256 0.35547 0.35547 0.35556 0.35556

Eigenvalues --- 0.35654 0.35682 0.35704 0.35704 0.35745

Eigenvalues --- 0.35869 0.35869 0.35869 0.35869 0.35870

Eigenvalues --- 0.35870 0.35870 0.35872 0.36030 0.36044

Eigenvalues --- 0.36044 0.36084 0.36811 0.36920 0.36920

Eigenvalues --- 0.37368 0.37404 0.37404 0.37514 0.38167

Eigenvalues --- 0.39638 0.39638 0.40122 0.40923 0.40932

Eigenvalues --- 0.40968 0.40968 0.41289 0.41289 0.41301

Eigenvalues --- 0.41353 0.43955 0.45712 0.45712 0.45827

Eigenvalues --- 0.45827 0.46072 0.46130 0.46197 0.46197

Eigenvalues --- 0.46306 0.46335 0.46423 0.46446 0.46446

Eigenvalues --- 0.46807 0.47123 0.50767 0.50767 0.50772

Eigenvalues --- 0.50774 0.52386 0.52741 0.52858 0.52858

Angle between quadratic step and forces= 54.58 degrees.

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.00027789 RMS(Int)= 0.00000003

Iteration 2 RMS(Cart)= 0.00000005 RMS(Int)= 0.00000000

ITry= 1 IFail=0 DXMaxC= 8.79D-04 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 5.20D-09 for atom 54.

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

(Linear) (Quad) (Total)

R1 2.74000 -0.00001 0.00000 -0.00005 -0.00005 2.73995

R2 2.57564 0.00002 0.00000 0.00003 0.00003 2.57566

R3 2.03920 0.00000 0.00000 0.00000 0.00000 2.03920

R4 2.58874 0.00002 0.00000 0.00005 0.00005 2.58879

R5 2.66784 -0.00001 0.00000 -0.00002 -0.00002 2.66781

R6 2.58874 0.00002 0.00000 0.00005 0.00005 2.58879

R7 3.95087 -0.00000 0.00000 -0.00001 -0.00001 3.95085

R8 2.74000 -0.00001 0.00000 -0.00005 -0.00005 2.73995

R9 2.66784 -0.00001 0.00000 -0.00002 -0.00002 2.66781

R10 2.03920 0.00000 0.00000 0.00000 0.00000 2.03920

R11 2.66784 -0.00001 0.00000 -0.00002 -0.00002 2.66781

R12 2.82229 0.00003 0.00000 0.00013 0.00013 2.82242

R13 2.58874 0.00002 0.00000 0.00005 0.00005 2.58879

R14 2.74000 -0.00001 0.00000 -0.00005 -0.00005 2.73995

R15 2.58874 0.00002 0.00000 0.00005 0.00005 2.58879

R16 3.95087 -0.00000 0.00000 -0.00001 -0.00001 3.95085

R17 2.74000 -0.00001 0.00000 -0.00005 -0.00005 2.73995

R18 2.66784 -0.00001 0.00000 -0.00002 -0.00002 2.66781

R19 2.57564 0.00002 0.00000 0.00003 0.00003 2.57566

R20 2.03920 0.00000 0.00000 0.00000 0.00000 2.03920

R21 2.03920 0.00000 0.00000 0.00000 0.00000 2.03920

R22 2.66784 -0.00001 0.00000 -0.00002 -0.00002 2.66781

R23 2.82229 0.00003 0.00000 0.00013 0.00013 2.82242

R24 2.74000 -0.00001 0.00000 -0.00005 -0.00005 2.73995

R25 2.58874 0.00002 0.00000 0.00005 0.00005 2.58879

R26 2.57564 0.00002 0.00000 0.00003 0.00003 2.57566

R27 2.03920 0.00000 0.00000 0.00000 0.00000 2.03920

R28 2.74000 -0.00001 0.00000 -0.00005 -0.00005 2.73995

R29 2.03920 0.00000 0.00000 0.00000 0.00000 2.03920

R30 2.58874 0.00002 0.00000 0.00005 0.00005 2.58879

R31 2.66784 -0.00001 0.00000 -0.00002 -0.00002 2.66781

R32 3.95087 -0.00000 0.00000 -0.00001 -0.00001 3.95085

R33 2.66784 -0.00001 0.00000 -0.00002 -0.00002 2.66781

R34 2.82229 0.00003 0.00000 0.00013 0.00013 2.82242

R35 2.74000 -0.00001 0.00000 -0.00005 -0.00005 2.73995

R36 2.58874 0.00002 0.00000 0.00005 0.00005 2.58879

R37 2.57564 0.00002 0.00000 0.00003 0.00003 2.57566

R38 2.03920 0.00000 0.00000 0.00000 0.00000 2.03920

R39 2.74000 -0.00001 0.00000 -0.00005 -0.00005 2.73995

R40 2.03920 0.00000 0.00000 0.00000 0.00000 2.03920

R41 2.58874 0.00002 0.00000 0.00005 0.00005 2.58879

R42 2.66784 -0.00001 0.00000 -0.00002 -0.00002 2.66781

R43 3.95087 -0.00000 0.00000 -0.00001 -0.00001 3.95085

R44 2.82229 0.00003 0.00000 0.00013 0.00013 2.82242

R45 2.64645 -0.00001 0.00000 -0.00003 -0.00003 2.64642

R46 2.64645 -0.00001 0.00000 -0.00003 -0.00003 2.64642

R47 2.63218 0.00001 0.00000 0.00003 0.00003 2.63222

R48 2.04952 -0.00000 0.00000 -0.00001 -0.00001 2.04951

R49 2.63475 -0.00000 0.00000 -0.00000 -0.00000 2.63475

R50 2.05046 -0.00000 0.00000 -0.00000 -0.00000 2.05046

R51 2.63475 -0.00000 0.00000 -0.00000 -0.00000 2.63475

R52 2.05028 0.00000 0.00000 0.00001 0.00001 2.05029

R53 2.63218 0.00001 0.00000 0.00003 0.00003 2.63222

R54 2.05046 -0.00000 0.00000 -0.00000 -0.00000 2.05046

R55 2.04952 -0.00000 0.00000 -0.00001 -0.00001 2.04951

R56 2.63475 -0.00000 0.00000 -0.00000 -0.00000 2.63475

R57 2.63475 -0.00000 0.00000 -0.00000 -0.00000 2.63475

R58 2.05028 0.00000 0.00000 0.00001 0.00001 2.05029

R59 2.63218 0.00001 0.00000 0.00003 0.00003 2.63222

R60 2.05046 -0.00000 0.00000 -0.00000 -0.00000 2.05046

R61 2.64645 -0.00001 0.00000 -0.00003 -0.00003 2.64642

R62 2.04952 -0.00000 0.00000 -0.00001 -0.00001 2.04951

R63 2.64645 -0.00001 0.00000 -0.00003 -0.00003 2.64642

R64 2.63218 0.00001 0.00000 0.00003 0.00003 2.63222

R65 2.04952 -0.00000 0.00000 -0.00001 -0.00001 2.04951

R66 2.05046 -0.00000 0.00000 -0.00000 -0.00000 2.05046

R67 2.64645 -0.00001 0.00000 -0.00003 -0.00003 2.64642

R68 2.64645 -0.00001 0.00000 -0.00003 -0.00003 2.64642

R69 2.63218 0.00001 0.00000 0.00003 0.00003 2.63222

R70 2.04952 -0.00000 0.00000 -0.00001 -0.00001 2.04951

R71 2.63475 -0.00000 0.00000 -0.00000 -0.00000 2.63475

R72 2.05046 -0.00000 0.00000 -0.00000 -0.00000 2.05046

R73 2.63475 -0.00000 0.00000 -0.00000 -0.00000 2.63475

R74 2.05028 0.00000 0.00000 0.00001 0.00001 2.05029

R75 2.63218 0.00001 0.00000 0.00003 0.00003 2.63222

R76 2.05046 -0.00000 0.00000 -0.00000 -0.00000 2.05046

R77 2.04952 -0.00000 0.00000 -0.00001 -0.00001 2.04951

R78 2.64645 -0.00001 0.00000 -0.00003 -0.00003 2.64642

R79 2.64645 -0.00001 0.00000 -0.00003 -0.00003 2.64642

R80 2.63218 0.00001 0.00000 0.00003 0.00003 2.63222

R81 2.04952 -0.00000 0.00000 -0.00001 -0.00001 2.04951

R82 2.63475 -0.00000 0.00000 -0.00000 -0.00000 2.63475

R83 2.05046 -0.00000 0.00000 -0.00000 -0.00000 2.05046

R84 2.63475 -0.00000 0.00000 -0.00000 -0.00000 2.63475

R85 2.05028 0.00000 0.00000 0.00001 0.00001 2.05029

R86 2.63218 0.00001 0.00000 0.00003 0.00003 2.63222

R87 2.05046 -0.00000 0.00000 -0.00000 -0.00000 2.05046

R88 2.04952 -0.00000 0.00000 -0.00001 -0.00001 2.04951

A1 1.87121 0.00000 0.00000 0.00001 0.00001 1.87122

A2 2.19523 -0.00001 0.00000 -0.00006 -0.00006 2.19518

A3 2.21659 0.00001 0.00000 0.00005 0.00005 2.21663

A4 1.89582 0.00000 0.00000 0.00001 0.00001 1.89583

A5 2.18767 0.00001 0.00000 0.00005 0.00005 2.18772

A6 2.19961 -0.00001 0.00000 -0.00005 -0.00005 2.19956

A7 1.89060 -0.00000 0.00000 -0.00003 -0.00003 1.89057

A8 2.19326 0.00000 0.00000 0.00001 0.00001 2.19327

A9 2.19326 0.00000 0.00000 0.00001 0.00001 2.19327

A10 1.89582 0.00000 0.00000 0.00001 0.00001 1.89583

A11 2.19961 -0.00001 0.00000 -0.00005 -0.00005 2.19956

A12 2.18767 0.00001 0.00000 0.00005 0.00005 2.18772

A13 1.87121 0.00000 0.00000 0.00001 0.00001 1.87122

A14 2.21659 0.00001 0.00000 0.00005 0.00005 2.21663

A15 2.19523 -0.00001 0.00000 -0.00006 -0.00006 2.19518

A16 2.20216 0.00001 0.00000 0.00007 0.00007 2.20223

A17 2.04051 -0.00001 0.00000 -0.00003 -0.00003 2.04048

A18 2.04051 -0.00001 0.00000 -0.00003 -0.00003 2.04048

A19 2.19961 -0.00001 0.00000 -0.00005 -0.00005 2.19956

A20 2.18767 0.00001 0.00000 0.00005 0.00005 2.18772

A21 1.89582 0.00000 0.00000 0.00001 0.00001 1.89583

A22 1.89060 -0.00000 0.00000 -0.00003 -0.00003 1.89057

A23 2.19326 0.00000 0.00000 0.00001 0.00001 2.19327

A24 2.19326 0.00000 0.00000 0.00001 0.00001 2.19327

A25 1.89582 0.00000 0.00000 0.00001 0.00001 1.89583

A26 2.19961 -0.00001 0.00000 -0.00005 -0.00005 2.19956

A27 2.18767 0.00001 0.00000 0.00005 0.00005 2.18772

A28 1.87121 0.00000 0.00000 0.00001 0.00001 1.87122

A29 2.19523 -0.00001 0.00000 -0.00006 -0.00006 2.19518

A30 2.21659 0.00001 0.00000 0.00005 0.00005 2.21663

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D5 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D6 -3.12324 -0.00000 0.00000 -0.00003 -0.00003 -3.12327

D7 3.12324 0.00000 0.00000 0.00003 0.00003 3.12327

D8 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D9 -0.01451 0.00000 0.00000 0.00003 0.00003 -0.01448

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D11 3.14070 -0.00000 0.00000 -0.00007 -0.00007 3.14063

D12 -0.11386 -0.00000 0.00000 -0.00008 -0.00008 -0.11394

D13 -3.06332 -0.00000 0.00000 -0.00007 -0.00007 -3.06339

D14 0.07827 -0.00000 0.00000 -0.00007 -0.00007 0.07820

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D16 -3.07915 0.00000 0.00000 0.00004 0.00004 -3.07910

D17 0.01451 -0.00000 0.00000 -0.00003 -0.00003 0.01448

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D38 2.02057 0.00000 0.00000 0.00023 0.00023 2.02080

D39 2.02057 0.00000 0.00000 0.00023 0.00023 2.02080

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D75 -2.02057 -0.00000 0.00000 -0.00023 -0.00023 -2.02080

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D172 -0.00467 0.00000 0.00000 -0.00000 -0.00000 -0.00467

D173 -0.00182 0.00000 0.00000 0.00001 0.00001 -0.00181

D174 3.13692 0.00000 0.00000 -0.00000 -0.00000 3.13692

D175 3.13978 0.00000 0.00000 0.00001 0.00001 3.13978

D176 -0.00467 0.00000 0.00000 -0.00000 -0.00000 -0.00467

D177 0.00366 -0.00000 0.00000 -0.00002 -0.00002 0.00364

D178 3.13612 0.00000 0.00000 0.00006 0.00006 3.13618

D179 -3.13509 -0.00000 0.00000 -0.00000 -0.00000 -3.13510

D180 -0.00263 0.00000 0.00000 0.00007 0.00007 -0.00256

D181 3.13977 0.00000 0.00000 0.00001 0.00001 3.13977

D182 -0.00183 0.00000 0.00000 0.00001 0.00001 -0.00182

D183 0.00725 -0.00000 0.00000 -0.00006 -0.00006 0.00719

D184 -3.13434 -0.00000 0.00000 -0.00006 -0.00006 -3.13440

D185 3.13977 0.00000 0.00000 0.00001 0.00001 3.13977

D186 0.00725 -0.00000 0.00000 -0.00006 -0.00006 0.00719

D187 -0.00183 0.00000 0.00000 0.00001 0.00001 -0.00182

D188 -3.13434 -0.00000 0.00000 -0.00006 -0.00006 -3.13440

D189 0.00366 -0.00000 0.00000 -0.00002 -0.00002 0.00364

D190 -3.13509 -0.00000 0.00000 -0.00000 -0.00000 -3.13510

D191 3.13612 0.00000 0.00000 0.00006 0.00006 3.13618

D192 -0.00263 0.00000 0.00000 0.00007 0.00007 -0.00256

D193 3.13977 0.00000 0.00000 0.00001 0.00001 3.13977

D194 0.00725 -0.00000 0.00000 -0.00006 -0.00006 0.00719

D195 -0.00183 0.00000 0.00000 0.00001 0.00001 -0.00182

D196 -3.13434 -0.00000 0.00000 -0.00006 -0.00006 -3.13440

D197 3.13977 0.00000 0.00000 0.00001 0.00001 3.13977

D198 0.00725 -0.00000 0.00000 -0.00006 -0.00006 0.00719

D199 -0.00183 0.00000 0.00000 0.00001 0.00001 -0.00182

D200 -3.13434 -0.00000 0.00000 -0.00006 -0.00006 -3.13440

D201 0.00366 -0.00000 0.00000 -0.00002 -0.00002 0.00364

D202 -3.13509 -0.00000 0.00000 -0.00000 -0.00000 -3.13510

D203 3.13612 0.00000 0.00000 0.00006 0.00006 3.13618

D204 -0.00263 0.00000 0.00000 0.00007 0.00007 -0.00256

D205 -0.00182 0.00000 0.00000 0.00001 0.00001 -0.00181

D206 3.13978 0.00000 0.00000 0.00001 0.00001 3.13978

D207 3.13692 0.00000 0.00000 -0.00000 -0.00000 3.13692

D208 -0.00467 0.00000 0.00000 -0.00000 -0.00000 -0.00467

D209 -0.00182 0.00000 0.00000 0.00001 0.00001 -0.00181

D210 3.13692 0.00000 0.00000 -0.00000 -0.00000 3.13692

D211 3.13978 0.00000 0.00000 0.00001 0.00001 3.13978

D212 -0.00467 0.00000 0.00000 -0.00000 -0.00000 -0.00467

D213 0.00366 -0.00000 0.00000 -0.00002 -0.00002 0.00364

D214 3.13612 0.00000 0.00000 0.00006 0.00006 3.13618

D215 -3.13509 -0.00000 0.00000 -0.00000 -0.00000 -3.13510

D216 -0.00263 0.00000 0.00000 0.00007 0.00007 -0.00256

D217 -3.13977 -0.00000 0.00000 -0.00001 -0.00001 -3.13977

D218 -0.00725 0.00000 0.00000 0.00006 0.00006 -0.00719

D219 0.00183 -0.00000 0.00000 -0.00001 -0.00001 0.00182

D220 3.13434 0.00000 0.00000 0.00006 0.00006 3.13440

D221 -3.13977 -0.00000 0.00000 -0.00001 -0.00001 -3.13977

D222 -0.00725 0.00000 0.00000 0.00006 0.00006 -0.00719

D223 0.00183 -0.00000 0.00000 -0.00001 -0.00001 0.00182

D224 3.13434 0.00000 0.00000 0.00006 0.00006 3.13440

D225 -0.00366 0.00000 0.00000 0.00002 0.00002 -0.00364

D226 3.13509 0.00000 0.00000 0.00000 0.00000 3.13510

D227 -3.13612 -0.00000 0.00000 -0.00006 -0.00006 -3.13618

D228 0.00263 -0.00000 0.00000 -0.00007 -0.00007 0.00256

D229 0.00182 -0.00000 0.00000 -0.00001 -0.00001 0.00181

D230 -3.13978 -0.00000 0.00000 -0.00001 -0.00001 -3.13978

D231 -3.13692 -0.00000 0.00000 0.00000 0.00000 -3.13692

D232 0.00467 -0.00000 0.00000 0.00000 0.00000 0.00467

D233 0.00182 -0.00000 0.00000 -0.00001 -0.00001 0.00181

D234 -3.13692 -0.00000 0.00000 0.00000 0.00000 -3.13692

D235 -3.13978 -0.00000 0.00000 -0.00001 -0.00001 -3.13978

D236 0.00467 -0.00000 0.00000 0.00000 0.00000 0.00467

D237 -0.00366 0.00000 0.00000 0.00002 0.00002 -0.00364

D238 -3.13612 -0.00000 0.00000 -0.00006 -0.00006 -3.13618

D239 3.13509 0.00000 0.00000 0.00000 0.00000 3.13510

D240 0.00263 -0.00000 0.00000 -0.00007 -0.00007 0.00256

Item Value Threshold Converged?

Maximum Force 0.000029 0.000450 YES

RMS Force 0.000006 0.000300 YES

Maximum Displacement 0.000879 0.001800 YES

RMS Displacement 0.000278 0.001200 YES

Predicted change in Energy=-4.648248D-08

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) 1.4499 -DE/DX = 0.0 !

! R2 R(1,5) 1.363 -DE/DX = 0.0 !

! R3 R(1,49) 1.0791 -DE/DX = 0.0 !

! R4 R(2,3) 1.3699 -DE/DX = 0.0 !

! R5 R(2,12) 1.4118 -DE/DX = 0.0 !

! R6 R(3,4) 1.3699 -DE/DX = 0.0 !

! R7 R(3,77) 2.0907 -DE/DX = 0.0 !

! R8 R(4,5) 1.4499 -DE/DX = 0.0 !

! R9 R(4,6) 1.4118 -DE/DX = 0.0 !

! R10 R(5,50) 1.0791 -DE/DX = 0.0 !

! R11 R(6,7) 1.4118 -DE/DX = 0.0 !

! R12 R(6,25) 1.4935 -DE/DX = 0.0 !

! R13 R(7,8) 1.3699 -DE/DX = 0.0 !

! R14 R(7,11) 1.4499 -DE/DX = 0.0 !

! R15 R(8,9) 1.3699 -DE/DX = 0.0 !

! R16 R(8,77) 2.0907 -DE/DX = 0.0 !

! R17 R(9,10) 1.4499 -DE/DX = 0.0 !

! R18 R(9,24) 1.4118 -DE/DX = 0.0 !

! R19 R(10,11) 1.363 -DE/DX = 0.0 !

! R20 R(10,51) 1.0791 -DE/DX = 0.0 !

! R21 R(11,52) 1.0791 -DE/DX = 0.0 !

! R22 R(12,13) 1.4118 -DE/DX = 0.0 !

! R23 R(12,34) 1.4935 -DE/DX = 0.0 !

! R24 R(13,14) 1.4499 -DE/DX = 0.0 !

! R25 R(13,17) 1.3699 -DE/DX = 0.0 !

! R26 R(14,15) 1.363 -DE/DX = 0.0 !

! R27 R(14,53) 1.0791 -DE/DX = 0.0 !

! R28 R(15,16) 1.4499 -DE/DX = 0.0 !

! R29 R(15,54) 1.0791 -DE/DX = 0.0 !

! R30 R(16,17) 1.3699 -DE/DX = 0.0 !

! R31 R(16,18) 1.4118 -DE/DX = 0.0 !

! R32 R(17,77) 2.0907 -DE/DX = 0.0 !

! R33 R(18,19) 1.4118 -DE/DX = 0.0 !

! R34 R(18,43) 1.4935 -DE/DX = 0.0 !

! R35 R(19,20) 1.4499 -DE/DX = 0.0 !

! R36 R(19,23) 1.3699 -DE/DX = 0.0 !

! R37 R(20,21) 1.363 -DE/DX = 0.0 !

! R38 R(20,55) 1.0791 -DE/DX = 0.0 !

! R39 R(21,22) 1.4499 -DE/DX = 0.0 !

! R40 R(21,56) 1.0791 -DE/DX = 0.0 !

! R41 R(22,23) 1.3699 -DE/DX = 0.0 !

! R42 R(22,24) 1.4118 -DE/DX = 0.0 !

! R43 R(23,77) 2.0907 -DE/DX = 0.0 !

! R44 R(24,37) 1.4935 -DE/DX = 0.0 !

! R45 R(25,26) 1.4004 -DE/DX = 0.0 !

! R46 R(25,30) 1.4004 -DE/DX = 0.0 !

! R47 R(26,27) 1.3929 -DE/DX = 0.0 !

! R48 R(26,57) 1.0846 -DE/DX = 0.0 !

! R49 R(27,28) 1.3943 -DE/DX = 0.0 !

! R50 R(27,58) 1.0851 -DE/DX = 0.0 !

! R51 R(28,29) 1.3943 -DE/DX = 0.0 !

! R52 R(28,59) 1.085 -DE/DX = 0.0 !

! R53 R(29,30) 1.3929 -DE/DX = 0.0 !

! R54 R(29,60) 1.0851 -DE/DX = 0.0 !

! R55 R(30,61) 1.0846 -DE/DX = 0.0 !

! R56 R(31,32) 1.3943 -DE/DX = 0.0 !

! R57 R(31,36) 1.3943 -DE/DX = 0.0 !

! R58 R(31,62) 1.085 -DE/DX = 0.0 !

! R59 R(32,33) 1.3929 -DE/DX = 0.0 !

! R60 R(32,63) 1.0851 -DE/DX = 0.0 !

! R61 R(33,34) 1.4004 -DE/DX = 0.0 !

! R62 R(33,64) 1.0846 -DE/DX = 0.0 !

! R63 R(34,35) 1.4004 -DE/DX = 0.0 !

! R64 R(35,36) 1.3929 -DE/DX = 0.0 !

! R65 R(35,65) 1.0846 -DE/DX = 0.0 !

! R66 R(36,66) 1.0851 -DE/DX = 0.0 !

! R67 R(37,38) 1.4004 -DE/DX = 0.0 !

! R68 R(37,42) 1.4004 -DE/DX = 0.0 !

! R69 R(38,39) 1.3929 -DE/DX = 0.0 !

! R70 R(38,67) 1.0846 -DE/DX = 0.0 !

! R71 R(39,40) 1.3943 -DE/DX = 0.0 !

! R72 R(39,68) 1.0851 -DE/DX = 0.0 !

! R73 R(40,41) 1.3943 -DE/DX = 0.0 !

! R74 R(40,69) 1.085 -DE/DX = 0.0 !

! R75 R(41,42) 1.3929 -DE/DX = 0.0 !

! R76 R(41,70) 1.0851 -DE/DX = 0.0 !

! R77 R(42,71) 1.0846 -DE/DX = 0.0 !

! R78 R(43,44) 1.4004 -DE/DX = 0.0 !

! R79 R(43,48) 1.4004 -DE/DX = 0.0 !

! R80 R(44,45) 1.3929 -DE/DX = 0.0 !

! R81 R(44,72) 1.0846 -DE/DX = 0.0 !

! R82 R(45,46) 1.3943 -DE/DX = 0.0 !

! R83 R(45,73) 1.0851 -DE/DX = 0.0 !

! R84 R(46,47) 1.3943 -DE/DX = 0.0 !

! R85 R(46,74) 1.085 -DE/DX = 0.0 !

! R86 R(47,48) 1.3929 -DE/DX = 0.0 !

! R87 R(47,75) 1.0851 -DE/DX = 0.0 !

! R88 R(48,76) 1.0846 -DE/DX = 0.0 !

! A1 A(2,1,5) 107.2123 -DE/DX = 0.0 !

! A2 A(2,1,49) 125.7776 -DE/DX = 0.0 !

! A3 A(5,1,49) 127.001 -DE/DX = 0.0 !

! A4 A(1,2,3) 108.6225 -DE/DX = 0.0 !

! A5 A(1,2,12) 125.3442 -DE/DX = 0.0 !

! A6 A(3,2,12) 126.0283 -DE/DX = 0.0 !

! A7 A(2,3,4) 108.3234 -DE/DX = 0.0 !

! A8 A(2,3,77) 125.6646 -DE/DX = 0.0 !

! A9 A(4,3,77) 125.6646 -DE/DX = 0.0 !

! A10 A(3,4,5) 108.6225 -DE/DX = 0.0 !

! A11 A(3,4,6) 126.0283 -DE/DX = 0.0 !

! A12 A(5,4,6) 125.3442 -DE/DX = 0.0 !

! A13 A(1,5,4) 107.2123 -DE/DX = 0.0 !

! A14 A(1,5,50) 127.001 -DE/DX = 0.0 !

! A15 A(4,5,50) 125.7776 -DE/DX = 0.0 !

! A16 A(4,6,7) 126.1744 -DE/DX = 0.0 !

! A17 A(4,6,25) 116.9128 -DE/DX = 0.0 !

! A18 A(7,6,25) 116.9128 -DE/DX = 0.0 !

! A19 A(6,7,8) 126.0283 -DE/DX = 0.0 !

! A20 A(6,7,11) 125.3442 -DE/DX = 0.0 !

! A21 A(8,7,11) 108.6225 -DE/DX = 0.0 !

! A22 A(7,8,9) 108.3234 -DE/DX = 0.0 !

! A23 A(7,8,77) 125.6646 -DE/DX = 0.0 !

! A24 A(9,8,77) 125.6646 -DE/DX = 0.0 !

! A25 A(8,9,10) 108.6225 -DE/DX = 0.0 !

! A26 A(8,9,24) 126.0283 -DE/DX = 0.0 !

! A27 A(10,9,24) 125.3442 -DE/DX = 0.0 !

! A28 A(9,10,11) 107.2123 -DE/DX = 0.0 !

! A29 A(9,10,51) 125.7776 -DE/DX = 0.0 !

! A30 A(11,10,51) 127.001 -DE/DX = 0.0 !

! A31 A(7,11,10) 107.2123 -DE/DX = 0.0 !

! A32 A(7,11,52) 125.7776 -DE/DX = 0.0 !

! A33 A(10,11,52) 127.001 -DE/DX = 0.0 !

! A34 A(2,12,13) 126.1744 -DE/DX = 0.0 !

! A35 A(2,12,34) 116.9128 -DE/DX = 0.0 !

! A36 A(13,12,34) 116.9128 -DE/DX = 0.0 !

! A37 A(12,13,14) 125.3442 -DE/DX = 0.0 !

! A38 A(12,13,17) 126.0283 -DE/DX = 0.0 !

! A39 A(14,13,17) 108.6225 -DE/DX = 0.0 !

! A40 A(13,14,15) 107.2123 -DE/DX = 0.0 !

! A41 A(13,14,53) 125.7776 -DE/DX = 0.0 !

! A42 A(15,14,53) 127.001 -DE/DX = 0.0 !

! A43 A(14,15,16) 107.2123 -DE/DX = 0.0 !

! A44 A(14,15,54) 127.001 -DE/DX = 0.0 !

! A45 A(16,15,54) 125.7776 -DE/DX = 0.0 !

! A46 A(15,16,17) 108.6225 -DE/DX = 0.0 !

! A47 A(15,16,18) 125.3442 -DE/DX = 0.0 !

! A48 A(17,16,18) 126.0283 -DE/DX = 0.0 !

! A49 A(13,17,16) 108.3234 -DE/DX = 0.0 !

! A50 A(13,17,77) 125.6646 -DE/DX = 0.0 !

! A51 A(16,17,77) 125.6646 -DE/DX = 0.0 !

! A52 A(16,18,19) 126.1744 -DE/DX = 0.0 !

! A53 A(16,18,43) 116.9128 -DE/DX = 0.0 !

! A54 A(19,18,43) 116.9128 -DE/DX = 0.0 !

! A55 A(18,19,20) 125.3442 -DE/DX = 0.0 !

! A56 A(18,19,23) 126.0283 -DE/DX = 0.0 !

! A57 A(20,19,23) 108.6225 -DE/DX = 0.0 !

! A58 A(19,20,21) 107.2123 -DE/DX = 0.0 !

! A59 A(19,20,55) 125.7776 -DE/DX = 0.0 !

! A60 A(21,20,55) 127.001 -DE/DX = 0.0 !

! A61 A(20,21,22) 107.2123 -DE/DX = 0.0 !

! A62 A(20,21,56) 127.001 -DE/DX = 0.0 !

! A63 A(22,21,56) 125.7776 -DE/DX = 0.0 !

! A64 A(21,22,23) 108.6225 -DE/DX = 0.0 !

! A65 A(21,22,24) 125.3442 -DE/DX = 0.0 !

! A66 A(23,22,24) 126.0283 -DE/DX = 0.0 !

! A67 A(19,23,22) 108.3234 -DE/DX = 0.0 !

! A68 A(19,23,77) 125.6646 -DE/DX = 0.0 !

! A69 A(22,23,77) 125.6646 -DE/DX = 0.0 !

! A70 A(9,24,22) 126.1744 -DE/DX = 0.0 !

! A71 A(9,24,37) 116.9128 -DE/DX = 0.0 !

! A72 A(22,24,37) 116.9128 -DE/DX = 0.0 !

! A73 A(6,25,26) 120.6585 -DE/DX = 0.0 !

! A74 A(6,25,30) 120.6585 -DE/DX = 0.0 !

! A75 A(26,25,30) 118.6829 -DE/DX = 0.0 !

! A76 A(25,26,27) 120.6797 -DE/DX = 0.0 !

! A77 A(25,26,57) 119.3697 -DE/DX = 0.0 !

! A78 A(27,26,57) 119.9486 -DE/DX = 0.0 !

! A79 A(26,27,28) 120.163 -DE/DX = 0.0 !

! A80 A(26,27,58) 119.7006 -DE/DX = 0.0 !

! A81 A(28,27,58) 120.1361 -DE/DX = 0.0 !

! A82 A(27,28,29) 119.6312 -DE/DX = 0.0 !

! A83 A(27,28,59) 120.1844 -DE/DX = 0.0 !

! A84 A(29,28,59) 120.1844 -DE/DX = 0.0 !

! A85 A(28,29,30) 120.163 -DE/DX = 0.0 !

! A86 A(28,29,60) 120.1361 -DE/DX = 0.0 !

! A87 A(30,29,60) 119.7006 -DE/DX = 0.0 !

! A88 A(25,30,29) 120.6797 -DE/DX = 0.0 !

! A89 A(25,30,61) 119.3697 -DE/DX = 0.0 !

! A90 A(29,30,61) 119.9486 -DE/DX = 0.0 !

! A91 A(32,31,36) 119.6312 -DE/DX = 0.0 !

! A92 A(32,31,62) 120.1844 -DE/DX = 0.0 !

! A93 A(36,31,62) 120.1844 -DE/DX = 0.0 !

! A94 A(31,32,33) 120.163 -DE/DX = 0.0 !

! A95 A(31,32,63) 120.1361 -DE/DX = 0.0 !

! A96 A(33,32,63) 119.7006 -DE/DX = 0.0 !

! A97 A(32,33,34) 120.6797 -DE/DX = 0.0 !

! A98 A(32,33,64) 119.9486 -DE/DX = 0.0 !

! A99 A(34,33,64) 119.3697 -DE/DX = 0.0 !

! A100 A(12,34,33) 120.6585 -DE/DX = 0.0 !

! A101 A(12,34,35) 120.6585 -DE/DX = 0.0 !

! A102 A(33,34,35) 118.6829 -DE/DX = 0.0 !

! A103 A(34,35,36) 120.6797 -DE/DX = 0.0 !

! A104 A(34,35,65) 119.3697 -DE/DX = 0.0 !

! A105 A(36,35,65) 119.9486 -DE/DX = 0.0 !

! A106 A(31,36,35) 120.163 -DE/DX = 0.0 !

! A107 A(31,36,66) 120.1361 -DE/DX = 0.0 !

! A108 A(35,36,66) 119.7006 -DE/DX = 0.0 !

! A109 A(24,37,38) 120.6585 -DE/DX = 0.0 !

! A110 A(24,37,42) 120.6585 -DE/DX = 0.0 !

! A111 A(38,37,42) 118.6829 -DE/DX = 0.0 !

! A112 A(37,38,39) 120.6797 -DE/DX = 0.0 !

! A113 A(37,38,67) 119.3697 -DE/DX = 0.0 !

! A114 A(39,38,67) 119.9486 -DE/DX = 0.0 !

! A115 A(38,39,40) 120.163 -DE/DX = 0.0 !

! A116 A(38,39,68) 119.7006 -DE/DX = 0.0 !

! A117 A(40,39,68) 120.1361 -DE/DX = 0.0 !

! A118 A(39,40,41) 119.6312 -DE/DX = 0.0 !

! A119 A(39,40,69) 120.1844 -DE/DX = 0.0 !

! A120 A(41,40,69) 120.1844 -DE/DX = 0.0 !

! A121 A(40,41,42) 120.163 -DE/DX = 0.0 !

! A122 A(40,41,70) 120.1361 -DE/DX = 0.0 !

! A123 A(42,41,70) 119.7006 -DE/DX = 0.0 !

! A124 A(37,42,41) 120.6797 -DE/DX = 0.0 !

! A125 A(37,42,71) 119.3697 -DE/DX = 0.0 !

! A126 A(41,42,71) 119.9486 -DE/DX = 0.0 !

! A127 A(18,43,44) 120.6585 -DE/DX = 0.0 !

! A128 A(18,43,48) 120.6585 -DE/DX = 0.0 !

! A129 A(44,43,48) 118.6829 -DE/DX = 0.0 !

! A130 A(43,44,45) 120.6797 -DE/DX = 0.0 !

! A131 A(43,44,72) 119.3697 -DE/DX = 0.0 !

! A132 A(45,44,72) 119.9486 -DE/DX = 0.0 !

! A133 A(44,45,46) 120.163 -DE/DX = 0.0 !

! A134 A(44,45,73) 119.7006 -DE/DX = 0.0 !

! A135 A(46,45,73) 120.1361 -DE/DX = 0.0 !

! A136 A(45,46,47) 119.6312 -DE/DX = 0.0 !

! A137 A(45,46,74) 120.1844 -DE/DX = 0.0 !

! A138 A(47,46,74) 120.1844 -DE/DX = 0.0 !

! A139 A(46,47,48) 120.163 -DE/DX = 0.0 !

! A140 A(46,47,75) 120.1361 -DE/DX = 0.0 !

! A141 A(48,47,75) 119.7006 -DE/DX = 0.0 !

! A142 A(43,48,47) 120.6797 -DE/DX = 0.0 !

! A143 A(43,48,76) 119.3697 -DE/DX = 0.0 !

! A144 A(47,48,76) 119.9486 -DE/DX = 0.0 !

! A145 A(3,77,8) 90.0099 -DE/DX = 0.0 !

! A146 A(3,77,17) 90.0099 -DE/DX = 0.0 !

! A147 A(8,77,23) 90.0099 -DE/DX = 0.0 !

! A148 A(17,77,23) 90.0099 -DE/DX = 0.0 !

! A149 L(3,77,23,17,-1) 180.0198 -DE/DX = 0.0 !

! A150 L(8,77,17,23,-1) 180.0198 -DE/DX = 0.0 !

! A151 L(3,77,23,17,-2) 178.495 -DE/DX = 0.0 !

! A152 L(8,77,17,23,-2) 178.495 -DE/DX = 0.0 !

! D1 D(5,1,2,3) 0.5095 -DE/DX = 0.0 !

! D2 D(5,1,2,12) 179.7358 -DE/DX = 0.0 !

! D3 D(49,1,2,3) -178.4553 -DE/DX = 0.0 !

! D4 D(49,1,2,12) 0.771 -DE/DX = 0.0 !

! D5 D(2,1,5,4) 0.0 -DE/DX = 0.0 !

! D6 D(2,1,5,50) -178.9484 -DE/DX = 0.0 !

! D7 D(49,1,5,4) 178.9484 -DE/DX = 0.0 !

! D8 D(49,1,5,50) 0.0 -DE/DX = 0.0 !

! D9 D(1,2,3,4) -0.8313 -DE/DX = 0.0 !

! D10 D(1,2,3,77) 172.6961 -DE/DX = 0.0 !

! D11 D(12,2,3,4) 179.9491 -DE/DX = 0.0 !

! D12 D(12,2,3,77) -6.5236 -DE/DX = 0.0 !

! D13 D(1,2,12,13) -175.5155 -DE/DX = 0.0 !

! D14 D(1,2,12,34) 4.4845 -DE/DX = 0.0 !

! D15 D(3,2,12,13) 3.5779 -DE/DX = 0.0 !

! D16 D(3,2,12,34) -176.4221 -DE/DX = 0.0 !

! D17 D(2,3,4,5) 0.8313 -DE/DX = 0.0 !

! D18 D(2,3,4,6) -179.9491 -DE/DX = 0.0 !

! D19 D(77,3,4,5) -172.6961 -DE/DX = 0.0 !

! D20 D(77,3,4,6) 6.5236 -DE/DX = 0.0 !

! D21 D(2,3,77,8) -175.4631 -DE/DX = 0.0 !

! D22 D(2,3,77,17) 3.0319 -DE/DX = 0.0 !

! D23 D(4,3,77,8) -3.0319 -DE/DX = 0.0 !

! D24 D(4,3,77,17) 175.4631 -DE/DX = 0.0 !

! D25 D(3,4,5,1) -0.5095 -DE/DX = 0.0 !

! D26 D(3,4,5,50) 178.4553 -DE/DX = 0.0 !

! D27 D(6,4,5,1) -179.7358 -DE/DX = 0.0 !

! D28 D(6,4,5,50) -0.771 -DE/DX = 0.0 !

! D29 D(3,4,6,7) -3.5779 -DE/DX = 0.0 !

! D30 D(3,4,6,25) 176.4221 -DE/DX = 0.0 !

! D31 D(5,4,6,7) 175.5155 -DE/DX = 0.0 !

! D32 D(5,4,6,25) -4.4845 -DE/DX = 0.0 !

! D33 D(4,6,7,8) -3.5779 -DE/DX = 0.0 !

! D34 D(4,6,7,11) 175.5155 -DE/DX = 0.0 !

! D35 D(25,6,7,8) 176.4221 -DE/DX = 0.0 !

! D36 D(25,6,7,11) -4.4845 -DE/DX = 0.0 !

! D37 D(4,6,25,26) -64.2296 -DE/DX = 0.0 !

! D38 D(4,6,25,30) 115.7704 -DE/DX = 0.0 !

! D39 D(7,6,25,26) 115.7704 -DE/DX = 0.0 !

! D40 D(7,6,25,30) -64.2296 -DE/DX = 0.0 !

! D41 D(6,7,8,9) -179.9491 -DE/DX = 0.0 !

! D42 D(6,7,8,77) 6.5236 -DE/DX = 0.0 !

! D43 D(11,7,8,9) 0.8313 -DE/DX = 0.0 !

! D44 D(11,7,8,77) -172.6961 -DE/DX = 0.0 !

! D45 D(6,7,11,10) -179.7358 -DE/DX = 0.0 !

! D46 D(6,7,11,52) -0.771 -DE/DX = 0.0 !

! D47 D(8,7,11,10) -0.5095 -DE/DX = 0.0 !

! D48 D(8,7,11,52) 178.4553 -DE/DX = 0.0 !

! D49 D(7,8,9,10) -0.8313 -DE/DX = 0.0 !

! D50 D(7,8,9,24) 179.9491 -DE/DX = 0.0 !

! D51 D(77,8,9,10) 172.6961 -DE/DX = 0.0 !

! D52 D(77,8,9,24) -6.5236 -DE/DX = 0.0 !

! D53 D(7,8,77,3) -3.0319 -DE/DX = 0.0 !

! D54 D(7,8,77,23) 175.4631 -DE/DX = 0.0 !

! D55 D(9,8,77,3) -175.4631 -DE/DX = 0.0 !

! D56 D(9,8,77,23) 3.0319 -DE/DX = 0.0 !

! D57 D(8,9,10,11) 0.5095 -DE/DX = 0.0 !

! D58 D(8,9,10,51) -178.4553 -DE/DX = 0.0 !

! D59 D(24,9,10,11) 179.7358 -DE/DX = 0.0 !

! D60 D(24,9,10,51) 0.771 -DE/DX = 0.0 !

! D61 D(8,9,24,22) 3.5779 -DE/DX = 0.0 !

! D62 D(8,9,24,37) -176.4221 -DE/DX = 0.0 !

! D63 D(10,9,24,22) -175.5155 -DE/DX = 0.0 !

! D64 D(10,9,24,37) 4.4845 -DE/DX = 0.0 !

! D65 D(9,10,11,7) 0.0 -DE/DX = 0.0 !

! D66 D(9,10,11,52) -178.9484 -DE/DX = 0.0 !

! D67 D(51,10,11,7) 178.9484 -DE/DX = 0.0 !

! D68 D(51,10,11,52) 0.0 -DE/DX = 0.0 !

! D69 D(2,12,13,14) -175.5155 -DE/DX = 0.0 !

! D70 D(2,12,13,17) 3.5779 -DE/DX = 0.0 !

! D71 D(34,12,13,14) 4.4845 -DE/DX = 0.0 !

! D72 D(34,12,13,17) -176.4221 -DE/DX = 0.0 !

! D73 D(2,12,34,33) 64.2296 -DE/DX = 0.0 !

! D74 D(2,12,34,35) -115.7704 -DE/DX = 0.0 !

! D75 D(13,12,34,33) -115.7704 -DE/DX = 0.0 !

! D76 D(13,12,34,35) 64.2296 -DE/DX = 0.0 !

! D77 D(12,13,14,15) 179.7358 -DE/DX = 0.0 !

! D78 D(12,13,14,53) 0.771 -DE/DX = 0.0 !

! D79 D(17,13,14,15) 0.5095 -DE/DX = 0.0 !

! D80 D(17,13,14,53) -178.4553 -DE/DX = 0.0 !

! D81 D(12,13,17,16) 179.9491 -DE/DX = 0.0 !

! D82 D(12,13,17,77) -6.5236 -DE/DX = 0.0 !

! D83 D(14,13,17,16) -0.8313 -DE/DX = 0.0 !

! D84 D(14,13,17,77) 172.6961 -DE/DX = 0.0 !

! D85 D(13,14,15,16) 0.0 -DE/DX = 0.0 !

! D86 D(13,14,15,54) -178.9484 -DE/DX = 0.0 !

! D87 D(53,14,15,16) 178.9484 -DE/DX = 0.0 !

! D88 D(53,14,15,54) 0.0 -DE/DX = 0.0 !

! D89 D(14,15,16,17) -0.5095 -DE/DX = 0.0 !

! D90 D(14,15,16,18) -179.7358 -DE/DX = 0.0 !

! D91 D(54,15,16,17) 178.4553 -DE/DX = 0.0 !

! D92 D(54,15,16,18) -0.771 -DE/DX = 0.0 !

! D93 D(15,16,17,13) 0.8313 -DE/DX = 0.0 !

! D94 D(15,16,17,77) -172.6961 -DE/DX = 0.0 !

! D95 D(18,16,17,13) -179.9491 -DE/DX = 0.0 !

! D96 D(18,16,17,77) 6.5236 -DE/DX = 0.0 !

! D97 D(15,16,18,19) 175.5155 -DE/DX = 0.0 !

! D98 D(15,16,18,43) -4.4845 -DE/DX = 0.0 !

! D99 D(17,16,18,19) -3.5779 -DE/DX = 0.0 !

! D100 D(17,16,18,43) 176.4221 -DE/DX = 0.0 !

! D101 D(13,17,77,3) 3.0319 -DE/DX = 0.0 !

! D102 D(13,17,77,23) -175.4631 -DE/DX = 0.0 !

! D103 D(16,17,77,3) 175.4631 -DE/DX = 0.0 !

! D104 D(16,17,77,23) -3.0319 -DE/DX = 0.0 !

! D105 D(16,18,19,20) 175.5155 -DE/DX = 0.0 !

! D106 D(16,18,19,23) -3.5779 -DE/DX = 0.0 !

! D107 D(43,18,19,20) -4.4845 -DE/DX = 0.0 !

! D108 D(43,18,19,23) 176.4221 -DE/DX = 0.0 !

! D109 D(16,18,43,44) -64.2296 -DE/DX = 0.0 !

! D110 D(16,18,43,48) 115.7704 -DE/DX = 0.0 !

! D111 D(19,18,43,44) 115.7704 -DE/DX = 0.0 !

! D112 D(19,18,43,48) -64.2296 -DE/DX = 0.0 !

! D113 D(18,19,20,21) -179.7358 -DE/DX = 0.0 !

! D114 D(18,19,20,55) -0.771 -DE/DX = 0.0 !

! D115 D(23,19,20,21) -0.5095 -DE/DX = 0.0 !

! D116 D(23,19,20,55) 178.4553 -DE/DX = 0.0 !

! D117 D(18,19,23,22) -179.9491 -DE/DX = 0.0 !

! D118 D(18,19,23,77) 6.5236 -DE/DX = 0.0 !

! D119 D(20,19,23,22) 0.8313 -DE/DX = 0.0 !

! D120 D(20,19,23,77) -172.6961 -DE/DX = 0.0 !

! D121 D(19,20,21,22) 0.0 -DE/DX = 0.0 !

! D122 D(19,20,21,56) 178.9484 -DE/DX = 0.0 !

! D123 D(55,20,21,22) -178.9484 -DE/DX = 0.0 !

! D124 D(55,20,21,56) 0.0 -DE/DX = 0.0 !

! D125 D(20,21,22,23) 0.5095 -DE/DX = 0.0 !

! D126 D(20,21,22,24) 179.7358 -DE/DX = 0.0 !

! D127 D(56,21,22,23) -178.4553 -DE/DX = 0.0 !

! D128 D(56,21,22,24) 0.771 -DE/DX = 0.0 !

! D129 D(21,22,23,19) -0.8313 -DE/DX = 0.0 !

! D130 D(21,22,23,77) 172.6961 -DE/DX = 0.0 !

! D131 D(24,22,23,19) 179.9491 -DE/DX = 0.0 !

! D132 D(24,22,23,77) -6.5236 -DE/DX = 0.0 !

! D133 D(21,22,24,9) -175.5155 -DE/DX = 0.0 !

! D134 D(21,22,24,37) 4.4845 -DE/DX = 0.0 !

! D135 D(23,22,24,9) 3.5779 -DE/DX = 0.0 !

! D136 D(23,22,24,37) -176.4221 -DE/DX = 0.0 !

! D137 D(19,23,77,8) 175.4631 -DE/DX = 0.0 !

! D138 D(19,23,77,17) -3.0319 -DE/DX = 0.0 !

! D139 D(22,23,77,8) 3.0319 -DE/DX = 0.0 !

! D140 D(22,23,77,17) -175.4631 -DE/DX = 0.0 !

! D141 D(9,24,37,38) 64.2296 -DE/DX = 0.0 !

! D142 D(9,24,37,42) -115.7704 -DE/DX = 0.0 !

! D143 D(22,24,37,38) -115.7704 -DE/DX = 0.0 !

! D144 D(22,24,37,42) 64.2296 -DE/DX = 0.0 !

! D145 D(6,25,26,27) -179.8953 -DE/DX = 0.0 !

! D146 D(6,25,26,57) -0.4155 -DE/DX = 0.0 !

! D147 D(30,25,26,27) 0.1047 -DE/DX = 0.0 !

! D148 D(30,25,26,57) 179.5845 -DE/DX = 0.0 !

! D149 D(6,25,30,29) -179.8953 -DE/DX = 0.0 !

! D150 D(6,25,30,61) -0.4155 -DE/DX = 0.0 !

! D151 D(26,25,30,29) 0.1047 -DE/DX = 0.0 !

! D152 D(26,25,30,61) 179.5845 -DE/DX = 0.0 !

! D153 D(25,26,27,28) -0.2097 -DE/DX = 0.0 !

! D154 D(25,26,27,58) 179.6276 -DE/DX = 0.0 !

! D155 D(57,26,27,28) -179.6865 -DE/DX = 0.0 !

! D156 D(57,26,27,58) 0.1508 -DE/DX = 0.0 !

! D157 D(26,27,28,29) 0.1041 -DE/DX = 0.0 !

! D158 D(26,27,28,59) -179.8959 -DE/DX = 0.0 !

! D159 D(58,27,28,29) -179.7325 -DE/DX = 0.0 !

! D160 D(58,27,28,59) 0.2675 -DE/DX = 0.0 !

! D161 D(27,28,29,30) 0.1041 -DE/DX = 0.0 !

! D162 D(27,28,29,60) -179.7325 -DE/DX = 0.0 !

! D163 D(59,28,29,30) -179.8959 -DE/DX = 0.0 !

! D164 D(59,28,29,60) 0.2675 -DE/DX = 0.0 !

! D165 D(28,29,30,25) -0.2097 -DE/DX = 0.0 !

! D166 D(28,29,30,61) -179.6865 -DE/DX = 0.0 !

! D167 D(60,29,30,25) 179.6276 -DE/DX = 0.0 !

! D168 D(60,29,30,61) 0.1508 -DE/DX = 0.0 !

! D169 D(36,31,32,33) -0.1041 -DE/DX = 0.0 !

! D170 D(36,31,32,63) 179.7325 -DE/DX = 0.0 !

! D171 D(62,31,32,33) 179.8959 -DE/DX = 0.0 !

! D172 D(62,31,32,63) -0.2675 -DE/DX = 0.0 !

! D173 D(32,31,36,35) -0.1041 -DE/DX = 0.0 !

! D174 D(32,31,36,66) 179.7325 -DE/DX = 0.0 !

! D175 D(62,31,36,35) 179.8959 -DE/DX = 0.0 !

! D176 D(62,31,36,66) -0.2675 -DE/DX = 0.0 !

! D177 D(31,32,33,34) 0.2097 -DE/DX = 0.0 !

! D178 D(31,32,33,64) 179.6865 -DE/DX = 0.0 !

! D179 D(63,32,33,34) -179.6276 -DE/DX = 0.0 !

! D180 D(63,32,33,64) -0.1508 -DE/DX = 0.0 !

! D181 D(32,33,34,12) 179.8953 -DE/DX = 0.0 !

! D182 D(32,33,34,35) -0.1047 -DE/DX = 0.0 !

! D183 D(64,33,34,12) 0.4155 -DE/DX = 0.0 !

! D184 D(64,33,34,35) -179.5845 -DE/DX = 0.0 !

! D185 D(12,34,35,36) 179.8953 -DE/DX = 0.0 !

! D186 D(12,34,35,65) 0.4155 -DE/DX = 0.0 !

! D187 D(33,34,35,36) -0.1047 -DE/DX = 0.0 !

! D188 D(33,34,35,65) -179.5845 -DE/DX = 0.0 !

! D189 D(34,35,36,31) 0.2097 -DE/DX = 0.0 !

! D190 D(34,35,36,66) -179.6276 -DE/DX = 0.0 !

! D191 D(65,35,36,31) 179.6865 -DE/DX = 0.0 !

! D192 D(65,35,36,66) -0.1508 -DE/DX = 0.0 !

! D193 D(24,37,38,39) 179.8953 -DE/DX = 0.0 !

! D194 D(24,37,38,67) 0.4155 -DE/DX = 0.0 !

! D195 D(42,37,38,39) -0.1047 -DE/DX = 0.0 !

! D196 D(42,37,38,67) -179.5845 -DE/DX = 0.0 !

! D197 D(24,37,42,41) 179.8953 -DE/DX = 0.0 !

! D198 D(24,37,42,71) 0.4155 -DE/DX = 0.0 !

! D199 D(38,37,42,41) -0.1047 -DE/DX = 0.0 !

! D200 D(38,37,42,71) -179.5845 -DE/DX = 0.0 !

! D201 D(37,38,39,40) 0.2097 -DE/DX = 0.0 !

! D202 D(37,38,39,68) -179.6276 -DE/DX = 0.0 !

! D203 D(67,38,39,40) 179.6865 -DE/DX = 0.0 !

! D204 D(67,38,39,68) -0.1508 -DE/DX = 0.0 !

! D205 D(38,39,40,41) -0.1041 -DE/DX = 0.0 !

! D206 D(38,39,40,69) 179.8959 -DE/DX = 0.0 !

! D207 D(68,39,40,41) 179.7325 -DE/DX = 0.0 !

! D208 D(68,39,40,69) -0.2675 -DE/DX = 0.0 !

! D209 D(39,40,41,42) -0.1041 -DE/DX = 0.0 !

! D210 D(39,40,41,70) 179.7325 -DE/DX = 0.0 !

! D211 D(69,40,41,42) 179.8959 -DE/DX = 0.0 !

! D212 D(69,40,41,70) -0.2675 -DE/DX = 0.0 !

! D213 D(40,41,42,37) 0.2097 -DE/DX = 0.0 !

! D214 D(40,41,42,71) 179.6865 -DE/DX = 0.0 !

! D215 D(70,41,42,37) -179.6276 -DE/DX = 0.0 !

! D216 D(70,41,42,71) -0.1508 -DE/DX = 0.0 !

! D217 D(18,43,44,45) -179.8953 -DE/DX = 0.0 !

! D218 D(18,43,44,72) -0.4155 -DE/DX = 0.0 !

! D219 D(48,43,44,45) 0.1047 -DE/DX = 0.0 !

! D220 D(48,43,44,72) 179.5845 -DE/DX = 0.0 !

! D221 D(18,43,48,47) -179.8953 -DE/DX = 0.0 !

! D222 D(18,43,48,76) -0.4155 -DE/DX = 0.0 !

! D223 D(44,43,48,47) 0.1047 -DE/DX = 0.0 !

! D224 D(44,43,48,76) 179.5845 -DE/DX = 0.0 !

! D225 D(43,44,45,46) -0.2097 -DE/DX = 0.0 !

! D226 D(43,44,45,73) 179.6276 -DE/DX = 0.0 !

! D227 D(72,44,45,46) -179.6865 -DE/DX = 0.0 !

! D228 D(72,44,45,73) 0.1508 -DE/DX = 0.0 !

! D229 D(44,45,46,47) 0.1041 -DE/DX = 0.0 !

! D230 D(44,45,46,74) -179.8959 -DE/DX = 0.0 !

! D231 D(73,45,46,47) -179.7325 -DE/DX = 0.0 !

! D232 D(73,45,46,74) 0.2675 -DE/DX = 0.0 !

! D233 D(45,46,47,48) 0.1041 -DE/DX = 0.0 !

! D234 D(45,46,47,75) -179.7325 -DE/DX = 0.0 !

! D235 D(74,46,47,48) -179.8959 -DE/DX = 0.0 !

! D236 D(74,46,47,75) 0.2675 -DE/DX = 0.0 !

! D237 D(46,47,48,43) -0.2097 -DE/DX = 0.0 !

! D238 D(46,47,48,76) -179.6865 -DE/DX = 0.0 !

! D239 D(75,47,48,43) 179.6276 -DE/DX = 0.0 !

! D240 D(75,47,48,76) 0.1508 -DE/DX = 0.0 !

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Leave Link 103 at Tue Aug 13 22:09:00 2019, MaxMem= 671088640 cpu: 0.7

(Enter /home/kira/g09/l9999.exe)

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435,-0.00001545,0.00000772,-0.00000419,0.00012579,-0.00038630,-0.00031

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IT TAKES GREATER CHARACTER TO CARRY OFF GOOD FORTUNE THAN BAD.

FRENCH PROVERB.

Job cpu time: 0 days 13 hours 17 minutes 40.0 seconds.

File lengths (MBytes): RWF= 2830 Int= 0 D2E= 0 Chk= 92 Scr= 1

Normal termination of Gaussian 09 at Tue Aug 13 22:09:01 2019.