Entering Gaussian System, Link 0=g09

Input=TPP3C1.com

Output=TPP3C1.log

Initial command:

/home/kira/g09/l1.exe "/home/kira/g09/scratch/Gau-13828.inp" -scrdir="/home/kira/g09/scratch/"

Entering Link 1 = /home/kira/g09/l1.exe PID= 13835.

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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

25-Aug-2019

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

%nprocshared=16

Will use up to 16 processors via shared memory.

%mem=32GB

%chk=TPP3C1.chk

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

#p opt=(GDIIS,calcall) b3lyp/6-311G\* scrf=(solvent=dmso,smd) empirical

dispersion=gd3bj

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

Warning! Use of Opt=GDIIS is deprecated since it is seldom a good choice.

1/10=4,14=-1,18=20,19=11,26=3,38=1/1,3;

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

3/5=4,6=6,7=1,11=2,16=1,25=1,30=1,70=32201,71=2,72=21,74=-5,124=41,140=1/1,2,3;

4//1;

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

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

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

10/6=1/2;

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

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

1/10=4,14=-1,18=20,19=11,26=3/3(3);

2/9=110/2;

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

99//99;

2/9=110/2;

3/5=4,6=6,7=1,11=2,16=1,25=1,30=1,70=32205,71=2,72=21,74=-5,124=41,140=1/1,2,3;

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

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

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

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

10/6=1/2;

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

1/10=4,14=-1,18=20,19=11,26=3/3(-8);

2/9=110/2;

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

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

99//99;

Leave Link 1 at Sun Aug 25 14:05:39 2019, MaxMem= 4294967296 cpu: 1.0

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

------

TPP3C1

------

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C 4.21591 -0.42395 0.67275

C 2.88859 -0.11233 1.12637

N 2.11682 0.03992 -0.00457

C 2.88377 -0.11313 -1.14059

C 4.21184 -0.42395 -0.69372

C 2.44433 0.0278 -2.46153

C 1.08805 0.20905 -2.87169

N -0.0081 0.01772 -2.06141

C -1.09442 0.21643 -2.86387

C -0.69626 0.58293 -4.19086

C 0.68078 0.57726 -4.19478

C 2.46007 0.0268 2.44819

C 1.09497 0.20885 2.86407

C 0.69905 0.57805 4.19107

C -0.678 0.58213 4.19454

C -1.0875 0.21663 2.87148

N 0.00736 0.01772 2.06141

C -2.44497 0.04101 2.46197

C -2.88531 -0.09401 1.14071

C -4.20964 -0.42011 0.69372

C -4.21371 -0.4201 -0.67278

C -2.89014 -0.09341 -1.1263

N -2.12081 0.06983 0.00457

C -2.46072 0.04002 -2.44865

C 3.48045 -0.01025 -3.52409

C 4.56011 0.8843 -3.51184

C 5.52388 0.84415 -4.51582

C 5.43099 -0.09784 -5.53893

C 4.3627 -0.99501 -5.55833

C 3.38966 -0.94552 -4.56581

C 5.45763 -0.09784 5.51307

C 5.54562 0.84415 4.48953

C 4.57686 0.8843 3.49038

C 3.49727 -0.01065 3.50699

C 3.41167 -0.94552 4.54973

C 4.38925 -0.99501 5.53759

C -3.49681 -0.00524 -3.50763

C -3.40454 -0.94079 -4.54946

C -4.38256 -0.99973 -5.53623

C -5.45832 -0.11138 -5.51194

C -5.55314 0.83128 -4.48962

C -4.58392 0.8808 -3.49138

C -3.47999 -0.00484 3.52472

C -3.38254 -0.94079 4.56548

C -4.35602 -0.99973 5.55692

C -5.43168 -0.11138 5.53778

C -5.5314 0.83127 4.51593

C -4.56717 0.8808 3.51287

H 5.05171 -0.63915 1.31833

H 5.04494 -0.63915 -1.34309

H -1.35303 0.82514 -5.01256

H 1.33392 0.81535 -5.02067

H 1.35712 0.81575 5.01303

H -1.32983 0.82473 5.02017

H -5.03918 -0.64845 1.34317

H -5.04594 -0.64845 -1.31845

H 4.63026 1.62477 -2.72327

H 6.34653 1.55114 -4.49895

H 6.18517 -0.13222 -6.31797

H 4.28692 -1.73448 -6.34852

H 2.56265 -1.64563 -4.58217

H 6.21553 -0.13223 6.2885

H 6.36838 1.55094 4.46853

H 4.64324 1.62457 2.70108

H 2.58435 -1.64543 4.57065

H 4.31745 -1.73448 6.32813

H -2.57203 -1.63446 -4.56991

H -4.30551 -1.73985 -6.32565

H -6.21669 -0.15319 -6.28654

H -6.38167 1.53129 -4.46887

H -4.65593 1.62155 -2.70305

H -2.55033 -1.63467 4.58136

H -4.275 -1.73986 6.34597

H -6.18634 -0.15319 6.316

H -6.35981 1.53148 4.49934

H -4.64294 1.62175 2.72529

H 1.11742 0.19455 -0.00178

H -1.12648 0.25294 0.00179

NAtoms= 78 NQM= 78 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 78

IAtWgt= 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

NucSpn= 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

NQMom= 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

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Leave Link 101 at Sun Aug 25 14:05:39 2019, MaxMem= 4294967296 cpu: 7.5

(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) 1.4369 calculate D2E/DX2 analytically !

! R2 R(1,5) 1.3665 calculate D2E/DX2 analytically !

! R3 R(1,49) 1.0778 calculate D2E/DX2 analytically !

! R4 R(2,3) 1.3776 calculate D2E/DX2 analytically !

! R5 R(2,12) 1.3965 calculate D2E/DX2 analytically !

! R6 R(3,4) 1.3792 calculate D2E/DX2 analytically !

! R7 R(3,77) 1.0113 calculate D2E/DX2 analytically !

! R8 R(4,5) 1.4353 calculate D2E/DX2 analytically !

! R9 R(4,6) 1.3992 calculate D2E/DX2 analytically !

! R10 R(5,50) 1.078 calculate D2E/DX2 analytically !

! R11 R(6,7) 1.4285 calculate D2E/DX2 analytically !

! R12 R(6,25) 1.4846 calculate D2E/DX2 analytically !

! R13 R(7,8) 1.3765 calculate D2E/DX2 analytically !

! R14 R(7,11) 1.4325 calculate D2E/DX2 analytically !

! R15 R(8,9) 1.3651 calculate D2E/DX2 analytically !

! R16 R(9,10) 1.4331 calculate D2E/DX2 analytically !

! R17 R(9,24) 1.4389 calculate D2E/DX2 analytically !

! R18 R(10,11) 1.3771 calculate D2E/DX2 analytically !

! R19 R(10,51) 1.0794 calculate D2E/DX2 analytically !

! R20 R(11,52) 1.0795 calculate D2E/DX2 analytically !

! R21 R(12,13) 1.4386 calculate D2E/DX2 analytically !

! R22 R(12,34) 1.4826 calculate D2E/DX2 analytically !

! R23 R(13,14) 1.4332 calculate D2E/DX2 analytically !

! R24 R(13,17) 1.3652 calculate D2E/DX2 analytically !

! R25 R(14,15) 1.3771 calculate D2E/DX2 analytically !

! R26 R(14,53) 1.0794 calculate D2E/DX2 analytically !

! R27 R(15,16) 1.4324 calculate D2E/DX2 analytically !

! R28 R(15,54) 1.0795 calculate D2E/DX2 analytically !

! R29 R(16,17) 1.3764 calculate D2E/DX2 analytically !

! R30 R(16,18) 1.4287 calculate D2E/DX2 analytically !

! R31 R(18,19) 1.3992 calculate D2E/DX2 analytically !

! R32 R(18,43) 1.4842 calculate D2E/DX2 analytically !

! R33 R(19,20) 1.4353 calculate D2E/DX2 analytically !

! R34 R(19,23) 1.3792 calculate D2E/DX2 analytically !

! R35 R(20,21) 1.3665 calculate D2E/DX2 analytically !

! R36 R(20,55) 1.078 calculate D2E/DX2 analytically !

! R37 R(21,22) 1.4368 calculate D2E/DX2 analytically !

! R38 R(21,56) 1.0778 calculate D2E/DX2 analytically !

! R39 R(22,23) 1.3775 calculate D2E/DX2 analytically !

! R40 R(22,24) 1.3967 calculate D2E/DX2 analytically !

! R41 R(23,78) 1.0111 calculate D2E/DX2 analytically !

! R42 R(24,37) 1.4822 calculate D2E/DX2 analytically !

! R43 R(25,26) 1.4022 calculate D2E/DX2 analytically !

! R44 R(25,30) 1.4029 calculate D2E/DX2 analytically !

! R45 R(26,27) 1.3923 calculate D2E/DX2 analytically !

! R46 R(26,57) 1.084 calculate D2E/DX2 analytically !

! R47 R(27,28) 1.3938 calculate D2E/DX2 analytically !

! R48 R(27,58) 1.0848 calculate D2E/DX2 analytically !

! R49 R(28,29) 1.3952 calculate D2E/DX2 analytically !

! R50 R(28,59) 1.0848 calculate D2E/DX2 analytically !

! R51 R(29,30) 1.3908 calculate D2E/DX2 analytically !

! R52 R(29,60) 1.0849 calculate D2E/DX2 analytically !

! R53 R(30,61) 1.0837 calculate D2E/DX2 analytically !

! R54 R(31,32) 1.3938 calculate D2E/DX2 analytically !

! R55 R(31,36) 1.3953 calculate D2E/DX2 analytically !

! R56 R(31,62) 1.0848 calculate D2E/DX2 analytically !

! R57 R(32,33) 1.3923 calculate D2E/DX2 analytically !

! R58 R(32,63) 1.0849 calculate D2E/DX2 analytically !

! R59 R(33,34) 1.4024 calculate D2E/DX2 analytically !

! R60 R(33,64) 1.0842 calculate D2E/DX2 analytically !

! R61 R(34,35) 1.4031 calculate D2E/DX2 analytically !

! R62 R(35,36) 1.3907 calculate D2E/DX2 analytically !

! R63 R(35,65) 1.0839 calculate D2E/DX2 analytically !

! R64 R(36,66) 1.0849 calculate D2E/DX2 analytically !

! R65 R(37,38) 1.4033 calculate D2E/DX2 analytically !

! R66 R(37,42) 1.4025 calculate D2E/DX2 analytically !

! R67 R(38,39) 1.3906 calculate D2E/DX2 analytically !

! R68 R(38,67) 1.0838 calculate D2E/DX2 analytically !

! R69 R(39,40) 1.3954 calculate D2E/DX2 analytically !

! R70 R(39,68) 1.0849 calculate D2E/DX2 analytically !

! R71 R(40,41) 1.3938 calculate D2E/DX2 analytically !

! R72 R(40,69) 1.0848 calculate D2E/DX2 analytically !

! R73 R(41,42) 1.3922 calculate D2E/DX2 analytically !

! R74 R(41,70) 1.0849 calculate D2E/DX2 analytically !

! R75 R(42,71) 1.0841 calculate D2E/DX2 analytically !

! R76 R(43,44) 1.4031 calculate D2E/DX2 analytically !

! R77 R(43,48) 1.4023 calculate D2E/DX2 analytically !

! R78 R(44,45) 1.3907 calculate D2E/DX2 analytically !

! R79 R(44,72) 1.0836 calculate D2E/DX2 analytically !

! R80 R(45,46) 1.3952 calculate D2E/DX2 analytically !

! R81 R(45,73) 1.0849 calculate D2E/DX2 analytically !

! R82 R(46,47) 1.3938 calculate D2E/DX2 analytically !

! R83 R(46,74) 1.0848 calculate D2E/DX2 analytically !

! R84 R(47,48) 1.3922 calculate D2E/DX2 analytically !

! R85 R(47,75) 1.0848 calculate D2E/DX2 analytically !

! R86 R(48,76) 1.084 calculate D2E/DX2 analytically !

! A1 A(2,1,5) 108.2367 calculate D2E/DX2 analytically !

! A2 A(2,1,49) 124.7878 calculate D2E/DX2 analytically !

! A3 A(5,1,49) 126.9624 calculate D2E/DX2 analytically !

! A4 A(1,2,3) 106.3979 calculate D2E/DX2 analytically !

! A5 A(1,2,12) 127.148 calculate D2E/DX2 analytically !

! A6 A(3,2,12) 126.4499 calculate D2E/DX2 analytically !

! A7 A(2,3,4) 110.6336 calculate D2E/DX2 analytically !

! A8 A(2,3,77) 124.6295 calculate D2E/DX2 analytically !

! A9 A(4,3,77) 124.6657 calculate D2E/DX2 analytically !

! A10 A(3,4,5) 106.3874 calculate D2E/DX2 analytically !

! A11 A(3,4,6) 126.2828 calculate D2E/DX2 analytically !

! A12 A(5,4,6) 127.3245 calculate D2E/DX2 analytically !

! A13 A(1,5,4) 108.3062 calculate D2E/DX2 analytically !

! A14 A(1,5,50) 126.8766 calculate D2E/DX2 analytically !

! A15 A(4,5,50) 124.8042 calculate D2E/DX2 analytically !

! A16 A(4,6,7) 125.5932 calculate D2E/DX2 analytically !

! A17 A(4,6,25) 116.9943 calculate D2E/DX2 analytically !

! A18 A(7,6,25) 117.4122 calculate D2E/DX2 analytically !

! A19 A(6,7,8) 124.7103 calculate D2E/DX2 analytically !

! A20 A(6,7,11) 124.5938 calculate D2E/DX2 analytically !

! A21 A(8,7,11) 110.6726 calculate D2E/DX2 analytically !

! A22 A(7,8,9) 105.5122 calculate D2E/DX2 analytically !

! A23 A(8,9,10) 111.1275 calculate D2E/DX2 analytically !

! A24 A(8,9,24) 124.6224 calculate D2E/DX2 analytically !

! A25 A(10,9,24) 124.2214 calculate D2E/DX2 analytically !

! A26 A(9,10,11) 106.2251 calculate D2E/DX2 analytically !

! A27 A(9,10,51) 126.385 calculate D2E/DX2 analytically !

! A28 A(11,10,51) 127.3858 calculate D2E/DX2 analytically !

! A29 A(7,11,10) 106.4235 calculate D2E/DX2 analytically !

! A30 A(7,11,52) 126.2499 calculate D2E/DX2 analytically !

! A31 A(10,11,52) 127.3211 calculate D2E/DX2 analytically !

! A32 A(2,12,13) 125.2682 calculate D2E/DX2 analytically !

! A33 A(2,12,34) 117.307 calculate D2E/DX2 analytically !

! A34 A(13,12,34) 117.4243 calculate D2E/DX2 analytically !

! A35 A(12,13,14) 124.2222 calculate D2E/DX2 analytically !

! A36 A(12,13,17) 124.6315 calculate D2E/DX2 analytically !

! A37 A(14,13,17) 111.1231 calculate D2E/DX2 analytically !

! A38 A(13,14,15) 106.2213 calculate D2E/DX2 analytically !

! A39 A(13,14,53) 126.3962 calculate D2E/DX2 analytically !

! A40 A(15,14,53) 127.3783 calculate D2E/DX2 analytically !

! A41 A(14,15,16) 106.4275 calculate D2E/DX2 analytically !

! A42 A(14,15,54) 127.3287 calculate D2E/DX2 analytically !

! A43 A(16,15,54) 126.2386 calculate D2E/DX2 analytically !

! A44 A(15,16,17) 110.676 calculate D2E/DX2 analytically !

! A45 A(15,16,18) 124.5925 calculate D2E/DX2 analytically !

! A46 A(17,16,18) 124.7029 calculate D2E/DX2 analytically !

! A47 A(13,17,16) 105.5128 calculate D2E/DX2 analytically !

! A48 A(16,18,19) 125.5575 calculate D2E/DX2 analytically !

! A49 A(16,18,43) 117.4611 calculate D2E/DX2 analytically !

! A50 A(19,18,43) 116.9813 calculate D2E/DX2 analytically !

! A51 A(18,19,20) 127.3284 calculate D2E/DX2 analytically !

! A52 A(18,19,23) 126.2968 calculate D2E/DX2 analytically !

! A53 A(20,19,23) 106.3741 calculate D2E/DX2 analytically !

! A54 A(19,20,21) 108.3114 calculate D2E/DX2 analytically !

! A55 A(19,20,55) 124.788 calculate D2E/DX2 analytically !

! A56 A(21,20,55) 126.8822 calculate D2E/DX2 analytically !

! A57 A(20,21,22) 108.2351 calculate D2E/DX2 analytically !

! A58 A(20,21,56) 126.9677 calculate D2E/DX2 analytically !

! A59 A(22,21,56) 124.7785 calculate D2E/DX2 analytically !

! A60 A(21,22,23) 106.398 calculate D2E/DX2 analytically !

! A61 A(21,22,24) 127.143 calculate D2E/DX2 analytically !

! A62 A(23,22,24) 126.4585 calculate D2E/DX2 analytically !

! A63 A(19,23,22) 110.6492 calculate D2E/DX2 analytically !

! A64 A(19,23,78) 124.6755 calculate D2E/DX2 analytically !

! A65 A(22,23,78) 124.6443 calculate D2E/DX2 analytically !

! A66 A(9,24,22) 125.231 calculate D2E/DX2 analytically !

! A67 A(9,24,37) 117.4728 calculate D2E/DX2 analytically !

! A68 A(22,24,37) 117.2961 calculate D2E/DX2 analytically !

! A69 A(6,25,26) 120.9836 calculate D2E/DX2 analytically !

! A70 A(6,25,30) 120.2236 calculate D2E/DX2 analytically !

! A71 A(26,25,30) 118.7923 calculate D2E/DX2 analytically !

! A72 A(25,26,27) 120.5516 calculate D2E/DX2 analytically !

! A73 A(25,26,57) 119.4712 calculate D2E/DX2 analytically !

! A74 A(27,26,57) 119.9655 calculate D2E/DX2 analytically !

! A75 A(26,27,28) 120.177 calculate D2E/DX2 analytically !

! A76 A(26,27,58) 119.664 calculate D2E/DX2 analytically !

! A77 A(28,27,58) 120.1589 calculate D2E/DX2 analytically !

! A78 A(27,28,29) 119.7248 calculate D2E/DX2 analytically !

! A79 A(27,28,59) 120.1461 calculate D2E/DX2 analytically !

! A80 A(29,28,59) 120.129 calculate D2E/DX2 analytically !

! A81 A(28,29,30) 120.1917 calculate D2E/DX2 analytically !

! A82 A(28,29,60) 120.1278 calculate D2E/DX2 analytically !

! A83 A(30,29,60) 119.6806 calculate D2E/DX2 analytically !

! A84 A(25,30,29) 120.5537 calculate D2E/DX2 analytically !

! A85 A(25,30,61) 119.4255 calculate D2E/DX2 analytically !

! A86 A(29,30,61) 120.0102 calculate D2E/DX2 analytically !

! A87 A(32,31,36) 119.7219 calculate D2E/DX2 analytically !

! A88 A(32,31,62) 120.1461 calculate D2E/DX2 analytically !

! A89 A(36,31,62) 120.132 calculate D2E/DX2 analytically !

! A90 A(31,32,33) 120.1695 calculate D2E/DX2 analytically !

! A91 A(31,32,63) 120.1596 calculate D2E/DX2 analytically !

! A92 A(33,32,63) 119.6708 calculate D2E/DX2 analytically !

! A93 A(32,33,34) 120.58 calculate D2E/DX2 analytically !

! A94 A(32,33,64) 119.9706 calculate D2E/DX2 analytically !

! A95 A(34,33,64) 119.4389 calculate D2E/DX2 analytically !

! A96 A(12,34,33) 120.9275 calculate D2E/DX2 analytically !

! A97 A(12,34,35) 120.3233 calculate D2E/DX2 analytically !

! A98 A(33,34,35) 118.7489 calculate D2E/DX2 analytically !

! A99 A(34,35,36) 120.5799 calculate D2E/DX2 analytically !

! A100 A(34,35,65) 119.4178 calculate D2E/DX2 analytically !

! A101 A(36,35,65) 119.9921 calculate D2E/DX2 analytically !

! A102 A(31,36,35) 120.1907 calculate D2E/DX2 analytically !

! A103 A(31,36,66) 120.1158 calculate D2E/DX2 analytically !

! A104 A(35,36,66) 119.6934 calculate D2E/DX2 analytically !

! A105 A(24,37,38) 120.3199 calculate D2E/DX2 analytically !

! A106 A(24,37,42) 120.9462 calculate D2E/DX2 analytically !

! A107 A(38,37,42) 118.7339 calculate D2E/DX2 analytically !

! A108 A(37,38,39) 120.5872 calculate D2E/DX2 analytically !

! A109 A(37,38,67) 119.4206 calculate D2E/DX2 analytically !

! A110 A(39,38,67) 119.9811 calculate D2E/DX2 analytically !

! A111 A(38,39,40) 120.1915 calculate D2E/DX2 analytically !

! A112 A(38,39,68) 119.6921 calculate D2E/DX2 analytically !

! A113 A(40,39,68) 120.1164 calculate D2E/DX2 analytically !

! A114 A(39,40,41) 119.7216 calculate D2E/DX2 analytically !

! A115 A(39,40,69) 120.1315 calculate D2E/DX2 analytically !

! A116 A(41,40,69) 120.1468 calculate D2E/DX2 analytically !

! A117 A(40,41,42) 120.1719 calculate D2E/DX2 analytically !

! A118 A(40,41,70) 120.1576 calculate D2E/DX2 analytically !

! A119 A(42,41,70) 119.6704 calculate D2E/DX2 analytically !

! A120 A(37,42,41) 120.5847 calculate D2E/DX2 analytically !

! A121 A(37,42,71) 119.4425 calculate D2E/DX2 analytically !

! A122 A(41,42,71) 119.9624 calculate D2E/DX2 analytically !

! A123 A(18,43,44) 120.2194 calculate D2E/DX2 analytically !

! A124 A(18,43,48) 121.0035 calculate D2E/DX2 analytically !

! A125 A(44,43,48) 118.777 calculate D2E/DX2 analytically !

! A126 A(43,44,45) 120.561 calculate D2E/DX2 analytically !

! A127 A(43,44,72) 119.4282 calculate D2E/DX2 analytically !

! A128 A(45,44,72) 119.9992 calculate D2E/DX2 analytically !

! A129 A(44,45,46) 120.1925 calculate D2E/DX2 analytically !

! A130 A(44,45,73) 119.6791 calculate D2E/DX2 analytically !

! A131 A(46,45,73) 120.1284 calculate D2E/DX2 analytically !

! A132 A(45,46,47) 119.7246 calculate D2E/DX2 analytically !

! A133 A(45,46,74) 120.1285 calculate D2E/DX2 analytically !

! A134 A(47,46,74) 120.1468 calculate D2E/DX2 analytically !

! A135 A(46,47,48) 120.1795 calculate D2E/DX2 analytically !

! A136 A(46,47,75) 120.1569 calculate D2E/DX2 analytically !

! A137 A(48,47,75) 119.6635 calculate D2E/DX2 analytically !

! A138 A(43,48,47) 120.5564 calculate D2E/DX2 analytically !

! A139 A(43,48,76) 119.4747 calculate D2E/DX2 analytically !

! A140 A(47,48,76) 119.9574 calculate D2E/DX2 analytically !

! D1 D(5,1,2,3) 1.1805 calculate D2E/DX2 analytically !

! D2 D(5,1,2,12) -178.1099 calculate D2E/DX2 analytically !

! D3 D(49,1,2,3) -177.583 calculate D2E/DX2 analytically !

! D4 D(49,1,2,12) 3.1266 calculate D2E/DX2 analytically !

! D5 D(2,1,5,4) -0.0142 calculate D2E/DX2 analytically !

! D6 D(2,1,5,50) -178.7483 calculate D2E/DX2 analytically !

! D7 D(49,1,5,4) 178.7148 calculate D2E/DX2 analytically !

! D8 D(49,1,5,50) -0.0192 calculate D2E/DX2 analytically !

! D9 D(1,2,3,4) -1.9539 calculate D2E/DX2 analytically !

! D10 D(1,2,3,77) 175.0962 calculate D2E/DX2 analytically !

! D11 D(12,2,3,4) 177.3429 calculate D2E/DX2 analytically !

! D12 D(12,2,3,77) -5.607 calculate D2E/DX2 analytically !

! D13 D(1,2,12,13) -173.4777 calculate D2E/DX2 analytically !

! D14 D(1,2,12,34) 6.7915 calculate D2E/DX2 analytically !

! D15 D(3,2,12,13) 7.3687 calculate D2E/DX2 analytically !

! D16 D(3,2,12,34) -172.3621 calculate D2E/DX2 analytically !

! D17 D(2,3,4,5) 1.9457 calculate D2E/DX2 analytically !

! D18 D(2,3,4,6) -177.27 calculate D2E/DX2 analytically !

! D19 D(77,3,4,5) -175.1031 calculate D2E/DX2 analytically !

! D20 D(77,3,4,6) 5.6813 calculate D2E/DX2 analytically !

! D21 D(3,4,5,1) -1.156 calculate D2E/DX2 analytically !

! D22 D(3,4,5,50) 177.6107 calculate D2E/DX2 analytically !

! D23 D(6,4,5,1) 178.0489 calculate D2E/DX2 analytically !

! D24 D(6,4,5,50) -3.1844 calculate D2E/DX2 analytically !

! D25 D(3,4,6,7) -7.4403 calculate D2E/DX2 analytically !

! D26 D(3,4,6,25) 172.3366 calculate D2E/DX2 analytically !

! D27 D(5,4,6,7) 173.506 calculate D2E/DX2 analytically !

! D28 D(5,4,6,25) -6.7172 calculate D2E/DX2 analytically !

! D29 D(4,6,7,8) -13.1057 calculate D2E/DX2 analytically !

! D30 D(4,6,7,11) 168.8142 calculate D2E/DX2 analytically !

! D31 D(25,6,7,8) 167.1183 calculate D2E/DX2 analytically !

! D32 D(25,6,7,11) -10.9618 calculate D2E/DX2 analytically !

! D33 D(4,6,25,26) -56.6939 calculate D2E/DX2 analytically !

! D34 D(4,6,25,30) 123.5658 calculate D2E/DX2 analytically !

! D35 D(7,6,25,26) 123.1016 calculate D2E/DX2 analytically !

! D36 D(7,6,25,30) -56.6386 calculate D2E/DX2 analytically !

! D37 D(6,7,8,9) -176.3801 calculate D2E/DX2 analytically !

! D38 D(11,7,8,9) 1.9307 calculate D2E/DX2 analytically !

! D39 D(6,7,11,10) 177.1313 calculate D2E/DX2 analytically !

! D40 D(6,7,11,52) -3.6744 calculate D2E/DX2 analytically !

! D41 D(8,7,11,10) -1.1819 calculate D2E/DX2 analytically !

! D42 D(8,7,11,52) 178.0124 calculate D2E/DX2 analytically !

! D43 D(7,8,9,10) -1.9679 calculate D2E/DX2 analytically !

! D44 D(7,8,9,24) 176.1507 calculate D2E/DX2 analytically !

! D45 D(8,9,10,11) 1.2764 calculate D2E/DX2 analytically !

! D46 D(8,9,10,51) -178.0358 calculate D2E/DX2 analytically !

! D47 D(24,9,10,11) -176.8512 calculate D2E/DX2 analytically !

! D48 D(24,9,10,51) 3.8367 calculate D2E/DX2 analytically !

! D49 D(8,9,24,22) 13.526 calculate D2E/DX2 analytically !

! D50 D(8,9,24,37) -166.4145 calculate D2E/DX2 analytically !

! D51 D(10,9,24,22) -168.5965 calculate D2E/DX2 analytically !

! D52 D(10,9,24,37) 11.4629 calculate D2E/DX2 analytically !

! D53 D(9,10,11,7) -0.0468 calculate D2E/DX2 analytically !

! D54 D(9,10,11,52) -179.2298 calculate D2E/DX2 analytically !

! D55 D(51,10,11,7) 179.2563 calculate D2E/DX2 analytically !

! D56 D(51,10,11,52) 0.0733 calculate D2E/DX2 analytically !

! D57 D(2,12,13,14) -168.7409 calculate D2E/DX2 analytically !

! D58 D(2,12,13,17) 13.1689 calculate D2E/DX2 analytically !

! D59 D(34,12,13,14) 10.9896 calculate D2E/DX2 analytically !

! D60 D(34,12,13,17) -167.1006 calculate D2E/DX2 analytically !

! D61 D(2,12,34,33) 56.5964 calculate D2E/DX2 analytically !

! D62 D(2,12,34,35) -123.5744 calculate D2E/DX2 analytically !

! D63 D(13,12,34,33) -123.1559 calculate D2E/DX2 analytically !

! D64 D(13,12,34,35) 56.6732 calculate D2E/DX2 analytically !

! D65 D(12,13,14,15) -177.0497 calculate D2E/DX2 analytically !

! D66 D(12,13,14,53) 3.6518 calculate D2E/DX2 analytically !

! D67 D(17,13,14,15) 1.2657 calculate D2E/DX2 analytically !

! D68 D(17,13,14,53) -178.0327 calculate D2E/DX2 analytically !

! D69 D(12,13,17,16) 176.3405 calculate D2E/DX2 analytically !

! D70 D(14,13,17,16) -1.9667 calculate D2E/DX2 analytically !

! D71 D(13,14,15,16) -0.0318 calculate D2E/DX2 analytically !

! D72 D(13,14,15,54) -179.2295 calculate D2E/DX2 analytically !

! D73 D(53,14,15,16) 179.2576 calculate D2E/DX2 analytically !

! D74 D(53,14,15,54) 0.0599 calculate D2E/DX2 analytically !

! D75 D(14,15,16,17) -1.1972 calculate D2E/DX2 analytically !

! D76 D(14,15,16,18) 176.9347 calculate D2E/DX2 analytically !

! D77 D(54,15,16,17) 178.0118 calculate D2E/DX2 analytically !

! D78 D(54,15,16,18) -3.8564 calculate D2E/DX2 analytically !

! D79 D(15,16,17,13) 1.9393 calculate D2E/DX2 analytically !

! D80 D(18,16,17,13) -176.19 calculate D2E/DX2 analytically !

! D81 D(15,16,18,19) 168.6605 calculate D2E/DX2 analytically !

! D82 D(15,16,18,43) -11.4378 calculate D2E/DX2 analytically !

! D83 D(17,16,18,19) -13.4656 calculate D2E/DX2 analytically !

! D84 D(17,16,18,43) 166.4361 calculate D2E/DX2 analytically !

! D85 D(16,18,19,20) 172.4261 calculate D2E/DX2 analytically !

! D86 D(16,18,19,23) -7.9362 calculate D2E/DX2 analytically !

! D87 D(43,18,19,20) -7.476 calculate D2E/DX2 analytically !

! D88 D(43,18,19,23) 172.1618 calculate D2E/DX2 analytically !

! D89 D(16,18,43,44) -56.0042 calculate D2E/DX2 analytically !

! D90 D(16,18,43,48) 123.8707 calculate D2E/DX2 analytically !

! D91 D(19,18,43,44) 123.906 calculate D2E/DX2 analytically !

! D92 D(19,18,43,48) -56.2191 calculate D2E/DX2 analytically !

! D93 D(18,19,20,21) 178.6267 calculate D2E/DX2 analytically !

! D94 D(18,19,20,55) -2.844 calculate D2E/DX2 analytically !

! D95 D(23,19,20,21) -1.069 calculate D2E/DX2 analytically !

! D96 D(23,19,20,55) 177.4602 calculate D2E/DX2 analytically !

! D97 D(18,19,23,22) -177.9088 calculate D2E/DX2 analytically !

! D98 D(18,19,23,78) 4.0411 calculate D2E/DX2 analytically !

! D99 D(20,19,23,22) 1.791 calculate D2E/DX2 analytically !

! D100 D(20,19,23,78) -176.2591 calculate D2E/DX2 analytically !

! D101 D(19,20,21,22) -0.0051 calculate D2E/DX2 analytically !

! D102 D(19,20,21,56) 178.4695 calculate D2E/DX2 analytically !

! D103 D(55,20,21,22) -178.495 calculate D2E/DX2 analytically !

! D104 D(55,20,21,56) -0.0204 calculate D2E/DX2 analytically !

! D105 D(20,21,22,23) 1.0787 calculate D2E/DX2 analytically !

! D106 D(20,21,22,24) -178.6721 calculate D2E/DX2 analytically !

! D107 D(56,21,22,23) -177.4374 calculate D2E/DX2 analytically !

! D108 D(56,21,22,24) 2.8118 calculate D2E/DX2 analytically !

! D109 D(21,22,23,19) -1.794 calculate D2E/DX2 analytically !

! D110 D(21,22,23,78) 176.2568 calculate D2E/DX2 analytically !

! D111 D(24,22,23,19) 177.959 calculate D2E/DX2 analytically !

! D112 D(24,22,23,78) -3.9902 calculate D2E/DX2 analytically !

! D113 D(21,22,24,9) -172.4126 calculate D2E/DX2 analytically !

! D114 D(21,22,24,37) 7.528 calculate D2E/DX2 analytically !

! D115 D(23,22,24,9) 7.8846 calculate D2E/DX2 analytically !

! D116 D(23,22,24,37) -172.1747 calculate D2E/DX2 analytically !

! D117 D(9,24,37,38) 56.0391 calculate D2E/DX2 analytically !

! D118 D(9,24,37,42) -123.9239 calculate D2E/DX2 analytically !

! D119 D(22,24,37,38) -123.9062 calculate D2E/DX2 analytically !

! D120 D(22,24,37,42) 56.1308 calculate D2E/DX2 analytically !

! D121 D(6,25,26,27) -179.7425 calculate D2E/DX2 analytically !

! D122 D(6,25,26,57) -0.9834 calculate D2E/DX2 analytically !

! D123 D(30,25,26,27) 0.0014 calculate D2E/DX2 analytically !

! D124 D(30,25,26,57) 178.7605 calculate D2E/DX2 analytically !

! D125 D(6,25,30,29) -179.4324 calculate D2E/DX2 analytically !

! D126 D(6,25,30,61) -0.6149 calculate D2E/DX2 analytically !

! D127 D(26,25,30,29) 0.8217 calculate D2E/DX2 analytically !

! D128 D(26,25,30,61) 179.6392 calculate D2E/DX2 analytically !

! D129 D(25,26,27,28) -0.6334 calculate D2E/DX2 analytically !

! D130 D(25,26,27,58) 179.2412 calculate D2E/DX2 analytically !

! D131 D(57,26,27,28) -179.3863 calculate D2E/DX2 analytically !

! D132 D(57,26,27,58) 0.4883 calculate D2E/DX2 analytically !

! D133 D(26,27,28,29) 0.4458 calculate D2E/DX2 analytically !

! D134 D(26,27,28,59) -179.6642 calculate D2E/DX2 analytically !

! D135 D(58,27,28,29) -179.4282 calculate D2E/DX2 analytically !

! D136 D(58,27,28,59) 0.4618 calculate D2E/DX2 analytically !

! D137 D(27,28,29,30) 0.375 calculate D2E/DX2 analytically !

! D138 D(27,28,29,60) -179.6605 calculate D2E/DX2 analytically !

! D139 D(59,28,29,30) -179.515 calculate D2E/DX2 analytically !

! D140 D(59,28,29,60) 0.4495 calculate D2E/DX2 analytically !

! D141 D(28,29,30,25) -1.0155 calculate D2E/DX2 analytically !

! D142 D(28,29,30,61) -179.8261 calculate D2E/DX2 analytically !

! D143 D(60,29,30,25) 179.0198 calculate D2E/DX2 analytically !

! D144 D(60,29,30,61) 0.2092 calculate D2E/DX2 analytically !

! D145 D(36,31,32,33) -0.4405 calculate D2E/DX2 analytically !

! D146 D(36,31,32,63) 179.4442 calculate D2E/DX2 analytically !

! D147 D(62,31,32,33) 179.6745 calculate D2E/DX2 analytically !

! D148 D(62,31,32,63) -0.4407 calculate D2E/DX2 analytically !

! D149 D(32,31,36,35) -0.3649 calculate D2E/DX2 analytically !

! D150 D(32,31,36,66) 179.654 calculate D2E/DX2 analytically !

! D151 D(62,31,36,35) 179.5201 calculate D2E/DX2 analytically !

! D152 D(62,31,36,66) -0.461 calculate D2E/DX2 analytically !

! D153 D(31,32,33,34) 0.5901 calculate D2E/DX2 analytically !

! D154 D(31,32,33,64) 179.4075 calculate D2E/DX2 analytically !

! D155 D(63,32,33,34) -179.2952 calculate D2E/DX2 analytically !

! D156 D(63,32,33,64) -0.4778 calculate D2E/DX2 analytically !

! D157 D(32,33,34,12) 179.8951 calculate D2E/DX2 analytically !

! D158 D(32,33,34,35) 0.0633 calculate D2E/DX2 analytically !

! D159 D(64,33,34,12) 1.0715 calculate D2E/DX2 analytically !

! D160 D(64,33,34,35) -178.7603 calculate D2E/DX2 analytically !

! D161 D(12,34,35,36) 179.2958 calculate D2E/DX2 analytically !

! D162 D(12,34,35,65) 0.4555 calculate D2E/DX2 analytically !

! D163 D(33,34,35,36) -0.8714 calculate D2E/DX2 analytically !

! D164 D(33,34,35,65) -179.7117 calculate D2E/DX2 analytically !

! D165 D(34,35,36,31) 1.0285 calculate D2E/DX2 analytically !

! D166 D(34,35,36,66) -178.9904 calculate D2E/DX2 analytically !

! D167 D(65,35,36,31) 179.8622 calculate D2E/DX2 analytically !

! D168 D(65,35,36,66) -0.1567 calculate D2E/DX2 analytically !

! D169 D(24,37,38,39) 179.1575 calculate D2E/DX2 analytically !

! D170 D(24,37,38,67) 0.3747 calculate D2E/DX2 analytically !

! D171 D(42,37,38,39) -0.8787 calculate D2E/DX2 analytically !

! D172 D(42,37,38,67) -179.6615 calculate D2E/DX2 analytically !

! D173 D(24,37,42,41) -179.9721 calculate D2E/DX2 analytically !

! D174 D(24,37,42,71) 1.2001 calculate D2E/DX2 analytically !

! D175 D(38,37,42,41) 0.0643 calculate D2E/DX2 analytically !

! D176 D(38,37,42,71) -178.7634 calculate D2E/DX2 analytically !

! D177 D(37,38,39,40) 1.0359 calculate D2E/DX2 analytically !

! D178 D(37,38,39,68) -178.9678 calculate D2E/DX2 analytically !

! D179 D(67,38,39,40) 179.8119 calculate D2E/DX2 analytically !

! D180 D(67,38,39,68) -0.1918 calculate D2E/DX2 analytically !

! D181 D(38,39,40,41) -0.366 calculate D2E/DX2 analytically !

! D182 D(38,39,40,69) 179.5257 calculate D2E/DX2 analytically !

! D183 D(68,39,40,41) 179.6378 calculate D2E/DX2 analytically !

! D184 D(68,39,40,69) -0.4705 calculate D2E/DX2 analytically !

! D185 D(39,40,41,42) -0.4457 calculate D2E/DX2 analytically !

! D186 D(39,40,41,70) 179.4409 calculate D2E/DX2 analytically !

! D187 D(69,40,41,42) 179.6625 calculate D2E/DX2 analytically !

! D188 D(69,40,41,70) -0.4508 calculate D2E/DX2 analytically !

! D189 D(40,41,42,37) 0.5953 calculate D2E/DX2 analytically !

! D190 D(40,41,42,71) 179.417 calculate D2E/DX2 analytically !

! D191 D(70,41,42,37) -179.2919 calculate D2E/DX2 analytically !

! D192 D(70,41,42,71) -0.4702 calculate D2E/DX2 analytically !

! D193 D(18,43,44,45) -179.2936 calculate D2E/DX2 analytically !

! D194 D(18,43,44,72) -0.5334 calculate D2E/DX2 analytically !

! D195 D(48,43,44,45) 0.8286 calculate D2E/DX2 analytically !

! D196 D(48,43,44,72) 179.5889 calculate D2E/DX2 analytically !

! D197 D(18,43,48,47) -179.876 calculate D2E/DX2 analytically !

! D198 D(18,43,48,76) -1.113 calculate D2E/DX2 analytically !

! D199 D(44,43,48,47) 0.0007 calculate D2E/DX2 analytically !

! D200 D(44,43,48,76) 178.7637 calculate D2E/DX2 analytically !

! D201 D(43,44,45,46) -1.0227 calculate D2E/DX2 analytically !

! D202 D(43,44,45,73) 178.9974 calculate D2E/DX2 analytically !

! D203 D(72,44,45,46) -179.7758 calculate D2E/DX2 analytically !

! D204 D(72,44,45,73) 0.2442 calculate D2E/DX2 analytically !

! D205 D(44,45,46,47) 0.3759 calculate D2E/DX2 analytically !

! D206 D(44,45,46,74) -179.5208 calculate D2E/DX2 analytically !

! D207 D(73,45,46,47) -179.6442 calculate D2E/DX2 analytically !

! D208 D(73,45,46,74) 0.4591 calculate D2E/DX2 analytically !

! D209 D(45,46,47,48) 0.451 calculate D2E/DX2 analytically !

! D210 D(45,46,47,75) -179.4248 calculate D2E/DX2 analytically !

! D211 D(74,46,47,48) -179.6523 calculate D2E/DX2 analytically !

! D212 D(74,46,47,75) 0.4719 calculate D2E/DX2 analytically !

! D213 D(46,47,48,43) -0.6387 calculate D2E/DX2 analytically !

! D214 D(46,47,48,76) -179.3957 calculate D2E/DX2 analytically !

! D215 D(75,47,48,43) 179.2378 calculate D2E/DX2 analytically !

! D216 D(75,47,48,76) 0.4807 calculate D2E/DX2 analytically !

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

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

Number of steps in this run= 452 maximum allowed number of steps= 468.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 25 14:05:39 2019, MaxMem= 4294967296 cpu: 0.4

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

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.672748 -4.215912 0.423954

2 6 0 1.126369 -2.888592 0.112334

3 7 0 -0.004568 -2.116815 -0.039918

4 6 0 -1.140586 -2.883769 0.113134

5 6 0 -0.693718 -4.211843 0.423954

6 6 0 -2.461534 -2.444325 -0.027804

7 6 0 -2.871695 -1.088052 -0.209050

8 7 0 -2.061413 0.008099 -0.017719

9 6 0 -2.863871 1.094422 -0.216427

10 6 0 -4.190859 0.696263 -0.582928

11 6 0 -4.194779 -0.680785 -0.577257

12 6 0 2.448194 -2.460071 -0.026802

13 6 0 2.864065 -1.094974 -0.208848

14 6 0 4.191071 -0.699046 -0.578055

15 6 0 4.194539 0.678003 -0.582126

16 6 0 2.871483 1.087502 -0.216625

17 7 0 2.061408 -0.007364 -0.017717

18 6 0 2.461973 2.444971 -0.041014

19 6 0 1.140710 2.885313 0.094014

20 6 0 0.693719 4.209639 0.420105

21 6 0 -0.672775 4.213708 0.420105

22 6 0 -1.126301 2.890137 0.093414

23 7 0 0.004570 2.120814 -0.069828

24 6 0 -2.448645 2.460719 -0.040016

25 6 0 -3.524086 -3.480453 0.010252

26 6 0 -3.511841 -4.560112 -0.884304

27 6 0 -4.515823 -5.523881 -0.844151

28 6 0 -5.538929 -5.430988 0.097841

29 6 0 -5.558333 -4.362702 0.995006

30 6 0 -4.565813 -3.389664 0.945520

31 6 0 5.513073 -5.457627 0.097845

32 6 0 4.489535 -5.545624 -0.844148

33 6 0 3.490376 -4.576863 -0.884302

34 6 0 3.506986 -3.497274 0.010654

35 6 0 4.549734 -3.411671 0.945523

36 6 0 5.537588 -4.389247 0.995010

37 6 0 -3.507632 3.496813 0.005242

38 6 0 -4.549455 3.404544 0.940790

39 6 0 -5.536227 4.382558 0.999729

40 6 0 -5.511940 5.458318 0.111380

41 6 0 -4.489618 5.553139 -0.831276

42 6 0 -3.491380 4.583922 -0.880799

43 6 0 3.524715 3.479990 0.004844

44 6 0 4.565484 3.382539 0.940793

45 6 0 5.556924 4.356020 0.999733

46 6 0 5.537784 5.431684 0.111384

47 6 0 4.515928 5.531396 -0.831273

48 6 0 3.512866 4.567165 -0.880797

49 1 0 1.318331 -5.051709 0.639146

50 1 0 -1.343093 -5.044942 0.639145

51 1 0 -5.012562 1.353030 -0.825137

52 1 0 -5.020673 -1.333916 -0.815349

53 1 0 5.013028 -1.357119 -0.815745

54 1 0 5.020173 1.329829 -0.824733

55 1 0 1.343169 5.039175 0.648450

56 1 0 -1.318450 5.045943 0.648449

57 1 0 -2.723275 -4.630264 -1.624774

58 1 0 -4.498952 -6.346525 -1.551142

59 1 0 -6.317970 -6.185173 0.132224

60 1 0 -6.348518 -4.286921 1.734477

61 1 0 -4.582172 -2.562654 1.645631

62 1 0 6.288497 -6.215531 0.132228

63 1 0 4.468528 -6.368378 -1.550939

64 1 0 2.701084 -4.643241 -1.624572

65 1 0 4.570650 -2.584351 1.645434

66 1 0 6.328125 -4.317447 1.734481

67 1 0 -4.569912 2.572026 1.634463

68 1 0 -6.325653 4.305514 1.739854

69 1 0 -6.286537 6.216688 0.153187

70 1 0 -4.468867 6.381669 -1.531285

71 1 0 -2.703055 4.655929 -1.621554

72 1 0 4.581358 2.550334 1.634666

73 1 0 6.345972 4.275000 1.739858

74 1 0 6.316001 6.186339 0.153191

75 1 0 4.499342 6.359815 -1.531482

76 1 0 2.725294 4.642943 -1.621752

77 1 0 -0.001777 -1.117419 -0.194551

78 1 0 0.001791 1.126483 -0.252939

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

Rotational constants (GHZ): 0.0590611 0.0581645 0.0301342

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

Standard basis: 6-311G(d) (5D, 7F)

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

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5359.8203598435 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2123118619 Hartrees.

Nuclear repulsion after empirical dispersion term = 5359.6080479816 Hartrees.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5741

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.91D-11

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 268

GePol: Fraction of low-weight points (<1% of avg) = 4.67%

GePol: Cavity surface area = 611.254 Ang\*\*2

GePol: Cavity volume = 627.808 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021257072 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5359.6059222744 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.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 25 14:05:41 2019, MaxMem= 4294967296 cpu: 2.6

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

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30513211896

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0000 S= 1.0000

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 570000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 98877243.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.66D-15 for 5735.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.77D-15 for 5727 53.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.66D-15 for 5729.

Iteration 1 A^-1\*A deviation from orthogonality is 5.00D-12 for 4207 4203.

E= -1913.36733578148

DIIS: error= 3.19D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1913.36733578148 IErMin= 1 ErrMin= 3.19D-02

ErrMax= 3.19D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.04D+00 BMatP= 4.04D+00

IDIUse=3 WtCom= 6.81D-01 WtEn= 3.19D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.034 Goal= None Shift= 0.000

GapD= 0.030 DampG=0.250 DampE=0.500 DampFc=0.2500 IDamp=-1.

Damping current iteration by 2.50D-01

RMSDP=1.94D-03 MaxDP=1.09D-01 OVMax= 2.50D-01

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.81D-04 CP: 9.90D-01

E= -1913.70354014021 Delta-E= -0.336204358732 Rises=F Damp=T

DIIS: error= 1.90D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1913.70354014021 IErMin= 2 ErrMin= 1.90D-02

ErrMax= 1.90D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.29D+00 BMatP= 4.04D+00

IDIUse=3 WtCom= 8.10D-01 WtEn= 1.90D-01

Coeff-Com: -0.109D+01 0.209D+01

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

Coeff: -0.883D+00 0.188D+01

Gap= 0.041 Goal= None Shift= 0.000

Gap= 0.088 Goal= None Shift= 0.000

RMSDP=6.90D-04 MaxDP=3.57D-02 DE=-3.36D-01 OVMax= 1.56D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.89D-04 CP: 9.77D-01 2.00D+00

E= -1914.29701311976 Delta-E= -0.593472979550 Rises=F Damp=F

DIIS: error= 7.70D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.29701311976 IErMin= 3 ErrMin= 7.70D-03

ErrMax= 7.70D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.17D-01 BMatP= 1.29D+00

IDIUse=3 WtCom= 9.23D-01 WtEn= 7.70D-02

Coeff-Com: -0.436D+00 0.815D+00 0.621D+00

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

Coeff: -0.402D+00 0.752D+00 0.650D+00

Gap= 0.037 Goal= None Shift= 0.000

Gap= 0.044 Goal= None Shift= 0.000

RMSDP=2.83D-04 MaxDP=1.90D-02 DE=-5.93D-01 OVMax= 6.05D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.02D-04 CP: 9.81D-01 2.02D+00 5.99D-01

E= -1914.31895904236 Delta-E= -0.021945922604 Rises=F Damp=F

DIIS: error= 3.34D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.31895904236 IErMin= 4 ErrMin= 3.34D-03

ErrMax= 3.34D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.28D-02 BMatP= 1.17D-01

IDIUse=3 WtCom= 9.67D-01 WtEn= 3.34D-02

Coeff-Com: -0.846D-01 0.154D+00 0.358D+00 0.573D+00

Coeff-En: 0.000D+00 0.000D+00 0.229D+00 0.771D+00

Coeff: -0.817D-01 0.149D+00 0.353D+00 0.579D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=1.21D-04 MaxDP=6.56D-03 DE=-2.19D-02 OVMax= 3.84D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 7.33D-05 CP: 9.79D-01 2.00D+00 6.91D-01 5.88D-01

E= -1914.32713672804 Delta-E= -0.008177685676 Rises=F Damp=F

DIIS: error= 1.01D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.32713672804 IErMin= 5 ErrMin= 1.01D-03

ErrMax= 1.01D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.91D-03 BMatP= 3.28D-02

IDIUse=3 WtCom= 9.90D-01 WtEn= 1.01D-02

Coeff-Com: -0.178D-01 0.298D-01 0.152D+00 0.327D+00 0.509D+00

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

Coeff: -0.176D-01 0.295D-01 0.151D+00 0.323D+00 0.514D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=4.24D-05 MaxDP=2.81D-03 DE=-8.18D-03 OVMax= 1.42D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.41D-05 CP: 9.79D-01 2.01D+00 7.11D-01 6.44D-01 5.90D-01

E= -1914.32777333597 Delta-E= -0.000636607933 Rises=F Damp=F

DIIS: error= 4.74D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.32777333597 IErMin= 6 ErrMin= 4.74D-04

ErrMax= 4.74D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.06D-04 BMatP= 2.91D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.74D-03

Coeff-Com: -0.179D-02 0.149D-02 0.456D-01 0.124D+00 0.308D+00 0.522D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.539D-01 0.946D+00

Coeff: -0.178D-02 0.149D-02 0.454D-01 0.124D+00 0.307D+00 0.524D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.051 Goal= None Shift= 0.000

RMSDP=1.48D-05 MaxDP=1.04D-03 DE=-6.37D-04 OVMax= 6.67D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.05D-05 CP: 9.79D-01 2.01D+00 7.09D-01 6.48D-01 7.02D-01

CP: 7.66D-01

E= -1914.32788195180 Delta-E= -0.000108615827 Rises=F Damp=F

DIIS: error= 1.81D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.32788195180 IErMin= 7 ErrMin= 1.81D-04

ErrMax= 1.81D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.82D-05 BMatP= 4.06D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.81D-03

Coeff-Com: 0.132D-02-0.310D-02 0.281D-02 0.228D-01 0.883D-01 0.269D+00

Coeff-Com: 0.618D+00

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

Coeff-En: 0.100D+01

Coeff: 0.131D-02-0.310D-02 0.280D-02 0.227D-01 0.882D-01 0.269D+00

Coeff: 0.619D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.051 Goal= None Shift= 0.000

RMSDP=7.35D-06 MaxDP=5.47D-04 DE=-1.09D-04 OVMax= 5.51D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 5.87D-06 CP: 9.79D-01 2.01D+00 7.10D-01 6.57D-01 7.10D-01

CP: 9.19D-01 1.10D+00

E= -1914.32790557115 Delta-E= -0.000023619352 Rises=F Damp=F

DIIS: error= 6.96D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.32790557115 IErMin= 8 ErrMin= 6.96D-05

ErrMax= 6.96D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.23D-05 BMatP= 4.82D-05

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

Coeff-Com: 0.135D-02-0.200D-02-0.190D-01-0.424D-01-0.980D-01-0.105D+00

Coeff-Com: 0.274D+00 0.992D+00

Coeff: 0.135D-02-0.200D-02-0.190D-01-0.424D-01-0.980D-01-0.105D+00

Coeff: 0.274D+00 0.992D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.052 Goal= None Shift= 0.000

RMSDP=9.84D-06 MaxDP=9.01D-04 DE=-2.36D-05 OVMax= 1.03D-02

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.56D-06 CP: 9.79D-01 2.01D+00 7.09D-01 6.62D-01 7.45D-01

CP: 1.07D+00 1.73D+00 1.75D+00

E= -1914.32792330242 Delta-E= -0.000017731274 Rises=F Damp=F

DIIS: error= 4.66D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.32792330242 IErMin= 9 ErrMin= 4.66D-05

ErrMax= 4.66D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.59D-06 BMatP= 1.23D-05

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

Coeff-Com: 0.290D-03-0.252D-03-0.932D-02-0.237D-01-0.615D-01-0.915D-01

Coeff-Com: 0.206D-01 0.460D+00 0.705D+00

Coeff: 0.290D-03-0.252D-03-0.932D-02-0.237D-01-0.615D-01-0.915D-01

Coeff: 0.206D-01 0.460D+00 0.705D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.052 Goal= None Shift= 0.000

RMSDP=5.87D-06 MaxDP=5.26D-04 DE=-1.77D-05 OVMax= 6.52D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.68D-06 CP: 9.79D-01 2.01D+00 7.10D-01 6.64D-01 7.53D-01

CP: 1.15D+00 2.06D+00 2.30D+00 1.60D+00

E= -1914.32792982454 Delta-E= -0.000006522118 Rises=F Damp=F

DIIS: error= 4.24D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.32792982454 IErMin=10 ErrMin= 4.24D-05

ErrMax= 4.24D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.58D-06 BMatP= 3.59D-06

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

Coeff-Com: -0.386D-03 0.655D-03 0.271D-02 0.446D-02 0.710D-02 0.628D-03

Coeff-Com: -0.979D-01-0.154D+00 0.332D+00 0.905D+00

Coeff: -0.386D-03 0.655D-03 0.271D-02 0.446D-02 0.710D-02 0.628D-03

Coeff: -0.979D-01-0.154D+00 0.332D+00 0.905D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.052 Goal= None Shift= 0.000

RMSDP=7.19D-06 MaxDP=6.01D-04 DE=-6.52D-06 OVMax= 8.26D-03

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.11D-06 CP: 9.79D-01 2.01D+00 7.10D-01 6.65D-01 7.66D-01

CP: 1.23D+00 2.43D+00 2.99D+00 2.59D+00 1.83D+00

E= -1914.32793609827 Delta-E= -0.000006273733 Rises=F Damp=F

DIIS: error= 3.62D-05 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.32793609827 IErMin=11 ErrMin= 3.62D-05

ErrMax= 3.62D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-06 BMatP= 1.58D-06

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

Coeff-Com: -0.172D-03 0.256D-03 0.301D-02 0.641D-02 0.150D-01 0.214D-01

Coeff-Com: -0.526D-01-0.150D+00-0.205D-01 0.388D+00 0.790D+00

Coeff: -0.172D-03 0.256D-03 0.301D-02 0.641D-02 0.150D-01 0.214D-01

Coeff: -0.526D-01-0.150D+00-0.205D-01 0.388D+00 0.790D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.052 Goal= None Shift= 0.000

RMSDP=5.30D-06 MaxDP=4.23D-04 DE=-6.27D-06 OVMax= 6.02D-03

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.14D-06 CP: 9.79D-01 2.01D+00 7.10D-01 6.66D-01 7.75D-01

CP: 1.29D+00 2.69D+00 3.00D+00 3.00D+00 2.69D+00

CP: 1.64D+00

E= -1914.32794015529 Delta-E= -0.000004057010 Rises=F Damp=F

DIIS: error= 3.38D-05 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.32794015529 IErMin=12 ErrMin= 3.38D-05

ErrMax= 3.38D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.09D-07 BMatP= 1.02D-06

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

Coeff-Com: 0.359D-03-0.624D-03 0.222D-03 0.180D-02 0.930D-02 0.312D-01

Coeff-Com: 0.629D-01 0.432D-01-0.518D+00-0.778D+00 0.647D+00 0.150D+01

Coeff: 0.359D-03-0.624D-03 0.222D-03 0.180D-02 0.930D-02 0.312D-01

Coeff: 0.629D-01 0.432D-01-0.518D+00-0.778D+00 0.647D+00 0.150D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.052 Goal= None Shift= 0.000

RMSDP=1.43D-05 MaxDP=1.16D-03 DE=-4.06D-06 OVMax= 1.64D-02

Cycle 13 Pass 1 IDiag 1:

RMSU= 7.52D-06 CP: 9.79D-01 2.01D+00 7.10D-01 6.69D-01 7.97D-01

CP: 1.43D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00

E= -1914.32794882743 Delta-E= -0.000008672143 Rises=F Damp=F

DIIS: error= 2.95D-05 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.32794882743 IErMin=13 ErrMin= 2.95D-05

ErrMax= 2.95D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.85D-07 BMatP= 7.09D-07

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

Coeff-Com: 0.345D-03-0.550D-03-0.140D-02-0.268D-02-0.236D-02 0.129D-01

Coeff-Com: 0.658D-01 0.130D+00-0.348D+00-0.758D+00-0.352D+00 0.133D+01

Coeff-Com: 0.930D+00

Coeff: 0.345D-03-0.550D-03-0.140D-02-0.268D-02-0.236D-02 0.129D-01

Coeff: 0.658D-01 0.130D+00-0.348D+00-0.758D+00-0.352D+00 0.133D+01

Coeff: 0.930D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.052 Goal= None Shift= 0.000

RMSDP=1.28D-05 MaxDP=1.02D-03 DE=-8.67D-06 OVMax= 1.46D-02

Cycle 14 Pass 1 IDiag 1:

RMSU= 4.69D-06 CP: 9.79D-01 2.01D+00 7.10D-01 6.71D-01 8.17D-01

CP: 1.56D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.52D+00

E= -1914.32795422002 Delta-E= -0.000005392594 Rises=F Damp=F

DIIS: error= 1.38D-05 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.32795422002 IErMin=14 ErrMin= 1.38D-05

ErrMax= 1.38D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.50D-07 BMatP= 6.85D-07

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

Coeff-Com: -0.158D-04 0.759D-04-0.119D-02-0.401D-02-0.103D-01-0.136D-01

Coeff-Com: -0.178D-01 0.712D-01 0.198D+00 0.132D+00-0.970D+00-0.106D+00

Coeff-Com: 0.608D+00 0.111D+01

Coeff: -0.158D-04 0.759D-04-0.119D-02-0.401D-02-0.103D-01-0.136D-01

Coeff: -0.178D-01 0.712D-01 0.198D+00 0.132D+00-0.970D+00-0.106D+00

Coeff: 0.608D+00 0.111D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.052 Goal= None Shift= 0.000

RMSDP=1.22D-05 MaxDP=9.90D-04 DE=-5.39D-06 OVMax= 1.39D-02

Cycle 15 Pass 1 IDiag 1:

RMSU= 7.27D-06 CP: 9.79D-01 2.01D+00 7.10D-01 6.73D-01 8.36D-01

CP: 1.68D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.95D+00

E= -1914.32795708090 Delta-E= -0.000002860882 Rises=F Damp=F

DIIS: error= 9.24D-06 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.32795708090 IErMin=15 ErrMin= 9.24D-06

ErrMax= 9.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.12D-08 BMatP= 2.50D-07

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

Coeff-Com: -0.101D-03 0.167D-03 0.405D-03 0.537D-03 0.113D-03-0.192D-02

Coeff-Com: -0.276D-01-0.287D-01 0.126D+00 0.226D+00-0.235D-01-0.378D+00

Coeff-Com: -0.263D+00 0.258D+00 0.111D+01

Coeff: -0.101D-03 0.167D-03 0.405D-03 0.537D-03 0.113D-03-0.192D-02

Coeff: -0.276D-01-0.287D-01 0.126D+00 0.226D+00-0.235D-01-0.378D+00

Coeff: -0.263D+00 0.258D+00 0.111D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.052 Goal= None Shift= 0.000

RMSDP=4.74D-06 MaxDP=3.80D-04 DE=-2.86D-06 OVMax= 5.32D-03

Cycle 16 Pass 1 IDiag 1:

RMSU= 3.40D-07 CP: 9.79D-01 2.01D+00 7.10D-01 6.74D-01 8.43D-01

CP: 1.73D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.32D+00 1.58D+00

E= -1914.32795760862 Delta-E= -0.000000527717 Rises=F Damp=F

DIIS: error= 6.43D-06 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1914.32795760862 IErMin=16 ErrMin= 6.43D-06

ErrMax= 6.43D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.63D-08 BMatP= 7.12D-08

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

Coeff-Com: -0.711D-04 0.966D-04 0.723D-03 0.193D-02 0.415D-02 0.480D-02

Coeff-Com: -0.111D-01-0.445D-01 0.538D-02 0.946D-01 0.388D+00-0.213D+00

Coeff-Com: -0.463D+00-0.254D+00 0.795D+00 0.692D+00

Coeff: -0.711D-04 0.966D-04 0.723D-03 0.193D-02 0.415D-02 0.480D-02

Coeff: -0.111D-01-0.445D-01 0.538D-02 0.946D-01 0.388D+00-0.213D+00

Coeff: -0.463D+00-0.254D+00 0.795D+00 0.692D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.052 Goal= None Shift= 0.000

RMSDP=2.15D-06 MaxDP=1.75D-04 DE=-5.28D-07 OVMax= 2.38D-03

Cycle 17 Pass 1 IDiag 1:

RMSU= 1.92D-07 CP: 9.79D-01 2.01D+00 7.10D-01 6.74D-01 8.46D-01

CP: 1.75D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.49D+00 1.84D+00

CP: 1.47D+00

E= -1914.32795773840 Delta-E= -0.000000129777 Rises=F Damp=F

DIIS: error= 2.70D-06 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1914.32795773840 IErMin=17 ErrMin= 2.70D-06

ErrMax= 2.70D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.26D-09 BMatP= 4.63D-08

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

Coeff-Com: 0.174D-04-0.345D-04 0.112D-03 0.521D-03 0.147D-02 0.214D-02

Coeff-Com: 0.574D-02-0.537D-02-0.441D-01-0.499D-01 0.123D+00 0.836D-01

Coeff-Com: -0.689D-01-0.164D+00-0.200D+00 0.270D+00 0.105D+01

Coeff: 0.174D-04-0.345D-04 0.112D-03 0.521D-03 0.147D-02 0.214D-02

Coeff: 0.574D-02-0.537D-02-0.441D-01-0.499D-01 0.123D+00 0.836D-01

Coeff: -0.689D-01-0.164D+00-0.200D+00 0.270D+00 0.105D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.052 Goal= None Shift= 0.000

RMSDP=1.33D-06 MaxDP=1.06D-04 DE=-1.30D-07 OVMax= 1.46D-03

Cycle 18 Pass 1 IDiag 1:

RMSU= 7.28D-08 CP: 9.79D-01 2.01D+00 7.10D-01 6.74D-01 8.48D-01

CP: 1.76D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.59D+00 2.01D+00

CP: 1.95D+00 1.32D+00

E= -1914.32795777091 Delta-E= -0.000000032516 Rises=F Damp=F

DIIS: error= 7.64D-07 at cycle 18 NSaved= 18.

NSaved=18 IEnMin=18 EnMin= -1914.32795777091 IErMin=18 ErrMin= 7.64D-07

ErrMax= 7.64D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.40D-09 BMatP= 8.26D-09

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

Coeff-Com: 0.158D-04-0.253D-04-0.614D-04-0.104D-03-0.864D-04-0.156D-03

Coeff-Com: 0.356D-02 0.416D-02-0.142D-01-0.258D-01-0.172D-01 0.610D-01

Coeff-Com: 0.366D-01-0.169D-01-0.198D+00-0.310D-02 0.385D+00 0.785D+00

Coeff: 0.158D-04-0.253D-04-0.614D-04-0.104D-03-0.864D-04-0.156D-03

Coeff: 0.356D-02 0.416D-02-0.142D-01-0.258D-01-0.172D-01 0.610D-01

Coeff: 0.366D-01-0.169D-01-0.198D+00-0.310D-02 0.385D+00 0.785D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.052 Goal= None Shift= 0.000

RMSDP=2.14D-07 MaxDP=1.69D-05 DE=-3.25D-08 OVMax= 2.26D-04

Cycle 19 Pass 1 IDiag 1:

RMSU= 2.58D-08 CP: 9.79D-01 2.01D+00 7.10D-01 6.74D-01 8.48D-01

CP: 1.76D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.60D+00 2.03D+00

CP: 2.07D+00 1.48D+00 1.21D+00

E= -1914.32795777283 Delta-E= -0.000000001919 Rises=F Damp=F

DIIS: error= 3.48D-07 at cycle 19 NSaved= 19.

NSaved=19 IEnMin=19 EnMin= -1914.32795777283 IErMin=19 ErrMin= 3.48D-07

ErrMax= 3.48D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.62D-10 BMatP= 1.40D-09

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

Coeff-Com: 0.224D-05-0.199D-05-0.587D-04-0.188D-03-0.402D-03-0.670D-03

Coeff-Com: 0.522D-03 0.337D-02 0.386D-02-0.560D-03-0.397D-01 0.997D-02

Coeff-Com: 0.312D-01 0.340D-01-0.452D-01-0.688D-01-0.796D-01 0.397D+00

Coeff-Com: 0.755D+00

Coeff: 0.224D-05-0.199D-05-0.587D-04-0.188D-03-0.402D-03-0.670D-03

Coeff: 0.522D-03 0.337D-02 0.386D-02-0.560D-03-0.397D-01 0.997D-02

Coeff: 0.312D-01 0.340D-01-0.452D-01-0.688D-01-0.796D-01 0.397D+00

Coeff: 0.755D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.052 Goal= None Shift= 0.000

RMSDP=1.56D-07 MaxDP=1.23D-05 DE=-1.92D-09 OVMax= 1.73D-04

Cycle 20 Pass 1 IDiag 1:

RMSU= 1.42D-08 CP: 9.79D-01 2.01D+00 7.10D-01 6.74D-01 8.48D-01

CP: 1.76D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.62D+00 2.05D+00

CP: 2.11D+00 1.51D+00 1.37D+00 1.21D+00

E= -1914.32795777328 Delta-E= -0.000000000447 Rises=F Damp=F

DIIS: error= 1.24D-07 at cycle 20 NSaved= 20.

NSaved=20 IEnMin=20 EnMin= -1914.32795777328 IErMin=20 ErrMin= 1.24D-07

ErrMax= 1.24D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.79D-11 BMatP= 4.62D-10

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

Coeff-Com: -0.232D-05 0.369D-05 0.701D-05 0.369D-05 0.115D-04-0.225D-04

Coeff-Com: -0.402D-03-0.436D-03 0.226D-02 0.325D-02 0.115D-02-0.761D-02

Coeff-Com: -0.495D-02 0.519D-02 0.298D-01-0.920D-02-0.781D-01-0.830D-01

Coeff-Com: 0.128D+00 0.101D+01

Coeff: -0.232D-05 0.369D-05 0.701D-05 0.369D-05 0.115D-04-0.225D-04

Coeff: -0.402D-03-0.436D-03 0.226D-02 0.325D-02 0.115D-02-0.761D-02

Coeff: -0.495D-02 0.519D-02 0.298D-01-0.920D-02-0.781D-01-0.830D-01

Coeff: 0.128D+00 0.101D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.052 Goal= None Shift= 0.000

RMSDP=1.10D-08 MaxDP=7.18D-07 DE=-4.47D-10 OVMax= 5.27D-06

Cycle 21 Pass 1 IDiag 1:

Restarting incremental Fock formation.

E= -1914.32795777205 Delta-E= 0.000000001225 Rises=F Damp=F

DIIS: error= 1.06D-07 at cycle 21 NSaved= 20.

NSaved=20 IEnMin=19 EnMin= -1914.32795777328 IErMin=20 ErrMin= 1.06D-07

ErrMax= 1.06D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.62D-11 BMatP= 3.79D-11

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

Coeff-Com: -0.108D-06 0.819D-06-0.208D-05-0.225D-05-0.157D-04-0.201D-03

Coeff-Com: -0.158D-03 0.112D-02 0.141D-02 0.543D-03-0.383D-02-0.232D-02

Coeff-Com: 0.267D-02 0.168D-01-0.213D-02-0.357D-01-0.744D-01 0.761D-02

Coeff-Com: 0.531D+00 0.558D+00

Coeff: -0.108D-06 0.819D-06-0.208D-05-0.225D-05-0.157D-04-0.201D-03

Coeff: -0.158D-03 0.112D-02 0.141D-02 0.543D-03-0.383D-02-0.232D-02

Coeff: 0.267D-02 0.168D-01-0.213D-02-0.357D-01-0.744D-01 0.761D-02

Coeff: 0.531D+00 0.558D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.052 Goal= None Shift= 0.000

RMSDP=1.02D-08 MaxDP=3.99D-07 DE= 1.23D-09 OVMax= 4.24D-06

Cycle 22 Pass 1 IDiag 1:

RMSU= 1.02D-08 CP: 1.00D+00

E= -1914.32795777209 Delta-E= -0.000000000038 Rises=F Damp=F

DIIS: error= 4.43D-08 at cycle 22 NSaved= 20.

NSaved=20 IEnMin=18 EnMin= -1914.32795777328 IErMin=20 ErrMin= 4.43D-08

ErrMax= 4.43D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.01D-12 BMatP= 1.62D-11

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

Coeff-Com: 0.391D-05 0.108D-04 0.230D-04 0.222D-04-0.880D-05-0.204D-03

Coeff-Com: -0.192D-03 0.518D-04 0.142D-02-0.203D-04-0.116D-02-0.164D-02

Coeff-Com: 0.471D-03 0.365D-02 0.896D-02-0.148D-01-0.441D-01-0.733D-01

Coeff-Com: 0.251D+00 0.870D+00

Coeff: 0.391D-05 0.108D-04 0.230D-04 0.222D-04-0.880D-05-0.204D-03

Coeff: -0.192D-03 0.518D-04 0.142D-02-0.203D-04-0.116D-02-0.164D-02

Coeff: 0.471D-03 0.365D-02 0.896D-02-0.148D-01-0.441D-01-0.733D-01

Coeff: 0.251D+00 0.870D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.052 Goal= None Shift= 0.000

RMSDP=9.40D-09 MaxDP=2.45D-07 DE=-3.82D-11 OVMax= 2.32D-06

Error on total polarization charges = 0.08254

SCF Done: E(UB3LYP) = -1914.32795777 A.U. after 22 cycles

NFock= 22 Conv=0.94D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0325 S= 1.0108

<L.S>= 0.000000000000E+00

KE= 1.906369195093D+03 PE=-1.516892867864D+04 EE= 5.988625603501D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.33

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0325, after 2.0006

Leave Link 502 at Sun Aug 25 14:16:12 2019, MaxMem= 4294967296 cpu: 9950.1

(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: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.10101438D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.38428478D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.10330201D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.52155683D-01

Leave Link 801 at Sun Aug 25 14:16:12 2019, MaxMem= 4294967296 cpu: 0.9

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

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

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

Leave Link 1101 at Sun Aug 25 14:16:20 2019, MaxMem= 4294967296 cpu: 115.8

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

Symmetrizing basis deriv contribution to polar:

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

Leave Link 1102 at Sun Aug 25 14:16:20 2019, MaxMem= 4294967296 cpu: 2.4

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

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 186

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 Sun Aug 25 14:35:56 2019, MaxMem= 4294967296 cpu: 18807.2

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

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 570000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 6.06D+03 4.98D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 5.42D+02 4.25D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 1.13D+01 4.92D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.42D-01 3.60D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 8.36D-04 2.38D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 6.80D-06 1.33D-04.

193 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 3.89D-08 1.21D-05.

74 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 1.78D-10 8.26D-07.

31 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 9.29D-13 4.13D-08.

3 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 1.24D-14 3.44D-09.

3 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 8.14D-15 4.33D-09.

3 vectors produced by pass 11 Test12= 2.55D-13 1.00D-09 XBig12= 9.36D-15 2.82D-09.

3 vectors produced by pass 12 Test12= 2.55D-13 1.00D-09 XBig12= 6.39D-15 2.38D-09.

3 vectors produced by pass 13 Test12= 2.55D-13 1.00D-09 XBig12= 5.57D-15 2.49D-09.

3 vectors produced by pass 14 Test12= 2.55D-13 1.00D-09 XBig12= 6.77D-15 2.52D-09.

3 vectors produced by pass 15 Test12= 2.55D-13 1.00D-09 XBig12= 7.41D-15 3.28D-09.

3 vectors produced by pass 16 Test12= 2.55D-13 1.00D-09 XBig12= 1.06D-14 3.92D-09.

3 vectors produced by pass 17 Test12= 2.55D-13 1.00D-09 XBig12= 4.63D-15 2.10D-09.

3 vectors produced by pass 18 Test12= 2.55D-13 1.00D-09 XBig12= 8.36D-15 3.96D-09.

2 vectors produced by pass 19 Test12= 2.55D-13 1.00D-09 XBig12= 4.62D-15 2.64D-09.

InvSVY: IOpt=1 It= 1 EMax= 5.68D-14

Solved reduced A of dimension 1737 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1235.20 Bohr\*\*3.

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

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

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

Leave Link 1002 at Sun Aug 25 18:30:30 2019, MaxMem= 4294967296 cpu: 225115.1

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

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

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Population analysis using the SCF density.

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Orbital symmetries:

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The electronic state is 3-A.

Alpha occ. eigenvalues -- -14.36189 -14.36142 -14.29531 -14.29529 -10.22752

Alpha occ. eigenvalues -- -10.22739 -10.22664 -10.22655 -10.21518 -10.21507

Alpha occ. eigenvalues -- -10.20942 -10.20932 -10.19709 -10.19702 -10.19494

Alpha occ. eigenvalues -- -10.19490 -10.19222 -10.19212 -10.19074 -10.19065

Alpha occ. eigenvalues -- -10.18128 -10.18123 -10.17984 -10.17981 -10.17846

Alpha occ. eigenvalues -- -10.17835 -10.17799 -10.17789 -10.17737 -10.17728

Alpha occ. eigenvalues -- -10.17687 -10.17679 -10.17671 -10.17660 -10.17580

Alpha occ. eigenvalues -- -10.17571 -10.17519 -10.17513 -10.17494 -10.17489

Alpha occ. eigenvalues -- -10.17447 -10.17443 -10.17430 -10.17426 -10.15551

Alpha occ. eigenvalues -- -10.15550 -10.15376 -10.15376 -0.99868 -0.99732

Alpha occ. eigenvalues -- -0.94742 -0.94465 -0.87608 -0.87173 -0.87065

Alpha occ. eigenvalues -- -0.86891 -0.83289 -0.82053 -0.81420 -0.80654

Alpha occ. eigenvalues -- -0.79891 -0.78966 -0.76078 -0.75511 -0.75387

Alpha occ. eigenvalues -- -0.75265 -0.75142 -0.75020 -0.74810 -0.74065

Alpha occ. eigenvalues -- -0.73656 -0.72418 -0.71700 -0.67161 -0.67038

Alpha occ. eigenvalues -- -0.62940 -0.61703 -0.61457 -0.61203 -0.61013

Alpha occ. eigenvalues -- -0.60977 -0.60576 -0.60452 -0.60224 -0.59946

Alpha occ. eigenvalues -- -0.59880 -0.57769 -0.57512 -0.56493 -0.55384

Alpha occ. eigenvalues -- -0.54815 -0.53040 -0.52659 -0.52483 -0.50981

Alpha occ. eigenvalues -- -0.50611 -0.50571 -0.50242 -0.49173 -0.47060

Alpha occ. eigenvalues -- -0.46856 -0.46471 -0.46305 -0.46177 -0.45830

Alpha occ. eigenvalues -- -0.45625 -0.45498 -0.45252 -0.44623 -0.44504

Alpha occ. eigenvalues -- -0.43943 -0.43545 -0.43134 -0.42946 -0.42712

Alpha occ. eigenvalues -- -0.42545 -0.42531 -0.42492 -0.42346 -0.42251

Alpha occ. eigenvalues -- -0.41828 -0.41000 -0.40512 -0.39725 -0.39703

Alpha occ. eigenvalues -- -0.39624 -0.38527 -0.38283 -0.38021 -0.37710

Alpha occ. eigenvalues -- -0.37293 -0.37058 -0.36716 -0.36495 -0.35652

Alpha occ. eigenvalues -- -0.35263 -0.35076 -0.35061 -0.34938 -0.34899

Alpha occ. eigenvalues -- -0.34838 -0.34601 -0.33154 -0.30573 -0.29556

Alpha occ. eigenvalues -- -0.28400 -0.27953 -0.27940 -0.27623 -0.27217

Alpha occ. eigenvalues -- -0.26280 -0.26242 -0.26170 -0.26122 -0.25660

Alpha occ. eigenvalues -- -0.25593 -0.25333 -0.24271 -0.24167 -0.21278

Alpha occ. eigenvalues -- -0.20957 -0.13898

Alpha virt. eigenvalues -- -0.10055 -0.05657 -0.01819 -0.01751 -0.01653

Alpha virt. eigenvalues -- -0.01414 -0.01282 -0.01274 -0.01247 -0.01166

Alpha virt. eigenvalues -- 0.02073 0.04649 0.05169 0.05256 0.05590

Alpha virt. eigenvalues -- 0.05614 0.05887 0.06865 0.07377 0.08161

Alpha virt. eigenvalues -- 0.08195 0.08401 0.09221 0.09471 0.09479

Alpha virt. eigenvalues -- 0.09804 0.09843 0.09962 0.10346 0.10370

Alpha virt. eigenvalues -- 0.10563 0.10577 0.10690 0.11018 0.11631

Alpha virt. eigenvalues -- 0.12532 0.12614 0.12802 0.12869 0.13075

Alpha virt. eigenvalues -- 0.13165 0.13171 0.13659 0.14114 0.14234

Alpha virt. eigenvalues -- 0.14272 0.14417 0.14754 0.15238 0.15816

Alpha virt. eigenvalues -- 0.16344 0.16525 0.17274 0.19133 0.20995

Alpha virt. eigenvalues -- 0.21046 0.22083 0.22559 0.23194 0.23354

Alpha virt. eigenvalues -- 0.23604 0.24112 0.24458 0.25171 0.25418

Alpha virt. eigenvalues -- 0.25922 0.26115 0.26313 0.26823 0.27598

Alpha virt. eigenvalues -- 0.27717 0.27728 0.27815 0.27898 0.28027

Alpha virt. eigenvalues -- 0.28703 0.28764 0.29401 0.29410 0.29465

Alpha virt. eigenvalues -- 0.29524 0.29713 0.30523 0.30745 0.30885

Alpha virt. eigenvalues -- 0.31006 0.31354 0.31483 0.33147 0.33759

Alpha virt. eigenvalues -- 0.34095 0.34724 0.35130 0.35219 0.35583

Alpha virt. eigenvalues -- 0.35758 0.35955 0.35980 0.36354 0.36748

Alpha virt. eigenvalues -- 0.36755 0.37173 0.37293 0.37539 0.37817

Alpha virt. eigenvalues -- 0.38203 0.38218 0.38491 0.38734 0.39237

Alpha virt. eigenvalues -- 0.39472 0.39931 0.40185 0.40261 0.40305

Alpha virt. eigenvalues -- 0.40600 0.40624 0.40901 0.41116 0.41221

Alpha virt. eigenvalues -- 0.41495 0.41628 0.41684 0.41732 0.41816

Alpha virt. eigenvalues -- 0.42524 0.42581 0.42659 0.42778 0.43212

Alpha virt. eigenvalues -- 0.43409 0.43536 0.43672 0.44184 0.44503

Alpha virt. eigenvalues -- 0.44591 0.44748 0.44804 0.44894 0.44953

Alpha virt. eigenvalues -- 0.45395 0.45506 0.45548 0.45616 0.45918

Alpha virt. eigenvalues -- 0.46545 0.46815 0.46852 0.47047 0.47288

Alpha virt. eigenvalues -- 0.47628 0.47841 0.48278 0.48744 0.49325

Alpha virt. eigenvalues -- 0.49422 0.49618 0.50519 0.50536 0.50578

Alpha virt. eigenvalues -- 0.51528 0.51707 0.52429 0.52532 0.52808

Alpha virt. eigenvalues -- 0.52956 0.53646 0.53968 0.53992 0.54054

Alpha virt. eigenvalues -- 0.54617 0.55309 0.55880 0.57362 0.57400

Alpha virt. eigenvalues -- 0.57542 0.57702 0.57793 0.58092 0.58335

Alpha virt. eigenvalues -- 0.59089 0.59426 0.59476 0.59869 0.59953

Alpha virt. eigenvalues -- 0.60052 0.60175 0.60499 0.60672 0.60726

Alpha virt. eigenvalues -- 0.60773 0.60924 0.61081 0.61353 0.61378

Alpha virt. eigenvalues -- 0.61709 0.61749 0.62119 0.62209 0.62489

Alpha virt. eigenvalues -- 0.62624 0.63131 0.63644 0.63839 0.64331

Alpha virt. eigenvalues -- 0.64438 0.64873 0.64911 0.65110 0.65273

Alpha virt. eigenvalues -- 0.65332 0.65484 0.65810 0.66069 0.66303

Alpha virt. eigenvalues -- 0.67267 0.67882 0.68140 0.68529 0.68905

Alpha virt. eigenvalues -- 0.69038 0.69663 0.69974 0.70126 0.70812

Alpha virt. eigenvalues -- 0.71703 0.71816 0.72186 0.72316 0.72900

Alpha virt. eigenvalues -- 0.72979 0.73375 0.73767 0.73911 0.73916

Alpha virt. eigenvalues -- 0.73983 0.74994 0.75046 0.75137 0.75824

Alpha virt. eigenvalues -- 0.76034 0.76124 0.76571 0.76956 0.77010

Alpha virt. eigenvalues -- 0.77785 0.78133 0.78533 0.78619 0.78729

Alpha virt. eigenvalues -- 0.78914 0.79373 0.79846 0.80268 0.80292

Alpha virt. eigenvalues -- 0.80448 0.81237 0.81461 0.81559 0.81923

Alpha virt. eigenvalues -- 0.83215 0.83258 0.83331 0.84627 0.84801

Alpha virt. eigenvalues -- 0.85041 0.85637 0.86917 0.87089 0.87209

Alpha virt. eigenvalues -- 0.87813 0.88330 0.88398 0.88679 0.88868

Alpha virt. eigenvalues -- 0.88929 0.90791 0.90844 0.91842 0.91956

Alpha virt. eigenvalues -- 0.92032 0.92784 0.93241 0.93487 0.93780

Alpha virt. eigenvalues -- 0.95095 0.95302 0.95490 0.95957 0.96136

Alpha virt. eigenvalues -- 0.97292 0.97522 0.98668 0.99193 0.99803

Alpha virt. eigenvalues -- 1.00561 1.01098 1.01445 1.01517 1.01749

Alpha virt. eigenvalues -- 1.02094 1.02744 1.02875 1.03199 1.04386

Alpha virt. eigenvalues -- 1.04744 1.06004 1.06891 1.07482 1.08653

Alpha virt. eigenvalues -- 1.08775 1.08874 1.08912 1.10158 1.11058

Alpha virt. eigenvalues -- 1.12005 1.13160 1.13242 1.13644 1.13715

Alpha virt. eigenvalues -- 1.14031 1.14099 1.14776 1.15428 1.15755

Alpha virt. eigenvalues -- 1.16048 1.16277 1.16359 1.16440 1.18436

Alpha virt. eigenvalues -- 1.18488 1.18824 1.19127 1.19919 1.20129

Alpha virt. eigenvalues -- 1.20412 1.20503 1.20791 1.21067 1.21103

Alpha virt. eigenvalues -- 1.21883 1.22812 1.22966 1.23140 1.24092

Alpha virt. eigenvalues -- 1.24901 1.25028 1.25083 1.25602 1.25651

Alpha virt. eigenvalues -- 1.26234 1.26785 1.27058 1.27606 1.28211

Alpha virt. eigenvalues -- 1.29232 1.29459 1.29944 1.30727 1.31942

Alpha virt. eigenvalues -- 1.32014 1.32050 1.33199 1.33955 1.35418

Alpha virt. eigenvalues -- 1.36806 1.38020 1.39292 1.39652 1.39896

Alpha virt. eigenvalues -- 1.40976 1.41567 1.41864 1.41906 1.43503

Alpha virt. eigenvalues -- 1.44796 1.44845 1.45384 1.46482 1.46716

Alpha virt. eigenvalues -- 1.47209 1.47298 1.47429 1.47561 1.47772

Alpha virt. eigenvalues -- 1.47979 1.48483 1.49017 1.49134 1.49349

Alpha virt. eigenvalues -- 1.51442 1.52612 1.52741 1.53008 1.53074

Alpha virt. eigenvalues -- 1.53521 1.53589 1.53756 1.55007 1.56852

Alpha virt. eigenvalues -- 1.57092 1.58491 1.61050 1.61438 1.61678

Alpha virt. eigenvalues -- 1.62006 1.62878 1.63835 1.64545 1.64730

Alpha virt. eigenvalues -- 1.67030 1.67149 1.67245 1.67870 1.68166

Alpha virt. eigenvalues -- 1.68796 1.69555 1.69896 1.70059 1.70933

Alpha virt. eigenvalues -- 1.71292 1.73267 1.73541 1.73916 1.74287

Alpha virt. eigenvalues -- 1.74526 1.74774 1.75225 1.75728 1.75788

Alpha virt. eigenvalues -- 1.76781 1.77259 1.78490 1.78624 1.78850

Alpha virt. eigenvalues -- 1.79561 1.79974 1.80245 1.80433 1.80891

Alpha virt. eigenvalues -- 1.81388 1.81503 1.81717 1.82476 1.82586

Alpha virt. eigenvalues -- 1.83391 1.84039 1.84116 1.85039 1.85156

Alpha virt. eigenvalues -- 1.85312 1.87003 1.87281 1.87481 1.87801

Alpha virt. eigenvalues -- 1.88486 1.88517 1.89795 1.89884 1.90523

Alpha virt. eigenvalues -- 1.91320 1.91582 1.91773 1.92026 1.92074

Alpha virt. eigenvalues -- 1.92303 1.92466 1.92876 1.93040 1.93320

Alpha virt. eigenvalues -- 1.93411 1.93474 1.93766 1.94295 1.94340

Alpha virt. eigenvalues -- 1.94371 1.95696 1.95837 1.96046 1.96094

Alpha virt. eigenvalues -- 1.96202 1.97043 1.97164 1.97521 1.99202

Alpha virt. eigenvalues -- 1.99342 2.00202 2.00721 2.01430 2.01726

Alpha virt. eigenvalues -- 2.05680 2.06344 2.06488 2.08251 2.08424

Alpha virt. eigenvalues -- 2.08652 2.09899 2.10372 2.12959 2.13479

Alpha virt. eigenvalues -- 2.13708 2.16372 2.17843 2.21675 2.22971

Alpha virt. eigenvalues -- 2.23529 2.23899 2.24357 2.24659 2.25204

Alpha virt. eigenvalues -- 2.25390 2.25981 2.26108 2.26169 2.26839

Alpha virt. eigenvalues -- 2.27107 2.27164 2.27249 2.27495 2.27587

Alpha virt. eigenvalues -- 2.27641 2.28183 2.28837 2.29251 2.29584

Alpha virt. eigenvalues -- 2.29657 2.30368 2.30917 2.31111 2.32141

Alpha virt. eigenvalues -- 2.32625 2.32686 2.32918 2.34482 2.34607

Alpha virt. eigenvalues -- 2.34657 2.35590 2.36033 2.36408 2.36421

Alpha virt. eigenvalues -- 2.37037 2.38392 2.38551 2.38797 2.39573

Alpha virt. eigenvalues -- 2.39773 2.40945 2.42971 2.43182 2.44421

Alpha virt. eigenvalues -- 2.44571 2.47116 2.47557 2.48154 2.50492

Alpha virt. eigenvalues -- 2.51234 2.51586 2.52131 2.52382 2.53868

Alpha virt. eigenvalues -- 2.55289 2.56578 2.56652 2.57658 2.57908

Alpha virt. eigenvalues -- 2.58355 2.59080 2.59340 2.59442 2.60739

Alpha virt. eigenvalues -- 2.61523 2.62021 2.62748 2.63588 2.64340

Alpha virt. eigenvalues -- 2.65245 2.65534 2.65868 2.66865 2.66995

Alpha virt. eigenvalues -- 2.69612 2.70017 2.70137 2.70441 2.70721

Alpha virt. eigenvalues -- 2.72024 2.72292 2.72709 2.73629 2.73722

Alpha virt. eigenvalues -- 2.74712 2.74833 2.76515 2.76541 2.76965

Alpha virt. eigenvalues -- 2.77854 2.78413 2.78528 2.78553 2.79327

Alpha virt. eigenvalues -- 2.82366 2.82803 2.83055 2.83140 2.83920

Alpha virt. eigenvalues -- 2.85375 2.85761 2.85892 2.86863 2.88981

Alpha virt. eigenvalues -- 2.89361 2.89868 2.90290 2.91882 2.94408

Alpha virt. eigenvalues -- 2.95044 2.95371 2.97287 2.97640 2.98031

Alpha virt. eigenvalues -- 2.98391 2.99708 3.02117 3.02689 3.02944

Alpha virt. eigenvalues -- 3.03192 3.03872 3.05291 3.05430 3.06831

Alpha virt. eigenvalues -- 3.07335 3.07785 3.07947 3.08028 3.09803

Alpha virt. eigenvalues -- 3.09819 3.12022 3.12138 3.13916 3.15013

Alpha virt. eigenvalues -- 3.15329 3.16264 3.16520 3.17734 3.19063

Alpha virt. eigenvalues -- 3.19514 3.21889 3.23826 3.23838 3.24814

Alpha virt. eigenvalues -- 3.25797 3.26053 3.26254 3.27060 3.27260

Alpha virt. eigenvalues -- 3.29251 3.29272 3.29617 3.30003 3.30200

Alpha virt. eigenvalues -- 3.30334 3.30595 3.30655 3.31166 3.31238

Alpha virt. eigenvalues -- 3.31408 3.31699 3.31745 3.33002 3.33018

Alpha virt. eigenvalues -- 3.33136 3.34015 3.35108 3.35302 3.35949

Alpha virt. eigenvalues -- 3.36800 3.37539 3.38798 3.39831 3.41429

Alpha virt. eigenvalues -- 3.42958 3.43172 3.44908 3.45297 3.48730

Alpha virt. eigenvalues -- 3.50599 3.50838 3.51523 3.56389 3.56950

Alpha virt. eigenvalues -- 3.57840 3.58195 3.58261 3.60068 3.60964

Alpha virt. eigenvalues -- 3.62024 3.63199 3.64671 3.64904 3.66329

Alpha virt. eigenvalues -- 3.71351 3.71632 3.71958 3.74195 3.75507

Alpha virt. eigenvalues -- 3.77186 3.80289 3.80968 3.82462 3.83646

Alpha virt. eigenvalues -- 3.87396 3.90280 3.90323 3.93011 3.93222

Alpha virt. eigenvalues -- 3.93885 3.95404 3.95613 3.96174 3.96402

Alpha virt. eigenvalues -- 3.98171 3.98909 4.02866 4.10446 4.28904

Alpha virt. eigenvalues -- 4.29730 4.36267 4.39980 4.47346 4.51326

Alpha virt. eigenvalues -- 4.54420 4.55142 4.62865 4.62893 4.66748

Alpha virt. eigenvalues -- 4.67863 4.78380 4.78393 4.78457 4.78470

Alpha virt. eigenvalues -- 5.08724 5.14748 5.16406 5.26352 23.24456

Alpha virt. eigenvalues -- 23.28042 23.28211 23.29921 23.45785 23.52104

Alpha virt. eigenvalues -- 23.54113 23.59579 23.74030 23.76777 23.77277

Alpha virt. eigenvalues -- 23.80095 23.80405 23.80517 23.80559 23.80814

Alpha virt. eigenvalues -- 23.85203 23.85852 23.86071 23.86606 23.90477

Alpha virt. eigenvalues -- 23.91352 23.94888 23.95974 23.98001 23.98060

Alpha virt. eigenvalues -- 23.99840 24.00159 24.04759 24.04864 24.04966

Alpha virt. eigenvalues -- 24.05093 24.06705 24.06932 24.08200 24.08318

Alpha virt. eigenvalues -- 24.12293 24.12507 24.12801 24.13300 24.15159

Alpha virt. eigenvalues -- 24.15199 24.15240 24.15304 35.55154 35.56049

Alpha virt. eigenvalues -- 35.62645 35.63177

Beta occ. eigenvalues -- -14.35896 -14.35849 -14.29316 -14.29314 -10.22849

Beta occ. eigenvalues -- -10.22836 -10.22647 -10.22637 -10.21176 -10.21166

Beta occ. eigenvalues -- -10.20429 -10.20420 -10.19683 -10.19677 -10.19413

Beta occ. eigenvalues -- -10.19410 -10.19252 -10.19242 -10.19122 -10.19112

Beta occ. eigenvalues -- -10.18158 -10.18153 -10.17924 -10.17920 -10.17803

Beta occ. eigenvalues -- -10.17793 -10.17757 -10.17748 -10.17676 -10.17669

Beta occ. eigenvalues -- -10.17641 -10.17630 -10.17629 -10.17622 -10.17539

Beta occ. eigenvalues -- -10.17532 -10.17529 -10.17523 -10.17503 -10.17498

Beta occ. eigenvalues -- -10.17463 -10.17459 -10.17440 -10.17436 -10.15498

Beta occ. eigenvalues -- -10.15498 -10.15280 -10.15279 -0.99503 -0.99374

Beta occ. eigenvalues -- -0.94277 -0.94014 -0.87346 -0.87015 -0.86866

Beta occ. eigenvalues -- -0.86746 -0.82828 -0.81564 -0.80860 -0.80301

Beta occ. eigenvalues -- -0.79684 -0.78606 -0.75875 -0.75371 -0.75289

Beta occ. eigenvalues -- -0.75207 -0.75061 -0.74813 -0.74722 -0.73882

Beta occ. eigenvalues -- -0.73430 -0.72210 -0.71194 -0.66786 -0.66596

Beta occ. eigenvalues -- -0.62728 -0.61573 -0.61385 -0.61119 -0.60918

Beta occ. eigenvalues -- -0.60856 -0.60448 -0.60350 -0.60044 -0.59783

Beta occ. eigenvalues -- -0.59774 -0.57517 -0.57440 -0.56293 -0.55207

Beta occ. eigenvalues -- -0.54651 -0.52836 -0.52516 -0.52417 -0.50828

Beta occ. eigenvalues -- -0.50464 -0.50425 -0.50060 -0.48981 -0.46952

Beta occ. eigenvalues -- -0.46685 -0.46082 -0.46053 -0.45992 -0.45642

Beta occ. eigenvalues -- -0.45459 -0.45370 -0.45188 -0.44539 -0.44279

Beta occ. eigenvalues -- -0.43378 -0.43034 -0.43005 -0.42828 -0.42622

Beta occ. eigenvalues -- -0.42503 -0.42454 -0.42414 -0.42211 -0.42105

Beta occ. eigenvalues -- -0.41732 -0.40791 -0.39634 -0.39626 -0.39505

Beta occ. eigenvalues -- -0.38819 -0.38394 -0.38059 -0.37892 -0.37572

Beta occ. eigenvalues -- -0.37141 -0.36943 -0.36543 -0.36222 -0.35555

Beta occ. eigenvalues -- -0.35166 -0.34973 -0.34888 -0.34842 -0.34796

Beta occ. eigenvalues -- -0.34721 -0.34460 -0.31646 -0.29142 -0.28084

Beta occ. eigenvalues -- -0.27927 -0.27668 -0.27060 -0.26993 -0.26603

Beta occ. eigenvalues -- -0.26169 -0.26116 -0.25993 -0.25972 -0.25424

Beta occ. eigenvalues -- -0.25281 -0.24542 -0.23369 -0.23164 -0.20589

Beta virt. eigenvalues -- -0.15373 -0.09054 -0.08381 -0.03819 -0.01623

Beta virt. eigenvalues -- -0.01586 -0.01494 -0.01310 -0.01128 -0.01117

Beta virt. eigenvalues -- -0.01004 -0.00876 0.03142 0.05298 0.05527

Beta virt. eigenvalues -- 0.05570 0.05627 0.05663 0.05909 0.07232

Beta virt. eigenvalues -- 0.07466 0.08184 0.08214 0.08422 0.09254

Beta virt. eigenvalues -- 0.09486 0.09500 0.09902 0.09990 0.10401

Beta virt. eigenvalues -- 0.10450 0.10500 0.10680 0.10828 0.11466

Beta virt. eigenvalues -- 0.11869 0.12197 0.12666 0.12742 0.12855

Beta virt. eigenvalues -- 0.12885 0.13150 0.13184 0.13240 0.13675

Beta virt. eigenvalues -- 0.14137 0.14275 0.14307 0.14452 0.15238

Beta virt. eigenvalues -- 0.15676 0.16323 0.16737 0.16811 0.17522

Beta virt. eigenvalues -- 0.19302 0.21082 0.21212 0.22308 0.22745

Beta virt. eigenvalues -- 0.23433 0.23589 0.23986 0.24265 0.24689

Beta virt. eigenvalues -- 0.25240 0.25532 0.26084 0.26262 0.26431

Beta virt. eigenvalues -- 0.26916 0.27747 0.27756 0.27811 0.27853

Beta virt. eigenvalues -- 0.27952 0.28051 0.28811 0.28848 0.29484

Beta virt. eigenvalues -- 0.29501 0.29551 0.29616 0.29817 0.30590

Beta virt. eigenvalues -- 0.30860 0.31018 0.31073 0.31547 0.31640

Beta virt. eigenvalues -- 0.33300 0.33923 0.34350 0.35006 0.35324

Beta virt. eigenvalues -- 0.35410 0.35703 0.36063 0.36266 0.36280

Beta virt. eigenvalues -- 0.36702 0.36956 0.37315 0.37401 0.37488

Beta virt. eigenvalues -- 0.37657 0.37933 0.38398 0.38452 0.38662

Beta virt. eigenvalues -- 0.38970 0.39453 0.39598 0.40111 0.40293

Beta virt. eigenvalues -- 0.40413 0.40466 0.40654 0.40766 0.41068

Beta virt. eigenvalues -- 0.41250 0.41350 0.41590 0.41808 0.41831

Beta virt. eigenvalues -- 0.41866 0.41886 0.42639 0.42752 0.42784

Beta virt. eigenvalues -- 0.42892 0.43337 0.43513 0.43616 0.43796

Beta virt. eigenvalues -- 0.44313 0.44599 0.44765 0.44853 0.44896

Beta virt. eigenvalues -- 0.44990 0.45133 0.45503 0.45638 0.45668

Beta virt. eigenvalues -- 0.45833 0.46085 0.46786 0.46970 0.47128

Beta virt. eigenvalues -- 0.47168 0.47491 0.47892 0.47893 0.48411

Beta virt. eigenvalues -- 0.48931 0.49492 0.49574 0.49731 0.50575

Beta virt. eigenvalues -- 0.50641 0.50764 0.51692 0.51923 0.52651

Beta virt. eigenvalues -- 0.52759 0.52968 0.53225 0.53785 0.54081

Beta virt. eigenvalues -- 0.54178 0.54197 0.54796 0.55412 0.56009

Beta virt. eigenvalues -- 0.57492 0.57558 0.57767 0.57810 0.58029

Beta virt. eigenvalues -- 0.58228 0.58486 0.59249 0.59545 0.59587

Beta virt. eigenvalues -- 0.59992 0.60021 0.60111 0.60279 0.60684

Beta virt. eigenvalues -- 0.60782 0.60832 0.60863 0.61056 0.61135

Beta virt. eigenvalues -- 0.61380 0.61436 0.61840 0.61893 0.62302

Beta virt. eigenvalues -- 0.62418 0.62658 0.62911 0.63383 0.63833

Beta virt. eigenvalues -- 0.63982 0.64419 0.64515 0.64959 0.65044

Beta virt. eigenvalues -- 0.65148 0.65365 0.65425 0.65569 0.65906

Beta virt. eigenvalues -- 0.66145 0.66448 0.67352 0.67983 0.68435

Beta virt. eigenvalues -- 0.68757 0.69015 0.69318 0.69828 0.70178

Beta virt. eigenvalues -- 0.70318 0.70956 0.71919 0.71927 0.72375

Beta virt. eigenvalues -- 0.72496 0.72999 0.73153 0.73571 0.73827

Beta virt. eigenvalues -- 0.74024 0.74101 0.74241 0.75118 0.75130

Beta virt. eigenvalues -- 0.75204 0.75883 0.76143 0.76218 0.76617

Beta virt. eigenvalues -- 0.77045 0.77405 0.78157 0.78304 0.78624

Beta virt. eigenvalues -- 0.78710 0.78914 0.78995 0.79460 0.79922

Beta virt. eigenvalues -- 0.80342 0.80384 0.80791 0.81425 0.81586

Beta virt. eigenvalues -- 0.81738 0.82019 0.83416 0.83506 0.83509

Beta virt. eigenvalues -- 0.84695 0.85084 0.85187 0.85693 0.87076

Beta virt. eigenvalues -- 0.87253 0.87343 0.87948 0.88482 0.88541

Beta virt. eigenvalues -- 0.88865 0.89030 0.89048 0.90994 0.91049

Beta virt. eigenvalues -- 0.91953 0.92120 0.92149 0.92995 0.93434

Beta virt. eigenvalues -- 0.93733 0.93919 0.95255 0.95464 0.95572

Beta virt. eigenvalues -- 0.96072 0.96254 0.97423 0.97714 0.98937

Beta virt. eigenvalues -- 0.99348 1.00007 1.00659 1.01182 1.01603

Beta virt. eigenvalues -- 1.01656 1.01972 1.02300 1.02877 1.02986

Beta virt. eigenvalues -- 1.03326 1.04533 1.04909 1.06107 1.07093

Beta virt. eigenvalues -- 1.07739 1.08839 1.08931 1.09058 1.09293

Beta virt. eigenvalues -- 1.10379 1.11354 1.12178 1.13345 1.13514

Beta virt. eigenvalues -- 1.13801 1.13865 1.14124 1.14223 1.14975

Beta virt. eigenvalues -- 1.15664 1.15948 1.16190 1.16419 1.16680

Beta virt. eigenvalues -- 1.16820 1.18559 1.18606 1.18916 1.19236

Beta virt. eigenvalues -- 1.20088 1.20215 1.20503 1.20630 1.20958

Beta virt. eigenvalues -- 1.21247 1.21455 1.22027 1.22954 1.23085

Beta virt. eigenvalues -- 1.23264 1.24211 1.25048 1.25164 1.25289

Beta virt. eigenvalues -- 1.25813 1.25861 1.26477 1.27057 1.27204

Beta virt. eigenvalues -- 1.27691 1.28521 1.29583 1.29713 1.30242

Beta virt. eigenvalues -- 1.31132 1.32134 1.32297 1.32314 1.33389

Beta virt. eigenvalues -- 1.34100 1.35530 1.37027 1.38200 1.39614

Beta virt. eigenvalues -- 1.39970 1.40297 1.41397 1.41631 1.41956

Beta virt. eigenvalues -- 1.41976 1.43760 1.44977 1.45128 1.45580

Beta virt. eigenvalues -- 1.46713 1.46954 1.47366 1.47573 1.47683

Beta virt. eigenvalues -- 1.47703 1.47956 1.48108 1.48621 1.49130

Beta virt. eigenvalues -- 1.49299 1.49497 1.51550 1.52747 1.52857

Beta virt. eigenvalues -- 1.53102 1.53216 1.53627 1.53863 1.54141

Beta virt. eigenvalues -- 1.55172 1.57302 1.57638 1.58610 1.61396

Beta virt. eigenvalues -- 1.61589 1.61819 1.62183 1.63154 1.64048

Beta virt. eigenvalues -- 1.64657 1.64838 1.67305 1.67506 1.67556

Beta virt. eigenvalues -- 1.68123 1.68284 1.69056 1.69714 1.70157

Beta virt. eigenvalues -- 1.70368 1.71115 1.71355 1.73781 1.73885

Beta virt. eigenvalues -- 1.74011 1.74673 1.74886 1.74918 1.75347

Beta virt. eigenvalues -- 1.75867 1.75950 1.76985 1.77581 1.78657

Beta virt. eigenvalues -- 1.78695 1.79251 1.79650 1.80076 1.80417

Beta virt. eigenvalues -- 1.80516 1.81086 1.81496 1.81693 1.81814

Beta virt. eigenvalues -- 1.82614 1.82679 1.83592 1.84144 1.84265

Beta virt. eigenvalues -- 1.85163 1.85361 1.85452 1.87305 1.87429

Beta virt. eigenvalues -- 1.87931 1.88069 1.88732 1.88781 1.89927

Beta virt. eigenvalues -- 1.90097 1.91076 1.91452 1.91674 1.91887

Beta virt. eigenvalues -- 1.92121 1.92198 1.92355 1.92537 1.92998

Beta virt. eigenvalues -- 1.93178 1.93426 1.93568 1.93626 1.94005

Beta virt. eigenvalues -- 1.94491 1.94511 1.94576 1.95833 1.96030

Beta virt. eigenvalues -- 1.96273 1.96343 1.96401 1.97324 1.97593

Beta virt. eigenvalues -- 1.97680 1.99387 1.99543 2.00572 2.00885

Beta virt. eigenvalues -- 2.01619 2.01967 2.06158 2.06653 2.06894

Beta virt. eigenvalues -- 2.08439 2.08861 2.09086 2.10182 2.10508

Beta virt. eigenvalues -- 2.13140 2.13725 2.13861 2.17068 2.17963

Beta virt. eigenvalues -- 2.21777 2.23104 2.23741 2.24026 2.24434

Beta virt. eigenvalues -- 2.24821 2.25418 2.25574 2.26041 2.26267

Beta virt. eigenvalues -- 2.26311 2.26921 2.27198 2.27280 2.27367

Beta virt. eigenvalues -- 2.27558 2.27641 2.27750 2.28244 2.29023

Beta virt. eigenvalues -- 2.29326 2.29717 2.29793 2.30411 2.31097

Beta virt. eigenvalues -- 2.31409 2.32225 2.32702 2.32770 2.33027

Beta virt. eigenvalues -- 2.34650 2.34786 2.34846 2.35677 2.36434

Beta virt. eigenvalues -- 2.36551 2.36609 2.37157 2.38632 2.38950

Beta virt. eigenvalues -- 2.39080 2.39814 2.39968 2.41068 2.43355

Beta virt. eigenvalues -- 2.43384 2.44697 2.44849 2.47307 2.47744

Beta virt. eigenvalues -- 2.48364 2.50861 2.51511 2.52310 2.52611

Beta virt. eigenvalues -- 2.52849 2.54085 2.55756 2.56792 2.57013

Beta virt. eigenvalues -- 2.57869 2.58114 2.58424 2.59150 2.59584

Beta virt. eigenvalues -- 2.59815 2.61298 2.61844 2.62425 2.63135

Beta virt. eigenvalues -- 2.63948 2.64534 2.65424 2.65593 2.65909

Beta virt. eigenvalues -- 2.67341 2.67420 2.69709 2.70078 2.70201

Beta virt. eigenvalues -- 2.70515 2.70942 2.72307 2.72445 2.73007

Beta virt. eigenvalues -- 2.73882 2.73988 2.74939 2.75090 2.76822

Beta virt. eigenvalues -- 2.76882 2.77208 2.78067 2.78569 2.78718

Beta virt. eigenvalues -- 2.78736 2.79505 2.82533 2.82950 2.83210

Beta virt. eigenvalues -- 2.83363 2.84226 2.85540 2.85918 2.86187

Beta virt. eigenvalues -- 2.87030 2.89093 2.89573 2.90129 2.90488

Beta virt. eigenvalues -- 2.91993 2.94481 2.95127 2.95442 2.97517

Beta virt. eigenvalues -- 2.98364 2.98506 2.98996 3.00354 3.02262

Beta virt. eigenvalues -- 3.02860 3.03503 3.03844 3.04673 3.05387

Beta virt. eigenvalues -- 3.05483 3.07267 3.07673 3.08004 3.08086

Beta virt. eigenvalues -- 3.08170 3.09889 3.10529 3.12116 3.12199

Beta virt. eigenvalues -- 3.13988 3.15103 3.15543 3.16347 3.16624

Beta virt. eigenvalues -- 3.17770 3.19179 3.19592 3.21982 3.23923

Beta virt. eigenvalues -- 3.23927 3.24883 3.25820 3.26072 3.26282

Beta virt. eigenvalues -- 3.27144 3.27368 3.29304 3.29315 3.29657

Beta virt. eigenvalues -- 3.30030 3.30290 3.30393 3.30609 3.30669

Beta virt. eigenvalues -- 3.31246 3.31384 3.31440 3.31782 3.31791

Beta virt. eigenvalues -- 3.33042 3.33095 3.33257 3.34216 3.35184

Beta virt. eigenvalues -- 3.35550 3.36146 3.36858 3.37611 3.38859

Beta virt. eigenvalues -- 3.39910 3.41529 3.43005 3.43218 3.45052

Beta virt. eigenvalues -- 3.45368 3.48818 3.50659 3.50905 3.51608

Beta virt. eigenvalues -- 3.56422 3.56987 3.57878 3.58229 3.58301

Beta virt. eigenvalues -- 3.60106 3.61095 3.62173 3.63325 3.64776

Beta virt. eigenvalues -- 3.64993 3.66422 3.71420 3.71726 3.72018

Beta virt. eigenvalues -- 3.74336 3.76023 3.77359 3.80702 3.81192

Beta virt. eigenvalues -- 3.83173 3.84212 3.88355 3.90530 3.91222

Beta virt. eigenvalues -- 3.93150 3.93373 3.93998 3.95560 3.95681

Beta virt. eigenvalues -- 3.96209 3.96443 3.98318 3.99049 4.03090

Beta virt. eigenvalues -- 4.10633 4.29214 4.30115 4.36618 4.40370

Beta virt. eigenvalues -- 4.47705 4.51620 4.54768 4.55434 4.63203

Beta virt. eigenvalues -- 4.63288 4.67046 4.68192 4.78422 4.78434

Beta virt. eigenvalues -- 4.78510 4.78522 5.08939 5.14957 5.16698

Beta virt. eigenvalues -- 5.26647 23.24489 23.28064 23.28238 23.29942

Beta virt. eigenvalues -- 23.45868 23.52160 23.54225 23.59639 23.74207

Beta virt. eigenvalues -- 23.76939 23.77440 23.80226 23.80471 23.80537

Beta virt. eigenvalues -- 23.80585 23.80837 23.85229 23.85875 23.86102

Beta virt. eigenvalues -- 23.86634 23.90544 23.91458 23.94950 23.96067

Beta virt. eigenvalues -- 23.98144 23.98198 23.99897 24.00213 24.04779

Beta virt. eigenvalues -- 24.04883 24.04990 24.05116 24.06812 24.07042

Beta virt. eigenvalues -- 24.08329 24.08447 24.12341 24.12531 24.12885

Beta virt. eigenvalues -- 24.13360 24.15191 24.15234 24.15277 24.15343

Beta virt. eigenvalues -- 35.55458 35.56353 35.62875 35.63406

Condensed to atoms (all electrons):

Atomic-Atomic Spin Densities.

Mulliken charges and spin densities:

1 2

1 C -0.260235 0.048633

2 C 0.337555 -0.068930

3 N -0.695610 0.130960

4 C 0.328202 0.010409

5 C -0.253950 -0.021073

6 C -0.050350 0.235651

7 C 0.167837 0.047707

8 N -0.473991 0.103969

9 C 0.173943 0.008495

10 C -0.286690 0.067415

11 C -0.277286 0.033872

12 C -0.064033 0.356724

13 C 0.177270 0.007700

14 C -0.285410 0.067970

15 C -0.278599 0.033185

16 C 0.164437 0.048133

17 N -0.474045 0.103977

18 C -0.044067 0.236036

19 C 0.325474 0.010192

20 C -0.254026 -0.021013

21 C -0.260283 0.048554

22 C 0.334956 -0.068982

23 N -0.693644 0.130814

24 C -0.057976 0.357555

25 C -0.100289 -0.026459

26 C -0.214577 0.026734

27 C -0.215659 -0.009888

28 C -0.213852 0.024397

29 C -0.217369 -0.009557

30 C -0.203960 0.023224

31 C -0.215997 0.034512

32 C -0.215947 -0.015695

33 C -0.216515 0.036802

34 C -0.099395 -0.039614

35 C -0.205399 0.032664

36 C -0.217597 -0.014323

37 C -0.098394 -0.040317

38 C -0.205417 0.033700

39 C -0.217714 -0.014903

40 C -0.215803 0.035807

41 C -0.215976 -0.016287

42 C -0.216838 0.037889

43 C -0.099372 -0.026911

44 C -0.203928 0.023953

45 C -0.217476 -0.009963

46 C -0.213586 0.025293

47 C -0.215676 -0.010296

48 C -0.214848 0.027493

49 H 0.255512 -0.001895

50 H 0.256590 0.001321

51 H 0.225817 -0.003832

52 H 0.226928 -0.002348

53 H 0.225922 -0.003855

54 H 0.226816 -0.002317

55 H 0.256569 0.001307

56 H 0.255506 -0.001904

57 H 0.234634 -0.001639

58 H 0.229089 0.000645

59 H 0.229257 -0.001285

60 H 0.228960 0.000831

61 H 0.231786 -0.001239

62 H 0.228366 -0.001848

63 H 0.228294 0.001068

64 H 0.233162 -0.002035

65 H 0.230336 -0.001630

66 H 0.228191 0.001171

67 H 0.230730 -0.001692

68 H 0.228254 0.001194

69 H 0.228447 -0.001916

70 H 0.228359 0.001090

71 H 0.233303 -0.002090

72 H 0.232214 -0.001289

73 H 0.229039 0.000847

74 H 0.229364 -0.001331

75 H 0.229170 0.000660

76 H 0.234798 -0.001679

77 H 0.417917 -0.005419

78 H 0.418772 -0.005096

Sum of Mulliken charges = -0.00000 2.00000

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

1 2

1 C -0.004722 0.046738

2 C 0.337555 -0.068930

3 N -0.277693 0.125541

4 C 0.328202 0.010409

5 C 0.002640 -0.019752

6 C -0.050350 0.235651

7 C 0.167837 0.047707

8 N -0.473991 0.103969

9 C 0.173943 0.008495

10 C -0.060873 0.063583

11 C -0.050358 0.031524

12 C -0.064033 0.356724

13 C 0.177270 0.007700

14 C -0.059487 0.064116

15 C -0.051783 0.030868

16 C 0.164437 0.048133

17 N -0.474045 0.103977

18 C -0.044067 0.236036

19 C 0.325474 0.010192

20 C 0.002543 -0.019706

21 C -0.004777 0.046651

22 C 0.334956 -0.068982

23 N -0.274872 0.125718

24 C -0.057976 0.357555

25 C -0.100289 -0.026459

26 C 0.020057 0.025095

27 C 0.013430 -0.009243

28 C 0.015405 0.023111

29 C 0.011591 -0.008726

30 C 0.027827 0.021985

31 C 0.012369 0.032664

32 C 0.012347 -0.014626

33 C 0.016647 0.034767

34 C -0.099395 -0.039614

35 C 0.024938 0.031034

36 C 0.010593 -0.013152

37 C -0.098394 -0.040317

38 C 0.025313 0.032008

39 C 0.010540 -0.013709

40 C 0.012644 0.033891

41 C 0.012383 -0.015198

42 C 0.016466 0.035799

43 C -0.099372 -0.026911

44 C 0.028285 0.022664

45 C 0.011563 -0.009116

46 C 0.015778 0.023962

47 C 0.013494 -0.009636

48 C 0.019950 0.025813

APT charges:

1

1 C 0.010889

2 C -0.145828

3 N -0.628112

4 C -0.509915

5 C 0.380618

6 C 1.750375

7 C -1.616657

8 N 0.239237

9 C -1.334789

10 C 0.058296

11 C 0.428960

12 C 1.132727

13 C -1.355190

14 C 0.059515

15 C 0.435799

16 C -1.628656

17 N 0.246877

18 C 1.772462

19 C -0.511465

20 C 0.392893

21 C 0.002195

22 C -0.119832

23 N -0.642030

24 C 1.117533

25 C -0.079856

26 C -0.039941

27 C -0.131079

28 C -0.037472

29 C -0.123259

30 C -0.034136

31 C -0.066695

32 C -0.107844

33 C -0.079811

34 C -0.000708

35 C -0.051132

36 C -0.111659

37 C -0.003352

38 C -0.050302

39 C -0.112521

40 C -0.068121

41 C -0.108942

42 C -0.079306

43 C -0.085419

44 C -0.032032

45 C -0.124959

46 C -0.036944

47 C -0.133215

48 C -0.038213

49 H 0.110410

50 H 0.114068

51 H 0.063102

52 H 0.069163

53 H 0.063112

54 H 0.068968

55 H 0.113750

56 H 0.110200

57 H 0.067190

58 H 0.029137

59 H 0.032629

60 H 0.028048

61 H 0.060638

62 H 0.031269

63 H 0.026276

64 H 0.067209

65 H 0.058006

66 H 0.023057

67 H 0.058444

68 H 0.022712

69 H 0.030921

70 H 0.026007

71 H 0.068142

72 H 0.060736

73 H 0.027847

74 H 0.032253

75 H 0.028996

76 H 0.067992

77 H 0.320516

78 H 0.320217

Sum of APT charges = 0.00000

APT charges with hydrogens summed into heavy atoms:

1

1 C 0.121299

2 C -0.145828

3 N -0.307596

4 C -0.509915

5 C 0.494686

6 C 1.750375

7 C -1.616657

8 N 0.239237

9 C -1.334789

10 C 0.121398

11 C 0.498123

12 C 1.132727

13 C -1.355190

14 C 0.122627

15 C 0.504767

16 C -1.628656

17 N 0.246877

18 C 1.772462

19 C -0.511465

20 C 0.506643

21 C 0.112395

22 C -0.119832

23 N -0.321812

24 C 1.117533

25 C -0.079856

26 C 0.027250

27 C -0.101942

28 C -0.004844

29 C -0.095211

30 C 0.026501

31 C -0.035426

32 C -0.081568

33 C -0.012601

34 C -0.000708

35 C 0.006875

36 C -0.088601

37 C -0.003352

38 C 0.008142

39 C -0.089809

40 C -0.037200

41 C -0.082935

42 C -0.011164

43 C -0.085419

44 C 0.028704

45 C -0.097113

46 C -0.004691

47 C -0.104219

48 C 0.029778

Electronic spatial extent (au): <R\*\*2>= 33165.8156

Charge= -0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0055 Y= 0.0597 Z= 0.2305 Tot= 0.2382

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

XX= -233.2372 YY= -198.9618 ZZ= -274.9028

XY= 2.9257 XZ= 0.0023 YZ= 0.1101

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

XX= 2.4634 YY= 36.7388 ZZ= -39.2022

XY= 2.9257 XZ= 0.0023 YZ= 0.1101

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

XXX= 0.1730 YYY= 2.4482 ZZZ= 4.9696 XYY= 0.1690

XXY= 0.4610 XXZ= 115.7953 XZZ= 0.0083 YZZ= -0.1603

YYZ= -89.3419 XYZ= -0.4168

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

XXXX= -21044.3031 YYYY= -19930.3406 ZZZZ= -1001.3928 XXXY= 80.4041

XXXZ= 0.1170 YYYX= 62.8395 YYYZ= 5.5643 ZZZX= 0.0113

ZZZY= 0.9020 XXYY= -5480.8337 XXZZ= -3931.4551 YYZZ= -3874.7865

XXYZ= 3.8800 YYXZ= 0.0375 ZZXY= 4.4040

N-N= 5.359605922274D+03 E-N=-1.516892868247D+04 KE= 1.906369195093D+03

Exact polarizability:1802.561 -78.5121448.150 -0.137 -0.375 454.894

Approx polarizability:1686.551 -84.3221399.671 0.086 -0.667 532.692

Isotropic Fermi Contact Couplings

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

1 C(13) 0.00324 1.82344 0.65065 0.60824

2 C(13) -0.01790 -10.06014 -3.58971 -3.35570

3 N(14) 0.01656 2.67521 0.95458 0.89236

4 C(13) -0.00915 -5.14585 -1.83617 -1.71647

5 C(13) -0.00340 -1.91282 -0.68254 -0.63805

6 C(13) 0.01028 5.78054 2.06264 1.92818

7 C(13) -0.00636 -3.57665 -1.27624 -1.19304

8 N(14) 0.00771 1.24629 0.44471 0.41572

9 C(13) -0.01213 -6.81634 -2.43224 -2.27369

10 C(13) 0.00127 0.71559 0.25534 0.23870

11 C(13) -0.00182 -1.02505 -0.36577 -0.34192

12 C(13) 0.01989 11.17813 3.98863 3.72862

13 C(13) -0.01214 -6.82507 -2.43536 -2.27660

14 C(13) 0.00131 0.73768 0.26322 0.24606

15 C(13) -0.00186 -1.04795 -0.37393 -0.34956

16 C(13) -0.00634 -3.56401 -1.27173 -1.18883

17 N(14) 0.00770 1.24468 0.44413 0.41518

18 C(13) 0.01027 5.77391 2.06027 1.92597

19 C(13) -0.00915 -5.14059 -1.83429 -1.71472

20 C(13) -0.00339 -1.90682 -0.68040 -0.63605

21 C(13) 0.00324 1.82260 0.65035 0.60795

22 C(13) -0.01790 -10.06157 -3.59022 -3.35618

23 N(14) 0.01657 2.67613 0.95491 0.89266

24 C(13) 0.01991 11.19085 3.99317 3.73287

25 C(13) -0.00822 -4.62310 -1.64964 -1.54210

26 C(13) 0.00824 4.62975 1.65201 1.54432

27 C(13) -0.00053 -0.29551 -0.10544 -0.09857

28 C(13) 0.00157 0.87974 0.31391 0.29345

29 C(13) -0.00081 -0.45679 -0.16300 -0.15237

30 C(13) 0.00680 3.81993 1.36305 1.27419

31 C(13) 0.00220 1.23580 0.44096 0.41222

32 C(13) -0.00099 -0.55899 -0.19946 -0.18646

33 C(13) 0.01100 6.18089 2.20549 2.06172

34 C(13) -0.01244 -6.99021 -2.49428 -2.33168

35 C(13) 0.01024 5.75425 2.05326 1.91941

36 C(13) -0.00108 -0.60577 -0.21615 -0.20206

37 C(13) -0.01249 -7.02023 -2.50499 -2.34170

38 C(13) 0.01019 5.72905 2.04427 1.91101

39 C(13) -0.00117 -0.65967 -0.23539 -0.22004

40 C(13) 0.00229 1.28524 0.45861 0.42871

41 C(13) -0.00109 -0.61369 -0.21898 -0.20471

42 C(13) 0.01099 6.17521 2.20347 2.05983

43 C(13) -0.00822 -4.61899 -1.64817 -1.54073

44 C(13) 0.00676 3.80124 1.35638 1.26796

45 C(13) -0.00088 -0.49350 -0.17609 -0.16462

46 C(13) 0.00163 0.91548 0.32667 0.30537

47 C(13) -0.00060 -0.33470 -0.11943 -0.11164

48 C(13) 0.00822 4.62152 1.64907 1.54157

49 H(1) -0.00064 -1.43997 -0.51382 -0.48032

50 H(1) 0.00030 0.66973 0.23898 0.22340

51 H(1) -0.00118 -2.64679 -0.94444 -0.88287

52 H(1) -0.00074 -1.66371 -0.59365 -0.55495

53 H(1) -0.00119 -2.66109 -0.94954 -0.88764

54 H(1) -0.00073 -1.64228 -0.58600 -0.54780

55 H(1) 0.00030 0.66604 0.23766 0.22217

56 H(1) -0.00064 -1.43915 -0.51352 -0.48005

57 H(1) -0.00040 -0.89476 -0.31927 -0.29846

58 H(1) 0.00020 0.45797 0.16341 0.15276

59 H(1) -0.00034 -0.75400 -0.26905 -0.25151

60 H(1) 0.00028 0.63281 0.22580 0.21108

61 H(1) -0.00032 -0.72188 -0.25758 -0.24079

62 H(1) -0.00049 -1.09034 -0.38906 -0.36370

63 H(1) 0.00033 0.74397 0.26547 0.24816

64 H(1) -0.00056 -1.25567 -0.44805 -0.41885

65 H(1) -0.00047 -1.04310 -0.37220 -0.34794

66 H(1) 0.00038 0.84706 0.30225 0.28255

67 H(1) -0.00048 -1.07203 -0.38253 -0.35759

68 H(1) 0.00039 0.86094 0.30721 0.28718

69 H(1) -0.00051 -1.13052 -0.40340 -0.37710

70 H(1) 0.00034 0.75261 0.26855 0.25104

71 H(1) -0.00058 -1.28991 -0.46027 -0.43027

72 H(1) -0.00033 -0.74231 -0.26487 -0.24761

73 H(1) 0.00029 0.64278 0.22936 0.21441

74 H(1) -0.00035 -0.78109 -0.27871 -0.26054

75 H(1) 0.00021 0.46283 0.16515 0.15438

76 H(1) -0.00041 -0.91844 -0.32772 -0.30636

77 H(1) -0.00215 -4.79942 -1.71255 -1.60092

78 H(1) -0.00217 -4.85980 -1.73410 -1.62105

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

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

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1 Atom -0.023529 -0.015371 0.038900

2 Atom 0.039336 0.013659 -0.052995

3 Atom -0.157464 -0.139093 0.296557

4 Atom -0.006250 -0.022044 0.028294

5 Atom 0.013593 0.012159 -0.025751

6 Atom -0.139755 -0.137150 0.276905

7 Atom -0.039387 -0.035022 0.074409

8 Atom -0.092403 -0.119359 0.211762

9 Atom -0.025124 -0.014839 0.039963

10 Atom -0.023658 -0.041848 0.065506

11 Atom -0.011893 -0.024656 0.036549

12 Atom -0.207001 -0.201576 0.408577

13 Atom -0.024709 -0.014240 0.038949

14 Atom -0.024100 -0.042051 0.066151

15 Atom -0.011388 -0.024345 0.035733

16 Atom -0.039661 -0.035443 0.075104

17 Atom -0.092523 -0.119431 0.211954

18 Atom -0.140394 -0.137410 0.277804

19 Atom -0.006065 -0.021539 0.027604

20 Atom 0.013558 0.012208 -0.025766

21 Atom -0.023507 -0.014238 0.037745

22 Atom 0.039486 0.013570 -0.053056

23 Atom -0.157611 -0.132619 0.290230

24 Atom -0.208165 -0.202156 0.410321

25 Atom 0.000625 -0.000072 -0.000552

26 Atom -0.009253 0.017578 -0.008326

27 Atom -0.000354 0.003551 -0.003197

28 Atom -0.000856 -0.002446 0.003302

29 Atom 0.001768 0.000830 -0.002598

30 Atom 0.017163 -0.005569 -0.011594

31 Atom -0.001712 -0.003371 0.005082

32 Atom 0.000394 0.003745 -0.004139

33 Atom -0.011351 0.024007 -0.012656

34 Atom 0.000941 0.000930 -0.001872

35 Atom 0.023427 -0.008648 -0.014779

36 Atom 0.002283 0.001362 -0.003645

37 Atom 0.001013 0.001105 -0.002117

38 Atom 0.023663 -0.008806 -0.014857

39 Atom 0.002257 0.001536 -0.003793

40 Atom -0.001674 -0.003877 0.005551

41 Atom 0.000393 0.003898 -0.004291

42 Atom -0.011406 0.023765 -0.012359

43 Atom 0.000662 0.000031 -0.000693

44 Atom 0.017312 -0.005648 -0.011664

45 Atom 0.001763 0.000937 -0.002700

46 Atom -0.000816 -0.002803 0.003619

47 Atom -0.000349 0.003632 -0.003282

48 Atom -0.009322 0.017352 -0.008030

49 Atom -0.000178 0.002796 -0.002618

50 Atom 0.001025 0.001714 -0.002740

51 Atom 0.005810 -0.002996 -0.002813

52 Atom 0.005038 -0.002284 -0.002753

53 Atom 0.005798 -0.002980 -0.002818

54 Atom 0.005035 -0.002289 -0.002747

55 Atom 0.001036 0.001706 -0.002741

56 Atom -0.000164 0.002780 -0.002616

57 Atom -0.000454 0.001856 -0.001402

58 Atom -0.000017 0.000597 -0.000580

59 Atom 0.000849 0.000741 -0.001589

60 Atom 0.000530 0.000145 -0.000676

61 Atom 0.000733 0.000016 -0.000750

62 Atom 0.001080 0.000979 -0.002059

63 Atom 0.000090 0.000613 -0.000703

64 Atom -0.000677 0.001908 -0.001231

65 Atom 0.000840 -0.000130 -0.000710

66 Atom 0.000544 0.000209 -0.000752

67 Atom 0.000789 -0.000062 -0.000727

68 Atom 0.000536 0.000228 -0.000764

69 Atom 0.001108 0.000990 -0.002098

70 Atom 0.000103 0.000606 -0.000709

71 Atom -0.000640 0.001905 -0.001265

72 Atom 0.000698 0.000064 -0.000762

73 Atom 0.000525 0.000157 -0.000682

74 Atom 0.000869 0.000746 -0.001616

75 Atom -0.000006 0.000592 -0.000586

76 Atom -0.000417 0.001856 -0.001439

77 Atom -0.006245 0.015388 -0.009142

78 Atom -0.006262 0.015117 -0.008855

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XY XZ YZ

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1 Atom 0.001180 -0.000490 0.020302

2 Atom 0.001522 -0.004316 -0.015497

3 Atom -0.000948 -0.003433 0.118806

4 Atom -0.000789 0.002135 0.010185

5 Atom -0.001752 0.000126 -0.007556

6 Atom -0.004514 -0.030498 0.045568

7 Atom -0.001302 -0.026923 0.004396

8 Atom -0.002623 -0.113575 0.005652

9 Atom 0.001268 -0.015325 -0.003005

10 Atom 0.000590 -0.039312 -0.000163

11 Atom -0.000082 -0.024544 0.000220

12 Atom 0.004328 0.045503 0.068019

13 Atom 0.001359 0.014880 0.003342

14 Atom 0.000757 0.039191 0.000726

15 Atom -0.000011 0.024569 0.000024

16 Atom -0.001090 0.027182 -0.003536

17 Atom -0.001186 0.113375 -0.001956

18 Atom -0.004017 0.026458 -0.044808

19 Atom -0.000766 -0.002249 -0.010986

20 Atom -0.001845 0.000146 0.007658

21 Atom 0.001306 0.000148 -0.021771

22 Atom 0.001667 0.003610 0.015857

23 Atom -0.001016 0.003367 -0.130368

24 Atom 0.003685 -0.040062 -0.067271

25 Atom 0.009848 -0.007278 0.006675

26 Atom -0.009444 0.007478 -0.012321

27 Atom 0.006046 -0.005306 0.003920

28 Atom -0.009273 0.014403 -0.013372

29 Atom 0.006015 -0.004851 0.004082

30 Atom -0.012943 0.006911 -0.006045

31 Atom 0.013325 -0.020168 -0.019103

32 Atom -0.008844 0.007891 0.006853

33 Atom 0.016657 -0.011021 -0.016347

34 Atom -0.013218 0.010973 0.010904

35 Atom 0.017614 -0.010959 -0.008935

36 Atom -0.008472 0.007173 0.006304

37 Atom -0.013432 -0.011293 -0.011202

38 Atom 0.018226 0.011726 0.009352

39 Atom -0.008636 -0.007488 -0.006513

40 Atom 0.013741 0.021080 0.019684

41 Atom -0.008995 -0.008256 -0.007006

42 Atom 0.017229 0.011689 0.017388

43 Atom 0.009998 0.007491 -0.006867

44 Atom -0.013382 -0.007441 0.006338

45 Atom 0.006130 0.005065 -0.004239

46 Atom -0.009561 -0.015038 0.013767

47 Atom 0.006144 0.005551 -0.004018

48 Atom -0.009809 -0.007913 0.013056

49 Atom -0.002017 0.000623 -0.001461

50 Atom -0.001378 0.000387 -0.000997

51 Atom -0.004738 0.002811 -0.001662

52 Atom 0.003432 0.002503 0.001298

53 Atom -0.004782 -0.002782 0.001675

54 Atom 0.003376 -0.002517 -0.001287

55 Atom -0.001376 -0.000389 0.001012

56 Atom -0.001990 -0.000672 0.001483

57 Atom 0.000385 -0.000702 0.003215

58 Atom 0.000999 -0.000121 0.000408

59 Atom 0.002001 0.000358 -0.000662

60 Atom 0.001116 -0.000542 -0.000120

61 Atom 0.000911 -0.002901 0.000068

62 Atom -0.002591 -0.000572 -0.000898

63 Atom -0.001230 0.000216 0.000391

64 Atom 0.000078 0.001270 0.003582

65 Atom -0.000546 0.003539 0.000572

66 Atom -0.001321 0.000574 -0.000034

67 Atom -0.000523 -0.003519 -0.000620

68 Atom -0.001333 -0.000576 0.000027

69 Atom -0.002662 0.000572 0.000957

70 Atom -0.001238 -0.000242 -0.000374

71 Atom 0.000125 -0.001320 -0.003550

72 Atom 0.000902 0.002889 -0.000105

73 Atom 0.001122 0.000544 0.000115

74 Atom 0.002049 -0.000357 0.000704

75 Atom 0.001003 0.000140 -0.000396

76 Atom 0.000357 0.000736 -0.003187

77 Atom -0.000280 -0.000047 -0.005210

78 Atom -0.000282 0.000048 0.005650

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Anisotropic Spin Dipole Couplings in Principal Axis System

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

Baa -0.0243 -3.258 -1.163 -1.087 0.8610 -0.4822 0.1616

1 C(13) Bbb -0.0214 -2.868 -1.023 -0.957 0.5086 0.8172 -0.2711

Bcc 0.0457 6.126 2.186 2.044 -0.0013 0.3157 0.9489

Baa -0.0566 -7.592 -2.709 -2.533 0.0405 0.2144 0.9759

2 C(13) Bbb 0.0168 2.258 0.806 0.753 -0.1059 0.9721 -0.2092

Bcc 0.0398 5.334 1.903 1.779 0.9936 0.0948 -0.0621

Baa -0.1694 -6.533 -2.331 -2.179 0.0059 0.9690 -0.2470

3 N(14) Bbb -0.1575 -6.074 -2.167 -2.026 1.0000 -0.0039 0.0086

Bcc 0.3269 12.607 4.498 4.205 -0.0074 0.2471 0.9690

Baa -0.0241 -3.235 -1.154 -1.079 0.0663 0.9790 -0.1930

4 C(13) Bbb -0.0063 -0.842 -0.300 -0.281 0.9964 -0.0753 -0.0394

Bcc 0.0304 4.077 1.455 1.360 0.0531 0.1897 0.9804

Baa -0.0272 -3.650 -1.303 -1.218 0.0051 0.1887 0.9820

5 C(13) Bbb 0.0119 1.591 0.568 0.531 0.7087 0.6922 -0.1367

Bcc 0.0153 2.059 0.735 0.687 0.7055 -0.6966 0.1302

Baa -0.1432 -19.221 -6.859 -6.411 0.6885 0.7247 -0.0286

6 C(13) Bbb -0.1409 -18.902 -6.745 -6.305 0.7216 -0.6806 0.1269

Bcc 0.2841 38.123 13.603 12.717 -0.0725 0.1080 0.9915

Baa -0.0454 -6.098 -2.176 -2.034 0.9755 0.0299 0.2180

7 C(13) Bbb -0.0352 -4.723 -1.685 -1.575 -0.0205 0.9988 -0.0451

Bcc 0.0806 10.821 3.861 3.609 -0.2191 0.0395 0.9749

Baa -0.1302 -5.021 -1.792 -1.675 0.9473 0.0659 0.3136

8 N(14) Bbb -0.1194 -4.606 -1.643 -1.536 -0.0572 0.9977 -0.0367

Bcc 0.2496 9.626 3.435 3.211 -0.3152 0.0168 0.9489

Baa -0.0286 -3.835 -1.368 -1.279 0.9754 -0.0427 0.2162

9 C(13) Bbb -0.0150 -2.012 -0.718 -0.671 0.0298 0.9976 0.0628

Bcc 0.0436 5.846 2.086 1.950 -0.2184 -0.0549 0.9743

Baa -0.0419 -5.625 -2.007 -1.876 -0.1355 0.9896 -0.0481

10 C(13) Bbb -0.0384 -5.159 -1.841 -1.721 0.9256 0.1437 0.3503

Bcc 0.0804 10.784 3.848 3.597 -0.3535 -0.0030 0.9354

Baa -0.0247 -3.309 -1.181 -1.104 -0.0021 1.0000 -0.0044

11 C(13) Bbb -0.0222 -2.973 -1.061 -0.992 0.9226 0.0037 0.3857

Bcc 0.0468 6.282 2.241 2.095 -0.3857 0.0033 0.9226

Baa -0.2106 -28.264 -10.085 -9.428 0.9152 0.3877 -0.1098

12 C(13) Bbb -0.2088 -28.015 -9.997 -9.345 -0.3963 0.9153 -0.0716

Bcc 0.4194 56.280 20.082 18.773 0.0728 0.1091 0.9914

Baa -0.0280 -3.763 -1.343 -1.255 0.9757 -0.0442 -0.2145

13 C(13) Bbb -0.0144 -1.937 -0.691 -0.646 0.0296 0.9971 -0.0707

Bcc 0.0425 5.700 2.034 1.901 0.2170 0.0626 0.9742

Baa -0.0421 -5.652 -2.017 -1.885 -0.1277 0.9910 0.0396

14 C(13) Bbb -0.0387 -5.191 -1.852 -1.731 0.9280 0.1335 -0.3479

Bcc 0.0808 10.843 3.869 3.617 0.3500 0.0077 0.9367

Baa -0.0243 -3.267 -1.166 -1.090 0.0071 1.0000 -0.0033

15 C(13) Bbb -0.0219 -2.934 -1.047 -0.979 0.9198 -0.0078 -0.3923

Bcc 0.0462 6.201 2.213 2.069 0.3923 0.0003 0.9198

Baa -0.0458 -6.143 -2.192 -2.049 0.9754 0.0281 -0.2185

16 C(13) Bbb -0.0356 -4.771 -1.702 -1.591 -0.0205 0.9991 0.0370

Bcc 0.0813 10.914 3.894 3.641 0.2194 -0.0316 0.9751

Baa -0.1301 -5.019 -1.791 -1.674 0.9482 0.0477 -0.3140

17 N(14) Bbb -0.1194 -4.606 -1.643 -1.536 -0.0434 0.9988 0.0207

Bcc 0.2495 9.624 3.434 3.210 0.3146 -0.0060 0.9492

Baa -0.1433 -19.232 -6.863 -6.415 0.6888 0.7242 0.0338

18 C(13) Bbb -0.1409 -18.914 -6.749 -6.309 0.7222 -0.6814 -0.1185

Bcc 0.2843 38.146 13.611 12.724 0.0628 -0.1060 0.9924

Baa -0.0240 -3.216 -1.148 -1.073 0.0682 0.9752 0.2107

19 C(13) Bbb -0.0061 -0.818 -0.292 -0.273 0.9961 -0.0785 0.0409

Bcc 0.0301 4.034 1.440 1.346 -0.0564 -0.2071 0.9767

Baa -0.0273 -3.658 -1.305 -1.220 -0.0121 -0.1910 0.9815

20 C(13) Bbb 0.0118 1.589 0.567 0.530 0.7199 0.6796 0.1412

Bcc 0.0154 2.068 0.738 0.690 -0.6940 0.7083 0.1293

Baa -0.0243 -3.258 -1.162 -1.087 0.8570 -0.4856 -0.1725

21 C(13) Bbb -0.0214 -2.869 -1.024 -0.957 0.5153 0.8046 0.2950

Bcc 0.0457 6.127 2.186 2.044 -0.0044 -0.3417 0.9398

Baa -0.0567 -7.614 -2.717 -2.540 -0.0328 -0.2191 0.9751

22 C(13) Bbb 0.0169 2.267 0.809 0.756 -0.1059 0.9709 0.2146

Bcc 0.0398 5.347 1.908 1.784 0.9938 0.0963 0.0551

Baa -0.1696 -6.540 -2.334 -2.182 0.0050 0.9621 0.2727

23 N(14) Bbb -0.1576 -6.080 -2.169 -2.028 1.0000 -0.0028 -0.0083

Bcc 0.3272 12.620 4.503 4.210 0.0073 -0.2728 0.9621

Baa -0.2110 -28.317 -10.104 -9.445 0.9194 0.3802 0.1004

24 C(13) Bbb -0.2092 -28.070 -10.016 -9.363 -0.3881 0.9186 0.0747

Bcc 0.4202 56.387 20.120 18.809 -0.0639 -0.1076 0.9921

Baa -0.0159 -2.135 -0.762 -0.712 -0.5932 0.5966 -0.5405

25 C(13) Bbb 0.0057 0.767 0.274 0.256 -0.2919 0.4662 0.8351

Bcc 0.0102 1.368 0.488 0.456 0.7502 0.6532 -0.1024

Baa -0.0164 -2.203 -0.786 -0.735 -0.6639 0.0849 0.7430

26 C(13) Bbb -0.0099 -1.325 -0.473 -0.442 0.6800 0.4820 0.5525

Bcc 0.0263 3.527 1.259 1.177 -0.3112 0.8721 -0.3777

Baa -0.0106 -1.425 -0.508 -0.475 0.6033 -0.4412 0.6644

27 C(13) Bbb 0.0027 0.358 0.128 0.119 -0.5410 0.3856 0.7474

Bcc 0.0080 1.067 0.381 0.356 0.5859 0.8103 0.0061

Baa -0.0143 -1.918 -0.685 -0.640 -0.4745 0.4691 0.7448

28 C(13) Bbb -0.0110 -1.470 -0.525 -0.490 0.6893 0.7243 -0.0170

Bcc 0.0253 3.389 1.209 1.130 0.5475 -0.5053 0.6670

Baa -0.0101 -1.350 -0.482 -0.450 0.5395 -0.5401 0.6460

29 C(13) Bbb 0.0026 0.354 0.126 0.118 -0.3442 0.5588 0.7545

Bcc 0.0074 0.996 0.355 0.332 0.7685 0.6294 -0.1156

Baa -0.0154 -2.065 -0.737 -0.689 0.0557 0.5757 0.8158

30 C(13) Bbb -0.0097 -1.308 -0.467 -0.436 0.4743 0.7037 -0.5290

Bcc 0.0251 3.373 1.204 1.125 0.8786 -0.4164 0.2338

Baa -0.0200 -2.681 -0.957 -0.894 0.4743 0.4733 0.7423

31 C(13) Bbb -0.0159 -2.132 -0.761 -0.711 -0.6952 0.7186 -0.0140

Bcc 0.0359 4.814 1.718 1.606 -0.5401 -0.5095 0.6699

Baa -0.0161 -2.157 -0.770 -0.720 -0.5757 -0.4845 0.6586

32 C(13) Bbb 0.0050 0.671 0.239 0.224 0.5263 0.3968 0.7520

Bcc 0.0111 1.486 0.530 0.496 -0.6257 0.7796 0.0266

Baa -0.0231 -3.094 -1.104 -1.032 0.6694 0.0210 0.7426

33 C(13) Bbb -0.0149 -2.004 -0.715 -0.668 0.6445 -0.5135 -0.5665

Bcc 0.0380 5.098 1.819 1.700 0.3694 0.8578 -0.3573

Baa -0.0234 -3.140 -1.120 -1.047 -0.5747 -0.5738 0.5836

34 C(13) Bbb 0.0092 1.240 0.443 0.414 0.4064 0.4188 0.8120

Bcc 0.0142 1.899 0.678 0.634 0.7103 -0.7038 0.0075

Baa -0.0212 -2.850 -1.017 -0.951 -0.0595 0.6317 0.7729

35 C(13) Bbb -0.0137 -1.842 -0.657 -0.615 -0.4826 0.6596 -0.5762

Bcc 0.0350 4.692 1.674 1.565 0.8738 0.4073 -0.2657

Baa -0.0148 -1.985 -0.708 -0.662 -0.5389 -0.5361 0.6498

36 C(13) Bbb 0.0044 0.590 0.211 0.197 0.3646 0.5470 0.7536

Bcc 0.0104 1.395 0.498 0.465 0.7594 -0.6430 0.0993

Baa -0.0240 -3.215 -1.147 -1.072 0.5730 0.5702 0.5887

37 C(13) Bbb 0.0095 1.270 0.453 0.424 -0.4128 -0.4198 0.8083

Bcc 0.0145 1.944 0.694 0.649 0.7080 -0.7062 -0.0051

Baa -0.0217 -2.916 -1.041 -0.973 0.0570 -0.6368 0.7690

38 C(13) Bbb -0.0143 -1.916 -0.684 -0.639 -0.4917 0.6524 0.5767

Bcc 0.0360 4.832 1.724 1.612 0.8689 0.4110 0.2759

Baa -0.0153 -2.050 -0.731 -0.684 0.5402 0.5305 0.6532

39 C(13) Bbb 0.0046 0.623 0.222 0.208 -0.3684 -0.5488 0.7504

Bcc 0.0106 1.427 0.509 0.476 0.7566 -0.6460 -0.1011

Baa -0.0207 -2.777 -0.991 -0.926 -0.4741 -0.4780 0.7394

40 C(13) Bbb -0.0166 -2.222 -0.793 -0.741 -0.6938 0.7199 0.0206

Bcc 0.0373 4.999 1.784 1.667 0.5421 0.5032 0.6730

Baa -0.0166 -2.223 -0.793 -0.742 0.5764 0.4798 0.6615

41 C(13) Bbb 0.0053 0.705 0.252 0.235 -0.5228 -0.4056 0.7498

Bcc 0.0113 1.518 0.542 0.506 -0.6280 0.7780 -0.0170

Baa -0.0236 -3.167 -1.130 -1.056 -0.6709 -0.0280 0.7410

42 C(13) Bbb -0.0154 -2.072 -0.739 -0.691 0.6391 -0.5286 0.5586

Bcc 0.0390 5.239 1.869 1.747 0.3761 0.8484 0.3725

Baa -0.0163 -2.183 -0.779 -0.728 -0.5917 0.5930 0.5460

43 C(13) Bbb 0.0059 0.786 0.281 0.262 0.2985 -0.4680 0.8318

Bcc 0.0104 1.397 0.498 0.466 0.7488 0.6552 0.1000

Baa -0.0157 -2.109 -0.753 -0.703 -0.0524 -0.5809 0.8123

44 C(13) Bbb -0.0101 -1.358 -0.485 -0.453 0.4836 0.6969 0.5296

Bcc 0.0258 3.467 1.237 1.156 0.8737 -0.4206 -0.2444

Baa -0.0104 -1.396 -0.498 -0.466 -0.5401 0.5349 0.6497

45 C(13) Bbb 0.0028 0.377 0.135 0.126 0.3478 -0.5611 0.7511

Bcc 0.0076 1.018 0.363 0.340 0.7663 0.6317 0.1170

Baa -0.0148 -1.984 -0.708 -0.662 0.4743 -0.4739 0.7419

46 C(13) Bbb -0.0114 -1.532 -0.547 -0.511 0.6878 0.7255 0.0237

Bcc 0.0262 3.517 1.255 1.173 -0.5495 0.4991 0.6701

Baa -0.0109 -1.469 -0.524 -0.490 -0.6032 0.4380 0.6666

47 C(13) Bbb 0.0028 0.382 0.136 0.127 0.5379 -0.3937 0.7454

Bcc 0.0081 1.087 0.388 0.363 0.5889 0.8082 0.0019

Baa -0.0168 -2.250 -0.803 -0.751 0.6659 -0.0919 0.7404

48 C(13) Bbb -0.0102 -1.366 -0.488 -0.456 0.6744 0.4985 -0.5446

Bcc 0.0269 3.616 1.290 1.206 -0.3190 0.8620 0.3939

Baa -0.0030 -1.597 -0.570 -0.533 -0.0522 0.2272 0.9724

49 H(1) Bbb -0.0012 -0.636 -0.227 -0.212 0.8988 0.4351 -0.0534

Bcc 0.0042 2.233 0.797 0.745 -0.4353 0.8712 -0.2270

Baa -0.0030 -1.577 -0.563 -0.526 -0.0255 0.2015 0.9792

50 H(1) Bbb -0.0000 -0.011 -0.004 -0.004 0.8060 0.5835 -0.0991

Bcc 0.0030 1.587 0.566 0.529 -0.5913 0.7867 -0.1773

Baa -0.0052 -2.756 -0.983 -0.919 0.3290 0.9106 0.2503

51 H(1) Bbb -0.0036 -1.929 -0.688 -0.644 -0.3434 -0.1315 0.9299

Bcc 0.0088 4.685 1.672 1.563 0.8797 -0.3919 0.2695

Baa -0.0039 -2.067 -0.737 -0.689 -0.1243 0.7748 -0.6198

52 H(1) Bbb -0.0033 -1.768 -0.631 -0.590 -0.4341 0.5193 0.7362

Bcc 0.0072 3.835 1.368 1.279 0.8923 0.3606 0.2718

Baa -0.0052 -2.769 -0.988 -0.924 0.3315 0.9089 -0.2529

53 H(1) Bbb -0.0036 -1.923 -0.686 -0.641 0.3430 0.1336 0.9298

Bcc 0.0088 4.692 1.674 1.565 0.8789 -0.3950 -0.2675

Baa -0.0039 -2.055 -0.733 -0.685 -0.1067 0.7593 0.6420

54 H(1) Bbb -0.0033 -1.762 -0.629 -0.588 0.4366 -0.5443 0.7163

Bcc 0.0072 3.817 1.362 1.273 0.8933 0.3567 -0.2734

Baa -0.0030 -1.581 -0.564 -0.527 0.0248 -0.2047 0.9785

55 H(1) Bbb -0.0000 -0.007 -0.002 -0.002 0.8050 0.5845 0.1019

Bcc 0.0030 1.587 0.566 0.530 -0.5928 0.7852 0.1793

Baa -0.0030 -1.605 -0.573 -0.535 0.0731 -0.2238 0.9719

56 H(1) Bbb -0.0012 -0.622 -0.222 -0.207 0.8974 0.4400 0.0338

Bcc 0.0042 2.227 0.794 0.743 -0.4352 0.8697 0.2330

Baa -0.0036 -1.911 -0.682 -0.637 0.2478 -0.5060 0.8262

57 H(1) Bbb -0.0003 -0.134 -0.048 -0.045 0.9688 0.1377 -0.2063

Bcc 0.0038 2.044 0.729 0.682 -0.0094 0.8515 0.5243

Baa -0.0010 -0.549 -0.196 -0.183 0.5840 -0.5160 0.6266

58 H(1) Bbb -0.0003 -0.182 -0.065 -0.061 -0.5766 0.2796 0.7677

Bcc 0.0014 0.731 0.261 0.244 0.5713 0.8097 0.1343

Baa -0.0022 -1.149 -0.410 -0.383 -0.4002 0.4584 0.7935

59 H(1) Bbb -0.0007 -0.349 -0.124 -0.116 0.5797 -0.5440 0.6066

Bcc 0.0028 1.497 0.534 0.499 0.7097 0.7028 -0.0480

Baa -0.0010 -0.555 -0.198 -0.185 0.5637 -0.4609 0.6854

60 H(1) Bbb -0.0005 -0.287 -0.102 -0.096 -0.3193 0.6437 0.6955

Bcc 0.0016 0.842 0.301 0.281 0.7618 0.6109 -0.2157

Baa -0.0031 -1.667 -0.595 -0.556 0.6185 -0.1959 0.7610

61 H(1) Bbb -0.0000 -0.006 -0.002 -0.002 -0.0507 0.9565 0.2874

Bcc 0.0031 1.673 0.597 0.558 0.7842 0.2163 -0.5816

Baa -0.0029 -1.540 -0.549 -0.514 0.4137 0.4600 0.7857

62 H(1) Bbb -0.0007 -0.397 -0.142 -0.132 -0.5727 -0.5394 0.6173

Bcc 0.0036 1.937 0.691 0.646 0.7077 -0.7053 0.0403

Baa -0.0012 -0.659 -0.235 -0.220 -0.5856 -0.5214 0.6207

63 H(1) Bbb -0.0004 -0.207 -0.074 -0.069 0.5245 0.3402 0.7805

Bcc 0.0016 0.865 0.309 0.289 -0.6181 0.7826 0.0743

Baa -0.0039 -2.082 -0.743 -0.695 -0.3077 -0.4963 0.8118

64 H(1) Bbb -0.0005 -0.248 -0.088 -0.083 0.9391 -0.2955 0.1753

Bcc 0.0044 2.330 0.831 0.777 0.1528 0.8163 0.5571

Baa -0.0037 -1.990 -0.710 -0.664 -0.6139 -0.2138 0.7599

65 H(1) Bbb 0.0000 0.022 0.008 0.007 -0.1201 0.9767 0.1778

Bcc 0.0037 1.968 0.702 0.657 0.7802 -0.0179 0.6253

Baa -0.0012 -0.666 -0.238 -0.222 -0.5797 -0.5107 0.6349

66 H(1) Bbb -0.0005 -0.289 -0.103 -0.096 0.3109 0.5816 0.7517

Bcc 0.0018 0.955 0.341 0.319 0.7532 -0.6332 0.1784

Baa -0.0037 -1.999 -0.713 -0.667 0.6140 0.2150 0.7595

67 H(1) Bbb 0.0001 0.062 0.022 0.021 -0.1312 0.9766 -0.1704

Bcc 0.0036 1.937 0.691 0.646 0.7783 -0.0050 -0.6278

Baa -0.0013 -0.674 -0.241 -0.225 0.5791 0.5055 0.6396

68 H(1) Bbb -0.0005 -0.288 -0.103 -0.096 -0.3193 -0.5813 0.7485

Bcc 0.0018 0.962 0.343 0.321 0.7501 -0.6377 -0.1752

Baa -0.0030 -1.586 -0.566 -0.529 -0.4140 -0.4667 0.7816

69 H(1) Bbb -0.0008 -0.401 -0.143 -0.134 0.5728 0.5338 0.6221

Bcc 0.0037 1.987 0.709 0.663 0.7075 -0.7052 -0.0464

Baa -0.0012 -0.665 -0.237 -0.222 0.5861 0.5174 0.6235

70 H(1) Bbb -0.0004 -0.202 -0.072 -0.067 -0.5171 -0.3535 0.7795

Bcc 0.0016 0.867 0.310 0.289 -0.6238 0.7793 -0.0604

Baa -0.0039 -2.085 -0.744 -0.695 0.3103 0.4907 0.8142

71 H(1) Bbb -0.0004 -0.235 -0.084 -0.078 0.9358 -0.3083 -0.1708

Bcc 0.0043 2.320 0.828 0.774 0.1672 0.8150 -0.5548

Baa -0.0031 -1.676 -0.598 -0.559 -0.6187 0.1990 0.7600

72 H(1) Bbb 0.0001 0.028 0.010 0.009 -0.0464 0.9564 -0.2882

Bcc 0.0031 1.649 0.588 0.550 0.7843 0.2136 0.5825

Baa -0.0011 -0.561 -0.200 -0.187 -0.5632 0.4576 0.6881

73 H(1) Bbb -0.0005 -0.285 -0.102 -0.095 0.3249 -0.6430 0.6935

Bcc 0.0016 0.846 0.302 0.282 0.7598 0.6141 0.2134

Baa -0.0022 -1.180 -0.421 -0.394 0.4007 -0.4653 0.7892

74 H(1) Bbb -0.0007 -0.351 -0.125 -0.117 -0.5794 0.5386 0.6117

Bcc 0.0029 1.531 0.546 0.511 0.7097 0.7024 0.0538

Baa -0.0010 -0.553 -0.197 -0.185 -0.5838 0.5123 0.6298

75 H(1) Bbb -0.0003 -0.176 -0.063 -0.059 0.5714 -0.2919 0.7670

Bcc 0.0014 0.730 0.260 0.243 0.5768 0.8077 -0.1223

Baa -0.0036 -1.915 -0.683 -0.639 -0.2488 0.5014 0.8287

76 H(1) Bbb -0.0002 -0.112 -0.040 -0.037 0.9684 0.1454 0.2028

Bcc 0.0038 2.026 0.723 0.676 -0.0188 0.8529 -0.5217

Baa -0.0102 -5.445 -1.943 -1.816 0.0258 0.1997 0.9795

77 H(1) Bbb -0.0062 -3.333 -1.189 -1.112 0.9996 0.0063 -0.0276

Bcc 0.0165 8.778 3.132 2.928 -0.0117 0.9798 -0.1994

Baa -0.0101 -5.401 -1.927 -1.802 -0.0282 -0.2186 0.9754

78 H(1) Bbb -0.0063 -3.341 -1.192 -1.114 0.9995 0.0052 0.0301

Bcc 0.0164 8.742 3.119 2.916 -0.0117 0.9758 0.2184

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

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Sun Aug 25 18:30:33 2019, MaxMem= 4294967296 cpu: 42.6

(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.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 186

Leave Link 701 at Sun Aug 25 18:32:02 2019, MaxMem= 4294967296 cpu: 1424.3

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

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

Leave Link 702 at Sun Aug 25 18:32:02 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

Leave Link 703 at Sun Aug 25 18:50:53 2019, MaxMem= 4294967296 cpu: 18095.5

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

Dipole = 2.15709586D-03 2.34843746D-02 9.06874693D-02

Polarizability= 1.80256053D+03-7.85121323D+01 1.44814987D+03

-1.36524673D-01-3.75228273D-01 4.54893505D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000167685 0.000077580 0.000335328

2 6 0.000430454 0.000016049 -0.000861899

3 7 0.000122945 0.000020757 0.000299086

4 6 0.000547452 -0.000434305 0.000599276

5 6 -0.000573072 0.000073548 -0.000934666

6 6 -0.001878322 0.000509471 -0.001296055

7 6 0.002575165 -0.000172204 -0.000118873

8 7 -0.001839410 0.000083925 0.000113123

9 6 0.001288836 -0.000358866 0.001345932

10 6 0.001415290 0.000401652 -0.000304067

11 6 0.000011109 -0.000198527 -0.000632456

12 6 0.000475850 -0.000150362 0.000312260

13 6 -0.001285769 -0.000335519 -0.001341817

14 6 -0.001400917 0.000399053 0.000305953

15 6 -0.000019426 -0.000207891 0.000635215

16 6 -0.002587981 -0.000158091 0.000124761

17 7 0.001841561 0.000088629 -0.000135461

18 6 0.001914687 0.000483264 0.001344483

19 6 -0.000589807 -0.000449184 -0.000711466

20 6 0.000585326 0.000092052 0.000967906

21 6 0.000162509 0.000067424 -0.000307200

22 6 -0.000398416 0.000028610 0.000757801

23 7 -0.000125212 0.000021033 -0.000240495

24 6 -0.000504315 -0.000118050 -0.000267045

25 6 -0.000055905 0.000184410 -0.000185607

26 6 0.000001744 -0.000000079 0.000090402

27 6 -0.000053519 0.000072144 0.000053891

28 6 -0.000128418 -0.000095110 0.000015901

29 6 0.000114349 0.000011825 -0.000048923

30 6 -0.000082206 0.000009594 0.000158866

31 6 0.000105817 0.000036622 0.000047280

32 6 0.000033499 -0.000051305 0.000008229

33 6 0.000027105 -0.000011188 0.000140563

34 6 0.000049107 -0.000113677 -0.000139821

35 6 0.000105270 0.000009097 0.000086912

36 6 -0.000065205 0.000023820 0.000007552

37 6 -0.000038487 -0.000123854 0.000154311

38 6 -0.000108734 0.000007087 -0.000090934

39 6 0.000067712 0.000026917 -0.000004442

40 6 -0.000111047 0.000039107 -0.000050518

41 6 -0.000031377 -0.000049815 -0.000007085

42 6 -0.000030448 -0.000006925 -0.000142135

43 6 0.000045298 0.000203417 0.000201740

44 6 0.000084306 0.000015202 -0.000164120

45 6 -0.000118808 0.000013488 0.000052656

46 6 0.000134178 -0.000091837 -0.000019151

47 6 0.000052416 0.000077913 -0.000054074

48 6 0.000002287 0.000000638 -0.000089347

49 1 0.000030538 0.000005057 -0.000006958

50 1 -0.000033435 0.000009575 -0.000023038

51 1 0.000017806 0.000023368 0.000036867

52 1 -0.000004801 -0.000002967 -0.000024240

53 1 -0.000017284 0.000023113 -0.000037443

54 1 0.000005825 -0.000000708 0.000023672

55 1 0.000029823 0.000011345 0.000021550

56 1 -0.000027909 0.000008540 0.000005939

57 1 0.000001436 0.000018404 0.000026667

58 1 -0.000016186 -0.000003104 0.000007505

59 1 0.000000487 -0.000004718 0.000012147

60 1 -0.000002764 0.000018207 0.000018422

61 1 -0.000004293 -0.000017346 0.000026634

62 1 0.000004023 -0.000004380 0.000010847

63 1 0.000020317 0.000003809 0.000011898

64 1 0.000008680 -0.000031102 0.000022842

65 1 -0.000003315 -0.000001310 0.000016047

66 1 0.000000612 -0.000016626 0.000027657

67 1 0.000002154 0.000000425 -0.000017881

68 1 -0.000001252 -0.000015050 -0.000028360

69 1 -0.000004044 -0.000000818 -0.000011354

70 1 -0.000018892 0.000006825 -0.000012031

71 1 -0.000007579 -0.000028304 -0.000022091

72 1 0.000002862 -0.000017150 -0.000028574

73 1 0.000001366 0.000020876 -0.000018609

74 1 -0.000000838 -0.000001823 -0.000012398

75 1 0.000016665 0.000000444 -0.000007203

76 1 -0.000000986 0.000021081 -0.000025260

77 1 0.000015748 0.000004424 0.000031087

78 1 -0.000014553 0.000002375 -0.000036109

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

Cartesian Forces: Max 0.002587981 RMS 0.000470096

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

Leave Link 716 at Sun Aug 25 18:50:53 2019, MaxMem= 4294967296 cpu: 2.6

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.002392854 RMS 0.000280042

Search for a local minimum.

Step number 1 out of a maximum of 452

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

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

ITU= 0

Eigenvalues --- -0.11888 0.00258 0.00345 0.00565 0.00615

Eigenvalues --- 0.00744 0.00780 0.01036 0.01059 0.01080

Eigenvalues --- 0.01094 0.01217 0.01221 0.01240 0.01305

Eigenvalues --- 0.01313 0.01368 0.01400 0.01454 0.01464

Eigenvalues --- 0.01480 0.01502 0.01514 0.01566 0.01570

Eigenvalues --- 0.01642 0.01687 0.01710 0.01724 0.01748

Eigenvalues --- 0.01752 0.01761 0.01770 0.01794 0.01853

Eigenvalues --- 0.01881 0.01946 0.01969 0.02065 0.02086

Eigenvalues --- 0.02144 0.02199 0.02254 0.02272 0.02291

Eigenvalues --- 0.02323 0.02357 0.02447 0.02461 0.02525

Eigenvalues --- 0.02553 0.02557 0.02599 0.02605 0.02610

Eigenvalues --- 0.02620 0.02628 0.02664 0.02743 0.02745

Eigenvalues --- 0.02792 0.02821 0.02868 0.02870 0.02871

Eigenvalues --- 0.02875 0.02985 0.03051 0.03490 0.03732

Eigenvalues --- 0.04187 0.04251 0.04623 0.04676 0.04685

Eigenvalues --- 0.04869 0.08015 0.09685 0.09752 0.09756

Eigenvalues --- 0.09933 0.09964 0.10474 0.10478 0.10696

Eigenvalues --- 0.10702 0.10706 0.10709 0.10713 0.10758

Eigenvalues --- 0.11403 0.11409 0.11414 0.11421 0.12010

Eigenvalues --- 0.12016 0.12017 0.12021 0.12281 0.12284

Eigenvalues --- 0.12287 0.12291 0.12778 0.12779 0.12785

Eigenvalues --- 0.12786 0.15268 0.16066 0.16455 0.16748

Eigenvalues --- 0.17132 0.17354 0.17410 0.17791 0.17990

Eigenvalues --- 0.18114 0.18159 0.18190 0.19087 0.19244

Eigenvalues --- 0.19336 0.19339 0.19350 0.19399 0.19408

Eigenvalues --- 0.19411 0.19548 0.19549 0.19550 0.19552

Eigenvalues --- 0.20536 0.20707 0.22121 0.22568 0.22947

Eigenvalues --- 0.23415 0.23559 0.24610 0.25184 0.25974

Eigenvalues --- 0.26412 0.26605 0.27534 0.27928 0.28100

Eigenvalues --- 0.28473 0.28657 0.28963 0.29258 0.30167

Eigenvalues --- 0.31130 0.31441 0.31652 0.33310 0.33493

Eigenvalues --- 0.33879 0.34618 0.34620 0.35482 0.35631

Eigenvalues --- 0.35635 0.35650 0.35661 0.35751 0.35759

Eigenvalues --- 0.35778 0.35790 0.35926 0.35929 0.35935

Eigenvalues --- 0.35938 0.35994 0.36000 0.36037 0.36054

Eigenvalues --- 0.36206 0.36252 0.36263 0.36320 0.36459

Eigenvalues --- 0.36729 0.36839 0.36994 0.37075 0.37574

Eigenvalues --- 0.37608 0.37934 0.38506 0.39243 0.39636

Eigenvalues --- 0.40165 0.40409 0.40919 0.41090 0.41121

Eigenvalues --- 0.41126 0.41160 0.41314 0.41401 0.41433

Eigenvalues --- 0.41446 0.41619 0.43526 0.43772 0.44467

Eigenvalues --- 0.45380 0.45870 0.45881 0.45940 0.45971

Eigenvalues --- 0.46178 0.46231 0.46242 0.46295 0.46402

Eigenvalues --- 0.48246 0.48430 0.48566 0.49152 0.49436

Eigenvalues --- 0.50764 0.50777 0.50792 0.50795 0.52592

Eigenvalues --- 0.53116 0.53139 0.55472

Eigenvalue 1 is -1.19D-01 should be greater than 0.000000 Eigenvector:

R30 R11 R29 R13 R15

1 -0.38165 -0.38047 0.30481 0.30453 -0.29569

R24 R17 R21 R9 R31

1 -0.29490 0.22485 0.22381 0.13040 0.12995

Angle between quadratic step and forces= 38.28 degrees.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.01526419 RMS(Int)= 0.00001633

Iteration 2 RMS(Cart)= 0.00004247 RMS(Int)= 0.00000117

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000117

ITry= 1 IFail=0 DXMaxC= 7.33D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.71533 -0.00002 0.00000 -0.00116 -0.00116 2.71417

R2 2.58226 0.00053 0.00000 0.00406 0.00406 2.58632

R3 2.03674 0.00002 0.00000 0.00005 0.00005 2.03679

R4 2.60333 -0.00020 0.00000 -0.00260 -0.00260 2.60073

R5 2.63900 0.00100 0.00000 0.00427 0.00427 2.64327

R6 2.60630 0.00015 0.00000 0.00193 0.00193 2.60823

R7 1.91107 -0.00001 0.00000 -0.00016 -0.00016 1.91091

R8 2.71232 -0.00077 0.00000 -0.00633 -0.00633 2.70599

R9 2.64418 0.00032 0.00000 0.00575 0.00575 2.64993

R10 2.03709 -0.00001 0.00000 -0.00003 -0.00003 2.03707

R11 2.69944 -0.00238 0.00000 -0.01917 -0.01917 2.68027

R12 2.80548 -0.00029 0.00000 -0.00028 -0.00028 2.80520

R13 2.60118 0.00130 0.00000 0.01363 0.01363 2.61481

R14 2.70699 -0.00022 0.00000 0.00089 0.00089 2.70789

R15 2.57968 -0.00120 0.00000 -0.01310 -0.01310 2.56658

R16 2.70815 0.00120 0.00000 0.00742 0.00742 2.71558

R17 2.71904 0.00133 0.00000 0.01050 0.01050 2.72954

R18 2.60228 -0.00058 0.00000 -0.00422 -0.00422 2.59806

R19 2.03986 -0.00003 0.00000 0.00007 0.00007 2.03993

R20 2.04000 0.00001 0.00000 -0.00019 -0.00019 2.03982

R21 2.71857 0.00132 0.00000 0.01043 0.01043 2.72899

R22 2.80179 0.00038 0.00000 0.00051 0.00051 2.80230

R23 2.70833 0.00120 0.00000 0.00741 0.00741 2.71574

R24 2.57979 -0.00119 0.00000 -0.01304 -0.01304 2.56675

R25 2.60226 -0.00058 0.00000 -0.00422 -0.00421 2.59805

R26 2.03983 -0.00003 0.00000 0.00007 0.00007 2.03990

R27 2.70684 -0.00022 0.00000 0.00090 0.00090 2.70774

R28 2.04004 0.00001 0.00000 -0.00019 -0.00019 2.03985

R29 2.60105 0.00131 0.00000 0.01368 0.01368 2.61473

R30 2.69990 -0.00239 0.00000 -0.01926 -0.01926 2.68064

R31 2.64418 0.00037 0.00000 0.00589 0.00589 2.65007

R32 2.80469 -0.00028 0.00000 -0.00022 -0.00022 2.80447

R33 2.71225 -0.00081 0.00000 -0.00644 -0.00644 2.70581

R34 2.60626 0.00013 0.00000 0.00184 0.00184 2.60810

R35 2.58231 0.00053 0.00000 0.00407 0.00408 2.58639

R36 2.03710 -0.00001 0.00000 -0.00003 -0.00003 2.03708

R37 2.71507 0.00000 0.00000 -0.00108 -0.00108 2.71399

R38 2.03675 0.00002 0.00000 0.00005 0.00005 2.03680

R39 2.60301 -0.00018 0.00000 -0.00249 -0.00249 2.60052

R40 2.63940 0.00096 0.00000 0.00415 0.00415 2.64355

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R42 2.80100 0.00037 0.00000 0.00049 0.00049 2.80149

R43 2.64969 -0.00008 0.00000 -0.00022 -0.00022 2.64947

R44 2.65112 -0.00015 0.00000 -0.00083 -0.00083 2.65030

R45 2.63103 -0.00011 0.00000 -0.00052 -0.00052 2.63050

R46 2.04846 0.00003 0.00000 -0.00002 -0.00002 2.04844

R47 2.63393 0.00007 0.00000 0.00039 0.00039 2.63432

R48 2.05004 -0.00001 0.00000 -0.00009 -0.00009 2.04995

R49 2.63650 -0.00007 0.00000 -0.00059 -0.00059 2.63591

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R55 2.63679 0.00003 0.00000 0.00024 0.00024 2.63703

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R57 2.63102 0.00010 0.00000 0.00034 0.00034 2.63136

R58 2.05009 0.00002 0.00000 0.00013 0.00013 2.05021

R59 2.65016 0.00009 0.00000 0.00044 0.00044 2.65060

R60 2.04875 -0.00004 0.00000 -0.00001 -0.00001 2.04874

R61 2.65144 0.00013 0.00000 0.00075 0.00075 2.65219

R62 2.62798 0.00005 0.00000 0.00007 0.00007 2.62805

R63 2.04822 0.00000 0.00000 0.00019 0.00019 2.04841

R64 2.05009 0.00003 0.00000 0.00016 0.00016 2.05025

R65 2.65179 0.00014 0.00000 0.00076 0.00076 2.65255

R66 2.65043 0.00010 0.00000 0.00045 0.00045 2.65088

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R68 2.04814 0.00000 0.00000 0.00020 0.00020 2.04834

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R73 2.63094 0.00010 0.00000 0.00035 0.00035 2.63129

R74 2.05007 0.00002 0.00000 0.00013 0.00013 2.05020

R75 2.04873 -0.00004 0.00000 -0.00000 -0.00000 2.04872

R76 2.65148 -0.00016 0.00000 -0.00085 -0.00085 2.65063

R77 2.64997 -0.00008 0.00000 -0.00024 -0.00024 2.64973

R78 2.62807 0.00001 0.00000 0.00031 0.00031 2.62839

R79 2.04778 0.00001 0.00000 -0.00008 -0.00008 2.04770

R80 2.63655 -0.00008 0.00000 -0.00061 -0.00061 2.63594

R81 2.05011 -0.00003 0.00000 -0.00014 -0.00014 2.04997

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A3 2.21591 -0.00002 0.00000 0.00030 0.00030 2.21621

A4 1.85699 -0.00016 0.00000 -0.00001 -0.00001 1.85699

A5 2.21915 0.00044 0.00000 0.00191 0.00192 2.22107

A6 2.20697 -0.00028 0.00000 -0.00189 -0.00189 2.20507

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A15 2.17824 -0.00001 0.00000 0.00001 0.00001 2.17826

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A23 1.93954 -0.00031 0.00000 0.00057 0.00057 1.94011

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A27 2.20584 -0.00031 0.00000 -0.00179 -0.00179 2.20405

A28 2.22330 -0.00030 0.00000 -0.00078 -0.00078 2.22252

A29 1.85744 -0.00051 0.00000 -0.00166 -0.00166 1.85578

A30 2.20348 0.00027 0.00000 0.00103 0.00103 2.20450

A31 2.22217 0.00024 0.00000 0.00063 0.00063 2.22280

A32 2.18634 -0.00017 0.00000 -0.00246 -0.00246 2.18388

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A34 2.04944 0.00006 0.00000 0.00118 0.00119 2.05063

A35 2.16809 0.00025 0.00000 -0.00063 -0.00063 2.16746

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A37 1.93946 -0.00030 0.00000 0.00059 0.00059 1.94005

A38 1.85391 0.00060 0.00000 0.00259 0.00259 1.85650

A39 2.20603 -0.00030 0.00000 -0.00178 -0.00178 2.20425

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A70 2.09830 -0.00003 0.00000 -0.00140 -0.00140 2.09690

A71 2.07332 0.00019 0.00000 0.00123 0.00123 2.07454

A72 2.10402 -0.00009 0.00000 -0.00073 -0.00073 2.10330

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A75 2.09748 -0.00003 0.00000 -0.00015 -0.00015 2.09734

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A78 2.08959 0.00006 0.00000 0.00052 0.00052 2.09011

A79 2.09694 -0.00004 0.00000 -0.00033 -0.00033 2.09662

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A91 2.09718 -0.00004 0.00000 -0.00019 -0.00019 2.09699

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A94 2.09388 -0.00006 0.00000 -0.00046 -0.00046 2.09342

A95 2.08460 -0.00005 0.00000 -0.00044 -0.00044 2.08417

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A103 2.09642 -0.00003 0.00000 -0.00016 -0.00016 2.09626

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A106 2.11091 0.00021 0.00000 0.00088 0.00088 2.11179

A107 2.07230 -0.00023 0.00000 -0.00164 -0.00164 2.07066

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A109 2.08428 -0.00004 0.00000 -0.00032 -0.00032 2.08396

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A111 2.09774 0.00004 0.00000 0.00023 0.00023 2.09797

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A113 2.09643 -0.00003 0.00000 -0.00016 -0.00016 2.09627

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D6 -3.11975 -0.00000 0.00000 0.00086 0.00086 -3.11889

D7 3.11916 0.00000 0.00000 0.00040 0.00040 3.11956

D8 -0.00034 0.00001 0.00000 0.00011 0.00011 -0.00022

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D10 3.05600 0.00001 0.00000 0.00043 0.00043 3.05643

D11 3.09522 0.00000 0.00000 0.00185 0.00184 3.09706

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D16 -3.00829 -0.00009 0.00000 0.00098 0.00098 -3.00731

D17 0.03396 -0.00001 0.00000 0.00022 0.00022 0.03418

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D21 -0.02018 0.00002 0.00000 -0.00083 -0.00083 -0.02101

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D31 2.91676 0.00016 0.00000 -0.00350 -0.00349 2.91327

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D71 -0.00056 -0.00009 0.00000 -0.00192 -0.00192 -0.00247

D72 -3.12814 -0.00003 0.00000 -0.00121 -0.00121 -3.12935

D73 3.12863 -0.00003 0.00000 -0.00040 -0.00040 3.12824

D74 0.00105 0.00003 0.00000 0.00031 0.00031 0.00136

D75 -0.02090 0.00007 0.00000 0.00160 0.00160 -0.01929

D76 3.08809 0.00007 0.00000 0.00322 0.00322 3.09131

D77 3.10689 0.00001 0.00000 0.00090 0.00090 3.10779

D78 -0.06731 0.00000 0.00000 0.00252 0.00252 -0.06479

D79 0.03385 -0.00000 0.00000 -0.00034 -0.00034 0.03350

D80 -3.07510 0.00001 0.00000 -0.00191 -0.00191 -3.07701

D81 2.94368 0.00020 0.00000 -0.00592 -0.00592 2.93776

D82 -0.19963 0.00018 0.00000 -0.00488 -0.00488 -0.20450

D83 -0.23502 0.00019 0.00000 -0.00414 -0.00414 -0.23916

D84 2.90486 0.00018 0.00000 -0.00310 -0.00310 2.90176

D85 3.00940 -0.00013 0.00000 0.00458 0.00458 3.01398

D86 -0.13851 -0.00014 0.00000 0.00324 0.00324 -0.13527

D87 -0.13048 -0.00011 0.00000 0.00354 0.00354 -0.12694

D88 3.00479 -0.00012 0.00000 0.00220 0.00220 3.00699

D89 -0.97746 -0.00007 0.00000 -0.00019 -0.00019 -0.97765

D90 2.16195 -0.00004 0.00000 0.00063 0.00063 2.16259

D91 2.16257 -0.00008 0.00000 0.00076 0.00076 2.16333

D92 -0.98121 -0.00005 0.00000 0.00159 0.00159 -0.97962

D93 3.11762 0.00002 0.00000 -0.00186 -0.00186 3.11577

D94 -0.04964 0.00000 0.00000 -0.00158 -0.00158 -0.05122

D95 -0.01866 0.00002 0.00000 -0.00074 -0.00074 -0.01939

D96 3.09727 0.00001 0.00000 -0.00046 -0.00046 3.09681

D97 -3.10509 -0.00000 0.00000 0.00132 0.00132 -3.10377

D98 0.07053 -0.00000 0.00000 0.00195 0.00195 0.07248

D99 0.03126 -0.00001 0.00000 0.00021 0.00021 0.03146

D100 -3.07630 -0.00001 0.00000 0.00084 0.00084 -3.07547

D101 -0.00009 -0.00002 0.00000 0.00101 0.00101 0.00092

D102 3.11488 0.00000 0.00000 0.00047 0.00047 3.11535

D103 -3.11532 -0.00001 0.00000 0.00072 0.00072 -3.11460

D104 -0.00036 0.00002 0.00000 0.00018 0.00018 -0.00018

D105 0.01883 0.00001 0.00000 -0.00088 -0.00088 0.01795

D106 -3.11842 0.00002 0.00000 -0.00227 -0.00227 -3.12069

D107 -3.09687 -0.00001 0.00000 -0.00035 -0.00034 -3.09721

D108 0.04908 0.00000 0.00000 -0.00174 -0.00174 0.04733

D109 -0.03131 0.00000 0.00000 0.00042 0.00042 -0.03089

D110 3.07626 0.00000 0.00000 -0.00020 -0.00020 3.07606

D111 3.10597 -0.00000 0.00000 0.00182 0.00182 3.10779

D112 -0.06964 -0.00000 0.00000 0.00120 0.00119 -0.06845

D113 -3.00917 -0.00011 0.00000 0.00322 0.00322 -3.00595

D114 0.13139 -0.00010 0.00000 0.00228 0.00228 0.13367

D115 0.13761 -0.00010 0.00000 0.00154 0.00154 0.13916

D116 -3.00502 -0.00009 0.00000 0.00061 0.00061 -3.00441

D117 0.97807 -0.00006 0.00000 -0.00176 -0.00177 0.97630

D118 -2.16288 -0.00004 0.00000 -0.00088 -0.00088 -2.16376

D119 -2.16257 -0.00007 0.00000 -0.00090 -0.00090 -2.16347

D120 0.97967 -0.00004 0.00000 -0.00001 -0.00001 0.97965

D121 -3.13710 0.00000 0.00000 -0.00156 -0.00156 -3.13866

D122 -0.01716 -0.00001 0.00000 -0.00178 -0.00178 -0.01894

D123 0.00003 0.00003 0.00000 -0.00062 -0.00062 -0.00059

D124 3.11996 0.00001 0.00000 -0.00083 -0.00083 3.11913

D125 -3.13169 0.00001 0.00000 0.00189 0.00189 -3.12979

D126 -0.01073 0.00000 0.00000 0.00155 0.00155 -0.00918

D127 0.01434 -0.00001 0.00000 0.00096 0.00096 0.01530

D128 3.13529 -0.00002 0.00000 0.00061 0.00061 3.13591

D129 -0.01105 -0.00003 0.00000 -0.00005 -0.00005 -0.01111

D130 3.12835 -0.00001 0.00000 0.00008 0.00008 3.12843

D131 -3.13088 -0.00001 0.00000 0.00016 0.00016 -3.13072

D132 0.00852 0.00000 0.00000 0.00029 0.00029 0.00881

D133 0.00778 0.00001 0.00000 0.00040 0.00040 0.00818

D134 -3.13573 0.00002 0.00000 0.00023 0.00023 -3.13550

D135 -3.13161 -0.00000 0.00000 0.00027 0.00027 -3.13134

D136 0.00806 0.00000 0.00000 0.00010 0.00010 0.00816

D137 0.00655 0.00001 0.00000 -0.00006 -0.00006 0.00649

D138 -3.13567 0.00000 0.00000 -0.00017 -0.00017 -3.13583

D139 -3.13313 0.00000 0.00000 0.00011 0.00011 -3.13302

D140 0.00785 -0.00000 0.00000 -0.00000 -0.00000 0.00784

D141 -0.01772 -0.00001 0.00000 -0.00062 -0.00062 -0.01834

D142 -3.13856 0.00001 0.00000 -0.00027 -0.00027 -3.13883

D143 3.12449 -0.00000 0.00000 -0.00051 -0.00051 3.12398

D144 0.00365 0.00001 0.00000 -0.00016 -0.00016 0.00349

D145 -0.00769 0.00001 0.00000 0.00019 0.00019 -0.00750

D146 3.13189 -0.00001 0.00000 -0.00001 -0.00001 3.13188

D147 3.13591 0.00002 0.00000 0.00018 0.00018 3.13609

D148 -0.00769 -0.00000 0.00000 -0.00002 -0.00002 -0.00772

D149 -0.00637 0.00002 0.00000 0.00002 0.00002 -0.00635

D150 3.13555 0.00001 0.00000 -0.00003 -0.00003 3.13553

D151 3.13322 0.00001 0.00000 0.00003 0.00003 3.13325

D152 -0.00805 0.00000 0.00000 -0.00002 -0.00002 -0.00806

D153 0.01030 -0.00003 0.00000 -0.00006 -0.00006 0.01024

D154 3.13125 -0.00001 0.00000 -0.00006 -0.00006 3.13119

D155 -3.12929 -0.00001 0.00000 0.00014 0.00014 -3.12915

D156 -0.00834 0.00001 0.00000 0.00014 0.00014 -0.00820

D157 3.13976 -0.00000 0.00000 -0.00113 -0.00113 3.13863

D158 0.00111 0.00002 0.00000 -0.00026 -0.00026 0.00085

D159 0.01870 -0.00002 0.00000 -0.00113 -0.00113 0.01757

D160 -3.11996 0.00000 0.00000 -0.00026 -0.00026 -3.12022

D161 3.12930 0.00003 0.00000 0.00133 0.00133 3.13063

D162 0.00795 0.00001 0.00000 0.00113 0.00113 0.00908

D163 -0.01521 0.00001 0.00000 0.00046 0.00046 -0.01475

D164 -3.13656 -0.00002 0.00000 0.00026 0.00026 -3.13630

D165 0.01795 -0.00002 0.00000 -0.00034 -0.00034 0.01761

D166 -3.12397 -0.00001 0.00000 -0.00029 -0.00029 -3.12426

D167 3.13919 -0.00000 0.00000 -0.00013 -0.00013 3.13905

D168 -0.00273 0.00001 0.00000 -0.00008 -0.00008 -0.00282

D169 3.12689 0.00003 0.00000 0.00128 0.00128 3.12817

D170 0.00654 0.00001 0.00000 0.00108 0.00108 0.00762

D171 -0.01534 0.00001 0.00000 0.00041 0.00041 -0.01492

D172 -3.13568 -0.00002 0.00000 0.00021 0.00021 -3.13547

D173 -3.14111 -0.00000 0.00000 -0.00108 -0.00108 3.14100

D174 0.02095 -0.00002 0.00000 -0.00110 -0.00110 0.01984

D175 0.00112 0.00002 0.00000 -0.00021 -0.00021 0.00091

D176 -3.12001 0.00000 0.00000 -0.00023 -0.00023 -3.12024

D177 0.01808 -0.00002 0.00000 -0.00032 -0.00032 0.01776

D178 -3.12358 -0.00001 0.00000 -0.00029 -0.00029 -3.12386

D179 3.13831 0.00000 0.00000 -0.00011 -0.00011 3.13820

D180 -0.00335 0.00001 0.00000 -0.00008 -0.00008 -0.00343

D181 -0.00639 0.00002 0.00000 0.00003 0.00003 -0.00636

D182 3.13332 0.00001 0.00000 0.00003 0.00003 3.13334

D183 3.13527 0.00001 0.00000 -0.00000 -0.00000 3.13527

D184 -0.00821 0.00000 0.00000 -0.00001 -0.00001 -0.00822

D185 -0.00778 0.00001 0.00000 0.00018 0.00018 -0.00760

D186 3.13183 -0.00001 0.00000 -0.00003 -0.00003 3.13181

D187 3.13570 0.00002 0.00000 0.00019 0.00019 3.13589

D188 -0.00787 0.00000 0.00000 -0.00002 -0.00002 -0.00789

D189 0.01039 -0.00003 0.00000 -0.00009 -0.00009 0.01030

D190 3.13142 -0.00001 0.00000 -0.00006 -0.00006 3.13135

D191 -3.12923 -0.00001 0.00000 0.00012 0.00012 -3.12911

D192 -0.00821 0.00001 0.00000 0.00014 0.00014 -0.00807

D193 -3.12926 0.00002 0.00000 0.00172 0.00172 -3.12755

D194 -0.00931 -0.00000 0.00000 0.00143 0.00143 -0.00788

D195 0.01446 -0.00001 0.00000 0.00091 0.00091 0.01538

D196 3.13442 -0.00002 0.00000 0.00062 0.00062 3.13504

D197 -3.13943 0.00000 0.00000 -0.00140 -0.00140 -3.14083

D198 -0.01943 -0.00001 0.00000 -0.00164 -0.00165 -0.02107

D199 0.00001 0.00003 0.00000 -0.00059 -0.00059 -0.00057

D200 3.12002 0.00001 0.00000 -0.00083 -0.00083 3.11918

D201 -0.01785 -0.00001 0.00000 -0.00059 -0.00059 -0.01844

D202 3.12409 -0.00000 0.00000 -0.00049 -0.00049 3.12360

D203 -3.13768 0.00001 0.00000 -0.00029 -0.00029 -3.13797

D204 0.00426 0.00001 0.00000 -0.00020 -0.00020 0.00407

D205 0.00656 0.00001 0.00000 -0.00006 -0.00006 0.00650

D206 -3.13323 0.00000 0.00000 0.00010 0.00010 -3.13312

D207 -3.13538 0.00001 0.00000 -0.00016 -0.00016 -3.13554

D208 0.00801 -0.00000 0.00000 0.00001 0.00001 0.00802

D209 0.00787 0.00001 0.00000 0.00039 0.00039 0.00827

D210 -3.13155 -0.00001 0.00000 0.00028 0.00028 -3.13128

D211 -3.13552 0.00002 0.00000 0.00023 0.00023 -3.13530

D212 0.00824 0.00000 0.00000 0.00011 0.00011 0.00835

D213 -0.01115 -0.00003 0.00000 -0.00006 -0.00006 -0.01121

D214 -3.13105 -0.00001 0.00000 0.00018 0.00018 -3.13086

D215 3.12829 -0.00001 0.00000 0.00005 0.00005 3.12834

D216 0.00839 0.00000 0.00000 0.00030 0.00030 0.00869

Item Value Threshold Converged?

Maximum Force 0.002393 0.000450 NO

RMS Force 0.000280 0.000300 YES

Maximum Displacement 0.073257 0.001800 NO

RMS Displacement 0.015258 0.001200 NO

Predicted change in Energy=-3.249324D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 25 18:50:53 2019, MaxMem= 4294967296 cpu: 2.8

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

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=0 Diff= 3.91D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.658247 -4.217977 0.420688

2 6 0 1.116788 -2.893343 0.107667

3 7 0 -0.009948 -2.117225 -0.041191

4 6 0 -1.149993 -2.879182 0.116028

5 6 0 -0.710315 -4.206296 0.425762

6 6 0 -2.472392 -2.433587 -0.022186

7 6 0 -2.876410 -1.086563 -0.206501

8 7 0 -2.061351 0.015627 -0.018156

9 6 0 -2.858529 1.096092 -0.222480

10 6 0 -4.188764 0.696908 -0.591472

11 6 0 -4.198494 -0.677830 -0.578501

12 6 0 2.441473 -2.467372 -0.034754

13 6 0 2.858734 -1.096617 -0.214786

14 6 0 4.189068 -0.699643 -0.586130

15 6 0 4.198333 0.675151 -0.582780

16 6 0 2.876188 1.086112 -0.213767

17 7 0 2.061262 -0.014843 -0.018090

18 6 0 2.472846 2.434294 -0.034996

19 6 0 1.150074 2.880815 0.097284

20 6 0 0.710278 4.204265 0.421723

21 6 0 -0.658320 4.215935 0.416599

22 6 0 -1.116764 2.894952 0.088807

23 7 0 0.010047 2.121244 -0.070624

24 6 0 -2.441904 2.468057 -0.047968

25 6 0 -3.537731 -3.466327 0.023453

26 6 0 -3.530912 -4.550406 -0.865618

27 6 0 -4.536907 -5.511240 -0.816206

28 6 0 -5.556003 -5.410531 0.129625

29 6 0 -5.569805 -4.337555 1.020792

30 6 0 -4.575255 -3.366898 0.961855

31 6 0 5.505495 -5.469241 0.072616

32 6 0 4.477837 -5.554468 -0.865070

33 6 0 3.479078 -4.584806 -0.899240

34 6 0 3.499120 -3.506305 -0.002676

35 6 0 4.546331 -3.424223 0.928107

36 6 0 5.533956 -4.402365 0.971648

37 6 0 -3.499811 3.505845 -0.008069

38 6 0 -4.545972 3.417138 0.923577

39 6 0 -5.532574 4.395708 0.976653

40 6 0 -5.504556 5.469915 0.086332

41 6 0 -4.478258 5.561898 -0.852213

42 6 0 -3.480354 4.591790 -0.895844

43 6 0 3.538397 3.465897 0.018254

44 6 0 4.574886 3.359998 0.957353

45 6 0 5.568458 4.330944 1.025415

46 6 0 5.555052 5.410932 0.142729

47 6 0 4.537257 5.518282 -0.803780

48 6 0 3.532101 4.557141 -0.862228

49 1 0 1.300243 -5.057066 0.633925

50 1 0 -1.363447 -5.035654 0.643945

51 1 0 -5.007871 1.355188 -0.838486

52 1 0 -5.026253 -1.329216 -0.814440

53 1 0 5.008494 -1.359231 -0.828475

54 1 0 5.025897 1.325267 -0.822945

55 1 0 1.363388 5.030154 0.652768

56 1 0 -1.300494 5.051550 0.642590

57 1 0 -2.745510 -4.626186 -1.608875

58 1 0 -4.524930 -6.337764 -1.518681

59 1 0 -6.336553 -6.162770 0.171228

60 1 0 -6.356907 -4.255919 1.762816

61 1 0 -4.586758 -2.535659 1.656969

62 1 0 6.280686 -6.227610 0.102343

63 1 0 4.453320 -6.375819 -1.573481

64 1 0 2.686873 -4.649643 -1.636522

65 1 0 4.570982 -2.598465 1.629899

66 1 0 6.327589 -4.332284 1.708089

67 1 0 -4.570027 2.586215 1.619210

68 1 0 -6.324991 4.320406 1.713886

69 1 0 -6.278970 6.228743 0.123536

70 1 0 -4.454165 6.388976 -1.553934

71 1 0 -2.689231 4.662206 -1.633762

72 1 0 4.585803 2.523826 1.646469

73 1 0 6.354386 4.244231 1.768102

74 1 0 6.334854 6.163510 0.191509

75 1 0 4.525672 6.350295 -1.499737

76 1 0 2.747751 4.638392 -1.605992

77 1 0 -0.002870 -1.118010 -0.196307

78 1 0 0.003120 1.126952 -0.253425

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

Rotational constants (GHZ): 0.0591333 0.0580823 0.0301311

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

Standard basis: 6-311G(d) (5D, 7F)

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

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5359.5705137074 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122973785 Hartrees.

Nuclear repulsion after empirical dispersion term = 5359.3582163288 Hartrees.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5741

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.15D-09

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 276

GePol: Fraction of low-weight points (<1% of avg) = 4.81%

GePol: Cavity surface area = 611.372 Ang\*\*2

GePol: Cavity volume = 627.925 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021246746 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5359.3560916542 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.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 25 18:50:56 2019, MaxMem= 4294967296 cpu: 2.4

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

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= 0.000000 -0.000000 0.000000

Rot= 0.999999 0.000002 -0.000000 0.001383 Ang= 0.16 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0325 S= 1.0108

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30466470113

Leave Link 401 at Sun Aug 25 18:51:01 2019, MaxMem= 4294967296 cpu: 83.2

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 580000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 98877243.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.99D-15 for 5703.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.56D-15 for 2769 2471.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.22D-15 for 5739.

Iteration 1 A^-1\*A deviation from orthogonality is 3.60D-10 for 3443 3441.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.78D-15 for 208.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.67D-15 for 4021 38.

Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 1155.

Iteration 2 A^-1\*A deviation from orthogonality is 4.07D-16 for 4320 4215.

E= -1914.32718551543

DIIS: error= 4.60D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.32718551543 IErMin= 1 ErrMin= 4.60D-04

ErrMax= 4.60D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.66D-03 BMatP= 1.66D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.60D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.631 Goal= None Shift= 0.000

Gap= 0.700 Goal= None Shift= 0.000

RMSDP=4.32D-05 MaxDP=1.64D-03 OVMax= 2.38D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.32D-05 CP: 1.00D+00

E= -1914.32791026266 Delta-E= -0.000724747222 Rises=F Damp=F

DIIS: error= 2.04D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.32791026266 IErMin= 2 ErrMin= 2.04D-04

ErrMax= 2.04D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-04 BMatP= 1.66D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.04D-03

Coeff-Com: 0.318D-01 0.968D+00

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

Coeff: 0.317D-01 0.968D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.053 Goal= None Shift= 0.000

RMSDP=2.53D-05 MaxDP=2.09D-03 DE=-7.25D-04 OVMax= 2.54D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.26D-05 CP: 1.00D+00 1.26D+00

E= -1914.32794705396 Delta-E= -0.000036791304 Rises=F Damp=F

DIIS: error= 4.86D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.32794705396 IErMin= 2 ErrMin= 2.04D-04

ErrMax= 4.86D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.27D-04 BMatP= 1.04D-04

IDIUse=3 WtCom= 3.12D-01 WtEn= 6.88D-01

Coeff-Com: -0.195D-01 0.628D+00 0.392D+00

Coeff-En: 0.000D+00 0.184D+00 0.816D+00

Coeff: -0.609D-02 0.322D+00 0.684D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.053 Goal= None Shift= 0.000

RMSDP=1.92D-05 MaxDP=1.12D-03 DE=-3.68D-05 OVMax= 1.05D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.69D-05 CP: 1.00D+00 1.46D+00 8.75D-01

E= -1914.32797301894 Delta-E= -0.000025964982 Rises=F Damp=F

DIIS: error= 3.88D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.32797301894 IErMin= 2 ErrMin= 2.04D-04

ErrMax= 3.88D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.47D-04 BMatP= 1.04D-04

IDIUse=3 WtCom= 3.37D-01 WtEn= 6.63D-01

Coeff-Com: -0.859D-02 0.111D+00 0.486D+00 0.412D+00

Coeff-En: 0.000D+00 0.000D+00 0.419D+00 0.581D+00

Coeff: -0.289D-02 0.373D-01 0.441D+00 0.524D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.053 Goal= None Shift= 0.000

RMSDP=1.73D-05 MaxDP=1.34D-03 DE=-2.60D-05 OVMax= 1.60D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.63D-06 CP: 1.00D+00 1.57D+00 1.57D+00 8.07D-01

E= -1914.32806483061 Delta-E= -0.000091811674 Rises=F Damp=F

DIIS: error= 2.34D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.32806483061 IErMin= 2 ErrMin= 2.04D-04

ErrMax= 2.34D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.22D-05 BMatP= 1.04D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.34D-03

Coeff-Com: 0.172D-02-0.663D-01 0.200D+00 0.388D+00 0.477D+00

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

Coeff: 0.172D-02-0.661D-01 0.199D+00 0.387D+00 0.479D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.053 Goal= None Shift= 0.000

RMSDP=1.01D-05 MaxDP=6.94D-04 DE=-9.18D-05 OVMax= 1.03D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.78D-06 CP: 1.00D+00 1.70D+00 1.81D+00 1.17D+00 1.13D+00

E= -1914.32809925889 Delta-E= -0.000034428273 Rises=F Damp=F

DIIS: error= 1.00D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.32809925889 IErMin= 6 ErrMin= 1.00D-04

ErrMax= 1.00D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.29D-06 BMatP= 4.22D-05

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

Coeff-Com: 0.204D-01-0.246D+00-0.595D+00-0.292D+00 0.406D-01 0.207D+01

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

Coeff: 0.204D-01-0.245D+00-0.594D+00-0.291D+00 0.405D-01 0.207D+01

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.053 Goal= None Shift= 0.000

RMSDP=4.70D-05 MaxDP=3.61D-03 DE=-3.44D-05 OVMax= 5.22D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 7.52D-06 CP: 1.00D+00 2.26D+00 3.00D+00 2.38D+00 3.00D+00

CP: 3.00D+00

E= -1914.32819248985 Delta-E= -0.000093230963 Rises=F Damp=F

DIIS: error= 6.36D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.32819248985 IErMin= 7 ErrMin= 6.36D-05

ErrMax= 6.36D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.15D-06 BMatP= 8.29D-06

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

Coeff-Com: 0.106D-01-0.680D-01-0.453D+00-0.422D+00-0.491D+00 0.115D+01

Coeff-Com: 0.127D+01

Coeff: 0.106D-01-0.680D-01-0.453D+00-0.422D+00-0.491D+00 0.115D+01

Coeff: 0.127D+01

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.054 Goal= None Shift= 0.000

RMSDP=4.67D-05 MaxDP=3.52D-03 DE=-9.32D-05 OVMax= 5.20D-02

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.48D-05 CP: 9.99D-01 2.79D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00

E= -1914.32823801233 Delta-E= -0.000045522477 Rises=F Damp=F

DIIS: error= 4.54D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.32823801233 IErMin= 8 ErrMin= 4.54D-05

ErrMax= 4.54D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.93D-06 BMatP= 5.15D-06

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

Coeff-Com: -0.535D-02 0.105D+00 0.149D+00 0.103D-01-0.266D+00-0.420D+00

Coeff-Com: 0.672D+00 0.755D+00

Coeff: -0.535D-02 0.105D+00 0.149D+00 0.103D-01-0.266D+00-0.420D+00

Coeff: 0.672D+00 0.755D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.054 Goal= None Shift= 0.000

RMSDP=4.71D-06 MaxDP=2.51D-04 DE=-4.55D-05 OVMax= 4.92D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.06D-06 CP: 9.99D-01 2.81D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.14D+00

E= -1914.32824128812 Delta-E= -0.000003275797 Rises=F Damp=F

DIIS: error= 2.84D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.32824128812 IErMin= 9 ErrMin= 2.84D-05

ErrMax= 2.84D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.57D-07 BMatP= 1.93D-06

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

Coeff-Com: -0.331D-02 0.436D-01 0.115D+00 0.806D-01 0.469D-02-0.318D+00

Coeff-Com: -0.697D-01 0.417D+00 0.731D+00

Coeff: -0.331D-02 0.436D-01 0.115D+00 0.806D-01 0.469D-02-0.318D+00

Coeff: -0.697D-01 0.417D+00 0.731D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.054 Goal= None Shift= 0.000

RMSDP=4.77D-06 MaxDP=3.05D-04 DE=-3.28D-06 OVMax= 5.44D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.08D-06 CP: 9.99D-01 2.86D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.29D+00 1.63D+00

E= -1914.32824340136 Delta-E= -0.000002113240 Rises=F Damp=F

DIIS: error= 1.79D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.32824340136 IErMin=10 ErrMin= 1.79D-05

ErrMax= 1.79D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.75D-07 BMatP= 9.57D-07

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

Coeff-Com: -0.747D-03-0.110D-01 0.530D-01 0.107D+00 0.189D+00-0.170D+00

Coeff-Com: -0.506D+00 0.878D-01 0.435D+00 0.816D+00

Coeff: -0.747D-03-0.110D-01 0.530D-01 0.107D+00 0.189D+00-0.170D+00

Coeff: -0.506D+00 0.878D-01 0.435D+00 0.816D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.054 Goal= None Shift= 0.000

RMSDP=5.06D-06 MaxDP=3.27D-04 DE=-2.11D-06 OVMax= 5.69D-03

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.03D-07 CP: 9.99D-01 2.90D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.45D+00 2.40D+00 1.58D+00

E= -1914.32824500063 Delta-E= -0.000001599263 Rises=F Damp=F

DIIS: error= 1.28D-05 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.32824500063 IErMin=11 ErrMin= 1.28D-05

ErrMax= 1.28D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.47D-07 BMatP= 5.75D-07

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

Coeff-Com: 0.758D-03-0.178D-01-0.189D-01 0.320D-01 0.100D+00-0.997D-02

Coeff-Com: -0.219D+00 0.107D-01-0.225D+00 0.390D+00 0.958D+00

Coeff: 0.758D-03-0.178D-01-0.189D-01 0.320D-01 0.100D+00-0.997D-02

Coeff: -0.219D+00 0.107D-01-0.225D+00 0.390D+00 0.958D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.054 Goal= None Shift= 0.000

RMSDP=4.87D-06 MaxDP=3.34D-04 DE=-1.60D-06 OVMax= 5.61D-03

Cycle 12 Pass 1 IDiag 1:

RMSU= 4.36D-07 CP: 9.99D-01 2.95D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.61D+00 2.95D+00 2.45D+00

CP: 1.58D+00

E= -1914.32824584786 Delta-E= -0.000000847231 Rises=F Damp=F

DIIS: error= 6.32D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.32824584786 IErMin=12 ErrMin= 6.32D-06

ErrMax= 6.32D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.66D-08 BMatP= 2.47D-07

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

Coeff-Com: 0.767D-03-0.722D-02-0.330D-01-0.161D-01 0.453D-03 0.423D-01

Coeff-Com: 0.254D-01 0.134D-01-0.308D+00-0.579D-01 0.618D+00 0.721D+00

Coeff: 0.767D-03-0.722D-02-0.330D-01-0.161D-01 0.453D-03 0.423D-01

Coeff: 0.254D-01 0.134D-01-0.308D+00-0.579D-01 0.618D+00 0.721D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.054 Goal= None Shift= 0.000

RMSDP=3.43D-06 MaxDP=2.43D-04 DE=-8.47D-07 OVMax= 3.95D-03

Cycle 13 Pass 1 IDiag 1:

RMSU= 8.74D-07 CP: 9.99D-01 2.98D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.72D+00 3.00D+00 2.98D+00

CP: 2.27D+00 1.56D+00

E= -1914.32824609233 Delta-E= -0.000000244472 Rises=F Damp=F

DIIS: error= 3.62D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.32824609233 IErMin=13 ErrMin= 3.62D-06

ErrMax= 3.62D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.13D-08 BMatP= 7.66D-08

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

Coeff-Com: -0.703D-05 0.317D-02-0.128D-02-0.149D-01-0.335D-01 0.236D-01

Coeff-Com: 0.801D-01 0.526D-03-0.940D-02-0.278D+00-0.151D+00 0.457D+00

Coeff-Com: 0.923D+00

Coeff: -0.703D-05 0.317D-02-0.128D-02-0.149D-01-0.335D-01 0.236D-01

Coeff: 0.801D-01 0.526D-03-0.940D-02-0.278D+00-0.151D+00 0.457D+00

Coeff: 0.923D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.054 Goal= None Shift= 0.000

RMSDP=1.23D-06 MaxDP=7.55D-05 DE=-2.44D-07 OVMax= 1.35D-03

Cycle 14 Pass 1 IDiag 1:

RMSU= 4.05D-07 CP: 9.99D-01 2.99D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.76D+00 3.00D+00 3.00D+00

CP: 2.45D+00 1.68D+00 1.68D+00

E= -1914.32824613414 Delta-E= -0.000000041809 Rises=F Damp=F

DIIS: error= 1.00D-06 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.32824613414 IErMin=14 ErrMin= 1.00D-06

ErrMax= 1.00D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.12D-09 BMatP= 2.13D-08

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

Coeff-Com: -0.238D-04 0.149D-02 0.171D-02-0.533D-02-0.140D-01 0.106D-01

Coeff-Com: 0.313D-01-0.238D-02 0.440D-01-0.112D+00-0.135D+00 0.966D-01

Coeff-Com: 0.371D+00 0.713D+00

Coeff: -0.238D-04 0.149D-02 0.171D-02-0.533D-02-0.140D-01 0.106D-01

Coeff: 0.313D-01-0.238D-02 0.440D-01-0.112D+00-0.135D+00 0.966D-01

Coeff: 0.371D+00 0.713D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.054 Goal= None Shift= 0.000

RMSDP=1.68D-07 MaxDP=1.06D-05 DE=-4.18D-08 OVMax= 1.54D-04

Cycle 15 Pass 1 IDiag 1:

RMSU= 7.03D-08 CP: 9.99D-01 2.99D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.75D+00 3.00D+00 3.00D+00

CP: 2.43D+00 1.64D+00 1.69D+00 1.06D+00

E= -1914.32824613587 Delta-E= -0.000000001731 Rises=F Damp=F

DIIS: error= 5.15D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.32824613587 IErMin=15 ErrMin= 5.15D-07

ErrMax= 5.15D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.21D-09 BMatP= 3.12D-09

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

Coeff-Com: -0.859D-05-0.223D-04 0.208D-03 0.546D-03 0.132D-02-0.184D-02

Coeff-Com: -0.328D-02-0.103D-02 0.215D-01 0.272D-01-0.186D-01-0.105D+00

Coeff-Com: -0.134D+00 0.408D+00 0.805D+00

Coeff: -0.859D-05-0.223D-04 0.208D-03 0.546D-03 0.132D-02-0.184D-02

Coeff: -0.328D-02-0.103D-02 0.215D-01 0.272D-01-0.186D-01-0.105D+00

Coeff: -0.134D+00 0.408D+00 0.805D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.054 Goal= None Shift= 0.000

RMSDP=2.31D-07 MaxDP=1.68D-05 DE=-1.73D-09 OVMax= 2.62D-04

Cycle 16 Pass 1 IDiag 1:

RMSU= 3.62D-08 CP: 9.99D-01 2.99D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.76D+00 3.00D+00 3.00D+00

CP: 2.48D+00 1.69D+00 1.77D+00 1.15D+00 8.77D-01

E= -1914.32824613700 Delta-E= -0.000000001130 Rises=F Damp=F

DIIS: error= 1.96D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1914.32824613700 IErMin=16 ErrMin= 1.96D-07

ErrMax= 1.96D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.00D-10 BMatP= 1.21D-09

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

Coeff-Com: 0.222D-05-0.285D-03-0.118D-03 0.126D-02 0.311D-02-0.203D-02

Coeff-Com: -0.692D-02-0.488D-03 0.276D-03 0.262D-01 0.168D-01-0.429D-01

Coeff-Com: -0.103D+00 0.111D-01 0.233D+00 0.864D+00

Coeff: 0.222D-05-0.285D-03-0.118D-03 0.126D-02 0.311D-02-0.203D-02

Coeff: -0.692D-02-0.488D-03 0.276D-03 0.262D-01 0.168D-01-0.429D-01

Coeff: -0.103D+00 0.111D-01 0.233D+00 0.864D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.054 Goal= None Shift= 0.000

RMSDP=4.33D-08 MaxDP=2.78D-06 DE=-1.13D-09 OVMax= 4.38D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 9.86D-09 CP: 9.99D-01 2.99D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.76D+00 3.00D+00 3.00D+00

CP: 2.47D+00 1.68D+00 1.77D+00 1.17D+00 1.06D+00

CP: 1.04D+00

E= -1914.32824613715 Delta-E= -0.000000000146 Rises=F Damp=F

DIIS: error= 1.56D-07 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1914.32824613715 IErMin=17 ErrMin= 1.56D-07

ErrMax= 1.56D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.38D-11 BMatP= 1.00D-10

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

Coeff-Com: 0.480D-05-0.166D-03-0.275D-03 0.490D-03 0.148D-02-0.671D-03

Coeff-Com: -0.323D-02 0.130D-03-0.310D-02 0.117D-01 0.124D-01-0.942D-02

Coeff-Com: -0.427D-01-0.489D-01 0.185D-01 0.494D+00 0.570D+00

Coeff: 0.480D-05-0.166D-03-0.275D-03 0.490D-03 0.148D-02-0.671D-03

Coeff: -0.323D-02 0.130D-03-0.310D-02 0.117D-01 0.124D-01-0.942D-02

Coeff: -0.427D-01-0.489D-01 0.185D-01 0.494D+00 0.570D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.054 Goal= None Shift= 0.000

RMSDP=4.97D-09 MaxDP=3.16D-07 DE=-1.46D-10 OVMax= 1.77D-06

Error on total polarization charges = 0.08255

SCF Done: E(UB3LYP) = -1914.32824614 A.U. after 17 cycles

NFock= 17 Conv=0.50D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0347 S= 1.0115

<L.S>= 0.000000000000E+00

KE= 1.906374202725D+03 PE=-1.516840980308D+04 EE= 5.988351262561D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.33

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0347, after 2.0007

Leave Link 502 at Sun Aug 25 18:59:03 2019, MaxMem= 4294967296 cpu: 7642.9

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

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

Range of M.O.s used for correlation: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.10507998D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.39088910D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.10751896D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.53713816D-01

Leave Link 801 at Sun Aug 25 18:59:03 2019, MaxMem= 4294967296 cpu: 0.8

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

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

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

Leave Link 1101 at Sun Aug 25 18:59:10 2019, MaxMem= 4294967296 cpu: 111.6

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

Symmetrizing basis deriv contribution to polar:

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

Leave Link 1102 at Sun Aug 25 18:59:11 2019, MaxMem= 4294967296 cpu: 2.0

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

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 184

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 Sun Aug 25 19:19:06 2019, MaxMem= 4294967296 cpu: 19119.4

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

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 580000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.72D+03 4.63D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 5.10D+02 3.84D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 1.10D+01 4.34D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.33D-01 3.49D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 7.81D-04 1.70D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 5.96D-06 1.28D-04.

194 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 3.54D-08 9.46D-06.

81 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 1.78D-10 6.44D-07.

40 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 9.24D-13 4.48D-08.

4 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 1.33D-14 3.40D-09.

2 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 5.56D-15 4.16D-09.

InvSVY: IOpt=1 It= 1 EMax= 6.39D-14

Solved reduced A of dimension 1728 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1212.47 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 Sun Aug 25 23:11:52 2019, MaxMem= 4294967296 cpu: 223389.2

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 184

Leave Link 701 at Sun Aug 25 23:13:20 2019, MaxMem= 4294967296 cpu: 1418.3

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

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

Leave Link 702 at Sun Aug 25 23:13:21 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

Leave Link 703 at Sun Aug 25 23:32:01 2019, MaxMem= 4294967296 cpu: 17919.4

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

Dipole = 5.28167095D-03 2.08089276D-02 3.53379253D-02

Polarizability= 1.72998165D+03-1.56202547D+02 1.44947760D+03

-5.65412556D-03-2.44563591D-01 4.57950423D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000533322 0.000138476 0.001554864

2 6 0.000610137 -0.000063537 -0.001650824

3 7 0.000147461 0.000294843 0.000050885

4 6 0.002189301 -0.001546580 0.002159294

5 6 -0.001501814 0.000181151 -0.001733854

6 6 -0.004079324 0.001249960 -0.002429155

7 6 0.005144042 -0.000760937 0.000570380

8 7 -0.003011705 0.000610180 0.000184382

9 6 0.001745873 -0.001028969 0.002596871

10 6 0.001333179 0.000897183 -0.001472026

11 6 -0.002041892 -0.000624966 -0.000893728

12 6 0.000563398 0.000036419 0.001605197

13 6 -0.001741075 -0.000979482 -0.002596520

14 6 -0.001326185 0.000902891 0.001468774

15 6 0.002040446 -0.000665948 0.000906185

16 6 -0.005150913 -0.000758548 -0.000572729

17 7 0.003011821 0.000638966 -0.000197091

18 6 0.004103361 0.001199873 0.002430965

19 6 -0.002208886 -0.001515580 -0.002161637

20 6 0.001509744 0.000182367 0.001738884

21 6 0.000536890 0.000144603 -0.001563863

22 6 -0.000600996 -0.000123653 0.001658942

23 7 -0.000148373 0.000296873 -0.000053307

24 6 -0.000584156 0.000124594 -0.001603641

25 6 0.000460914 0.000616247 -0.000265510

26 6 0.000057492 -0.000034144 0.000108674

27 6 -0.000091732 0.000122031 -0.000016499

28 6 -0.000102348 -0.000110611 -0.000002031

29 6 0.000164633 0.000078634 -0.000106443

30 6 -0.000054453 -0.000118367 0.000246672

31 6 0.000058622 -0.000037466 0.000072282

32 6 0.000014907 -0.000046974 -0.000140923

33 6 0.000048896 -0.000023523 0.000219453

34 6 -0.000425532 -0.000206117 -0.000273874

35 6 0.000184874 0.000082003 0.000004010

36 6 -0.000097074 0.000059978 0.000073772

37 6 0.000434150 -0.000217572 0.000277573

38 6 -0.000185769 0.000084715 -0.000003857

39 6 0.000096441 0.000064103 -0.000072862

40 6 -0.000060980 -0.000036420 -0.000074826

41 6 -0.000012771 -0.000045513 0.000142422

42 6 -0.000049542 -0.000021740 -0.000221474

43 6 -0.000471436 0.000662188 0.000272346

44 6 0.000055668 -0.000116216 -0.000250229

45 6 -0.000168029 0.000080476 0.000109820

46 6 0.000106402 -0.000107343 0.000001382

47 6 0.000091832 0.000128379 0.000016563

48 6 -0.000056358 -0.000031462 -0.000106078

49 1 0.000003778 0.000063404 0.000016813

50 1 0.000056221 0.000046449 0.000045137

51 1 -0.000031006 0.000065568 0.000052611

52 1 -0.000007608 0.000075735 0.000057692

53 1 0.000031839 0.000067295 -0.000053213

54 1 0.000009050 0.000080912 -0.000059095

55 1 -0.000057840 0.000046827 -0.000045423

56 1 -0.000005515 0.000068922 -0.000017466

57 1 0.000026225 -0.000028737 0.000007039

58 1 -0.000016454 0.000015993 -0.000022299

59 1 0.000024727 -0.000023477 0.000022099

60 1 -0.000026758 0.000020757 -0.000013732

61 1 0.000059107 -0.000067635 0.000085954

62 1 -0.000002388 -0.000002545 0.000004686

63 1 0.000018345 -0.000005053 -0.000002833

64 1 0.000026119 -0.000024529 -0.000026643

65 1 -0.000045332 -0.000005734 0.000036546

66 1 0.000003461 0.000000472 0.000015680

67 1 0.000045145 -0.000004478 -0.000038668

68 1 -0.000004064 0.000002388 -0.000015768

69 1 0.000002535 0.000000654 -0.000004845

70 1 -0.000017422 -0.000001435 0.000003146

71 1 -0.000026094 -0.000023734 0.000027877

72 1 -0.000061866 -0.000070070 -0.000089520

73 1 0.000025444 0.000023515 0.000013796

74 1 -0.000025516 -0.000021045 -0.000022881

75 1 0.000016518 0.000018944 0.000022539

76 1 -0.000024887 -0.000027453 -0.000008349

77 1 0.000035020 0.000023449 0.000079643

78 1 -0.000036601 0.000029175 -0.000078139

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

Cartesian Forces: Max 0.005150913 RMS 0.000967026

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

Leave Link 716 at Sun Aug 25 23:32:01 2019, MaxMem= 4294967296 cpu: 1.9

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.002829482 RMS 0.000386168

Search for a local minimum.

Step number 2 out of a maximum of 452

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

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -2.88D-04 DEPred=-3.25D-04 R= 8.87D-01

TightC=F SS= 1.41D+00 RLast= 5.25D-02 DXNew= 5.0454D-01 1.5762D-01

Trust test= 8.87D-01 RLast= 5.25D-02 DXMaxT set to 3.00D-01

ITU= 1 0

Eigenvalues --- -0.05375 0.00110 0.00316 0.00597 0.00606

Eigenvalues --- 0.00775 0.00786 0.01013 0.01044 0.01109

Eigenvalues --- 0.01131 0.01222 0.01227 0.01246 0.01315

Eigenvalues --- 0.01340 0.01359 0.01385 0.01443 0.01448

Eigenvalues --- 0.01501 0.01521 0.01536 0.01559 0.01580

Eigenvalues --- 0.01651 0.01691 0.01719 0.01724 0.01747

Eigenvalues --- 0.01760 0.01767 0.01771 0.01795 0.01844

Eigenvalues --- 0.01880 0.01890 0.01980 0.02124 0.02141

Eigenvalues --- 0.02182 0.02205 0.02248 0.02283 0.02297

Eigenvalues --- 0.02339 0.02357 0.02447 0.02481 0.02531

Eigenvalues --- 0.02553 0.02558 0.02590 0.02599 0.02617

Eigenvalues --- 0.02624 0.02633 0.02683 0.02748 0.02749

Eigenvalues --- 0.02801 0.02821 0.02868 0.02870 0.02872

Eigenvalues --- 0.02882 0.03018 0.03077 0.03520 0.03802

Eigenvalues --- 0.04209 0.04271 0.04543 0.04663 0.04670

Eigenvalues --- 0.04827 0.08053 0.09706 0.09767 0.09810

Eigenvalues --- 0.09932 0.09965 0.10471 0.10484 0.10691

Eigenvalues --- 0.10698 0.10702 0.10716 0.10721 0.10760

Eigenvalues --- 0.11400 0.11408 0.11420 0.11427 0.12003

Eigenvalues --- 0.12010 0.12019 0.12019 0.12274 0.12280

Eigenvalues --- 0.12294 0.12300 0.12779 0.12782 0.12784

Eigenvalues --- 0.12786 0.14579 0.15937 0.16080 0.16692

Eigenvalues --- 0.17062 0.17347 0.17357 0.17428 0.17947

Eigenvalues --- 0.18079 0.18178 0.18241 0.19057 0.19205

Eigenvalues --- 0.19346 0.19361 0.19373 0.19377 0.19404

Eigenvalues --- 0.19423 0.19546 0.19548 0.19552 0.19553

Eigenvalues --- 0.20088 0.20566 0.22147 0.22234 0.22610

Eigenvalues --- 0.23612 0.23780 0.24421 0.24907 0.25543

Eigenvalues --- 0.25855 0.26880 0.27560 0.27762 0.28169

Eigenvalues --- 0.28348 0.28748 0.29003 0.29269 0.30604

Eigenvalues --- 0.31081 0.31493 0.31679 0.33245 0.33314

Eigenvalues --- 0.33885 0.34586 0.34594 0.35597 0.35610

Eigenvalues --- 0.35654 0.35668 0.35735 0.35737 0.35766

Eigenvalues --- 0.35780 0.35871 0.35910 0.35915 0.35947

Eigenvalues --- 0.35950 0.35984 0.35987 0.36044 0.36096

Eigenvalues --- 0.36173 0.36250 0.36263 0.36346 0.36435

Eigenvalues --- 0.36618 0.36779 0.37106 0.37136 0.37489

Eigenvalues --- 0.37536 0.38096 0.38193 0.39278 0.39433

Eigenvalues --- 0.40095 0.40471 0.41020 0.41039 0.41087

Eigenvalues --- 0.41199 0.41228 0.41257 0.41373 0.41498

Eigenvalues --- 0.41522 0.41744 0.43338 0.43587 0.45584

Eigenvalues --- 0.45804 0.45816 0.45822 0.45988 0.46174

Eigenvalues --- 0.46186 0.46195 0.46306 0.46348 0.47082

Eigenvalues --- 0.47717 0.47859 0.48299 0.49236 0.49315

Eigenvalues --- 0.50730 0.50735 0.50829 0.50832 0.52339

Eigenvalues --- 0.52608 0.53544 0.55549

Eigenvalue 1 is -5.38D-02 should be greater than 0.000000 Eigenvector:

R30 R11 R13 R29 R31

1 0.34910 0.34826 -0.21982 -0.21974 -0.19704

R9 R15 R24 R33 R8

1 -0.19687 0.19598 0.19510 0.18168 0.18123

DIIS coeff's: 1.95916 -0.95916

Cosine: 0.993 > 0.970

Length: 1.620

GDIIS step was calculated using 2 of the last 2 vectors.

Iteration 1 RMS(Cart)= 0.23122934 RMS(Int)= 0.00310746

Iteration 2 RMS(Cart)= 0.01170280 RMS(Int)= 0.00021923

Iteration 3 RMS(Cart)= 0.00002633 RMS(Int)= 0.00021918

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00021918

ITry= 1 IFail=0 DXMaxC= 1.15D+00 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.71417 -0.00079 -0.00111 -0.01807 -0.01912 2.69505

R2 2.58632 0.00124 0.00390 0.02679 0.03093 2.61725

R3 2.03679 0.00000 0.00005 -0.00046 -0.00041 2.03638

R4 2.60073 -0.00021 -0.00249 -0.00607 -0.00874 2.59199

R5 2.64327 0.00113 0.00409 0.02266 0.02675 2.67002

R6 2.60823 0.00002 0.00185 0.00171 0.00337 2.61160

R7 1.91091 -0.00003 -0.00015 -0.00063 -0.00078 1.91013

R8 2.70599 -0.00138 -0.00607 -0.03341 -0.03939 2.66661

R9 2.64993 0.00199 0.00551 0.04303 0.04857 2.69850

R10 2.03707 0.00001 -0.00002 0.00048 0.00045 2.03752

R11 2.68027 -0.00283 -0.01839 -0.06879 -0.08716 2.59311

R12 2.80520 0.00030 -0.00027 0.00499 0.00472 2.80991

R13 2.61481 0.00192 0.01307 0.04638 0.05917 2.67398

R14 2.70789 0.00101 0.00086 0.02232 0.02331 2.73120

R15 2.56658 -0.00161 -0.01257 -0.04257 -0.05539 2.51119

R16 2.71558 0.00142 0.00712 0.03311 0.04028 2.75585

R17 2.72954 0.00031 0.01007 0.01097 0.02099 2.75053

R18 2.59806 -0.00126 -0.00404 -0.02675 -0.03047 2.56759

R19 2.03993 -0.00001 0.00007 -0.00001 0.00006 2.03999

R20 2.03982 -0.00003 -0.00018 -0.00027 -0.00045 2.03937

R21 2.72899 0.00031 0.01000 0.01059 0.02056 2.74956

R22 2.80230 -0.00016 0.00049 -0.00527 -0.00478 2.79752

R23 2.71574 0.00141 0.00711 0.03320 0.04036 2.75609

R24 2.56675 -0.00160 -0.01251 -0.04238 -0.05514 2.51161

R25 2.59805 -0.00126 -0.00404 -0.02682 -0.03055 2.56750

R26 2.03990 -0.00001 0.00006 0.00001 0.00007 2.03997

R27 2.70774 0.00101 0.00087 0.02249 0.02349 2.73123

R28 2.03985 -0.00003 -0.00018 -0.00027 -0.00045 2.03940

R29 2.61473 0.00192 0.01312 0.04629 0.05914 2.67387

R30 2.68064 -0.00283 -0.01848 -0.06887 -0.08732 2.59332

R31 2.65007 0.00199 0.00565 0.04292 0.04859 2.69866

R32 2.80447 0.00031 -0.00021 0.00512 0.00490 2.80937

R33 2.70581 -0.00138 -0.00618 -0.03335 -0.03944 2.66637

R34 2.60810 0.00002 0.00176 0.00182 0.00338 2.61148

R35 2.58639 0.00124 0.00391 0.02686 0.03101 2.61740

R36 2.03708 0.00001 -0.00003 0.00051 0.00049 2.03756

R37 2.71399 -0.00080 -0.00103 -0.01826 -0.01923 2.69476

R38 2.03680 0.00000 0.00005 -0.00050 -0.00045 2.03635

R39 2.60052 -0.00022 -0.00239 -0.00611 -0.00868 2.59184

R40 2.64355 0.00113 0.00399 0.02290 0.02687 2.67042

R41 1.91048 -0.00003 -0.00014 -0.00061 -0.00075 1.90973

R42 2.80149 -0.00016 0.00047 -0.00545 -0.00498 2.79651

R43 2.64947 -0.00001 -0.00021 -0.00013 -0.00034 2.64914

R44 2.65030 -0.00009 -0.00079 -0.00217 -0.00296 2.64733

R45 2.63050 -0.00004 -0.00050 -0.00136 -0.00186 2.62864

R46 2.04844 -0.00001 -0.00002 -0.00025 -0.00027 2.04817

R47 2.63432 0.00006 0.00037 0.00152 0.00189 2.63621

R48 2.04995 -0.00000 -0.00009 -0.00005 -0.00014 2.04980

R49 2.63591 -0.00010 -0.00057 -0.00180 -0.00237 2.63354

R50 2.05003 0.00000 -0.00003 0.00004 0.00002 2.05004

R51 2.62854 0.00010 0.00028 0.00190 0.00218 2.63072

R52 2.04998 -0.00000 -0.00013 -0.00007 -0.00020 2.04978

R53 2.04778 -0.00000 -0.00008 -0.00017 -0.00025 2.04753

R54 2.63385 0.00003 -0.00008 0.00057 0.00049 2.63433

R55 2.63703 -0.00002 0.00023 -0.00038 -0.00015 2.63688

R56 2.05010 0.00000 0.00004 -0.00003 0.00001 2.05011

R57 2.63136 -0.00001 0.00033 0.00014 0.00047 2.63183

R58 2.05021 0.00001 0.00012 0.00024 0.00036 2.05057

R59 2.65060 0.00006 0.00042 0.00189 0.00231 2.65292

R60 2.04874 0.00001 -0.00001 0.00006 0.00005 2.04880

R61 2.65219 0.00005 0.00072 0.00192 0.00264 2.65482

R62 2.62805 0.00003 0.00007 -0.00001 0.00005 2.62811

R63 2.04841 0.00004 0.00019 0.00085 0.00104 2.04945

R64 2.05025 0.00001 0.00016 0.00017 0.00032 2.05057

R65 2.65255 0.00005 0.00073 0.00204 0.00277 2.65532

R66 2.65088 0.00006 0.00043 0.00194 0.00237 2.65324

R67 2.62788 0.00003 0.00006 0.00004 0.00011 2.62798

R68 2.04834 0.00004 0.00019 0.00086 0.00105 2.04939

R69 2.63708 -0.00002 0.00024 -0.00038 -0.00015 2.63694

R70 2.05025 0.00001 0.00016 0.00017 0.00033 2.05058

R71 2.63386 0.00003 -0.00008 0.00055 0.00047 2.63433

R72 2.05009 0.00000 0.00004 -0.00002 0.00002 2.05011

R73 2.63129 -0.00001 0.00033 0.00008 0.00041 2.63170

R74 2.05020 0.00001 0.00012 0.00025 0.00037 2.05057

R75 2.04872 0.00001 -0.00000 0.00000 -0.00000 2.04872

R76 2.65063 -0.00009 -0.00082 -0.00224 -0.00306 2.64757

R77 2.64973 -0.00002 -0.00023 -0.00019 -0.00041 2.64932

R78 2.62839 0.00010 0.00030 0.00191 0.00221 2.63059

R79 2.04770 -0.00000 -0.00008 -0.00017 -0.00024 2.04746

R80 2.63594 -0.00010 -0.00058 -0.00184 -0.00243 2.63351

R81 2.04997 -0.00000 -0.00013 -0.00007 -0.00020 2.04977

R82 2.63433 0.00006 0.00037 0.00154 0.00191 2.63624

R83 2.05002 0.00000 -0.00003 0.00004 0.00001 2.05003

R84 2.63042 -0.00004 -0.00051 -0.00132 -0.00183 2.62859

R85 2.04993 -0.00000 -0.00009 -0.00005 -0.00014 2.04978

R86 2.04841 -0.00001 -0.00003 -0.00022 -0.00024 2.04816

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A2 2.17845 0.00009 0.00047 0.00325 0.00377 2.18222

A3 2.21621 0.00013 0.00028 0.00167 0.00200 2.21820

A4 1.85699 0.00002 -0.00001 0.00163 0.00160 1.85859

A5 2.22107 0.00006 0.00184 0.00684 0.00949 2.23056

A6 2.20507 -0.00007 -0.00182 -0.00858 -0.01122 2.19385

A7 1.93114 0.00011 0.00021 -0.00008 0.00037 1.93150

A8 2.17501 -0.00013 -0.00018 -0.00390 -0.00422 2.17078

A9 2.17580 0.00002 -0.00003 0.00349 0.00332 2.17912

A10 1.85736 0.00009 0.00053 0.00413 0.00458 1.86194

A11 2.20469 -0.00019 0.00061 -0.00504 -0.00516 2.19953

A12 2.22103 0.00010 -0.00115 0.00118 0.00068 2.22171

A13 1.89035 -0.00000 0.00005 -0.00082 -0.00086 1.88949

A14 2.21436 -0.00006 -0.00006 -0.00186 -0.00189 2.21247

A15 2.17826 0.00007 0.00001 0.00250 0.00254 2.18080

A16 2.19349 0.00030 0.00141 0.00672 0.00718 2.20067

A17 2.04057 -0.00048 -0.00131 -0.01592 -0.01678 2.02379

A18 2.04912 0.00019 -0.00010 0.00925 0.00960 2.05872

A19 2.17855 0.00025 0.00186 0.00450 0.00564 2.18419

A20 2.17420 0.00035 -0.00036 0.01100 0.01127 2.18547

A21 1.93007 -0.00060 -0.00146 -0.01609 -0.01765 1.91242

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A26 1.85657 0.00001 0.00248 0.00047 0.00289 1.85946

A27 2.20405 -0.00005 -0.00171 -0.00406 -0.00575 2.19830

A28 2.22252 0.00004 -0.00075 0.00362 0.00290 2.22541

A29 1.85578 0.00026 -0.00160 0.00586 0.00428 1.86006

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A31 2.22280 -0.00012 0.00060 -0.00106 -0.00048 2.22232

A32 2.18388 -0.00047 -0.00236 -0.01541 -0.01893 2.16495

A33 2.04867 0.00041 0.00123 0.01652 0.01831 2.06698

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A68 2.04847 0.00042 0.00122 0.01717 0.01896 2.06744

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A71 2.07454 0.00009 0.00118 0.00232 0.00350 2.07804

A72 2.10330 -0.00006 -0.00070 -0.00122 -0.00192 2.10138

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D2 -3.11094 0.00005 -0.00224 0.01895 0.01660 -3.09434

D3 -3.09968 -0.00006 -0.00026 0.00138 0.00105 -3.09863

D4 0.05296 -0.00001 -0.00154 0.01155 0.01002 0.06298

D5 0.00090 -0.00005 0.00110 -0.01260 -0.01137 -0.01047

D6 -3.11889 -0.00004 0.00083 -0.00374 -0.00286 -3.12175

D7 3.11956 0.00001 0.00039 -0.00497 -0.00458 3.11498

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D11 3.09706 -0.00000 0.00177 -0.01123 -0.00939 3.08767

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D13 -3.02419 -0.00020 0.00342 -0.07210 -0.06837 -3.09257

D14 0.12113 -0.00019 0.00249 -0.06283 -0.06007 0.06106

D15 0.13056 -0.00015 0.00187 -0.06008 -0.05790 0.07265

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D19 -3.05583 -0.00005 0.00028 0.00393 0.00425 -3.05159

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D21 -0.02101 0.00008 -0.00080 0.01172 0.01081 -0.01020

D22 3.09934 0.00007 -0.00053 0.00303 0.00242 3.10176

D23 3.10589 0.00002 -0.00159 0.03078 0.02922 3.13511

D24 -0.05695 0.00001 -0.00132 0.02209 0.02083 -0.03612

D25 -0.12680 -0.00038 0.00294 -0.03540 -0.03205 -0.15885

D26 3.01007 -0.00030 0.00213 -0.02512 -0.02262 2.98745

D27 3.03229 -0.00031 0.00388 -0.05818 -0.05395 2.97835

D28 -0.11403 -0.00023 0.00307 -0.04790 -0.04451 -0.15854

D29 -0.23308 0.00053 -0.00416 0.00943 0.00564 -0.22743

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D32 -0.19664 0.00043 -0.00510 0.02509 0.02032 -0.17631

D33 -0.98766 -0.00021 0.00176 -0.00124 0.00054 -0.98712

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D46 -3.10688 0.00012 0.00042 -0.00356 -0.00310 -3.10998

D47 -3.08259 0.00008 0.00388 -0.00766 -0.00388 -3.08647

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D50 -2.90297 0.00008 0.00145 0.08326 0.08499 -2.81798

D51 -2.94435 0.00021 -0.00172 0.10190 0.10037 -2.84398

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D98 0.07248 -0.00000 0.00187 -0.01491 -0.01306 0.05942

D99 0.03146 -0.00007 0.00020 -0.00631 -0.00615 0.02532

D100 -3.07547 -0.00005 0.00080 0.00448 0.00533 -3.07014

D101 0.00092 -0.00005 0.00097 -0.01212 -0.01103 -0.01011

D102 3.11535 0.00002 0.00045 -0.00473 -0.00428 3.11106

D103 -3.11460 -0.00004 0.00069 -0.00370 -0.00295 -3.11755

D104 -0.00018 0.00003 0.00017 0.00369 0.00380 0.00362

D105 0.01795 0.00001 -0.00084 0.00821 0.00719 0.02514

D106 -3.12069 0.00006 -0.00218 0.01790 0.01560 -3.10509

D107 -3.09721 -0.00006 -0.00033 0.00105 0.00065 -3.09656

D108 0.04733 -0.00001 -0.00167 0.01073 0.00906 0.05639

D109 -0.03089 0.00004 0.00041 -0.00087 -0.00045 -0.03134

D110 3.07606 0.00003 -0.00019 -0.01147 -0.01168 3.06438

D111 3.10779 -0.00001 0.00174 -0.01041 -0.00859 3.09920

D112 -0.06845 -0.00003 0.00115 -0.02101 -0.01981 -0.08826

D113 -3.00595 -0.00019 0.00308 -0.07344 -0.07003 -3.07598

D114 0.13367 -0.00020 0.00219 -0.06302 -0.06055 0.07312

D115 0.13916 -0.00013 0.00148 -0.06193 -0.06013 0.07902

D116 -3.00441 -0.00013 0.00058 -0.05151 -0.05065 -3.05506

D117 0.97630 -0.00019 -0.00169 -0.01825 -0.01991 0.95639

D118 -2.16376 -0.00018 -0.00084 -0.01717 -0.01798 -2.18173

D119 -2.16347 -0.00019 -0.00086 -0.02786 -0.02875 -2.19222

D120 0.97965 -0.00018 -0.00001 -0.02677 -0.02682 0.95284

D121 -3.13866 0.00007 -0.00150 0.00392 0.00242 -3.13624

D122 -0.01894 0.00001 -0.00170 0.00155 -0.00015 -0.01909

D123 -0.00059 0.00010 -0.00059 0.00456 0.00396 0.00337

D124 3.11913 0.00004 -0.00080 0.00219 0.00139 3.12052

D125 -3.12979 -0.00004 0.00182 -0.00309 -0.00127 -3.13107

D126 -0.00918 -0.00006 0.00149 -0.00353 -0.00204 -0.01122

D127 0.01530 -0.00007 0.00092 -0.00372 -0.00280 0.01249

D128 3.13591 -0.00009 0.00059 -0.00416 -0.00357 3.13234

D129 -0.01111 -0.00008 -0.00005 -0.00293 -0.00298 -0.01409

D130 3.12843 -0.00005 0.00007 -0.00193 -0.00186 3.12657

D131 -3.13072 -0.00002 0.00015 -0.00054 -0.00038 -3.13110

D132 0.00881 0.00001 0.00028 0.00046 0.00074 0.00955

D133 0.00818 0.00002 0.00038 0.00039 0.00077 0.00895

D134 -3.13550 0.00004 0.00022 0.00089 0.00111 -3.13439

D135 -3.13134 -0.00000 0.00026 -0.00062 -0.00036 -3.13170

D136 0.00816 0.00001 0.00010 -0.00012 -0.00002 0.00814

D137 0.00649 0.00001 -0.00006 0.00046 0.00040 0.00689

D138 -3.13583 0.00001 -0.00016 0.00083 0.00067 -3.13516

D139 -3.13302 -0.00001 0.00010 -0.00004 0.00006 -3.13296

D140 0.00784 -0.00001 -0.00000 0.00033 0.00033 0.00818

D141 -0.01834 0.00002 -0.00059 0.00126 0.00066 -0.01768

D142 -3.13883 0.00003 -0.00026 0.00172 0.00146 -3.13737

D143 3.12398 0.00002 -0.00049 0.00088 0.00039 3.12437

D144 0.00349 0.00004 -0.00016 0.00135 0.00119 0.00468

D145 -0.00750 0.00003 0.00018 -0.00155 -0.00138 -0.00888

D146 3.13188 0.00000 -0.00001 -0.00380 -0.00383 3.12805

D147 3.13609 0.00003 0.00017 0.00070 0.00087 3.13696

D148 -0.00772 0.00001 -0.00002 -0.00155 -0.00158 -0.00930

D149 -0.00635 0.00004 0.00002 0.00285 0.00288 -0.00346

D150 3.13553 0.00001 -0.00003 0.00307 0.00306 3.13858

D151 3.13325 0.00003 0.00003 0.00061 0.00064 3.13389

D152 -0.00806 0.00000 -0.00002 0.00083 0.00081 -0.00725

D153 0.01024 -0.00007 -0.00006 -0.00508 -0.00516 0.00508

D154 3.13119 -0.00000 -0.00006 -0.00292 -0.00300 3.12820

D155 -3.12915 -0.00004 0.00013 -0.00284 -0.00272 -3.13187

D156 -0.00820 0.00002 0.00014 -0.00068 -0.00056 -0.00875

D157 3.13863 0.00003 -0.00108 0.01037 0.00928 -3.13527

D158 0.00085 0.00004 -0.00025 0.01022 0.00996 0.01080

D159 0.01757 -0.00003 -0.00109 0.00826 0.00716 0.02473

D160 -3.12022 -0.00003 -0.00025 0.00811 0.00784 -3.11238

D161 3.13063 0.00003 0.00127 -0.00914 -0.00788 3.12275

D162 0.00908 -0.00002 0.00108 -0.00808 -0.00701 0.00207

D163 -0.01475 0.00003 0.00044 -0.00894 -0.00849 -0.02324

D164 -3.13630 -0.00003 0.00025 -0.00788 -0.00761 3.13927

D165 0.01761 -0.00007 -0.00032 0.00251 0.00220 0.01981

D166 -3.12426 -0.00003 -0.00028 0.00230 0.00203 -3.12223

D167 3.13905 -0.00001 -0.00013 0.00147 0.00135 3.14040

D168 -0.00282 0.00003 -0.00008 0.00126 0.00118 -0.00164

D169 3.12817 0.00003 0.00123 -0.00737 -0.00616 3.12201

D170 0.00762 -0.00002 0.00103 -0.00705 -0.00603 0.00158

D171 -0.01492 0.00003 0.00040 -0.00841 -0.00801 -0.02293

D172 -3.13547 -0.00003 0.00020 -0.00809 -0.00788 3.13983

D173 3.14100 0.00003 -0.00104 0.00876 0.00771 -3.13447

D174 0.01984 -0.00003 -0.00106 0.00711 0.00604 0.02588

D175 0.00091 0.00004 -0.00020 0.00983 0.00962 0.01053

D176 -3.12024 -0.00003 -0.00022 0.00818 0.00794 -3.11230

D177 0.01776 -0.00007 -0.00030 0.00213 0.00184 0.01960

D178 -3.12386 -0.00003 -0.00027 0.00199 0.00172 -3.12214

D179 3.13820 -0.00001 -0.00011 0.00184 0.00174 3.13994

D180 -0.00343 0.00003 -0.00008 0.00170 0.00163 -0.00180

D181 -0.00636 0.00004 0.00003 0.00294 0.00298 -0.00338

D182 3.13334 0.00004 0.00002 0.00055 0.00057 3.13391

D183 3.13527 0.00001 -0.00000 0.00309 0.00309 3.13836

D184 -0.00822 0.00000 -0.00001 0.00069 0.00069 -0.00753

D185 -0.00760 0.00003 0.00017 -0.00150 -0.00133 -0.00893

D186 3.13181 0.00000 -0.00003 -0.00395 -0.00399 3.12782

D187 3.13589 0.00004 0.00018 0.00090 0.00108 3.13697

D188 -0.00789 0.00001 -0.00002 -0.00156 -0.00158 -0.00947

D189 0.01030 -0.00007 -0.00008 -0.00498 -0.00508 0.00522

D190 3.13135 -0.00000 -0.00006 -0.00328 -0.00336 3.12799

D191 -3.12911 -0.00004 0.00011 -0.00254 -0.00244 -3.13155

D192 -0.00807 0.00003 0.00014 -0.00084 -0.00071 -0.00878

D193 -3.12755 -0.00004 0.00165 -0.00211 -0.00046 -3.12800

D194 -0.00788 -0.00006 0.00137 -0.00288 -0.00151 -0.00938

D195 0.01538 -0.00007 0.00088 -0.00331 -0.00244 0.01294

D196 3.13504 -0.00009 0.00060 -0.00408 -0.00349 3.13156

D197 -3.14083 0.00007 -0.00134 0.00297 0.00163 -3.13920

D198 -0.02107 0.00001 -0.00158 0.00083 -0.00075 -0.02182

D199 -0.00057 0.00010 -0.00056 0.00419 0.00363 0.00305

D200 3.11918 0.00004 -0.00080 0.00205 0.00125 3.12043

D201 -0.01844 0.00002 -0.00056 0.00106 0.00049 -0.01794

D202 3.12360 0.00002 -0.00047 0.00074 0.00026 3.12387

D203 -3.13797 0.00004 -0.00028 0.00186 0.00157 -3.13640

D204 0.00407 0.00004 -0.00019 0.00153 0.00134 0.00541

D205 0.00650 0.00001 -0.00006 0.00041 0.00035 0.00684

D206 -3.13312 -0.00001 0.00010 -0.00010 0.00001 -3.13312

D207 -3.13554 0.00001 -0.00015 0.00073 0.00058 -3.13497

D208 0.00802 -0.00001 0.00001 0.00023 0.00024 0.00826

D209 0.00827 0.00002 0.00038 0.00047 0.00085 0.00912

D210 -3.13128 -0.00000 0.00027 -0.00059 -0.00032 -3.13159

D211 -3.13530 0.00004 0.00022 0.00098 0.00119 -3.13410

D212 0.00835 0.00001 0.00011 -0.00008 0.00002 0.00837

D213 -0.01121 -0.00008 -0.00006 -0.00281 -0.00286 -0.01407

D214 -3.13086 -0.00002 0.00018 -0.00064 -0.00046 -3.13132

D215 3.12834 -0.00005 0.00005 -0.00175 -0.00170 3.12664

D216 0.00869 0.00001 0.00029 0.00041 0.00070 0.00939

Item Value Threshold Converged?

Maximum Force 0.002829 0.000450 NO

RMS Force 0.000386 0.000300 NO

Maximum Displacement 1.152995 0.001800 NO

RMS Displacement 0.236174 0.001200 NO

Predicted change in Energy=-3.525511D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Aug 25 23:32:01 2019, MaxMem= 4294967296 cpu: 2.6

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

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.02D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.296107 -4.244770 0.449549

2 6 0 0.872463 -2.975451 0.148587

3 7 0 -0.173165 -2.114884 -0.069200

4 6 0 -1.380856 -2.778817 0.033731

5 6 0 -1.080529 -4.116354 0.368434

6 6 0 -2.673973 -2.204773 -0.159812

7 6 0 -2.951501 -0.869065 -0.307576

8 7 0 -2.047840 0.185498 -0.036376

9 6 0 -2.744276 1.304774 -0.203938

10 6 0 -4.108676 1.029910 -0.639368

11 6 0 -4.230171 -0.321965 -0.700700

12 6 0 2.243567 -2.646193 0.059222

13 6 0 2.743945 -1.304232 -0.197288

14 6 0 4.108661 -1.031799 -0.633681

15 6 0 4.229283 0.319611 -0.705165

16 6 0 2.950146 0.868967 -0.316674

17 7 0 2.046686 -0.183906 -0.038638

18 6 0 2.673849 2.205635 -0.174328

19 6 0 1.380523 2.781485 0.012999

20 6 0 1.081131 4.115792 0.360656

21 6 0 -0.295525 4.244583 0.442173

22 6 0 -0.872771 2.978837 0.128869

23 7 0 0.172227 2.120277 -0.099116

24 6 0 -2.244303 2.648466 0.047164

25 6 0 -3.811858 -3.161290 -0.195723

26 6 0 -3.832804 -4.219341 -1.115129

27 6 0 -4.905050 -5.104971 -1.144800

28 6 0 -5.961849 -4.956123 -0.246408

29 6 0 -5.946222 -3.910644 0.674935

30 6 0 -4.883389 -3.011752 0.694221

31 6 0 5.143944 -5.769981 0.578144

32 6 0 4.156340 -5.894385 -0.397806

33 6 0 3.211874 -4.886064 -0.573591

34 6 0 3.240316 -3.728776 0.220580

35 6 0 4.253165 -3.609195 1.186760

36 6 0 5.187064 -4.622997 1.371645

37 6 0 -3.241164 3.728952 0.216779

38 6 0 -4.254333 3.601930 1.182056

39 6 0 -5.187961 4.614370 1.375087

40 6 0 -5.144573 5.767943 0.591156

41 6 0 -4.156819 5.900101 -0.383619

42 6 0 -3.212608 4.893102 -0.567605

43 6 0 3.813069 3.160397 -0.201773

44 6 0 4.880991 3.004184 0.691553

45 6 0 5.943923 3.903026 0.683494

46 6 0 5.963598 4.955161 -0.230142

47 6 0 4.910778 5.110655 -1.132099

48 6 0 3.838275 4.225082 -1.113529

49 1 0 0.852089 -5.131001 0.707839

50 1 0 -1.812553 -4.885679 0.555024

51 1 0 -4.861375 1.768605 -0.869864

52 1 0 -5.101156 -0.888152 -0.993042

53 1 0 4.862011 -1.771555 -0.858520

54 1 0 5.100122 0.884304 -1.000866

55 1 0 1.813808 4.881714 0.558466

56 1 0 -0.850852 5.127738 0.712068

57 1 0 -3.017146 -4.330444 -1.820162

58 1 0 -4.916059 -5.911295 -1.870274

59 1 0 -6.794351 -5.651410 -0.266058

60 1 0 -6.762059 -3.793089 1.380028

61 1 0 -4.869238 -2.201192 1.413096

62 1 0 5.876601 -6.557901 0.717199

63 1 0 4.122447 -6.777000 -1.028140

64 1 0 2.454871 -4.985433 -1.343339

65 1 0 4.292508 -2.721239 1.808186

66 1 0 5.950360 -4.518327 2.135780

67 1 0 -4.294025 2.709233 1.796578

68 1 0 -5.951216 4.503616 2.138411

69 1 0 -5.877109 6.554808 0.736684

70 1 0 -4.122661 6.787748 -1.006829

71 1 0 -2.455857 4.999036 -1.336669

72 1 0 4.863380 2.189027 1.405074

73 1 0 6.756542 3.780379 1.391421

74 1 0 6.796143 5.650582 -0.240992

75 1 0 4.925143 5.922203 -1.851651

76 1 0 3.025690 4.341586 -1.821234

77 1 0 -0.071608 -1.121489 -0.225913

78 1 0 0.069384 1.131575 -0.281246

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

Rotational constants (GHZ): 0.0598434 0.0573352 0.0302247

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

Standard basis: 6-311G(d) (5D, 7F)

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

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5359.8086552340 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2121859385 Hartrees.

Nuclear repulsion after empirical dispersion term = 5359.5964692954 Hartrees.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5716

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.14D-09

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 332

GePol: Fraction of low-weight points (<1% of avg) = 5.81%

GePol: Cavity surface area = 612.967 Ang\*\*2

GePol: Cavity volume = 629.580 Ang\*\*3

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

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

PCM non-electrostatic energy = -0.0020960925 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5359.5943732029 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.

NBasis= 954 RedAO= T EigKep= 1.30D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 941 941 941 941 941 MxSgAt= 78 MxSgA2= 78.

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Aug 25 23:32:03 2019, MaxMem= 4294967296 cpu: 2.8

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

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= -0.000000 -0.000000 0.000000

Rot= 0.999336 -0.000005 0.000031 0.036440 Ang= -4.18 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0348 S= 1.0115

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30176207063

Leave Link 401 at Sun Aug 25 23:32:08 2019, MaxMem= 4294967296 cpu: 82.8

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 590000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 98017968.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.55D-15 for 5693.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.33D-15 for 2666 2389.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.33D-15 for 5693.

Iteration 1 A^-1\*A deviation from orthogonality is 2.68D-11 for 3393 3390.

E= -1914.23234603391

DIIS: error= 8.73D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.23234603391 IErMin= 1 ErrMin= 8.73D-03

ErrMax= 8.73D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.24D-01 BMatP= 2.24D-01

IDIUse=3 WtCom= 9.13D-01 WtEn= 8.73D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.630 Goal= None Shift= 0.000

Gap= 0.702 Goal= None Shift= 0.000

GapD= 0.630 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=3.31D-04 MaxDP=8.68D-03 OVMax= 1.63D-01

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.30D-04 CP: 9.97D-01

E= -1914.32400972805 Delta-E= -0.091663694147 Rises=F Damp=F

DIIS: error= 1.07D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.32400972805 IErMin= 2 ErrMin= 1.07D-03

ErrMax= 1.07D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.72D-03 BMatP= 2.24D-01

IDIUse=3 WtCom= 9.89D-01 WtEn= 1.07D-02

Coeff-Com: -0.468D-01 0.105D+01

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

Coeff: -0.463D-01 0.105D+01

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.061 Goal= None Shift= 0.000

RMSDP=1.20D-04 MaxDP=6.50D-03 DE=-9.17D-02 OVMax= 1.08D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.06D-04 CP: 9.96D-01 1.17D+00

E= -1914.32585414742 Delta-E= -0.001844419370 Rises=F Damp=F

DIIS: error= 1.54D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.32585414742 IErMin= 2 ErrMin= 1.07D-03

ErrMax= 1.54D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.80D-03 BMatP= 3.72D-03

IDIUse=3 WtCom= 9.85D-01 WtEn= 1.54D-02

Coeff-Com: -0.327D-01 0.553D+00 0.480D+00

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

Coeff: -0.322D-01 0.544D+00 0.488D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.062 Goal= None Shift= 0.000

RMSDP=6.08D-05 MaxDP=3.28D-03 DE=-1.84D-03 OVMax= 5.15D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.63D-05 CP: 9.96D-01 1.24D+00 1.10D+00

E= -1914.32716232712 Delta-E= -0.001308179698 Rises=F Damp=F

DIIS: error= 7.46D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.32716232712 IErMin= 4 ErrMin= 7.46D-04

ErrMax= 7.46D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.55D-04 BMatP= 3.72D-03

IDIUse=3 WtCom= 9.93D-01 WtEn= 7.46D-03

Coeff-Com: -0.692D-02 0.803D-01 0.313D+00 0.614D+00

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

Coeff: -0.687D-02 0.797D-01 0.310D+00 0.617D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=4.93D-05 MaxDP=3.10D-03 DE=-1.31D-03 OVMax= 5.05D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.10D-05 CP: 9.95D-01 1.28D+00 1.48D+00 1.18D+00

E= -1914.32776370725 Delta-E= -0.000601380133 Rises=F Damp=F

DIIS: error= 6.38D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.32776370725 IErMin= 5 ErrMin= 6.38D-04

ErrMax= 6.38D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.85D-04 BMatP= 8.55D-04

IDIUse=3 WtCom= 9.94D-01 WtEn= 6.38D-03

Coeff-Com: 0.297D-02-0.683D-01 0.127D+00 0.338D+00 0.601D+00

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

Coeff: 0.295D-02-0.679D-01 0.126D+00 0.336D+00 0.603D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=3.69D-05 MaxDP=2.19D-03 DE=-6.01D-04 OVMax= 3.98D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.05D-05 CP: 9.95D-01 1.32D+00 1.73D+00 1.51D+00 1.36D+00

E= -1914.32803830020 Delta-E= -0.000274592949 Rises=F Damp=F

DIIS: error= 5.07D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.32803830020 IErMin= 6 ErrMin= 5.07D-04

ErrMax= 5.07D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.90D-05 BMatP= 1.85D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.07D-03

Coeff-Com: 0.654D-02-0.929D-01-0.764D-01-0.253D+00 0.244D+00 0.117D+01

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

Coeff: 0.651D-02-0.924D-01-0.760D-01-0.252D+00 0.243D+00 0.117D+01

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=6.03D-05 MaxDP=3.68D-03 DE=-2.75D-04 OVMax= 6.66D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 8.97D-06 CP: 9.95D-01 1.37D+00 2.15D+00 1.97D+00 2.46D+00

CP: 2.12D+00

E= -1914.32830171092 Delta-E= -0.000263410714 Rises=F Damp=F

DIIS: error= 2.16D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.32830171092 IErMin= 7 ErrMin= 2.16D-04

ErrMax= 2.16D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.22D-05 BMatP= 6.90D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.16D-03

Coeff-Com: 0.150D-02-0.133D-01-0.341D-01-0.192D+00-0.986D-01 0.468D+00

Coeff-Com: 0.869D+00

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

Coeff-En: 0.100D+01

Coeff: 0.150D-02-0.133D-01-0.340D-01-0.192D+00-0.984D-01 0.467D+00

Coeff: 0.869D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=2.65D-05 MaxDP=1.60D-03 DE=-2.63D-04 OVMax= 2.91D-02

Cycle 8 Pass 1 IDiag 1:

RMSU= 3.98D-06 CP: 9.94D-01 1.39D+00 2.32D+00 2.16D+00 2.96D+00

CP: 2.94D+00 1.39D+00

E= -1914.32835595158 Delta-E= -0.000054240664 Rises=F Damp=F

DIIS: error= 1.20D-04 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.32835595158 IErMin= 8 ErrMin= 1.20D-04

ErrMax= 1.20D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-05 BMatP= 2.22D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.20D-03

Coeff-Com: -0.141D-02 0.245D-01 0.249D-01-0.919D-02-0.117D+00-0.106D+00

Coeff-Com: 0.514D+00 0.671D+00

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

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

Coeff: -0.141D-02 0.244D-01 0.248D-01-0.918D-02-0.117D+00-0.106D+00

Coeff: 0.513D+00 0.671D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=7.65D-06 MaxDP=4.92D-04 DE=-5.42D-05 OVMax= 8.13D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.45D-06 CP: 9.94D-01 1.39D+00 2.36D+00 2.21D+00 3.00D+00

CP: 3.00D+00 1.63D+00 1.27D+00

E= -1914.32836935747 Delta-E= -0.000013405886 Rises=F Damp=F

DIIS: error= 8.43D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.32836935747 IErMin= 9 ErrMin= 8.43D-05

ErrMax= 8.43D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.03D-06 BMatP= 1.05D-05

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

Coeff-Com: -0.451D-03 0.352D-02 0.187D-01 0.548D-01 0.109D-01-0.141D+00

Coeff-Com: -0.215D+00 0.184D+00 0.108D+01

Coeff: -0.451D-03 0.352D-02 0.187D-01 0.548D-01 0.109D-01-0.141D+00

Coeff: -0.215D+00 0.184D+00 0.108D+01

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=8.83D-06 MaxDP=5.54D-04 DE=-1.34D-05 OVMax= 9.59D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.55D-06 CP: 9.94D-01 1.40D+00 2.41D+00 2.26D+00 3.00D+00

CP: 3.00D+00 1.87D+00 1.95D+00 2.06D+00

E= -1914.32837921418 Delta-E= -0.000009856717 Rises=F Damp=F

DIIS: error= 5.37D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.32837921418 IErMin=10 ErrMin= 5.37D-05

ErrMax= 5.37D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.19D-06 BMatP= 3.03D-06

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

Coeff-Com: 0.434D-03-0.107D-01 0.305D-02 0.447D-01 0.611D-01-0.514D-01

Coeff-Com: -0.438D+00-0.148D+00 0.825D+00 0.715D+00

Coeff: 0.434D-03-0.107D-01 0.305D-02 0.447D-01 0.611D-01-0.514D-01

Coeff: -0.438D+00-0.148D+00 0.825D+00 0.715D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.75D-06 MaxDP=4.79D-04 DE=-9.86D-06 OVMax= 8.47D-03

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.36D-06 CP: 9.94D-01 1.40D+00 2.45D+00 2.32D+00 3.00D+00

CP: 3.00D+00 2.08D+00 2.40D+00 3.00D+00 1.58D+00

E= -1914.32838457829 Delta-E= -0.000005364110 Rises=F Damp=F

DIIS: error= 2.98D-05 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.32838457829 IErMin=11 ErrMin= 2.98D-05

ErrMax= 2.98D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.12D-07 BMatP= 2.19D-06

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

Coeff-Com: 0.303D-03-0.550D-02-0.175D-02 0.424D-02 0.255D-01 0.250D-01

Coeff-Com: -0.128D+00-0.105D+00-0.113D+00 0.320D+00 0.978D+00

Coeff: 0.303D-03-0.550D-02-0.175D-02 0.424D-02 0.255D-01 0.250D-01

Coeff: -0.128D+00-0.105D+00-0.113D+00 0.320D+00 0.978D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.68D-06 MaxDP=2.78D-04 DE=-5.36D-06 OVMax= 4.99D-03

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.73D-06 CP: 9.94D-01 1.41D+00 2.47D+00 2.34D+00 3.00D+00

CP: 3.00D+00 2.21D+00 2.79D+00 3.00D+00 2.08D+00

CP: 1.43D+00

E= -1914.32838641913 Delta-E= -0.000001840841 Rises=F Damp=F

DIIS: error= 1.24D-05 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.32838641913 IErMin=12 ErrMin= 1.24D-05

ErrMax= 1.24D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.90D-07 BMatP= 5.12D-07

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

Coeff-Com: 0.488D-04 0.369D-03-0.278D-02-0.177D-01-0.103D-01 0.314D-01

Coeff-Com: 0.904D-01 0.143D-01-0.332D+00-0.112D+00 0.441D+00 0.897D+00

Coeff: 0.488D-04 0.369D-03-0.278D-02-0.177D-01-0.103D-01 0.314D-01

Coeff: 0.904D-01 0.143D-01-0.332D+00-0.112D+00 0.441D+00 0.897D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.09D-06 MaxDP=1.82D-04 DE=-1.84D-06 OVMax= 3.35D-03

Cycle 13 Pass 1 IDiag 1:

RMSU= 3.68D-07 CP: 9.94D-01 1.41D+00 2.49D+00 2.36D+00 3.00D+00

CP: 3.00D+00 2.29D+00 2.97D+00 3.00D+00 2.41D+00

CP: 1.94D+00 1.59D+00

E= -1914.32838694401 Delta-E= -0.000000524871 Rises=F Damp=F

DIIS: error= 6.68D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.32838694401 IErMin=13 ErrMin= 6.68D-06

ErrMax= 6.68D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.94D-08 BMatP= 1.90D-07

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

Coeff-Com: -0.119D-03 0.254D-02 0.121D-02-0.652D-02-0.960D-02 0.125D-02

Coeff-Com: 0.866D-01 0.466D-01-0.120D+00-0.190D+00-0.122D+00 0.516D+00

Coeff-Com: 0.794D+00

Coeff: -0.119D-03 0.254D-02 0.121D-02-0.652D-02-0.960D-02 0.125D-02

Coeff: 0.866D-01 0.466D-01-0.120D+00-0.190D+00-0.122D+00 0.516D+00

Coeff: 0.794D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=8.19D-07 MaxDP=5.32D-05 DE=-5.25D-07 OVMax= 8.13D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 4.02D-07 CP: 9.94D-01 1.41D+00 2.49D+00 2.36D+00 3.00D+00

CP: 3.00D+00 2.32D+00 3.00D+00 3.00D+00 2.46D+00

CP: 2.01D+00 1.81D+00 8.61D-01

E= -1914.32838705177 Delta-E= -0.000000107764 Rises=F Damp=F

DIIS: error= 2.54D-06 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.32838705177 IErMin=14 ErrMin= 2.54D-06

ErrMax= 2.54D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.53D-08 BMatP= 6.94D-08

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

Coeff-Com: -0.556D-04 0.931D-03 0.998D-03 0.305D-03-0.225D-02-0.590D-02

Coeff-Com: 0.182D-01 0.173D-01 0.213D-01-0.694D-01-0.144D+00 0.507D-04

Coeff-Com: 0.377D+00 0.786D+00

Coeff: -0.556D-04 0.931D-03 0.998D-03 0.305D-03-0.225D-02-0.590D-02

Coeff: 0.182D-01 0.173D-01 0.213D-01-0.694D-01-0.144D+00 0.507D-04

Coeff: 0.377D+00 0.786D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.65D-07 MaxDP=3.06D-05 DE=-1.08D-07 OVMax= 5.62D-04

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.36D-07 CP: 9.94D-01 1.41D+00 2.49D+00 2.37D+00 3.00D+00

CP: 3.00D+00 2.33D+00 3.00D+00 3.00D+00 2.52D+00

CP: 2.11D+00 1.93D+00 1.04D+00 1.33D+00

E= -1914.32838707649 Delta-E= -0.000000024720 Rises=F Damp=F

DIIS: error= 1.03D-06 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.32838707649 IErMin=15 ErrMin= 1.03D-06

ErrMax= 1.03D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.04D-09 BMatP= 1.53D-08

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

Coeff-Com: 0.285D-05-0.208D-03 0.304D-03 0.190D-02 0.151D-02-0.290D-02

Coeff-Com: -0.135D-01-0.272D-02 0.454D-01 0.985D-02-0.425D-01-0.162D+00

Coeff-Com: 0.109D-01 0.424D+00 0.729D+00

Coeff: 0.285D-05-0.208D-03 0.304D-03 0.190D-02 0.151D-02-0.290D-02

Coeff: -0.135D-01-0.272D-02 0.454D-01 0.985D-02-0.425D-01-0.162D+00

Coeff: 0.109D-01 0.424D+00 0.729D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.03D-07 MaxDP=1.12D-05 DE=-2.47D-08 OVMax= 1.87D-04

Cycle 16 Pass 1 IDiag 1:

RMSU= 4.30D-08 CP: 9.94D-01 1.41D+00 2.49D+00 2.37D+00 3.00D+00

CP: 3.00D+00 2.33D+00 3.00D+00 3.00D+00 2.54D+00

CP: 2.15D+00 1.98D+00 1.10D+00 1.52D+00 1.21D+00

E= -1914.32838708100 Delta-E= -0.000000004506 Rises=F Damp=F

DIIS: error= 4.55D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1914.32838708100 IErMin=16 ErrMin= 4.55D-07

ErrMax= 4.55D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.18D-10 BMatP= 4.04D-09

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

Coeff-Com: 0.104D-04-0.239D-03-0.376D-04 0.724D-03 0.902D-03-0.345D-03

Coeff-Com: -0.882D-02-0.388D-02 0.145D-01 0.151D-01 0.106D-01-0.690D-01

Coeff-Com: -0.552D-01 0.151D-01 0.294D+00 0.787D+00

Coeff: 0.104D-04-0.239D-03-0.376D-04 0.724D-03 0.902D-03-0.345D-03

Coeff: -0.882D-02-0.388D-02 0.145D-01 0.151D-01 0.106D-01-0.690D-01

Coeff: -0.552D-01 0.151D-01 0.294D+00 0.787D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.00D-07 MaxDP=5.76D-06 DE=-4.51D-09 OVMax= 1.05D-04

Cycle 17 Pass 1 IDiag 1:

RMSU= 1.97D-08 CP: 9.94D-01 1.41D+00 2.49D+00 2.37D+00 3.00D+00

CP: 3.00D+00 2.34D+00 3.00D+00 3.00D+00 2.55D+00

CP: 2.16D+00 2.00D+00 1.14D+00 1.56D+00 1.35D+00

CP: 1.14D+00

E= -1914.32838708175 Delta-E= -0.000000000754 Rises=F Damp=F

DIIS: error= 2.78D-07 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1914.32838708175 IErMin=17 ErrMin= 2.78D-07

ErrMax= 2.78D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.33D-10 BMatP= 6.18D-10

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

Coeff-Com: 0.345D-05-0.497D-04-0.664D-04-0.131D-03 0.938D-04 0.541D-03

Coeff-Com: -0.364D-03-0.105D-02-0.430D-02 0.286D-02 0.138D-01 0.788D-02

Coeff-Com: -0.210D-01-0.860D-01-0.394D-01 0.292D+00 0.835D+00

Coeff: 0.345D-05-0.497D-04-0.664D-04-0.131D-03 0.938D-04 0.541D-03

Coeff: -0.364D-03-0.105D-02-0.430D-02 0.286D-02 0.138D-01 0.788D-02

Coeff: -0.210D-01-0.860D-01-0.394D-01 0.292D+00 0.835D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.71D-08 MaxDP=1.67D-06 DE=-7.54D-10 OVMax= 2.46D-05

Cycle 18 Pass 1 IDiag 1:

RMSU= 1.07D-08 CP: 9.94D-01 1.41D+00 2.49D+00 2.37D+00 3.00D+00

CP: 3.00D+00 2.34D+00 3.00D+00 3.00D+00 2.55D+00

CP: 2.17D+00 2.00D+00 1.15D+00 1.58D+00 1.39D+00

CP: 1.29D+00 1.21D+00

E= -1914.32838708192 Delta-E= -0.000000000170 Rises=F Damp=F

DIIS: error= 1.78D-07 at cycle 18 NSaved= 18.

NSaved=18 IEnMin=18 EnMin= -1914.32838708192 IErMin=18 ErrMin= 1.78D-07

ErrMax= 1.78D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.23D-11 BMatP= 1.33D-10

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

Coeff-Com: -0.141D-06 0.281D-04-0.412D-04-0.322D-03-0.188D-03 0.519D-03

Coeff-Com: 0.235D-02 0.328D-03-0.683D-02-0.282D-02 0.547D-02 0.247D-01

Coeff-Com: 0.303D-02-0.579D-01-0.107D+00-0.662D-01 0.479D+00 0.725D+00

Coeff: -0.141D-06 0.281D-04-0.412D-04-0.322D-03-0.188D-03 0.519D-03

Coeff: 0.235D-02 0.328D-03-0.683D-02-0.282D-02 0.547D-02 0.247D-01

Coeff: 0.303D-02-0.579D-01-0.107D+00-0.662D-01 0.479D+00 0.725D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.88D-08 MaxDP=1.12D-06 DE=-1.70D-10 OVMax= 1.82D-05

Cycle 19 Pass 1 IDiag 1:

RMSU= 5.41D-09 CP: 9.94D-01 1.41D+00 2.49D+00 2.37D+00 3.00D+00

CP: 3.00D+00 2.34D+00 3.00D+00 3.00D+00 2.55D+00

CP: 2.17D+00 2.01D+00 1.15D+00 1.58D+00 1.42D+00

CP: 1.36D+00 1.51D+00 1.24D+00

E= -1914.32838708196 Delta-E= -0.000000000044 Rises=F Damp=F

DIIS: error= 7.57D-08 at cycle 19 NSaved= 19.

NSaved=19 IEnMin=19 EnMin= -1914.32838708196 IErMin=19 ErrMin= 7.57D-08

ErrMax= 7.57D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.63D-11 BMatP= 6.23D-11

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

Coeff-Com: -0.134D-05 0.322D-04 0.115D-04-0.104D-03-0.123D-03 0.614D-04

Coeff-Com: 0.132D-02 0.499D-03-0.179D-02-0.262D-02-0.249D-02 0.100D-01

Coeff-Com: 0.107D-01 0.409D-02-0.373D-01-0.159D+00-0.895D-01 0.367D+00

Coeff-Com: 0.899D+00

Coeff: -0.134D-05 0.322D-04 0.115D-04-0.104D-03-0.123D-03 0.614D-04

Coeff: 0.132D-02 0.499D-03-0.179D-02-0.262D-02-0.249D-02 0.100D-01

Coeff: 0.107D-01 0.409D-02-0.373D-01-0.159D+00-0.895D-01 0.367D+00

Coeff: 0.899D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=8.28D-09 MaxDP=5.93D-07 DE=-4.37D-11 OVMax= 5.72D-06

Error on total polarization charges = 0.08258

SCF Done: E(UB3LYP) = -1914.32838708 A.U. after 19 cycles

NFock= 19 Conv=0.83D-08 -V/T= 2.0041

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0349 S= 1.0116

<L.S>= 0.000000000000E+00

KE= 1.906427270107D+03 PE=-1.516882463620D+04 EE= 5.988474605807D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0349, after 2.0008

Leave Link 502 at Sun Aug 25 23:40:54 2019, MaxMem= 4294967296 cpu: 8332.1

(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: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.46857340D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.63750495D-01

Leave Link 801 at Sun Aug 25 23:40:54 2019, MaxMem= 4294967296 cpu: 0.9

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

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

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

Leave Link 1101 at Sun Aug 25 23:41:01 2019, MaxMem= 4294967296 cpu: 112.1

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

Symmetrizing basis deriv contribution to polar:

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

Leave Link 1102 at Sun Aug 25 23:41:01 2019, MaxMem= 4294967296 cpu: 2.1

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

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 190

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 Mon Aug 26 00:01:00 2019, MaxMem= 4294967296 cpu: 19174.9

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

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 590000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 4.54D+03 3.33D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 3.63D+02 2.58D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 6.40D+00 3.83D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 7.76D-02 2.91D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 4.72D-04 1.69D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 3.14D-06 1.01D-04.

189 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 1.70D-08 6.56D-06.

79 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 6.69D-11 3.97D-07.

32 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 3.52D-13 2.08D-08.

4 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 7.59D-15 2.73D-09.

3 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 3.06D-15 1.87D-09.

3 vectors produced by pass 11 Test12= 2.55D-13 1.00D-09 XBig12= 6.27D-15 2.35D-09.

3 vectors produced by pass 12 Test12= 2.55D-13 1.00D-09 XBig12= 7.15D-15 2.52D-09.

3 vectors produced by pass 13 Test12= 2.55D-13 1.00D-09 XBig12= 8.49D-15 2.20D-09.

3 vectors produced by pass 14 Test12= 2.55D-13 1.00D-09 XBig12= 4.67D-15 1.99D-09.

3 vectors produced by pass 15 Test12= 2.55D-13 1.00D-09 XBig12= 8.54D-15 2.63D-09.

3 vectors produced by pass 16 Test12= 2.55D-13 1.00D-09 XBig12= 7.15D-15 2.93D-09.

3 vectors produced by pass 17 Test12= 2.55D-13 1.00D-09 XBig12= 8.49D-15 2.52D-09.

3 vectors produced by pass 18 Test12= 2.55D-13 1.00D-09 XBig12= 7.03D-15 2.20D-09.

3 vectors produced by pass 19 Test12= 2.55D-13 1.00D-09 XBig12= 9.37D-15 3.04D-09.

3 vectors produced by pass 20 Test12= 2.55D-13 1.00D-09 XBig12= 5.20D-15 1.82D-09.

3 vectors produced by pass 21 Test12= 2.55D-13 1.00D-09 XBig12= 9.23D-15 2.84D-09.

3 vectors produced by pass 22 Test12= 2.55D-13 1.00D-09 XBig12= 1.01D-14 3.41D-09.

3 vectors produced by pass 23 Test12= 2.55D-13 1.00D-09 XBig12= 1.03D-14 2.88D-09.

3 vectors produced by pass 24 Test12= 2.55D-13 1.00D-09 XBig12= 6.74D-15 2.06D-09.

3 vectors produced by pass 25 Test12= 2.55D-13 1.00D-09 XBig12= 5.31D-15 2.13D-09.

1 vectors produced by pass 26 Test12= 2.55D-13 1.00D-09 XBig12= 2.94D-15 1.44D-09.

InvSVY: IOpt=1 It= 1 EMax= 1.42D-14

Solved reduced A of dimension 1760 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1128.21 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 Mon Aug 26 03:57:38 2019, MaxMem= 4294967296 cpu: 227095.4

(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.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 190

Leave Link 701 at Mon Aug 26 03:59:07 2019, MaxMem= 4294967296 cpu: 1421.6

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

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

Leave Link 702 at Mon Aug 26 03:59:07 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

Leave Link 703 at Mon Aug 26 04:17:45 2019, MaxMem= 4294967296 cpu: 17887.9

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

Dipole = 3.96592380D-03 8.89375290D-03-2.73201014D-01

Polarizability= 1.40753019D+03-1.66760695D+02 1.52196824D+03

-1.24269488D-03-3.34359085D-01 4.55124630D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.001869515 0.000388006 0.001939895

2 6 0.004012601 -0.002151554 0.001621916

3 7 -0.001182239 0.002138795 -0.004943869

4 6 -0.001698542 -0.003020325 0.003631559

5 6 0.000983558 -0.001228267 -0.000447464

6 6 0.009764345 0.000863083 0.001942681

7 6 -0.013289542 -0.001970479 0.002608063

8 7 0.012588936 0.003125785 0.002570449

9 6 -0.015605393 -0.002806075 -0.002582647

10 6 -0.001098412 -0.000144103 -0.001686848

11 6 -0.002664185 -0.001554869 -0.001414106

12 6 -0.007880371 0.003083827 0.003027570

13 6 0.015588218 -0.002703944 0.002568050

14 6 0.001124007 -0.000080836 0.001649084

15 6 0.002637319 -0.001698895 0.001430333

16 6 0.013334718 -0.002153222 -0.002567436

17 7 -0.012613582 0.003285366 -0.002551893

18 6 -0.009796743 0.000971690 -0.001963091

19 6 0.001671239 -0.002974677 -0.003645328

20 6 -0.000972057 -0.001286243 0.000443876

21 6 0.001872021 0.000365219 -0.001930534

22 6 -0.003973258 -0.002316744 -0.001690372

23 7 0.001200904 0.002148233 0.004962034

24 6 0.007849580 0.003258077 -0.002981916

25 6 0.000280647 0.001995802 0.000610026

26 6 -0.000108846 -0.000249967 -0.000303542

27 6 -0.000000871 0.000133173 -0.000211848

28 6 0.000296019 0.000099961 -0.000075336

29 6 -0.000321266 0.000100934 -0.000172903

30 6 0.001066215 -0.000396882 0.000335945

31 6 -0.000249934 -0.000154918 -0.000023351

32 6 -0.000201069 0.000293432 -0.000288110

33 6 0.000108583 -0.000360124 -0.000696020

34 6 0.000139326 0.000147765 0.000241455

35 6 -0.000305475 -0.000410101 -0.000274130

36 6 0.000051480 0.000640505 0.000414468

37 6 -0.000158375 0.000193893 -0.000267027

38 6 0.000310208 -0.000374015 0.000272256

39 6 -0.000043331 0.000630249 -0.000405649

40 6 0.000247924 -0.000162770 0.000013378

41 6 0.000205999 0.000308084 0.000289208

42 6 -0.000140615 -0.000341111 0.000696105

43 6 -0.000273385 0.002107898 -0.000600982

44 6 -0.001100016 -0.000431416 -0.000337615

45 6 0.000329166 0.000118364 0.000179077

46 6 -0.000308100 0.000105387 0.000078119

47 6 0.000019249 0.000155281 0.000222344

48 6 0.000114126 -0.000265590 0.000289263

49 1 0.000351155 0.000305219 -0.000112022

50 1 0.000180752 0.000350931 0.000310917

51 1 -0.000191060 0.000356424 0.000174358

52 1 0.000056884 0.000521223 0.000371566

53 1 0.000198456 0.000344686 -0.000180766

54 1 -0.000044677 0.000540407 -0.000373280

55 1 -0.000180625 0.000351234 -0.000313155

56 1 -0.000367952 0.000284495 0.000108045

57 1 0.000208954 -0.000114503 0.000113057

58 1 0.000049617 0.000059792 -0.000089165

59 1 0.000073736 -0.000052532 0.000046665

60 1 -0.000018110 0.000022294 -0.000100650

61 1 0.000099674 -0.000316144 0.000024135

62 1 0.000023579 -0.000031098 -0.000070414

63 1 -0.000100956 0.000016412 -0.000024938

64 1 0.000076545 -0.000144352 -0.000049186

65 1 0.000135628 -0.000049549 -0.000154786

66 1 -0.000095636 0.000091435 -0.000040484

67 1 -0.000135012 -0.000046888 0.000167997

68 1 0.000092754 0.000095147 0.000041556

69 1 -0.000021012 -0.000026087 0.000075457

70 1 0.000096979 0.000009486 0.000021849

71 1 -0.000046129 -0.000139800 0.000071501

72 1 -0.000097811 -0.000315509 -0.000032680

73 1 0.000015621 0.000025193 0.000102808

74 1 -0.000076524 -0.000047776 -0.000044679

75 1 -0.000052957 0.000060524 0.000086858

76 1 -0.000209437 -0.000121412 -0.000122141

77 1 -0.000174246 0.000317357 -0.000042517

78 1 0.000210540 0.000231706 0.000058958

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

Cartesian Forces: Max 0.015605393 RMS 0.002800790

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

Leave Link 716 at Mon Aug 26 04:17:45 2019, MaxMem= 4294967296 cpu: 1.9

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.012328454 RMS 0.001437511

Search for a local minimum.

Step number 3 out of a maximum of 452

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

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -1.41D-04 DEPred=-3.53D-03 R= 4.00D-02

Trust test= 4.00D-02 RLast= 4.26D-01 DXMaxT set to 1.50D-01

ITU= -1 1 0

Eigenvalues --- 0.00230 0.00246 0.00535 0.00586 0.00627

Eigenvalues --- 0.00675 0.00835 0.00958 0.01038 0.01106

Eigenvalues --- 0.01137 0.01221 0.01233 0.01295 0.01302

Eigenvalues --- 0.01358 0.01377 0.01418 0.01426 0.01478

Eigenvalues --- 0.01604 0.01614 0.01656 0.01674 0.01690

Eigenvalues --- 0.01703 0.01732 0.01735 0.01760 0.01766

Eigenvalues --- 0.01778 0.01785 0.01795 0.01799 0.01829

Eigenvalues --- 0.01841 0.01926 0.02089 0.02173 0.02199

Eigenvalues --- 0.02215 0.02284 0.02304 0.02336 0.02356

Eigenvalues --- 0.02367 0.02406 0.02462 0.02539 0.02544

Eigenvalues --- 0.02559 0.02569 0.02626 0.02631 0.02666

Eigenvalues --- 0.02680 0.02716 0.02781 0.02789 0.02808

Eigenvalues --- 0.02811 0.02862 0.02866 0.02873 0.02881

Eigenvalues --- 0.02935 0.02943 0.03720 0.04019 0.04253

Eigenvalues --- 0.04333 0.04378 0.04443 0.04541 0.04623

Eigenvalues --- 0.07950 0.08514 0.09642 0.09748 0.09782

Eigenvalues --- 0.09877 0.10239 0.10417 0.10424 0.10663

Eigenvalues --- 0.10722 0.10730 0.10731 0.10735 0.10739

Eigenvalues --- 0.11400 0.11404 0.11409 0.11419 0.11966

Eigenvalues --- 0.11981 0.11989 0.11990 0.12313 0.12316

Eigenvalues --- 0.12318 0.12327 0.12756 0.12759 0.12777

Eigenvalues --- 0.12789 0.15601 0.15795 0.16360 0.16804

Eigenvalues --- 0.17472 0.17607 0.17733 0.17807 0.18185

Eigenvalues --- 0.18277 0.18375 0.18846 0.19240 0.19277

Eigenvalues --- 0.19348 0.19390 0.19413 0.19427 0.19444

Eigenvalues --- 0.19464 0.19541 0.19543 0.19560 0.19562

Eigenvalues --- 0.19933 0.20479 0.22022 0.22062 0.22364

Eigenvalues --- 0.23355 0.23638 0.23881 0.24576 0.25010

Eigenvalues --- 0.26063 0.26851 0.27180 0.27255 0.28309

Eigenvalues --- 0.28345 0.28970 0.29023 0.29809 0.30696

Eigenvalues --- 0.30777 0.31911 0.31962 0.32356 0.32485

Eigenvalues --- 0.33567 0.34429 0.34853 0.35414 0.35544

Eigenvalues --- 0.35597 0.35643 0.35685 0.35707 0.35715

Eigenvalues --- 0.35732 0.35773 0.35832 0.35869 0.35890

Eigenvalues --- 0.35902 0.35913 0.35970 0.35973 0.36000

Eigenvalues --- 0.36049 0.36116 0.36123 0.36212 0.36355

Eigenvalues --- 0.36441 0.36521 0.37169 0.37218 0.37339

Eigenvalues --- 0.37373 0.37999 0.38066 0.38264 0.38332

Eigenvalues --- 0.39944 0.40432 0.41050 0.41103 0.41136

Eigenvalues --- 0.41185 0.41244 0.41268 0.41454 0.41500

Eigenvalues --- 0.41594 0.41845 0.43901 0.44038 0.45383

Eigenvalues --- 0.45673 0.45694 0.45879 0.46027 0.46084

Eigenvalues --- 0.46148 0.46178 0.46229 0.46416 0.46430

Eigenvalues --- 0.46542 0.46743 0.46937 0.50592 0.50607

Eigenvalues --- 0.50902 0.50912 0.51608 0.52123 0.54874

Eigenvalues --- 0.54968 0.56758 0.57403

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 1.00877 -0.00877

Cosine: 1.000 > 0.970

Length: 1.004

GDIIS step was calculated using 2 of the last 3 vectors.

Maximum step size ( 0.150) exceeded in Quadratic search.

-- Step size scaled by 0.337

Iteration 1 RMS(Cart)= 0.14699147 RMS(Int)= 0.00199402

Iteration 2 RMS(Cart)= 0.00621963 RMS(Int)= 0.00024337

Iteration 3 RMS(Cart)= 0.00000825 RMS(Int)= 0.00024337

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00024337

ITry= 1 IFail=0 DXMaxC= 7.30D-01 DCOld= 1.00D+10 DXMaxT= 1.50D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.69505 -0.00216 -0.00006 -0.02739 -0.02739 2.66767

R2 2.61725 0.00035 0.00009 0.02281 0.02317 2.64042

R3 2.03638 0.00014 -0.00000 0.00004 0.00004 2.03642

R4 2.59199 0.00317 -0.00003 -0.00073 -0.00095 2.59104

R5 2.67002 -0.00095 0.00008 0.03460 0.03467 2.70469

R6 2.61160 -0.00287 0.00001 -0.00403 -0.00423 2.60737

R7 1.91013 0.00022 -0.00000 0.00061 0.00060 1.91073

R8 2.66661 0.00148 -0.00012 -0.01943 -0.01944 2.64717

R9 2.69850 0.00140 0.00014 0.02603 0.02622 2.72471

R10 2.03752 -0.00012 0.00000 -0.00028 -0.00028 2.03724

R11 2.59311 0.01228 -0.00026 -0.00400 -0.00424 2.58887

R12 2.80991 0.00104 0.00001 0.00005 0.00007 2.80998

R13 2.67398 -0.00543 0.00017 -0.01912 -0.01925 2.65473

R14 2.73120 0.00355 0.00007 0.02063 0.02080 2.75200

R15 2.51119 0.00964 -0.00016 0.02382 0.02342 2.53461

R16 2.75585 -0.00080 0.00012 0.01547 0.01567 2.77152

R17 2.75053 -0.00916 0.00006 -0.05615 -0.05614 2.69439

R18 2.56759 0.00026 -0.00009 -0.01521 -0.01498 2.55261

R19 2.03999 0.00007 0.00000 -0.00090 -0.00090 2.03908

R20 2.03937 -0.00011 -0.00000 -0.00029 -0.00029 2.03908

R21 2.74956 -0.00913 0.00006 -0.05542 -0.05538 2.69418

R22 2.79752 -0.00099 -0.00001 0.00291 0.00289 2.80041

R23 2.75609 -0.00083 0.00012 0.01523 0.01543 2.77153

R24 2.51161 0.00964 -0.00016 0.02369 0.02330 2.53491

R25 2.56750 0.00028 -0.00009 -0.01510 -0.01488 2.55262

R26 2.03997 0.00006 0.00000 -0.00086 -0.00086 2.03910

R27 2.73123 0.00355 0.00007 0.02064 0.02080 2.75204

R28 2.03940 -0.00011 -0.00000 -0.00031 -0.00031 2.03909

R29 2.67387 -0.00548 0.00017 -0.01923 -0.01931 2.65456

R30 2.59332 0.01233 -0.00026 -0.00396 -0.00419 2.58914

R31 2.69866 0.00140 0.00014 0.02596 0.02613 2.72479

R32 2.80937 0.00104 0.00001 0.00007 0.00009 2.80946

R33 2.66637 0.00149 -0.00012 -0.01929 -0.01929 2.64709

R34 2.61148 -0.00286 0.00001 -0.00401 -0.00425 2.60723

R35 2.61740 0.00035 0.00009 0.02277 0.02314 2.64054

R36 2.03756 -0.00012 0.00000 -0.00028 -0.00028 2.03728

R37 2.69476 -0.00215 -0.00006 -0.02731 -0.02731 2.66744

R38 2.03635 0.00015 -0.00000 0.00012 0.00012 2.03646

R39 2.59184 0.00321 -0.00003 -0.00071 -0.00095 2.59089

R40 2.67042 -0.00100 0.00008 0.03444 0.03448 2.70490

R41 1.90973 0.00025 -0.00000 0.00069 0.00069 1.91042

R42 2.79651 -0.00100 -0.00001 0.00341 0.00340 2.79991

R43 2.64914 0.00020 -0.00000 0.00011 0.00011 2.64924

R44 2.64733 0.00038 -0.00001 -0.00048 -0.00049 2.64684

R45 2.62864 0.00034 -0.00001 -0.00009 -0.00010 2.62854

R46 2.04817 0.00002 -0.00000 0.00024 0.00024 2.04841

R47 2.63621 -0.00014 0.00001 0.00053 0.00053 2.63674

R48 2.04980 0.00007 -0.00000 0.00013 0.00013 2.04993

R49 2.63354 0.00008 -0.00001 -0.00048 -0.00049 2.63305

R50 2.05004 0.00002 0.00000 0.00000 0.00000 2.05005

R51 2.63072 0.00015 0.00001 0.00074 0.00075 2.63147

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R54 2.63433 0.00013 0.00000 0.00127 0.00128 2.63561

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R56 2.05011 -0.00003 0.00000 0.00004 0.00004 2.05014

R57 2.63183 -0.00055 0.00000 -0.00136 -0.00136 2.63047

R58 2.05057 -0.00007 0.00000 -0.00009 -0.00009 2.05048

R59 2.65292 -0.00046 0.00001 -0.00018 -0.00017 2.65274

R60 2.04880 -0.00006 0.00000 0.00004 0.00004 2.04884

R61 2.65482 -0.00025 0.00001 -0.00187 -0.00187 2.65296

R62 2.62811 0.00003 0.00000 0.00131 0.00131 2.62942

R63 2.04945 -0.00008 0.00000 -0.00037 -0.00036 2.04908

R64 2.05057 -0.00008 0.00000 -0.00010 -0.00010 2.05047

R65 2.65532 -0.00029 0.00001 -0.00207 -0.00206 2.65326

R66 2.65324 -0.00046 0.00001 -0.00037 -0.00037 2.65288

R67 2.62798 0.00002 0.00000 0.00138 0.00138 2.62936

R68 2.04939 -0.00008 0.00000 -0.00032 -0.00031 2.04908

R69 2.63694 -0.00007 -0.00000 -0.00160 -0.00160 2.63534

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R71 2.63433 0.00015 0.00000 0.00125 0.00126 2.63558

R72 2.05011 -0.00004 0.00000 0.00004 0.00004 2.05015

R73 2.63170 -0.00055 0.00000 -0.00127 -0.00127 2.63043

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R75 2.04872 -0.00004 -0.00000 0.00008 0.00008 2.04880

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R77 2.64932 0.00019 -0.00000 0.00010 0.00010 2.64942

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A3 2.21820 -0.00011 0.00001 -0.00230 -0.00224 2.21596

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A6 2.19385 -0.00008 -0.00003 -0.00178 -0.00266 2.19119

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A9 2.17912 0.00036 0.00001 0.00324 0.00311 2.18223

A10 1.86194 0.00058 0.00001 0.00562 0.00559 1.86753

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A13 1.88949 -0.00012 -0.00000 -0.00499 -0.00508 1.88441

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A16 2.20067 -0.00131 0.00002 0.00289 0.00193 2.20260

A17 2.02379 -0.00077 -0.00005 -0.00904 -0.00862 2.01516

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A21 1.91242 -0.00050 -0.00005 0.00168 0.00151 1.91393

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A25 2.14943 -0.00121 -0.00005 0.00084 0.00171 2.15115

A26 1.85946 -0.00130 0.00001 0.00272 0.00263 1.86209

A27 2.19830 0.00047 -0.00002 -0.00126 -0.00129 2.19701

A28 2.22541 0.00083 0.00001 -0.00156 -0.00156 2.22385

A29 1.86006 0.00226 0.00001 0.00190 0.00186 1.86192

A30 2.20076 -0.00132 -0.00001 -0.00233 -0.00233 2.19844

A31 2.22232 -0.00095 -0.00000 0.00037 0.00038 2.22270

A32 2.16495 0.00088 -0.00006 0.01077 0.00945 2.17439

A33 2.06698 -0.00085 0.00005 -0.02350 -0.02293 2.04405

A34 2.05120 -0.00003 0.00000 0.01298 0.01348 2.06468

A35 2.14937 -0.00121 -0.00005 0.00087 0.00168 2.15104

A36 2.18460 0.00195 0.00003 0.00851 0.00762 2.19222

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A38 1.85940 -0.00130 0.00001 0.00273 0.00266 1.86205

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A104 2.08939 -0.00008 0.00000 -0.00024 -0.00024 2.08915

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D2 -3.09434 0.00015 0.00005 -0.00476 -0.00482 -3.09916

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D5 -0.01047 0.00007 -0.00003 0.00549 0.00561 -0.00487

D6 -3.12175 -0.00025 -0.00001 -0.00498 -0.00488 -3.12663

D7 3.11498 0.00026 -0.00001 0.00842 0.00842 3.12340

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D13 -3.09257 -0.00017 -0.00020 0.06711 0.06719 -3.02538

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D47 -3.08647 -0.00035 -0.00001 -0.02076 -0.02084 -3.10730

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D49 0.33106 -0.00100 0.00028 -0.14797 -0.14756 0.18349

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D58 0.32158 -0.00092 0.00027 -0.14019 -0.13976 0.18182

D59 0.28018 -0.00058 0.00026 -0.09783 -0.09699 0.18319

D60 -2.83195 -0.00111 0.00025 -0.11556 -0.11484 -2.94678

D61 0.96218 -0.00055 -0.00007 0.02590 0.02575 0.98793

D62 -2.18397 -0.00069 -0.00008 0.03440 0.03425 -2.14972

D63 -2.16818 -0.00038 -0.00005 0.00247 0.00250 -2.16568

D64 0.96887 -0.00052 -0.00005 0.01097 0.01099 0.97986

D65 -3.09014 -0.00029 -0.00001 -0.01916 -0.01925 -3.10939

D66 0.05802 -0.00008 -0.00002 -0.00389 -0.00390 0.05412

D67 0.02554 0.00022 0.00000 -0.00332 -0.00347 0.02207

D68 -3.10949 0.00043 -0.00001 0.01195 0.01189 -3.09760

D69 3.07625 0.00015 0.00000 0.01483 0.01491 3.09115

D70 -0.03880 -0.00031 -0.00001 -0.00126 -0.00122 -0.04002

D71 -0.00040 -0.00016 0.00001 0.00589 0.00603 0.00563

D72 -3.13321 0.00031 -0.00001 0.01338 0.01341 -3.11981

D73 3.13450 -0.00038 0.00002 -0.00968 -0.00963 3.12486

D74 0.00169 0.00009 0.00000 -0.00220 -0.00226 -0.00057

D75 -0.02300 -0.00008 -0.00001 -0.00723 -0.00736 -0.03036

D76 3.06611 0.00038 -0.00007 0.01112 0.01092 3.07703

D77 3.10996 -0.00054 0.00001 -0.01458 -0.01459 3.09537

D78 -0.08412 -0.00008 -0.00006 0.00377 0.00369 -0.08043

D79 0.03815 0.00016 0.00001 0.00512 0.00514 0.04328

D80 -3.05098 -0.00037 0.00008 -0.01242 -0.01265 -3.06363

D81 2.96884 0.00110 0.00009 0.05153 0.05202 3.02086

D82 -0.18354 0.00109 0.00006 0.04422 0.04464 -0.13890

D83 -0.23325 0.00165 0.00002 0.07227 0.07285 -0.16040

D84 2.89755 0.00164 -0.00001 0.06496 0.06547 2.96302

D85 2.96142 -0.00055 -0.00016 0.00339 0.00363 2.96505

D86 -0.16568 -0.00099 -0.00009 -0.01505 -0.01457 -0.18026

D87 -0.16958 -0.00056 -0.00013 0.01049 0.01073 -0.15884

D88 2.98650 -0.00101 -0.00006 -0.00795 -0.00747 2.97904

D89 -0.97182 -0.00062 0.00002 -0.03375 -0.03373 -1.00555

D90 2.17044 -0.00047 0.00002 -0.03084 -0.03081 2.13963

D91 2.16007 -0.00062 -0.00001 -0.04026 -0.04028 2.11980

D92 -0.98085 -0.00048 -0.00000 -0.03735 -0.03735 -1.01821

D93 -3.13806 -0.00035 0.00009 -0.01706 -0.01696 3.12816

D94 -0.02984 -0.00003 0.00006 -0.00592 -0.00577 -0.03561

D95 -0.00870 0.00001 0.00003 -0.00153 -0.00158 -0.01028

D96 3.09952 0.00034 0.00001 0.00960 0.00961 3.10913

D97 -3.12831 0.00023 -0.00007 0.01221 0.01208 -3.11623

D98 0.05942 0.00013 -0.00004 0.00487 0.00483 0.06425

D99 0.02532 -0.00014 -0.00002 -0.00305 -0.00305 0.02227

D100 -3.07014 -0.00025 0.00002 -0.01039 -0.01030 -3.08044

D101 -0.01011 0.00006 -0.00003 0.00517 0.00529 -0.00482

D102 3.11106 0.00029 -0.00001 0.00963 0.00962 3.12068

D103 -3.11755 -0.00028 -0.00001 -0.00635 -0.00624 -3.12379

D104 0.00362 -0.00005 0.00001 -0.00189 -0.00192 0.00170

D105 0.02514 -0.00015 0.00002 -0.00687 -0.00701 0.01813

D106 -3.10509 0.00023 0.00005 -0.00049 -0.00058 -3.10568

D107 -3.09656 -0.00037 0.00000 -0.01111 -0.01114 -3.10770

D108 0.05639 0.00001 0.00003 -0.00474 -0.00472 0.05167

D109 -0.03134 0.00016 -0.00000 0.00605 0.00617 -0.02517

D110 3.06438 0.00026 -0.00003 0.01339 0.01341 3.07779

D111 3.09920 -0.00021 -0.00003 -0.00018 -0.00011 3.09910

D112 -0.08826 -0.00011 -0.00006 0.00716 0.00713 -0.08113

D113 -3.07598 -0.00018 -0.00021 0.06565 0.06575 -3.01024

D114 0.07312 0.00001 -0.00018 0.04090 0.04117 0.11429

D115 0.07902 0.00026 -0.00018 0.07313 0.07325 0.15228

D116 -3.05506 0.00046 -0.00015 0.04839 0.04868 -3.00638

D117 0.95639 -0.00052 -0.00006 0.01619 0.01619 0.97258

D118 -2.18173 -0.00038 -0.00005 0.00791 0.00793 -2.17380

D119 -2.19222 -0.00070 -0.00008 0.03933 0.03918 -2.15305

D120 0.95284 -0.00056 -0.00008 0.03106 0.03092 0.98375

D121 -3.13624 0.00012 0.00001 0.00483 0.00484 -3.13140

D122 -0.01909 0.00009 -0.00000 0.00703 0.00703 -0.01206

D123 0.00337 0.00027 0.00001 0.00836 0.00837 0.01174

D124 3.12052 0.00023 0.00000 0.01056 0.01056 3.13108

D125 -3.13107 -0.00016 -0.00000 -0.00569 -0.00569 -3.13676

D126 -0.01122 -0.00009 -0.00001 -0.00223 -0.00224 -0.01346

D127 0.01249 -0.00031 -0.00001 -0.00919 -0.00919 0.00330

D128 3.13234 -0.00024 -0.00001 -0.00573 -0.00574 3.12660

D129 -0.01409 -0.00011 -0.00001 -0.00325 -0.00326 -0.01734

D130 3.12657 -0.00008 -0.00001 -0.00247 -0.00248 3.12409

D131 -3.13110 -0.00007 -0.00000 -0.00546 -0.00546 -3.13657

D132 0.00955 -0.00005 0.00000 -0.00469 -0.00469 0.00487

D133 0.00895 -0.00002 0.00000 -0.00116 -0.00116 0.00779

D134 -3.13439 0.00004 0.00000 0.00030 0.00030 -3.13409

D135 -3.13170 -0.00004 -0.00000 -0.00194 -0.00194 -3.13364

D136 0.00814 0.00002 -0.00000 -0.00048 -0.00048 0.00767

D137 0.00689 -0.00002 0.00000 0.00033 0.00033 0.00722

D138 -3.13516 0.00004 0.00000 0.00054 0.00055 -3.13462

D139 -3.13296 -0.00009 0.00000 -0.00113 -0.00113 -3.13409

D140 0.00818 -0.00002 0.00000 -0.00092 -0.00092 0.00726

D141 -0.01768 0.00018 0.00000 0.00490 0.00490 -0.01278

D142 -3.13737 0.00011 0.00000 0.00141 0.00142 -3.13595

D143 3.12437 0.00012 0.00000 0.00469 0.00469 3.12906

D144 0.00468 0.00004 0.00000 0.00120 0.00121 0.00589

D145 -0.00888 0.00007 -0.00000 0.00290 0.00289 -0.00598

D146 3.12805 0.00001 -0.00001 0.00385 0.00383 3.13188

D147 3.13696 0.00002 0.00000 -0.00122 -0.00121 3.13574

D148 -0.00930 -0.00003 -0.00000 -0.00027 -0.00028 -0.00957

D149 -0.00346 0.00006 0.00001 -0.00231 -0.00230 -0.00577

D150 3.13858 -0.00002 0.00001 -0.00333 -0.00332 3.13526

D151 3.13389 0.00010 0.00000 0.00180 0.00181 3.13569

D152 -0.00725 0.00002 0.00000 0.00079 0.00079 -0.00647

D153 0.00508 0.00002 -0.00002 0.00410 0.00408 0.00916

D154 3.12820 -0.00008 -0.00001 0.00628 0.00626 3.13446

D155 -3.13187 0.00007 -0.00001 0.00316 0.00315 -3.12873

D156 -0.00875 -0.00002 -0.00000 0.00533 0.00533 -0.00343

D157 -3.13527 -0.00036 0.00003 -0.00302 -0.00301 -3.13828

D158 0.01080 -0.00022 0.00003 -0.01139 -0.01137 -0.00056

D159 0.02473 -0.00026 0.00002 -0.00520 -0.00519 0.01954

D160 -3.11238 -0.00012 0.00002 -0.01358 -0.01355 -3.12593

D161 3.12275 0.00049 -0.00002 0.00381 0.00377 3.12651

D162 0.00207 0.00025 -0.00002 0.00325 0.00321 0.00528

D163 -0.02324 0.00035 -0.00003 0.01200 0.01198 -0.01126

D164 3.13927 0.00010 -0.00002 0.01143 0.01142 -3.13249

D165 0.01981 -0.00028 0.00001 -0.00529 -0.00529 0.01453

D166 -3.12223 -0.00020 0.00001 -0.00428 -0.00427 -3.12650

D167 3.14040 -0.00004 0.00000 -0.00474 -0.00474 3.13566

D168 -0.00164 0.00005 0.00000 -0.00373 -0.00373 -0.00537

D169 3.12201 0.00049 -0.00002 0.00455 0.00451 3.12651

D170 0.00158 0.00025 -0.00002 0.00375 0.00371 0.00530

D171 -0.02293 0.00035 -0.00002 0.01251 0.01249 -0.01044

D172 3.13983 0.00011 -0.00002 0.01171 0.01170 -3.13165

D173 -3.13447 -0.00035 0.00002 -0.00390 -0.00390 -3.13837

D174 0.02588 -0.00026 0.00002 -0.00629 -0.00629 0.01959

D175 0.01053 -0.00021 0.00003 -0.01205 -0.01203 -0.00149

D176 -3.11230 -0.00012 0.00002 -0.01444 -0.01441 -3.12671

D177 0.01960 -0.00028 0.00001 -0.00528 -0.00528 0.01432

D178 -3.12214 -0.00019 0.00001 -0.00444 -0.00443 -3.12657

D179 3.13994 -0.00004 0.00001 -0.00450 -0.00450 3.13544

D180 -0.00180 0.00004 0.00000 -0.00365 -0.00365 -0.00545

D181 -0.00338 0.00006 0.00001 -0.00272 -0.00271 -0.00609

D182 3.13391 0.00010 0.00000 0.00172 0.00173 3.13564

D183 3.13836 -0.00002 0.00001 -0.00358 -0.00357 3.13480

D184 -0.00753 0.00002 0.00000 0.00087 0.00087 -0.00666

D185 -0.00893 0.00006 -0.00000 0.00317 0.00316 -0.00577

D186 3.12782 0.00001 -0.00001 0.00441 0.00439 3.13221

D187 3.13697 0.00002 0.00000 -0.00128 -0.00128 3.13569

D188 -0.00947 -0.00003 -0.00000 -0.00004 -0.00005 -0.00952

D189 0.00522 0.00002 -0.00002 0.00438 0.00436 0.00958

D190 3.12799 -0.00008 -0.00001 0.00676 0.00674 3.13473

D191 -3.13155 0.00007 -0.00001 0.00315 0.00313 -3.12842

D192 -0.00878 -0.00002 -0.00000 0.00552 0.00552 -0.00326

D193 -3.12800 -0.00018 -0.00000 -0.00658 -0.00658 -3.13458

D194 -0.00938 -0.00010 -0.00000 -0.00297 -0.00298 -0.01236

D195 0.01294 -0.00032 -0.00001 -0.00944 -0.00945 0.00349

D196 3.13156 -0.00024 -0.00001 -0.00584 -0.00585 3.12571

D197 -3.13920 0.00014 0.00000 0.00578 0.00579 -3.13341

D198 -0.02182 0.00010 -0.00000 0.00788 0.00788 -0.01394

D199 0.00305 0.00028 0.00001 0.00866 0.00867 0.01173

D200 3.12043 0.00024 0.00000 0.01076 0.01076 3.13119

D201 -0.01794 0.00019 0.00000 0.00494 0.00495 -0.01300

D202 3.12387 0.00013 0.00000 0.00469 0.00470 3.12856

D203 -3.13640 0.00010 0.00000 0.00131 0.00131 -3.13509

D204 0.00541 0.00004 0.00000 0.00106 0.00106 0.00647

D205 0.00684 -0.00002 0.00000 0.00045 0.00045 0.00729

D206 -3.13312 -0.00009 0.00000 -0.00111 -0.00111 -3.13423

D207 -3.13497 0.00004 0.00000 0.00070 0.00070 -3.13427

D208 0.00826 -0.00002 0.00000 -0.00086 -0.00086 0.00740

D209 0.00912 -0.00002 0.00000 -0.00123 -0.00122 0.00790

D210 -3.13159 -0.00005 -0.00000 -0.00216 -0.00216 -3.13375

D211 -3.13410 0.00004 0.00000 0.00033 0.00034 -3.13377

D212 0.00837 0.00002 0.00000 -0.00060 -0.00060 0.00777

D213 -0.01407 -0.00012 -0.00001 -0.00340 -0.00341 -0.01748

D214 -3.13132 -0.00007 -0.00000 -0.00551 -0.00551 -3.13683

D215 3.12664 -0.00009 -0.00001 -0.00247 -0.00247 3.12417

D216 0.00939 -0.00005 0.00000 -0.00457 -0.00457 0.00482

Item Value Threshold Converged?

Maximum Force 0.012328 0.000450 NO

RMS Force 0.001438 0.000300 NO

Maximum Displacement 0.729782 0.001800 NO

RMS Displacement 0.147394 0.001200 NO

Predicted change in Energy=-3.078309D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Mon Aug 26 04:17:46 2019, MaxMem= 4294967296 cpu: 2.5

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

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.33D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.733206 -4.187042 0.435378

2 6 0 1.165102 -2.876638 0.136858

3 7 0 0.037861 -2.118672 -0.049650

4 6 0 -1.093212 -2.897508 0.083851

5 6 0 -0.663501 -4.193512 0.396944

6 6 0 -2.452861 -2.447425 -0.082680

7 6 0 -2.864505 -1.147319 -0.213438

8 7 0 -2.059833 -0.010173 -0.031958

9 6 0 -2.881768 1.041982 -0.159877

10 6 0 -4.245683 0.611515 -0.484578

11 6 0 -4.228069 -0.738667 -0.520832

12 6 0 2.512137 -2.408536 0.014863

13 6 0 2.881697 -1.042197 -0.155884

14 6 0 4.245258 -0.612994 -0.483736

15 6 0 4.227476 0.737032 -0.525526

16 6 0 2.864237 1.146885 -0.218198

17 7 0 2.059804 0.010582 -0.031185

18 6 0 2.453189 2.447663 -0.090817

19 6 0 1.093313 2.898021 0.073460

20 6 0 0.663927 4.190863 0.399601

21 6 0 -0.732841 4.184283 0.438142

22 6 0 -1.164961 2.877111 0.126614

23 7 0 -0.037962 2.121133 -0.068634

24 6 0 -2.512322 2.408909 0.007330

25 6 0 -3.484067 -3.518686 -0.093233

26 6 0 -3.437379 -4.550284 -1.041392

27 6 0 -4.412923 -5.541742 -1.051735

28 6 0 -5.436304 -5.528770 -0.103368

29 6 0 -5.484000 -4.513487 0.849708

30 6 0 -4.518649 -3.509896 0.850893

31 6 0 5.637776 -5.341734 0.268317

32 6 0 4.641340 -5.467356 -0.699432

33 6 0 3.623829 -4.521399 -0.785823

34 6 0 3.589232 -3.423679 0.088470

35 6 0 4.604397 -3.304503 1.050825

36 6 0 5.613345 -4.257975 1.145630

37 6 0 -3.589091 3.423669 0.085495

38 6 0 -4.604199 3.300914 1.047696

39 6 0 -5.612897 4.254187 1.146614

40 6 0 -5.637284 5.341653 0.273902

41 6 0 -4.640740 5.471330 -0.693180

42 6 0 -3.623389 4.525613 -0.783595

43 6 0 3.484546 3.518430 -0.097223

44 6 0 4.519806 3.504601 0.846265

45 6 0 5.484210 4.509028 0.851000

46 6 0 5.435170 5.530225 -0.095649

47 6 0 4.411330 5.548305 -1.043466

48 6 0 3.436595 4.556065 -1.038846

49 1 0 1.379059 -5.019100 0.663054

50 1 0 -1.310459 -5.033739 0.591054

51 1 0 -5.085128 1.261656 -0.676853

52 1 0 -5.051291 -1.398254 -0.747902

53 1 0 5.084626 -1.263800 -0.674131

54 1 0 5.050339 1.395849 -0.756143

55 1 0 1.311221 5.028322 0.604374

56 1 0 -1.378691 5.013381 0.676473

57 1 0 -2.645925 -4.559733 -1.782004

58 1 0 -4.374583 -6.325367 -1.800868

59 1 0 -6.192474 -6.306624 -0.108394

60 1 0 -6.273059 -4.500759 1.593998

61 1 0 -4.553019 -2.723252 1.595574

62 1 0 6.427137 -6.082708 0.337948

63 1 0 4.657820 -6.302614 -1.391853

64 1 0 2.856321 -4.621995 -1.544965

65 1 0 4.587630 -2.467020 1.739383

66 1 0 6.380853 -4.154771 1.905660

67 1 0 -4.587607 2.460739 1.732963

68 1 0 -6.380231 4.147974 1.906413

69 1 0 -6.426543 6.082429 0.346787

70 1 0 -4.656928 6.309650 -1.381911

71 1 0 -2.855889 4.629975 -1.542209

72 1 0 4.554955 2.713888 1.586545

73 1 0 6.273436 4.492473 1.595032

74 1 0 6.190553 6.308853 -0.096003

75 1 0 4.371961 6.336675 -1.787535

76 1 0 2.644674 4.569672 -1.778877

77 1 0 0.039527 -1.120897 -0.213341

78 1 0 -0.040209 1.127397 -0.254382

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

Rotational constants (GHZ): 0.0593600 0.0576567 0.0301056

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

Standard basis: 6-311G(d) (5D, 7F)

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

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5357.1794691289 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122734518 Hartrees.

Nuclear repulsion after empirical dispersion term = 5356.9671956770 Hartrees.

Force inversion solution in PCM.

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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 : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5762

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.60D-10

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 286

GePol: Fraction of low-weight points (<1% of avg) = 4.96%

GePol: Cavity surface area = 612.155 Ang\*\*2

GePol: Cavity volume = 628.390 Ang\*\*3

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

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

PCM non-electrostatic energy = -0.0021167130 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5356.9650789640 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.

NBasis= 954 RedAO= T EigKep= 1.27D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

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

DipDrv: MaxL=1.

Leave Link 303 at Mon Aug 26 04:17:48 2019, MaxMem= 4294967296 cpu: 2.4

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

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= 0.000000 0.000000 -0.000000

Rot= 0.998890 0.000031 -0.000036 -0.047102 Ang= 5.40 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0350 S= 1.0116

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30375797042

Leave Link 401 at Mon Aug 26 04:17:53 2019, MaxMem= 4294967296 cpu: 86.7

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 580000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 99601932.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.55D-15 for 5747.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.94D-15 for 3040 2807.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.88D-15 for 5747.

Iteration 1 A^-1\*A deviation from orthogonality is 9.00D-11 for 4685 4674.

E= -1914.27010982073

DIIS: error= 5.45D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.27010982073 IErMin= 1 ErrMin= 5.45D-03

ErrMax= 5.45D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.31D-01 BMatP= 1.31D-01

IDIUse=3 WtCom= 9.46D-01 WtEn= 5.45D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.637 Goal= None Shift= 0.000

Gap= 0.705 Goal= None Shift= 0.000

GapD= 0.637 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=2.77D-04 MaxDP=7.74D-03 OVMax= 1.05D-01

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.77D-04 CP: 9.99D-01

E= -1914.32901114269 Delta-E= -0.058901321961 Rises=F Damp=F

DIIS: error= 8.42D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.32901114269 IErMin= 2 ErrMin= 8.42D-04

ErrMax= 8.42D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.96D-03 BMatP= 1.31D-01

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.42D-03

Coeff-Com: -0.573D-01 0.106D+01

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

Coeff: -0.568D-01 0.106D+01

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=7.65D-05 MaxDP=4.27D-03 DE=-5.89D-02 OVMax= 6.66D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 6.68D-05 CP: 9.99D-01 1.13D+00

E= -1914.33021191414 Delta-E= -0.001200771456 Rises=F Damp=F

DIIS: error= 6.99D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33021191414 IErMin= 3 ErrMin= 6.99D-04

ErrMax= 6.99D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.12D-03 BMatP= 1.96D-03

IDIUse=3 WtCom= 9.93D-01 WtEn= 6.99D-03

Coeff-Com: -0.321D-01 0.474D+00 0.558D+00

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

Coeff: -0.318D-01 0.471D+00 0.561D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.32D-05 MaxDP=1.59D-03 DE=-1.20D-03 OVMax= 2.64D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.07D-05 CP: 9.99D-01 1.17D+00 1.10D+00

E= -1914.33061473204 Delta-E= -0.000402817893 Rises=F Damp=F

DIIS: error= 5.16D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33061473204 IErMin= 4 ErrMin= 5.16D-04

ErrMax= 5.16D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.99D-04 BMatP= 1.12D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.16D-03

Coeff-Com: -0.643D-02 0.674D-01 0.327D+00 0.612D+00

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

Coeff: -0.639D-02 0.671D-01 0.325D+00 0.614D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.74D-05 MaxDP=1.88D-03 DE=-4.03D-04 OVMax= 2.83D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.42D-05 CP: 9.99D-01 1.20D+00 1.43D+00 1.17D+00

E= -1914.33084425030 Delta-E= -0.000229518260 Rises=F Damp=F

DIIS: error= 3.88D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33084425030 IErMin= 5 ErrMin= 3.88D-04

ErrMax= 3.88D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.62D-05 BMatP= 2.99D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.88D-03

Coeff-Com: 0.145D-02-0.370D-01 0.109D+00 0.343D+00 0.583D+00

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

Coeff: 0.144D-02-0.369D-01 0.109D+00 0.342D+00 0.584D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.95D-05 MaxDP=1.30D-03 DE=-2.30D-04 OVMax= 2.03D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.02D-06 CP: 9.99D-01 1.22D+00 1.63D+00 1.51D+00 1.25D+00

E= -1914.33096295901 Delta-E= -0.000118708710 Rises=F Damp=F

DIIS: error= 3.49D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33096295901 IErMin= 6 ErrMin= 3.49D-04

ErrMax= 3.49D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.39D-05 BMatP= 7.62D-05

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.49D-03

Coeff-Com: 0.569D-02-0.752D-01-0.134D+00-0.169D+00 0.298D+00 0.107D+01

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

Coeff: 0.567D-02-0.750D-01-0.134D+00-0.168D+00 0.297D+00 0.107D+01

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.57D-05 MaxDP=2.82D-03 DE=-1.19D-04 OVMax= 3.95D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.60D-06 CP: 9.99D-01 1.26D+00 2.01D+00 2.07D+00 2.16D+00

CP: 1.83D+00

E= -1914.33111656734 Delta-E= -0.000153608335 Rises=F Damp=F

DIIS: error= 1.79D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33111656734 IErMin= 7 ErrMin= 1.79D-04

ErrMax= 1.79D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.12D-05 BMatP= 3.39D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.79D-03

Coeff-Com: 0.182D-02-0.949D-02-0.126D+00-0.278D+00-0.314D+00 0.594D+00

Coeff-Com: 0.113D+01

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

Coeff-En: 0.100D+01

Coeff: 0.182D-02-0.948D-02-0.126D+00-0.277D+00-0.314D+00 0.593D+00

Coeff: 0.113D+01

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=3.59D-05 MaxDP=2.88D-03 DE=-1.54D-04 OVMax= 3.87D-02

Cycle 8 Pass 1 IDiag 1:

RMSU= 4.26D-06 CP: 9.98D-01 1.29D+00 2.39D+00 2.64D+00 3.00D+00

CP: 3.00D+00 1.83D+00

E= -1914.33120309719 Delta-E= -0.000086529848 Rises=F Damp=F

DIIS: error= 7.34D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33120309719 IErMin= 8 ErrMin= 7.34D-05

ErrMax= 7.34D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.87D-06 BMatP= 2.12D-05

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

Coeff-Com: -0.218D-02 0.408D-01-0.274D-02-0.638D-01-0.375D+00-0.155D+00

Coeff-Com: 0.781D+00 0.778D+00

Coeff: -0.218D-02 0.408D-01-0.274D-02-0.638D-01-0.375D+00-0.155D+00

Coeff: 0.781D+00 0.778D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.73D-05 MaxDP=1.54D-03 DE=-8.65D-05 OVMax= 1.89D-02

Cycle 9 Pass 1 IDiag 1:

RMSU= 7.44D-06 CP: 9.98D-01 1.31D+00 2.55D+00 2.93D+00 3.00D+00

CP: 3.00D+00 2.51D+00 1.83D+00

E= -1914.33122007803 Delta-E= -0.000016980842 Rises=F Damp=F

DIIS: error= 2.25D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33122007803 IErMin= 9 ErrMin= 2.25D-05

ErrMax= 2.25D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.21D-06 BMatP= 8.87D-06

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

Coeff-Com: -0.465D-03 0.413D-02 0.156D-01 0.506D-01 0.368D-01-0.105D+00

Coeff-Com: -0.141D+00 0.844D-01 0.105D+01

Coeff: -0.465D-03 0.413D-02 0.156D-01 0.506D-01 0.368D-01-0.105D+00

Coeff: -0.141D+00 0.844D-01 0.105D+01

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=2.63D-06 MaxDP=2.11D-04 DE=-1.70D-05 OVMax= 2.06D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.44D-06 CP: 9.98D-01 1.31D+00 2.57D+00 2.96D+00 3.00D+00

CP: 3.00D+00 2.64D+00 2.08D+00 1.13D+00

E= -1914.33122180163 Delta-E= -0.000001723603 Rises=F Damp=F

DIIS: error= 1.96D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33122180163 IErMin=10 ErrMin= 1.96D-05

ErrMax= 1.96D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.66D-07 BMatP= 1.21D-06

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

Coeff-Com: 0.459D-03-0.115D-01 0.933D-02 0.507D-01 0.144D+00 0.963D-03

Coeff-Com: -0.351D+00-0.202D+00 0.691D+00 0.667D+00

Coeff: 0.459D-03-0.115D-01 0.933D-02 0.507D-01 0.144D+00 0.963D-03

Coeff: -0.351D+00-0.202D+00 0.691D+00 0.667D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.32D-06 MaxDP=1.03D-04 DE=-1.72D-06 OVMax= 8.54D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 8.99D-07 CP: 9.98D-01 1.31D+00 2.57D+00 2.97D+00 3.00D+00

CP: 3.00D+00 2.71D+00 2.16D+00 1.18D+00 1.28D+00

E= -1914.33122237218 Delta-E= -0.000000570545 Rises=F Damp=F

DIIS: error= 9.97D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33122237218 IErMin=11 ErrMin= 9.97D-06

ErrMax= 9.97D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.80D-07 BMatP= 8.66D-07

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

Coeff-Com: 0.324D-03-0.618D-02 0.142D-02 0.926D-02 0.470D-01 0.322D-01

Coeff-Com: -0.133D+00-0.108D+00 0.712D-01 0.333D+00 0.752D+00

Coeff: 0.324D-03-0.618D-02 0.142D-02 0.926D-02 0.470D-01 0.322D-01

Coeff: -0.133D+00-0.108D+00 0.712D-01 0.333D+00 0.752D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.27D-06 MaxDP=9.71D-05 DE=-5.71D-07 OVMax= 1.28D-03

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.37D-07 CP: 9.98D-01 1.31D+00 2.58D+00 2.99D+00 3.00D+00

CP: 3.00D+00 2.75D+00 2.25D+00 1.25D+00 1.44D+00

CP: 9.06D-01

E= -1914.33122257409 Delta-E= -0.000000201911 Rises=F Damp=F

DIIS: error= 5.66D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.33122257409 IErMin=12 ErrMin= 5.66D-06

ErrMax= 5.66D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.81D-08 BMatP= 1.80D-07

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

Coeff-Com: 0.434D-04-0.140D-04-0.182D-02-0.990D-02-0.202D-01 0.203D-01

Coeff-Com: 0.255D-01 0.722D-02-0.151D+00-0.105D-01 0.448D+00 0.693D+00

Coeff: 0.434D-04-0.140D-04-0.182D-02-0.990D-02-0.202D-01 0.203D-01

Coeff: 0.255D-01 0.722D-02-0.151D+00-0.105D-01 0.448D+00 0.693D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=6.77D-07 MaxDP=5.20D-05 DE=-2.02D-07 OVMax= 6.92D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 2.04D-07 CP: 9.98D-01 1.31D+00 2.59D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.77D+00 2.29D+00 1.28D+00 1.44D+00

CP: 1.05D+00 1.19D+00

E= -1914.33122262997 Delta-E= -0.000000055876 Rises=F Damp=F

DIIS: error= 2.24D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.33122262997 IErMin=13 ErrMin= 2.24D-06

ErrMax= 2.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.21D-08 BMatP= 6.81D-08

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

Coeff-Com: -0.597D-04 0.141D-02-0.941D-03-0.424D-02-0.177D-01-0.179D-03

Coeff-Com: 0.345D-01 0.301D-01-0.775D-01-0.102D+00-0.218D-01 0.314D+00

Coeff-Com: 0.845D+00

Coeff: -0.597D-04 0.141D-02-0.941D-03-0.424D-02-0.177D-01-0.179D-03

Coeff: 0.345D-01 0.301D-01-0.775D-01-0.102D+00-0.218D-01 0.314D+00

Coeff: 0.845D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=3.31D-07 MaxDP=2.24D-05 DE=-5.59D-08 OVMax= 3.29D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.27D-07 CP: 9.98D-01 1.31D+00 2.59D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.78D+00 2.31D+00 1.29D+00 1.48D+00

CP: 1.10D+00 1.47D+00 1.25D+00

E= -1914.33122264439 Delta-E= -0.000000014421 Rises=F Damp=F

DIIS: error= 1.09D-06 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.33122264439 IErMin=14 ErrMin= 1.09D-06

ErrMax= 1.09D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.72D-09 BMatP= 1.21D-08

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

Coeff-Com: -0.344D-04 0.655D-03-0.265D-03-0.916D-04-0.477D-02-0.282D-02

Coeff-Com: 0.111D-01 0.141D-01-0.159D-01-0.510D-01-0.911D-01 0.311D-01

Coeff-Com: 0.382D+00 0.726D+00

Coeff: -0.344D-04 0.655D-03-0.265D-03-0.916D-04-0.477D-02-0.282D-02

Coeff: 0.111D-01 0.141D-01-0.159D-01-0.510D-01-0.911D-01 0.311D-01

Coeff: 0.382D+00 0.726D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=9.50D-08 MaxDP=7.35D-06 DE=-1.44D-08 OVMax= 7.54D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 4.41D-08 CP: 9.98D-01 1.31D+00 2.59D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.78D+00 2.32D+00 1.29D+00 1.50D+00

CP: 1.14D+00 1.57D+00 1.37D+00 1.25D+00

E= -1914.33122264676 Delta-E= -0.000000002373 Rises=F Damp=F

DIIS: error= 5.20D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.33122264676 IErMin=15 ErrMin= 5.20D-07

ErrMax= 5.20D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.71D-10 BMatP= 2.72D-09

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

Coeff-Com: -0.209D-05-0.249D-04 0.503D-04 0.101D-02 0.184D-02-0.115D-02

Coeff-Com: -0.338D-02 0.475D-03 0.948D-02-0.101D-02-0.400D-01-0.586D-01

Coeff-Com: -0.206D-01 0.383D+00 0.729D+00

Coeff: -0.209D-05-0.249D-04 0.503D-04 0.101D-02 0.184D-02-0.115D-02

Coeff: -0.338D-02 0.475D-03 0.948D-02-0.101D-02-0.400D-01-0.586D-01

Coeff: -0.206D-01 0.383D+00 0.729D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=5.16D-08 MaxDP=4.32D-06 DE=-2.37D-09 OVMax= 4.76D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.88D-08 CP: 9.98D-01 1.31D+00 2.59D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.79D+00 2.32D+00 1.30D+00 1.50D+00

CP: 1.14D+00 1.61D+00 1.42D+00 1.44D+00 1.12D+00

E= -1914.33122264734 Delta-E= -0.000000000575 Rises=F Damp=F

DIIS: error= 2.62D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1914.33122264734 IErMin=16 ErrMin= 2.62D-07

ErrMax= 2.62D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.35D-10 BMatP= 7.71D-10

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

Coeff-Com: 0.527D-05-0.128D-03 0.735D-04 0.415D-03 0.158D-02-0.322D-04

Coeff-Com: -0.360D-02-0.225D-02 0.709D-02 0.985D-02 0.104D-02-0.337D-01

Coeff-Com: -0.883D-01 0.155D-01 0.312D+00 0.780D+00

Coeff: 0.527D-05-0.128D-03 0.735D-04 0.415D-03 0.158D-02-0.322D-04

Coeff: -0.360D-02-0.225D-02 0.709D-02 0.985D-02 0.104D-02-0.337D-01

Coeff: -0.883D-01 0.155D-01 0.312D+00 0.780D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=3.33D-08 MaxDP=2.68D-06 DE=-5.75D-10 OVMax= 3.47D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 9.10D-09 CP: 9.98D-01 1.31D+00 2.59D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.79D+00 2.32D+00 1.30D+00 1.50D+00

CP: 1.14D+00 1.63D+00 1.45D+00 1.56D+00 1.32D+00

CP: 1.14D+00

E= -1914.33122264749 Delta-E= -0.000000000149 Rises=F Damp=F

DIIS: error= 1.37D-07 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1914.33122264749 IErMin=17 ErrMin= 1.37D-07

ErrMax= 1.37D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.45D-11 BMatP= 1.35D-10

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

Coeff-Com: 0.296D-05-0.539D-04 0.217D-04-0.589D-04 0.315D-03 0.190D-03

Coeff-Com: -0.813D-03-0.114D-02 0.128D-02 0.541D-02 0.109D-01-0.199D-02

Coeff-Com: -0.382D-01-0.916D-01-0.445D-01 0.404D+00 0.756D+00

Coeff: 0.296D-05-0.539D-04 0.217D-04-0.589D-04 0.315D-03 0.190D-03

Coeff: -0.813D-03-0.114D-02 0.128D-02 0.541D-02 0.109D-01-0.199D-02

Coeff: -0.382D-01-0.916D-01-0.445D-01 0.404D+00 0.756D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.04D-08 MaxDP=6.97D-07 DE=-1.49D-10 OVMax= 8.04D-06

Cycle 18 Pass 1 IDiag 1:

RMSU= 5.55D-09 CP: 9.98D-01 1.31D+00 2.59D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.79D+00 2.32D+00 1.30D+00 1.50D+00

CP: 1.14D+00 1.63D+00 1.45D+00 1.59D+00 1.40D+00

CP: 1.37D+00 1.13D+00

E= -1914.33122264753 Delta-E= -0.000000000045 Rises=F Damp=F

DIIS: error= 6.95D-08 at cycle 18 NSaved= 18.

NSaved=18 IEnMin=18 EnMin= -1914.33122264753 IErMin=18 ErrMin= 6.95D-08

ErrMax= 6.95D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-11 BMatP= 4.45D-11

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

Coeff-Com: 0.143D-06 0.578D-05-0.126D-04-0.135D-03-0.215D-03 0.696D-04

Coeff-Com: 0.570D-03-0.188D-04-0.117D-02 0.383D-03 0.510D-02 0.745D-02

Coeff-Com: 0.218D-02-0.484D-01-0.102D+00 0.213D-01 0.359D+00 0.756D+00

Coeff: 0.143D-06 0.578D-05-0.126D-04-0.135D-03-0.215D-03 0.696D-04

Coeff: 0.570D-03-0.188D-04-0.117D-02 0.383D-03 0.510D-02 0.745D-02

Coeff: 0.218D-02-0.484D-01-0.102D+00 0.213D-01 0.359D+00 0.756D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=5.26D-09 MaxDP=2.97D-07 DE=-4.46D-11 OVMax= 4.93D-06

Error on total polarization charges = 0.08270

SCF Done: E(UB3LYP) = -1914.33122265 A.U. after 18 cycles

NFock= 18 Conv=0.53D-08 -V/T= 2.0041

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0433 S= 1.0144

<L.S>= 0.000000000000E+00

KE= 1.906429531814D+03 PE=-1.516356278450D+04 EE= 5.985836951075D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.33

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0433, after 2.0011

Leave Link 502 at Mon Aug 26 04:26:11 2019, MaxMem= 4294967296 cpu: 7878.8

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

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

Range of M.O.s used for correlation: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.10640313D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.50091175D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.10321330D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.65065226D-01

Leave Link 801 at Mon Aug 26 04:26:11 2019, MaxMem= 4294967296 cpu: 0.9

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

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

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

Leave Link 1101 at Mon Aug 26 04:26:18 2019, MaxMem= 4294967296 cpu: 110.9

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

Symmetrizing basis deriv contribution to polar:

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

Leave Link 1102 at Mon Aug 26 04:26:18 2019, MaxMem= 4294967296 cpu: 2.3

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

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 189

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 Mon Aug 26 04:46:00 2019, MaxMem= 4294967296 cpu: 18904.4

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

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 580000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 4.89D+03 3.99D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 3.91D+02 2.74D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 7.52D+00 3.63D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 8.94D-02 3.20D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 5.85D-04 1.72D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.46D-06 1.33D-04.

191 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 2.10D-08 7.85D-06.

83 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.35D-11 5.36D-07.

34 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 4.41D-13 3.03D-08.

3 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 6.74D-15 2.94D-09.

3 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 2.40D-15 1.68D-09.

3 vectors produced by pass 11 Test12= 2.55D-13 1.00D-09 XBig12= 7.18D-15 3.58D-09.

3 vectors produced by pass 12 Test12= 2.55D-13 1.00D-09 XBig12= 7.76D-15 3.31D-09.

3 vectors produced by pass 13 Test12= 2.55D-13 1.00D-09 XBig12= 7.62D-15 3.02D-09.

3 vectors produced by pass 14 Test12= 2.55D-13 1.00D-09 XBig12= 4.20D-15 1.66D-09.

3 vectors produced by pass 15 Test12= 2.55D-13 1.00D-09 XBig12= 8.97D-15 3.32D-09.

3 vectors produced by pass 16 Test12= 2.55D-13 1.00D-09 XBig12= 5.75D-15 2.28D-09.

3 vectors produced by pass 17 Test12= 2.55D-13 1.00D-09 XBig12= 7.36D-15 2.87D-09.

3 vectors produced by pass 18 Test12= 2.55D-13 1.00D-09 XBig12= 5.69D-15 2.26D-09.

3 vectors produced by pass 19 Test12= 2.55D-13 1.00D-09 XBig12= 7.52D-15 2.20D-09.

3 vectors produced by pass 20 Test12= 2.55D-13 1.00D-09 XBig12= 6.63D-15 2.41D-09.

3 vectors produced by pass 21 Test12= 2.55D-13 1.00D-09 XBig12= 6.69D-15 2.23D-09.

1 vectors produced by pass 22 Test12= 2.55D-13 1.00D-09 XBig12= 3.61D-15 2.07D-09.

InvSVY: IOpt=1 It= 1 EMax= 8.53D-14

Solved reduced A of dimension 1755 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1110.00 Bohr\*\*3.

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

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

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

Leave Link 1002 at Mon Aug 26 08:34:19 2019, MaxMem= 4294967296 cpu: 219115.9

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 189

Leave Link 701 at Mon Aug 26 08:35:48 2019, MaxMem= 4294967296 cpu: 1426.9

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

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

Leave Link 702 at Mon Aug 26 08:35:48 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

Leave Link 703 at Mon Aug 26 08:54:04 2019, MaxMem= 4294967296 cpu: 17527.5

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

Dipole = 5.36044533D-04 9.96816770D-03-2.97903273D-01

Polarizability= 1.28482593D+03-8.80105457D+01 1.58789720D+03

1.68879256D-02-9.04790744D-02 4.57277964D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000021378 -0.000079883 -0.000868552

2 6 0.001526930 -0.000433387 0.004591066

3 7 -0.001491721 0.001444504 -0.004793141

4 6 -0.004631720 -0.000730139 0.000327082

5 6 0.002970955 -0.001364689 0.002311265

6 6 0.011369861 -0.000098737 0.004537218

7 6 -0.014433758 -0.000669251 0.001170428

8 7 0.011977687 0.001295268 0.001686086

9 6 -0.010836062 -0.000655114 -0.004681862

10 6 -0.002470766 0.000100439 -0.000034090

11 6 -0.000457419 -0.001016979 0.000009409

12 6 -0.003481252 0.000969415 -0.000451906

13 6 0.010826875 -0.000611071 0.004649666

14 6 0.002487285 0.000105023 0.000021258

15 6 0.000440673 -0.001099945 -0.000006844

16 6 0.014435876 -0.000760017 -0.001139569

17 7 -0.011913124 0.001396592 -0.001659668

18 6 -0.011355498 -0.000037699 -0.004537849

19 6 0.004590741 -0.000700046 -0.000327083

20 6 -0.002949774 -0.001432452 -0.002314324

21 6 -0.000015995 -0.000086934 0.000874872

22 6 -0.001503185 -0.000499685 -0.004633983

23 7 0.001469166 0.001483877 0.004778210

24 6 0.003414725 0.001039688 0.000467862

25 6 0.000195824 0.001072687 0.000402127

26 6 -0.000263956 -0.000235729 -0.000362558

27 6 0.000145572 -0.000012988 -0.000109797

28 6 0.000253237 0.000262618 -0.000067188

29 6 -0.000234363 -0.000036848 -0.000077786

30 6 0.000801919 -0.000168124 -0.000026665

31 6 -0.000098943 -0.000068977 -0.000211619

32 6 -0.000175636 0.000153185 -0.000004784

33 6 -0.000100367 -0.000255075 -0.000756952

34 6 0.000247324 -0.000161157 0.000527985

35 6 -0.000171733 -0.000386261 -0.000233547

36 6 -0.000034569 0.000411361 0.000214261

37 6 -0.000250217 -0.000165151 -0.000565829

38 6 0.000196186 -0.000351317 0.000221614

39 6 0.000047079 0.000390963 -0.000207724

40 6 0.000085515 -0.000078172 0.000204564

41 6 0.000172871 0.000143907 0.000020277

42 6 0.000063237 -0.000209013 0.000755036

43 6 -0.000202848 0.001127145 -0.000406613

44 6 -0.000821410 -0.000187524 0.000030876

45 6 0.000242609 -0.000027772 0.000076110

46 6 -0.000264983 0.000269828 0.000079784

47 6 -0.000139686 -0.000018325 0.000110768

48 6 0.000272317 -0.000229192 0.000357622

49 1 0.000251070 0.000162405 -0.000037215

50 1 0.000140081 0.000174255 0.000249129

51 1 -0.000232538 0.000296922 0.000056539

52 1 0.000114470 0.000209971 0.000221319

53 1 0.000231192 0.000297159 -0.000065152

54 1 -0.000111173 0.000224602 -0.000222957

55 1 -0.000136902 0.000174402 -0.000241521

56 1 -0.000255348 0.000159071 0.000051788

57 1 0.000095494 -0.000079015 0.000092231

58 1 0.000072684 0.000031133 -0.000050378

59 1 0.000077837 -0.000023653 0.000025871

60 1 -0.000002464 -0.000008944 -0.000072774

61 1 -0.000014994 -0.000135171 0.000035893

62 1 -0.000008995 -0.000010011 -0.000040314

63 1 -0.000066992 -0.000036444 -0.000063304

64 1 0.000033080 -0.000065818 0.000003411

65 1 0.000138919 -0.000035279 -0.000049103

66 1 -0.000048333 0.000063872 -0.000058479

67 1 -0.000150653 -0.000030293 0.000059267

68 1 0.000045722 0.000068053 0.000061206

69 1 0.000010241 -0.000005797 0.000043494

70 1 0.000073921 -0.000040181 0.000063124

71 1 0.000007372 -0.000065907 0.000021027

72 1 0.000022993 -0.000129694 -0.000046386

73 1 0.000003794 -0.000006565 0.000076102

74 1 -0.000080787 -0.000022884 -0.000024791

75 1 -0.000073293 0.000035739 0.000050120

76 1 -0.000093043 -0.000081455 -0.000100667

77 1 0.000132202 0.000071793 -0.000098232

78 1 -0.000132414 0.000008883 0.000115239

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

Cartesian Forces: Max 0.014435876 RMS 0.002551729

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

Leave Link 716 at Mon Aug 26 08:54:04 2019, MaxMem= 4294967296 cpu: 2.1

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.012442156 RMS 0.001293933

Search for a local minimum.

Step number 4 out of a maximum of 452

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

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -2.84D-03 DEPred=-3.08D-03 R= 9.21D-01

TightC=F SS= 1.41D+00 RLast= 4.70D-01 DXNew= 2.5227D-01 1.4098D+00

Trust test= 9.21D-01 RLast= 4.70D-01 DXMaxT set to 2.52D-01

ITU= 1 -1 1 0

Eigenvalues --- 0.00184 0.00345 0.00503 0.00613 0.00771

Eigenvalues --- 0.00799 0.00975 0.01046 0.01053 0.01113

Eigenvalues --- 0.01167 0.01200 0.01233 0.01295 0.01296

Eigenvalues --- 0.01302 0.01366 0.01405 0.01435 0.01481

Eigenvalues --- 0.01493 0.01551 0.01576 0.01623 0.01701

Eigenvalues --- 0.01709 0.01735 0.01741 0.01754 0.01762

Eigenvalues --- 0.01769 0.01773 0.01801 0.01823 0.01889

Eigenvalues --- 0.01890 0.01906 0.02075 0.02086 0.02191

Eigenvalues --- 0.02200 0.02252 0.02272 0.02279 0.02335

Eigenvalues --- 0.02341 0.02396 0.02488 0.02504 0.02514

Eigenvalues --- 0.02538 0.02552 0.02596 0.02599 0.02605

Eigenvalues --- 0.02615 0.02667 0.02754 0.02762 0.02773

Eigenvalues --- 0.02781 0.02869 0.02871 0.02872 0.02886

Eigenvalues --- 0.03045 0.03054 0.03873 0.04148 0.04248

Eigenvalues --- 0.04302 0.04376 0.04479 0.04524 0.04583

Eigenvalues --- 0.08643 0.09651 0.09684 0.09841 0.09854

Eigenvalues --- 0.09892 0.10425 0.10454 0.10626 0.10683

Eigenvalues --- 0.10684 0.10718 0.10722 0.10727 0.11370

Eigenvalues --- 0.11373 0.11420 0.11424 0.11688 0.11972

Eigenvalues --- 0.11979 0.11999 0.12031 0.12266 0.12268

Eigenvalues --- 0.12304 0.12306 0.12740 0.12745 0.12798

Eigenvalues --- 0.12802 0.15745 0.15838 0.16414 0.17236

Eigenvalues --- 0.17297 0.17408 0.17793 0.17873 0.17946

Eigenvalues --- 0.18289 0.18370 0.18715 0.19262 0.19299

Eigenvalues --- 0.19357 0.19364 0.19368 0.19409 0.19428

Eigenvalues --- 0.19447 0.19541 0.19543 0.19555 0.19557

Eigenvalues --- 0.20390 0.21652 0.21949 0.22131 0.22729

Eigenvalues --- 0.23244 0.23881 0.23908 0.25118 0.25535

Eigenvalues --- 0.26511 0.26564 0.26776 0.27377 0.28433

Eigenvalues --- 0.28576 0.28602 0.28643 0.29950 0.30930

Eigenvalues --- 0.31403 0.32233 0.32437 0.32812 0.32848

Eigenvalues --- 0.34146 0.34404 0.35398 0.35490 0.35528

Eigenvalues --- 0.35588 0.35595 0.35650 0.35653 0.35725

Eigenvalues --- 0.35749 0.35789 0.35811 0.35895 0.35896

Eigenvalues --- 0.35930 0.35935 0.35939 0.35945 0.36035

Eigenvalues --- 0.36041 0.36140 0.36197 0.36281 0.36313

Eigenvalues --- 0.36746 0.36980 0.37229 0.37419 0.37447

Eigenvalues --- 0.37554 0.37887 0.38041 0.38780 0.38885

Eigenvalues --- 0.40341 0.40534 0.40851 0.41034 0.41046

Eigenvalues --- 0.41061 0.41175 0.41202 0.41425 0.41487

Eigenvalues --- 0.41667 0.41930 0.42607 0.42935 0.45316

Eigenvalues --- 0.45529 0.45808 0.45843 0.46117 0.46140

Eigenvalues --- 0.46184 0.46217 0.46219 0.46363 0.46373

Eigenvalues --- 0.47061 0.47302 0.48598 0.50637 0.50650

Eigenvalues --- 0.50880 0.50883 0.51855 0.52417 0.54803

Eigenvalues --- 0.54926 0.57799 0.58971

Cosine: 0.957 < 0.970

Cut down GDIIS temporarily because of the cosine check. E 9

DIIS coeff's: 1.64943 -0.64943

Cosine: 0.957 > 0.500

Length: 1.093

GDIIS step was calculated using 2 of the last 4 vectors.

Iteration 1 RMS(Cart)= 0.11279727 RMS(Int)= 0.00168490

Iteration 2 RMS(Cart)= 0.00520559 RMS(Int)= 0.00031038

Iteration 3 RMS(Cart)= 0.00000567 RMS(Int)= 0.00031037

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00031037

ITry= 1 IFail=0 DXMaxC= 4.47D-01 DCOld= 1.00D+10 DXMaxT= 2.52D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.66767 -0.00009 -0.01779 -0.00152 -0.01923 2.64844

R2 2.64042 -0.00153 0.01505 -0.00454 0.01088 2.65130

R3 2.03642 0.00014 0.00003 0.00046 0.00049 2.03691

R4 2.59104 0.00337 -0.00062 0.00728 0.00640 2.59744

R5 2.70469 -0.00285 0.02252 -0.00024 0.02226 2.72695

R6 2.60737 -0.00246 -0.00275 -0.00787 -0.01090 2.59646

R7 1.91073 -0.00012 0.00039 -0.00126 -0.00087 1.90986

R8 2.64717 0.00357 -0.01262 0.01194 -0.00054 2.64663

R9 2.72471 -0.00106 0.01702 -0.00803 0.00905 2.73377

R10 2.03724 -0.00008 -0.00018 0.00021 0.00003 2.03727

R11 2.58887 0.01244 -0.00275 0.03736 0.03463 2.62351

R12 2.80998 0.00095 0.00004 -0.00522 -0.00517 2.80481

R13 2.65473 -0.00548 -0.01250 -0.04002 -0.05295 2.60178

R14 2.75200 0.00190 0.01351 0.00249 0.01612 2.76812

R15 2.53461 0.00878 0.01521 0.03567 0.05054 2.58514

R16 2.77152 -0.00190 0.01018 -0.01224 -0.00192 2.76961

R17 2.69439 -0.00469 -0.03646 -0.02367 -0.06017 2.63423

R18 2.55261 0.00167 -0.00973 0.00634 -0.00291 2.54970

R19 2.03908 0.00015 -0.00059 0.00083 0.00024 2.03933

R20 2.03908 -0.00006 -0.00019 0.00014 -0.00006 2.03902

R21 2.69418 -0.00475 -0.03597 -0.02405 -0.06003 2.63414

R22 2.80041 -0.00066 0.00188 -0.00002 0.00185 2.80226

R23 2.77153 -0.00192 0.01002 -0.01211 -0.00194 2.76958

R24 2.53491 0.00872 0.01513 0.03555 0.05034 2.58525

R25 2.55262 0.00167 -0.00967 0.00629 -0.00292 2.54970

R26 2.03910 0.00015 -0.00056 0.00078 0.00022 2.03932

R27 2.75204 0.00188 0.01351 0.00246 0.01608 2.76812

R28 2.03909 -0.00006 -0.00020 0.00014 -0.00006 2.03903

R29 2.65456 -0.00548 -0.01254 -0.03992 -0.05285 2.60171

R30 2.58914 0.01244 -0.00272 0.03726 0.03456 2.62370

R31 2.72479 -0.00105 0.01697 -0.00798 0.00901 2.73380

R32 2.80946 0.00095 0.00006 -0.00538 -0.00533 2.80413

R33 2.64709 0.00356 -0.01253 0.01170 -0.00067 2.64642

R34 2.60723 -0.00246 -0.00276 -0.00801 -0.01112 2.59611

R35 2.64054 -0.00153 0.01503 -0.00444 0.01098 2.65152

R36 2.03728 -0.00008 -0.00018 0.00026 0.00008 2.03736

R37 2.66744 -0.00006 -0.01774 -0.00152 -0.01918 2.64827

R38 2.03646 0.00013 0.00008 0.00040 0.00047 2.03694

R39 2.59089 0.00337 -0.00061 0.00723 0.00630 2.59719

R40 2.70490 -0.00286 0.02239 -0.00013 0.02221 2.72711

R41 1.91042 -0.00013 0.00045 -0.00148 -0.00103 1.90938

R42 2.79991 -0.00067 0.00221 -0.00037 0.00183 2.80174

R43 2.64924 0.00003 0.00007 0.00197 0.00203 2.65128

R44 2.64684 0.00037 -0.00032 0.00291 0.00258 2.64942

R45 2.62854 0.00028 -0.00006 -0.00067 -0.00073 2.62781

R46 2.04841 0.00002 0.00016 -0.00027 -0.00011 2.04829

R47 2.63674 -0.00018 0.00035 -0.00036 -0.00001 2.63673

R48 2.04993 0.00007 0.00008 0.00013 0.00021 2.05014

R49 2.63305 0.00021 -0.00032 0.00096 0.00064 2.63370

R50 2.05005 0.00004 0.00000 0.00005 0.00005 2.05010

R51 2.63147 0.00019 0.00049 -0.00019 0.00030 2.63177

R52 2.04993 0.00006 0.00010 0.00006 0.00016 2.05009

R53 2.04801 0.00010 0.00031 0.00017 0.00048 2.04850

R54 2.63561 -0.00005 0.00083 0.00011 0.00095 2.63656

R55 2.63534 -0.00002 -0.00100 -0.00050 -0.00149 2.63385

R56 2.05014 -0.00003 0.00002 -0.00007 -0.00004 2.05010

R57 2.63047 -0.00039 -0.00088 -0.00111 -0.00199 2.62848

R58 2.05048 -0.00007 -0.00006 -0.00025 -0.00031 2.05017

R59 2.65274 -0.00049 -0.00011 -0.00029 -0.00041 2.65233

R60 2.04884 -0.00005 0.00003 -0.00049 -0.00046 2.04837

R61 2.65296 -0.00019 -0.00121 -0.00108 -0.00230 2.65066

R62 2.62942 -0.00006 0.00085 0.00030 0.00115 2.63057

R63 2.04908 -0.00009 -0.00024 -0.00049 -0.00072 2.04836

R64 2.05047 -0.00008 -0.00006 -0.00028 -0.00034 2.05013

R65 2.65326 -0.00022 -0.00134 -0.00103 -0.00237 2.65089

R66 2.65288 -0.00049 -0.00024 -0.00014 -0.00038 2.65249

R67 2.62936 -0.00007 0.00090 0.00026 0.00115 2.63051

R68 2.04908 -0.00010 -0.00020 -0.00055 -0.00075 2.04832

R69 2.63534 -0.00000 -0.00104 -0.00046 -0.00149 2.63385

R70 2.05049 -0.00009 -0.00006 -0.00029 -0.00035 2.05013

R71 2.63558 -0.00003 0.00082 0.00019 0.00101 2.63659

R72 2.05015 -0.00004 0.00003 -0.00008 -0.00005 2.05010

R73 2.63043 -0.00040 -0.00083 -0.00120 -0.00203 2.62840

R74 2.05050 -0.00008 -0.00005 -0.00029 -0.00033 2.05017

R75 2.04880 -0.00003 0.00005 -0.00048 -0.00043 2.04837

R76 2.64705 0.00037 -0.00033 0.00290 0.00256 2.64961

R77 2.64942 0.00002 0.00007 0.00194 0.00200 2.65142

R78 2.63139 0.00019 0.00051 -0.00021 0.00030 2.63169

R79 2.04796 0.00010 0.00032 0.00018 0.00050 2.04846

R80 2.63303 0.00022 -0.00031 0.00100 0.00069 2.63372

R81 2.04992 0.00006 0.00010 0.00007 0.00018 2.05010

R82 2.63678 -0.00018 0.00035 -0.00033 0.00003 2.63681

R83 2.05004 0.00004 0.00000 0.00006 0.00007 2.05011

R84 2.62847 0.00029 -0.00008 -0.00067 -0.00074 2.62773

R85 2.04991 0.00008 0.00008 0.00015 0.00023 2.05015

R86 2.04839 0.00002 0.00015 -0.00024 -0.00009 2.04830

A1 1.88001 -0.00009 -0.00171 0.00157 -0.00026 1.87975

A2 2.18713 0.00021 0.00319 -0.00052 0.00269 2.18982

A3 2.21596 -0.00011 -0.00146 -0.00092 -0.00235 2.21361

A4 1.86543 0.00049 0.00444 -0.00048 0.00389 1.86932

A5 2.22631 -0.00092 -0.00276 0.00265 0.00096 2.22726

A6 2.19119 0.00042 -0.00173 -0.00263 -0.00559 2.18560

A7 1.92703 -0.00079 -0.00291 0.00053 -0.00202 1.92501

A8 2.17266 0.00049 0.00122 0.00075 0.00178 2.17444

A9 2.18223 0.00030 0.00202 -0.00165 0.00016 2.18239

A10 1.86753 0.00029 0.00363 -0.00085 0.00267 1.87019

A11 2.19647 -0.00068 -0.00199 -0.00133 -0.00435 2.19212

A12 2.21915 0.00039 -0.00166 0.00205 0.00120 2.22036

A13 1.88441 0.00011 -0.00330 -0.00092 -0.00430 1.88011

A14 2.21247 -0.00031 -0.00000 0.00152 0.00150 2.21397

A15 2.18612 0.00020 0.00346 -0.00048 0.00296 2.18908

A16 2.20260 -0.00134 0.00125 -0.01432 -0.01440 2.18820

A17 2.01516 -0.00039 -0.00560 0.00544 0.00049 2.01565

A18 2.06534 0.00173 0.00430 0.00892 0.01389 2.07923

A19 2.19412 -0.00087 0.00645 -0.00667 -0.00123 2.19289

A20 2.17461 0.00110 -0.00705 -0.00126 -0.00724 2.16737

A21 1.91393 -0.00022 0.00098 0.00801 0.00880 1.92273

A22 1.84590 0.00041 0.00188 0.00107 0.00327 1.84917

A23 1.93988 -0.00076 -0.00590 -0.00698 -0.01296 1.92693

A24 2.19209 0.00120 0.00501 -0.00149 0.00221 2.19429

A25 2.15115 -0.00044 0.00111 0.00850 0.01082 2.16196

A26 1.86209 -0.00124 0.00171 -0.00133 0.00030 1.86239

A27 2.19701 0.00045 -0.00084 -0.00108 -0.00198 2.19503

A28 2.22385 0.00079 -0.00102 0.00228 0.00119 2.22504

A29 1.86192 0.00181 0.00121 -0.00097 0.00020 1.86212

A30 2.19844 -0.00111 -0.00151 -0.00003 -0.00154 2.19690

A31 2.22270 -0.00070 0.00025 0.00097 0.00122 2.22393

A32 2.17439 0.00088 0.00613 0.00414 0.00863 2.18302

A33 2.04405 -0.00129 -0.01489 -0.00594 -0.02009 2.02396

A34 2.06468 0.00042 0.00875 0.00194 0.01143 2.07610

A35 2.15104 -0.00044 0.00109 0.00856 0.01079 2.16184

A36 2.19222 0.00119 0.00495 -0.00156 0.00217 2.19439

A37 1.93987 -0.00075 -0.00586 -0.00698 -0.01292 1.92695

A38 1.86205 -0.00124 0.00172 -0.00133 0.00033 1.86239

A39 2.19710 0.00045 -0.00094 -0.00097 -0.00198 2.19512

A40 2.22380 0.00080 -0.00092 0.00217 0.00117 2.22497

A41 1.86196 0.00180 0.00116 -0.00097 0.00015 1.86211

A42 2.22281 -0.00070 0.00023 0.00100 0.00122 2.22403

A43 2.19829 -0.00110 -0.00144 -0.00006 -0.00151 2.19679

A44 1.91399 -0.00022 0.00098 0.00803 0.00881 1.92281

A45 2.17444 0.00109 -0.00684 -0.00131 -0.00712 2.16732

A46 2.19419 -0.00086 0.00635 -0.00663 -0.00132 2.19287

A47 1.84586 0.00041 0.00189 0.00105 0.00326 1.84912

A48 2.20194 -0.00132 0.00110 -0.01439 -0.01471 2.18723

A49 2.06605 0.00172 0.00436 0.00941 0.01448 2.08054

A50 2.01506 -0.00040 -0.00552 0.00501 0.00019 2.01525

A51 2.21917 0.00040 -0.00156 0.00197 0.00130 2.22047

A52 2.19654 -0.00069 -0.00206 -0.00121 -0.00442 2.19212

A53 1.86747 0.00029 0.00367 -0.00080 0.00277 1.87024

A54 1.88440 0.00011 -0.00331 -0.00099 -0.00439 1.88001

A55 2.18600 0.00020 0.00346 -0.00072 0.00273 2.18873

A56 2.21254 -0.00030 0.00004 0.00184 0.00186 2.21441

A57 1.87998 -0.00009 -0.00177 0.00164 -0.00027 1.87971

A58 2.21624 -0.00013 -0.00131 -0.00108 -0.00235 2.21389

A59 2.18684 0.00022 0.00312 -0.00041 0.00274 2.18958

A60 1.86545 0.00047 0.00453 -0.00063 0.00382 1.86927

A61 2.22619 -0.00089 -0.00298 0.00307 0.00126 2.22745

A62 2.19140 0.00042 -0.00160 -0.00275 -0.00571 2.18569

A63 1.92714 -0.00078 -0.00300 0.00065 -0.00197 1.92518

A64 2.18248 0.00028 0.00201 -0.00184 -0.00003 2.18245

A65 2.17285 0.00050 0.00117 0.00102 0.00200 2.17485

A66 2.17398 0.00088 0.00635 0.00371 0.00824 2.18223

A67 2.06517 0.00047 0.00887 0.00252 0.01220 2.07737

A68 2.04391 -0.00134 -0.01528 -0.00607 -0.02052 2.02339

A69 2.10811 -0.00017 -0.00072 -0.00794 -0.00866 2.09945

A70 2.09779 0.00075 0.00122 0.01255 0.01377 2.11156

A71 2.07728 -0.00058 -0.00049 -0.00460 -0.00511 2.07217

A72 2.10154 0.00043 0.00010 0.00376 0.00385 2.10538

A73 2.08613 -0.00020 0.00006 -0.00117 -0.00110 2.08503

A74 2.09530 -0.00022 -0.00013 -0.00258 -0.00271 2.09260

A75 2.09753 0.00002 0.00033 -0.00059 -0.00026 2.09727

A76 2.08892 0.00005 -0.00009 0.00039 0.00030 2.08922

A77 2.09673 -0.00007 -0.00024 0.00020 -0.00004 2.09669

A78 2.09070 -0.00018 -0.00039 -0.00104 -0.00143 2.08927

A79 2.09604 0.00006 0.00010 0.00064 0.00073 2.09677

A80 2.09645 0.00012 0.00029 0.00041 0.00069 2.09714

A81 2.09671 0.00008 -0.00009 0.00121 0.00111 2.09782

A82 2.09759 -0.00006 0.00011 -0.00071 -0.00060 2.09699

A83 2.08888 -0.00002 -0.00002 -0.00050 -0.00051 2.08837

A84 2.10246 0.00024 0.00055 0.00127 0.00180 2.10426

A85 2.08420 -0.00010 -0.00014 -0.00051 -0.00064 2.08356

A86 2.09638 -0.00014 -0.00037 -0.00079 -0.00115 2.09523

A87 2.08747 0.00013 0.00047 0.00111 0.00157 2.08904

A88 2.09768 -0.00007 -0.00040 -0.00043 -0.00082 2.09686

A89 2.09803 -0.00006 -0.00007 -0.00068 -0.00075 2.09728

A90 2.09913 -0.00011 -0.00007 -0.00064 -0.00072 2.09841

A91 2.09586 0.00012 -0.00009 0.00050 0.00041 2.09627

A92 2.08819 -0.00001 0.00017 0.00015 0.00032 2.08851

A93 2.10688 -0.00014 -0.00070 -0.00130 -0.00202 2.10486

A94 2.09193 0.00006 0.00083 0.00051 0.00134 2.09327

A95 2.08426 0.00008 -0.00011 0.00076 0.00066 2.08492

A96 2.12075 -0.00140 -0.00373 -0.00582 -0.00955 2.11120

A97 2.09610 0.00082 0.00250 0.00275 0.00525 2.10135

A98 2.06633 0.00058 0.00123 0.00306 0.00425 2.07058

A99 2.10933 -0.00047 -0.00048 -0.00244 -0.00294 2.10639

A100 2.08252 0.00026 -0.00018 0.00114 0.00098 2.08350

A101 2.09116 0.00021 0.00066 0.00127 0.00194 2.09311

A102 2.09713 0.00001 -0.00037 0.00022 -0.00016 2.09697

A103 2.09690 0.00004 0.00052 -0.00018 0.00034 2.09725

A104 2.08915 -0.00005 -0.00015 -0.00004 -0.00019 2.08896

A105 2.09636 0.00084 0.00244 0.00282 0.00525 2.10160

A106 2.12081 -0.00145 -0.00378 -0.00594 -0.00973 2.11108

A107 2.06601 0.00061 0.00134 0.00310 0.00441 2.07042

A108 2.10942 -0.00048 -0.00050 -0.00246 -0.00298 2.10644

A109 2.08263 0.00026 -0.00022 0.00117 0.00096 2.08359

A110 2.09096 0.00022 0.00073 0.00124 0.00198 2.09293

A111 2.09721 0.00000 -0.00042 0.00020 -0.00023 2.09698

A112 2.08908 -0.00004 -0.00012 -0.00002 -0.00014 2.08894

A113 2.09690 0.00004 0.00054 -0.00019 0.00036 2.09726

A114 2.08741 0.00013 0.00052 0.00114 0.00165 2.08906

A115 2.09801 -0.00006 -0.00009 -0.00068 -0.00077 2.09724

A116 2.09776 -0.00007 -0.00042 -0.00046 -0.00088 2.09688

A117 2.09913 -0.00011 -0.00010 -0.00061 -0.00073 2.09841

A118 2.09589 0.00012 -0.00012 0.00047 0.00035 2.09624

A119 2.08815 -0.00001 0.00022 0.00015 0.00038 2.08853

A120 2.10708 -0.00016 -0.00076 -0.00137 -0.00214 2.10494

A121 2.08454 0.00004 -0.00006 0.00039 0.00034 2.08488

A122 2.09145 0.00012 0.00084 0.00094 0.00179 2.09323

A123 2.09751 0.00077 0.00148 0.01265 0.01414 2.11165

A124 2.10856 -0.00019 -0.00098 -0.00810 -0.00907 2.09949

A125 2.07711 -0.00058 -0.00051 -0.00455 -0.00507 2.07204

A126 2.10254 0.00024 0.00053 0.00125 0.00176 2.10431

A127 2.08434 -0.00012 -0.00010 -0.00067 -0.00076 2.08358

A128 2.09614 -0.00012 -0.00038 -0.00062 -0.00099 2.09515

A129 2.09669 0.00008 -0.00006 0.00122 0.00115 2.09784

A130 2.08888 -0.00002 -0.00003 -0.00052 -0.00055 2.08833

A131 2.09762 -0.00007 0.00009 -0.00070 -0.00061 2.09701

A132 2.09074 -0.00019 -0.00040 -0.00108 -0.00149 2.08925

A133 2.09642 0.00012 0.00029 0.00044 0.00073 2.09715

A134 2.09602 0.00007 0.00011 0.00065 0.00076 2.09678

A135 2.09753 0.00002 0.00031 -0.00054 -0.00024 2.09729

A136 2.09669 -0.00007 -0.00023 0.00020 -0.00004 2.09665

A137 2.08897 0.00005 -0.00007 0.00035 0.00027 2.08924

A138 2.10160 0.00043 0.00015 0.00371 0.00384 2.10544

A139 2.08610 -0.00021 0.00000 -0.00125 -0.00124 2.08486

A140 2.09527 -0.00022 -0.00012 -0.00244 -0.00256 2.09271

D1 0.01896 -0.00004 -0.00538 0.00538 -0.00016 0.01879

D2 -3.09916 0.00016 -0.00313 0.02616 0.02295 -3.07621

D3 -3.10959 -0.00021 -0.00712 -0.00505 -0.01224 -3.12182

D4 0.05549 -0.00001 -0.00486 0.01573 0.01088 0.06636

D5 -0.00487 0.00001 0.00364 -0.00284 0.00095 -0.00392

D6 -3.12663 -0.00020 -0.00317 -0.00943 -0.01249 -3.13912

D7 3.12340 0.00017 0.00547 0.00782 0.01328 3.13668

D8 0.00164 -0.00003 -0.00134 0.00122 -0.00016 0.00148

D9 -0.02648 0.00005 0.00518 -0.00610 -0.00080 -0.02727

D10 3.06331 0.00014 0.01143 -0.01381 -0.00237 3.06095

D11 3.09224 -0.00017 0.00297 -0.02625 -0.02310 3.06914

D12 -0.10116 -0.00007 0.00922 -0.03396 -0.02467 -0.12583

D13 -3.02538 -0.00013 0.04363 0.01740 0.06130 -2.96407

D14 0.10337 0.00009 0.02748 0.03062 0.05850 0.16187

D15 0.14383 0.00011 0.04622 0.04179 0.08821 0.23204

D16 -3.01061 0.00033 0.03007 0.05501 0.08541 -2.92520

D17 0.02355 -0.00006 -0.00303 0.00434 0.00130 0.02485

D18 -3.10956 0.00021 0.00485 0.02072 0.02541 -3.08414

D19 -3.06589 -0.00016 -0.00929 0.01201 0.00282 -3.06307

D20 0.08419 0.00011 -0.00141 0.02839 0.02693 0.11112

D21 -0.01102 0.00001 -0.00053 -0.00087 -0.00146 -0.01247

D22 3.11112 0.00020 0.00608 0.00564 0.01172 3.12284

D23 3.12194 -0.00028 -0.00855 -0.01755 -0.02611 3.09583

D24 -0.03911 -0.00008 -0.00194 -0.01105 -0.01293 -0.05204

D25 -0.17165 -0.00069 -0.00832 -0.08778 -0.09552 -0.26717

D26 2.98343 -0.00078 -0.00261 -0.09182 -0.09390 2.88953

D27 2.98013 -0.00037 0.00116 -0.06811 -0.06659 2.91354

D28 -0.14798 -0.00045 0.00686 -0.07215 -0.06497 -0.21295

D29 -0.15714 0.00069 0.04565 0.00747 0.05361 -0.10353

D30 3.02262 0.00040 0.03413 0.00415 0.03864 3.06126

D31 2.97062 0.00075 0.03978 0.01158 0.05183 3.02245

D32 -0.13281 0.00046 0.02825 0.00826 0.03687 -0.09595

D33 -1.02443 -0.00015 -0.02423 0.05483 0.03059 -0.99385

D34 2.11560 -0.00025 -0.02655 0.05483 0.02828 2.14388

D35 2.12952 -0.00020 -0.01900 0.05131 0.03232 2.16185

D36 -1.01363 -0.00030 -0.02131 0.05132 0.03001 -0.98362

D37 -3.06490 -0.00023 -0.00610 0.00192 -0.00453 -3.06943

D38 0.04334 0.00005 0.00371 0.00470 0.00838 0.05172

D39 3.07842 0.00026 0.00500 -0.00245 0.00248 3.08090

D40 -0.07920 -0.00004 0.00064 -0.00438 -0.00375 -0.08294

D41 -0.03027 0.00003 -0.00514 -0.00506 -0.01034 -0.04061

D42 3.09529 -0.00027 -0.00950 -0.00699 -0.01657 3.07873

D43 -0.04019 -0.00022 -0.00105 -0.00289 -0.00387 -0.04406

D44 3.08907 0.00010 0.01051 -0.00050 0.01000 3.09907

D45 0.02230 0.00020 -0.00221 -0.00033 -0.00273 0.01958

D46 -3.09730 0.00027 0.00824 0.00562 0.01375 -3.08355

D47 -3.10730 -0.00013 -0.01353 -0.00257 -0.01622 -3.12352

D48 0.05628 -0.00005 -0.00308 0.00338 0.00025 0.05654

D49 0.18349 -0.00015 -0.09583 0.04195 -0.05377 0.12973

D50 -2.94084 -0.00036 -0.07979 0.03076 -0.04868 -2.98952

D51 -2.97185 0.00021 -0.08304 0.04450 -0.03828 -3.01013

D52 0.18700 -0.00000 -0.06700 0.03331 -0.03319 0.15380

D53 0.00545 -0.00021 0.00411 0.00266 0.00683 0.01228

D54 -3.11982 0.00009 0.00856 0.00464 0.01322 -3.10661

D55 3.12461 -0.00029 -0.00655 -0.00347 -0.01007 3.11454

D56 -0.00067 0.00001 -0.00210 -0.00148 -0.00368 -0.00435

D57 -2.97139 0.00021 -0.07917 0.04292 -0.03599 -3.00738

D58 0.18182 -0.00013 -0.09076 0.04015 -0.05049 0.13133

D59 0.18319 0.00000 -0.06299 0.02961 -0.03290 0.15029

D60 -2.94678 -0.00033 -0.07458 0.02684 -0.04740 -2.99418

D61 0.98793 -0.00037 0.01672 -0.02749 -0.01081 0.97712

D62 -2.14972 -0.00034 0.02224 -0.02520 -0.00302 -2.15274

D63 -2.16568 -0.00017 0.00162 -0.01511 -0.01343 -2.17911

D64 0.97986 -0.00013 0.00714 -0.01282 -0.00564 0.97422

D65 -3.10939 -0.00010 -0.01250 -0.00252 -0.01515 -3.12454

D66 0.05412 -0.00003 -0.00253 0.00356 0.00098 0.05511

D67 0.02207 0.00021 -0.00225 -0.00009 -0.00253 0.01955

D68 -3.09760 0.00028 0.00772 0.00599 0.01360 -3.08399

D69 3.09115 0.00007 0.00968 -0.00034 0.00934 3.10049

D70 -0.04002 -0.00023 -0.00079 -0.00291 -0.00363 -0.04365

D71 0.00563 -0.00021 0.00392 0.00233 0.00631 0.01194

D72 -3.11981 0.00010 0.00871 0.00492 0.01365 -3.10615

D73 3.12486 -0.00029 -0.00626 -0.00392 -0.01023 3.11463

D74 -0.00057 0.00002 -0.00147 -0.00133 -0.00289 -0.00347

D75 -0.03036 0.00002 -0.00478 -0.00472 -0.00963 -0.03999

D76 3.07703 0.00027 0.00709 -0.00216 0.00487 3.08190

D77 3.09537 -0.00028 -0.00947 -0.00725 -0.01680 3.07857

D78 -0.08043 -0.00003 0.00240 -0.00469 -0.00229 -0.08272

D79 0.04328 0.00006 0.00334 0.00451 0.00781 0.05110

D80 -3.06363 -0.00024 -0.00821 0.00178 -0.00682 -3.07044

D81 3.02086 0.00044 0.03378 0.00524 0.03938 3.06024

D82 -0.13890 0.00052 0.02899 0.00753 0.03689 -0.10201

D83 -0.16040 0.00074 0.04731 0.00851 0.05630 -0.10411

D84 2.96302 0.00083 0.04252 0.01080 0.05381 3.01683

D85 2.96505 -0.00037 0.00236 -0.07472 -0.07198 2.89306

D86 -0.18026 -0.00070 -0.00947 -0.09190 -0.10076 -0.28101

D87 -0.15884 -0.00047 0.00697 -0.07701 -0.06971 -0.22856

D88 2.97904 -0.00080 -0.00485 -0.09418 -0.09849 2.88055

D89 -1.00555 -0.00031 -0.02191 0.05159 0.02969 -0.97586

D90 2.13963 -0.00021 -0.02001 0.05222 0.03222 2.17185

D91 2.11980 -0.00024 -0.02616 0.05343 0.02727 2.14707

D92 -1.01821 -0.00015 -0.02426 0.05406 0.02979 -0.98842

D93 3.12816 -0.00030 -0.01101 -0.01502 -0.02604 3.10212

D94 -0.03561 -0.00009 -0.00375 -0.00892 -0.01261 -0.04822

D95 -0.01028 -0.00002 -0.00103 -0.00046 -0.00154 -0.01183

D96 3.10913 0.00019 0.00624 0.00564 0.01189 3.12101

D97 -3.11623 0.00025 0.00784 0.01793 0.02560 -3.09063

D98 0.06425 0.00013 0.00314 0.02244 0.02553 0.08978

D99 0.02227 -0.00002 -0.00198 0.00362 0.00162 0.02389

D100 -3.08044 -0.00014 -0.00669 0.00813 0.00156 -3.07888

D101 -0.00482 0.00001 0.00344 -0.00280 0.00079 -0.00403

D102 3.12068 0.00019 0.00625 0.00735 0.01357 3.13425

D103 -3.12379 -0.00021 -0.00405 -0.00897 -0.01291 -3.13670

D104 0.00170 -0.00003 -0.00125 0.00118 -0.00012 0.00158

D105 0.01813 -0.00003 -0.00455 0.00491 0.00018 0.01832

D106 -3.10568 0.00019 -0.00038 0.02365 0.02318 -3.08250

D107 -3.10770 -0.00020 -0.00724 -0.00501 -0.01232 -3.12002

D108 0.05167 0.00002 -0.00306 0.01374 0.01067 0.06235

D109 -0.02517 0.00002 0.00401 -0.00535 -0.00121 -0.02637

D110 3.07779 0.00013 0.00871 -0.00991 -0.00119 3.07660

D111 3.09910 -0.00021 -0.00007 -0.02355 -0.02342 3.07568

D112 -0.08113 -0.00010 0.00463 -0.02811 -0.02340 -0.10453

D113 -3.01024 -0.00014 0.04270 0.02295 0.06592 -2.94431

D114 0.11429 0.00008 0.02674 0.03410 0.06126 0.17556

D115 0.15228 0.00012 0.04757 0.04497 0.09273 0.24500

D116 -3.00638 0.00034 0.03162 0.05611 0.08807 -2.91831

D117 0.97258 -0.00013 0.01052 -0.01628 -0.00573 0.96685

D118 -2.17380 -0.00017 0.00515 -0.02054 -0.01533 -2.18913

D119 -2.15305 -0.00034 0.02544 -0.02673 -0.00135 -2.15440

D120 0.98375 -0.00039 0.02008 -0.03099 -0.01095 0.97280

D121 -3.13140 -0.00002 0.00314 0.00336 0.00653 -3.12487

D122 -0.01206 0.00004 0.00457 0.00406 0.00864 -0.00342

D123 0.01174 0.00008 0.00543 0.00334 0.00877 0.02051

D124 3.13108 0.00014 0.00686 0.00404 0.01088 -3.14122

D125 -3.13676 -0.00004 -0.00370 -0.00466 -0.00834 3.13809

D126 -0.01346 0.00000 -0.00145 -0.00629 -0.00773 -0.02119

D127 0.00330 -0.00014 -0.00597 -0.00465 -0.01062 -0.00732

D128 3.12660 -0.00010 -0.00373 -0.00629 -0.01001 3.11659

D129 -0.01734 0.00001 -0.00211 0.00012 -0.00200 -0.01935

D130 3.12409 0.00001 -0.00161 0.00054 -0.00108 3.12301

D131 -3.13657 -0.00005 -0.00355 -0.00060 -0.00415 -3.14071

D132 0.00487 -0.00005 -0.00304 -0.00018 -0.00322 0.00165

D133 0.00779 -0.00005 -0.00075 -0.00235 -0.00311 0.00468

D134 -3.13409 0.00001 0.00020 0.00073 0.00093 -3.13315

D135 -3.13364 -0.00005 -0.00126 -0.00277 -0.00404 -3.13768

D136 0.00767 0.00001 -0.00031 0.00031 0.00000 0.00767

D137 0.00722 -0.00002 0.00022 0.00101 0.00123 0.00845

D138 -3.13462 0.00003 0.00035 0.00297 0.00334 -3.13128

D139 -3.13409 -0.00007 -0.00073 -0.00207 -0.00281 -3.13690

D140 0.00726 -0.00003 -0.00059 -0.00012 -0.00071 0.00656

D141 -0.01278 0.00011 0.00318 0.00251 0.00572 -0.00706

D142 -3.13595 0.00006 0.00092 0.00416 0.00510 -3.13085

D143 3.12906 0.00006 0.00305 0.00056 0.00362 3.13268

D144 0.00589 0.00001 0.00078 0.00221 0.00300 0.00889

D145 -0.00598 0.00001 0.00188 -0.00270 -0.00083 -0.00681

D146 3.13188 0.00002 0.00249 0.00038 0.00285 3.13474

D147 3.13574 0.00000 -0.00079 -0.00178 -0.00256 3.13319

D148 -0.00957 0.00001 -0.00018 0.00131 0.00112 -0.00845

D149 -0.00577 0.00005 -0.00150 0.00184 0.00035 -0.00541

D150 3.13526 -0.00002 -0.00216 -0.00009 -0.00224 3.13302

D151 3.13569 0.00006 0.00117 0.00091 0.00209 3.13778

D152 -0.00647 -0.00001 0.00051 -0.00102 -0.00051 -0.00697

D153 0.00916 0.00004 0.00265 0.00420 0.00682 0.01598

D154 3.13446 -0.00002 0.00407 0.00112 0.00515 3.13961

D155 -3.12873 0.00003 0.00204 0.00113 0.00316 -3.12557

D156 -0.00343 -0.00003 0.00346 -0.00196 0.00149 -0.00194

D157 -3.13828 -0.00012 -0.00195 -0.00246 -0.00446 3.14045

D158 -0.00056 -0.00015 -0.00738 -0.00472 -0.01211 -0.01268

D159 0.01954 -0.00006 -0.00337 0.00061 -0.00280 0.01673

D160 -3.12593 -0.00009 -0.00880 -0.00165 -0.01046 -3.13639

D161 3.12651 0.00019 0.00245 0.00164 0.00403 3.13054

D162 0.00528 0.00007 0.00208 0.00281 0.00486 0.01014

D163 -0.01126 0.00022 0.00778 0.00388 0.01167 0.00041

D164 -3.13249 0.00011 0.00742 0.00506 0.01250 -3.11999

D165 0.01453 -0.00018 -0.00343 -0.00250 -0.00593 0.00860

D166 -3.12650 -0.00010 -0.00277 -0.00058 -0.00335 -3.12985

D167 3.13566 -0.00006 -0.00308 -0.00369 -0.00677 3.12888

D168 -0.00537 0.00001 -0.00242 -0.00177 -0.00419 -0.00956

D169 3.12651 0.00016 0.00293 -0.00115 0.00172 3.12823

D170 0.00530 0.00006 0.00241 0.00136 0.00373 0.00902

D171 -0.01044 0.00021 0.00811 0.00300 0.01113 0.00069

D172 -3.13165 0.00011 0.00760 0.00551 0.01314 -3.11851

D173 -3.13837 -0.00010 -0.00253 0.00044 -0.00213 -3.14051

D174 0.01959 -0.00005 -0.00408 0.00295 -0.00117 0.01842

D175 -0.00149 -0.00014 -0.00781 -0.00374 -0.01156 -0.01305

D176 -3.12671 -0.00009 -0.00936 -0.00123 -0.01060 -3.13731

D177 0.01432 -0.00018 -0.00343 -0.00231 -0.00573 0.00859

D178 -3.12657 -0.00010 -0.00287 -0.00004 -0.00290 -3.12947

D179 3.13544 -0.00007 -0.00292 -0.00483 -0.00776 3.12768

D180 -0.00545 0.00001 -0.00237 -0.00256 -0.00493 -0.01038

D181 -0.00609 0.00006 -0.00176 0.00224 0.00049 -0.00560

D182 3.13564 0.00007 0.00112 0.00128 0.00241 3.13805

D183 3.13480 -0.00002 -0.00232 -0.00004 -0.00235 3.13245

D184 -0.00666 -0.00001 0.00057 -0.00100 -0.00044 -0.00709

D185 -0.00577 0.00001 0.00205 -0.00300 -0.00095 -0.00672

D186 3.13221 0.00002 0.00285 -0.00001 0.00282 3.13503

D187 3.13569 0.00000 -0.00083 -0.00205 -0.00287 3.13282

D188 -0.00952 0.00001 -0.00003 0.00094 0.00090 -0.00862

D189 0.00958 0.00003 0.00283 0.00380 0.00660 0.01617

D190 3.13473 -0.00002 0.00438 0.00127 0.00562 3.14035

D191 -3.12842 0.00002 0.00204 0.00082 0.00284 -3.12557

D192 -0.00326 -0.00003 0.00358 -0.00170 0.00186 -0.00140

D193 -3.13458 -0.00005 -0.00427 -0.00403 -0.00828 3.14032

D194 -0.01236 -0.00000 -0.00193 -0.00591 -0.00782 -0.02018

D195 0.00349 -0.00015 -0.00613 -0.00465 -0.01078 -0.00729

D196 3.12571 -0.00009 -0.00380 -0.00653 -0.01032 3.11539

D197 -3.13341 -0.00000 0.00376 0.00286 0.00664 -3.12677

D198 -0.01394 0.00005 0.00511 0.00367 0.00880 -0.00514

D199 0.01173 0.00009 0.00563 0.00344 0.00907 0.02080

D200 3.13119 0.00014 0.00699 0.00425 0.01123 -3.14076

D201 -0.01300 0.00011 0.00321 0.00238 0.00561 -0.00738

D202 3.12856 0.00006 0.00305 0.00053 0.00359 3.13216

D203 -3.13509 0.00006 0.00085 0.00428 0.00515 -3.12994

D204 0.00647 0.00001 0.00069 0.00243 0.00313 0.00960

D205 0.00729 -0.00002 0.00029 0.00116 0.00146 0.00875

D206 -3.13423 -0.00008 -0.00072 -0.00212 -0.00285 -3.13708

D207 -3.13427 0.00003 0.00046 0.00302 0.00349 -3.13078

D208 0.00740 -0.00003 -0.00056 -0.00027 -0.00082 0.00658

D209 0.00790 -0.00005 -0.00079 -0.00240 -0.00320 0.00470

D210 -3.13375 -0.00005 -0.00141 -0.00273 -0.00414 -3.13790

D211 -3.13377 0.00001 0.00022 0.00089 0.00111 -3.13266

D212 0.00777 0.00001 -0.00039 0.00056 0.00016 0.00793

D213 -0.01748 0.00001 -0.00221 0.00004 -0.00219 -0.01966

D214 -3.13683 -0.00005 -0.00358 -0.00079 -0.00437 -3.14120

D215 3.12417 0.00000 -0.00160 0.00037 -0.00124 3.12293

D216 0.00482 -0.00005 -0.00297 -0.00046 -0.00343 0.00139

Item Value Threshold Converged?

Maximum Force 0.012442 0.000450 NO

RMS Force 0.001294 0.000300 NO

Maximum Displacement 0.446974 0.001800 NO

RMS Displacement 0.113997 0.001200 NO

Predicted change in Energy=-1.701459D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Mon Aug 26 08:54:04 2019, MaxMem= 4294967296 cpu: 2.6

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

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=2 Diff= 4.48D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 2.006568 -3.706477 0.601108

2 6 0 2.004220 -2.351966 0.241286

3 7 0 0.695884 -1.995731 0.016296

4 6 0 -0.129436 -3.081095 0.185634

5 6 0 0.679510 -4.160247 0.563180

6 6 0 -1.559190 -3.094274 -0.034411

7 6 0 -2.364038 -1.969649 -0.156118

8 7 0 -1.955916 -0.667421 0.026165

9 6 0 -3.081434 0.100160 -0.098131

10 6 0 -4.237524 -0.737856 -0.428590

11 6 0 -3.793241 -2.011027 -0.474523

12 6 0 3.144457 -1.484413 0.069295

13 6 0 3.081546 -0.101339 -0.092534

14 6 0 4.237731 0.735307 -0.426070

15 6 0 3.793695 2.008407 -0.476204

16 6 0 2.364452 1.968326 -0.157819

17 7 0 1.956158 0.666902 0.029457

18 6 0 1.559538 3.093548 -0.040991

19 6 0 0.129567 3.079905 0.177733

20 6 0 -0.677322 4.154226 0.572635

21 6 0 -2.004478 3.700323 0.609935

22 6 0 -2.003983 2.350779 0.232237

23 7 0 -0.696840 1.997494 -0.003295

24 6 0 -3.144656 1.483665 0.060224

25 6 0 -2.181074 -4.439701 -0.112204

26 6 0 -1.731480 -5.373469 -1.057899

27 6 0 -2.322265 -6.628922 -1.150221

28 6 0 -3.357407 -6.982106 -0.283851

29 6 0 -3.800677 -6.068897 0.671104

30 6 0 -3.220600 -4.805533 0.754507

31 6 0 6.984095 -3.397811 0.151785

32 6 0 6.018610 -3.807194 -0.768456

33 6 0 4.770510 -3.193757 -0.793629

34 6 0 4.471892 -2.145063 0.090130

35 6 0 5.452008 -1.739916 1.008123

36 6 0 6.695515 -2.364682 1.041715

37 6 0 -4.471388 2.144962 0.085202

38 6 0 -5.451007 1.737054 1.002689

39 6 0 -6.692987 2.364460 1.041825

40 6 0 -6.980712 3.403110 0.158068

41 6 0 -6.015778 3.815499 -0.761439

42 6 0 -4.769126 3.199468 -0.792051

43 6 0 2.180634 4.439082 -0.116360

44 6 0 3.221820 4.803087 0.749296

45 6 0 3.799440 6.067788 0.669885

46 6 0 3.352389 6.984227 -0.280216

47 6 0 2.315635 6.632952 -1.145498

48 6 0 1.727046 5.376254 -1.056879

49 1 0 2.879611 -4.283490 0.859355

50 1 0 0.329656 -5.154957 0.787685

51 1 0 -5.236255 -0.383063 -0.631713

52 1 0 -4.361242 -2.895282 -0.718890

53 1 0 5.236453 0.379747 -0.627869

54 1 0 4.361645 2.891736 -0.724038

55 1 0 -0.325524 5.145125 0.810769

56 1 0 -2.876223 4.273339 0.881194

57 1 0 -0.928215 -5.103354 -1.733669

58 1 0 -1.974256 -7.333092 -1.898561

59 1 0 -3.812688 -7.964516 -0.351125

60 1 0 -4.598514 -6.339393 1.354636

61 1 0 -3.560424 -4.100676 1.504702

62 1 0 7.954363 -3.882534 0.175353

63 1 0 6.238286 -4.606388 -1.468491

64 1 0 4.024602 -3.514353 -1.511816

65 1 0 5.227179 -0.944813 1.709694

66 1 0 7.437777 -2.045611 1.765741

67 1 0 -5.226588 0.938394 1.700310

68 1 0 -7.434608 2.043350 1.765606

69 1 0 -7.949748 3.890054 0.186156

70 1 0 -6.234752 4.619205 -1.456507

71 1 0 -4.023441 3.522912 -1.509188

72 1 0 3.564078 4.096076 1.496320

73 1 0 4.598221 6.336864 1.352881

74 1 0 3.805664 7.967784 -0.344279

75 1 0 1.964560 7.339736 -1.889937

76 1 0 0.922224 5.107709 -1.731426

77 1 0 0.384840 -1.057437 -0.194131

78 1 0 -0.388127 1.065018 -0.240142

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

Rotational constants (GHZ): 0.0587858 0.0583659 0.0301339

Leave Link 202 at Mon Aug 26 08:54:04 2019, MaxMem= 4294967296 cpu: 0.1

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

Standard basis: 6-311G(d) (5D, 7F)

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

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5358.9736707670 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2123042062 Hartrees.

Nuclear repulsion after empirical dispersion term = 5358.7613665608 Hartrees.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5811

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.21D-10

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 375

GePol: Fraction of low-weight points (<1% of avg) = 6.45%

GePol: Cavity surface area = 610.855 Ang\*\*2

GePol: Cavity volume = 628.009 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021250161 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5358.7592415447 Hartrees.

Leave Link 301 at Mon Aug 26 08:54:04 2019, MaxMem= 4294967296 cpu: 2.3

(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.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Mon Aug 26 08:54:06 2019, MaxMem= 4294967296 cpu: 27.4

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

DipDrv: MaxL=1.

Leave Link 303 at Mon Aug 26 08:54:06 2019, MaxMem= 4294967296 cpu: 2.3

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

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= -0.000000 0.000000 -0.000000

Rot= 0.987394 0.000013 -0.000001 -0.158281 Ang= 18.21 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0434 S= 1.0144

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30480546631

Leave Link 401 at Mon Aug 26 08:54:12 2019, MaxMem= 4294967296 cpu: 84.8

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 580000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 101303163.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.09D-14 for 5792.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.21D-15 for 5795 5734.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.12D-14 for 5792.

Iteration 1 A^-1\*A deviation from orthogonality is 1.15D-10 for 5075 1395.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.89D-15 for 5567.

Iteration 2 A\*A^-1 deviation from orthogonality is 4.00D-15 for 5114 1404.

Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 1144.

Iteration 2 A^-1\*A deviation from orthogonality is 5.00D-16 for 5197 3238.

E= -1914.28230564399

DIIS: error= 6.13D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.28230564399 IErMin= 1 ErrMin= 6.13D-03

ErrMax= 6.13D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.18D-01 BMatP= 1.18D-01

IDIUse=3 WtCom= 9.39D-01 WtEn= 6.13D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.644 Goal= None Shift= 0.000

Gap= 0.707 Goal= None Shift= 0.000

GapD= 0.644 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=2.49D-04 MaxDP=6.78D-03 OVMax= 7.18D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.49D-04 CP: 9.99D-01

E= -1914.33111454134 Delta-E= -0.048808897344 Rises=F Damp=F

DIIS: error= 8.23D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33111454134 IErMin= 2 ErrMin= 8.23D-04

ErrMax= 8.23D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.84D-03 BMatP= 1.18D-01

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.23D-03

Coeff-Com: -0.479D-01 0.105D+01

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

Coeff: -0.475D-01 0.105D+01

Gap= 0.051 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.18D-05 MaxDP=5.19D-03 DE=-4.88D-02 OVMax= 6.17D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 6.66D-05 CP: 9.99D-01 1.11D+00

E= -1914.33183309187 Delta-E= -0.000718550530 Rises=F Damp=F

DIIS: error= 1.28D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33183309187 IErMin= 2 ErrMin= 8.23D-04

ErrMax= 1.28D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.13D-03 BMatP= 1.84D-03

IDIUse=3 WtCom= 2.18D-01 WtEn= 7.82D-01

Coeff-Com: -0.348D-01 0.577D+00 0.458D+00

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

Coeff: -0.760D-02 0.126D+00 0.882D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=6.23D-05 MaxDP=4.61D-03 DE=-7.19D-04 OVMax= 2.67D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.87D-05 CP: 9.99D-01 1.16D+00 7.58D-01

E= -1914.33127463665 Delta-E= 0.000558455215 Rises=F Damp=F

DIIS: error= 1.54D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 3 EnMin= -1914.33183309187 IErMin= 2 ErrMin= 8.23D-04

ErrMax= 1.54D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.80D-03 BMatP= 1.84D-03

IDIUse=3 WtCom= 2.03D-01 WtEn= 7.97D-01

Coeff-Com: -0.951D-02 0.117D+00 0.563D+00 0.329D+00

Coeff-En: 0.000D+00 0.000D+00 0.625D+00 0.375D+00

Coeff: -0.193D-02 0.238D-01 0.612D+00 0.366D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=4.08D-05 MaxDP=3.30D-03 DE= 5.58D-04 OVMax= 2.48D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.58D-05 CP: 9.98D-01 1.16D+00 1.21D+00 6.18D-01

E= -1914.33266693086 Delta-E= -0.001392294205 Rises=F Damp=F

DIIS: error= 3.45D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33266693086 IErMin= 5 ErrMin= 3.45D-04

ErrMax= 3.45D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-04 BMatP= 1.84D-03

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.45D-03

Coeff-Com: 0.919D-03-0.369D-01 0.294D+00 0.207D+00 0.535D+00

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

Coeff: 0.916D-03-0.368D-01 0.293D+00 0.207D+00 0.537D+00

Gap= 0.052 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.52D-05 MaxDP=1.15D-03 DE=-1.39D-03 OVMax= 1.51D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.17D-06 CP: 9.98D-01 1.18D+00 1.38D+00 7.46D-01 1.14D+00

E= -1914.33276362459 Delta-E= -0.000096693733 Rises=F Damp=F

DIIS: error= 3.04D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33276362459 IErMin= 6 ErrMin= 3.04D-04

ErrMax= 3.04D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.40D-05 BMatP= 1.04D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.04D-03

Coeff-Com: 0.728D-02-0.103D+00-0.220D+00-0.790D-01 0.201D+00 0.119D+01

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

Coeff: 0.726D-02-0.103D+00-0.219D+00-0.787D-01 0.201D+00 0.119D+01

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=3.35D-05 MaxDP=2.92D-03 DE=-9.67D-05 OVMax= 3.52D-02

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.09D-06 CP: 9.98D-01 1.21D+00 1.73D+00 1.02D+00 1.94D+00

CP: 1.99D+00

E= -1914.33289808302 Delta-E= -0.000134458433 Rises=F Damp=F

DIIS: error= 1.49D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33289808302 IErMin= 7 ErrMin= 1.49D-04

ErrMax= 1.49D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.58D-05 BMatP= 3.40D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.49D-03

Coeff-Com: 0.274D-02-0.244D-01-0.235D+00-0.114D+00-0.198D+00 0.478D+00

Coeff-Com: 0.109D+01

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

Coeff-En: 0.100D+01

Coeff: 0.274D-02-0.244D-01-0.235D+00-0.114D+00-0.197D+00 0.477D+00

Coeff: 0.109D+01

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.68D-05 MaxDP=2.24D-03 DE=-1.34D-04 OVMax= 2.81D-02

Cycle 8 Pass 1 IDiag 1:

RMSU= 3.25D-06 CP: 9.98D-01 1.23D+00 2.01D+00 1.25D+00 2.58D+00

CP: 3.00D+00 1.71D+00

E= -1914.33294978017 Delta-E= -0.000051697147 Rises=F Damp=F

DIIS: error= 6.67D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33294978017 IErMin= 8 ErrMin= 6.67D-05

ErrMax= 6.67D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.02D-06 BMatP= 1.58D-05

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

Coeff-Com: -0.167D-02 0.339D-01-0.355D-01-0.203D-01-0.189D+00-0.237D+00

Coeff-Com: 0.714D+00 0.736D+00

Coeff: -0.167D-02 0.339D-01-0.355D-01-0.203D-01-0.189D+00-0.237D+00

Coeff: 0.714D+00 0.736D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.07D-05 MaxDP=9.19D-04 DE=-5.17D-05 OVMax= 1.16D-02

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.25D-06 CP: 9.98D-01 1.24D+00 2.11D+00 1.34D+00 2.86D+00

CP: 3.00D+00 2.23D+00 1.51D+00

E= -1914.33295843085 Delta-E= -0.000008650683 Rises=F Damp=F

DIIS: error= 2.63D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33295843085 IErMin= 9 ErrMin= 2.63D-05

ErrMax= 2.63D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.84D-07 BMatP= 7.02D-06

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

Coeff-Com: -0.443D-03 0.403D-02 0.339D-01 0.209D-01 0.475D-01-0.869D-01

Coeff-Com: -0.178D+00 0.741D-01 0.108D+01

Coeff: -0.443D-03 0.403D-02 0.339D-01 0.209D-01 0.475D-01-0.869D-01

Coeff: -0.178D+00 0.741D-01 0.108D+01

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.43D-06 MaxDP=1.74D-04 DE=-8.65D-06 OVMax= 2.12D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.11D-06 CP: 9.98D-01 1.24D+00 2.12D+00 1.35D+00 2.90D+00

CP: 3.00D+00 2.40D+00 1.85D+00 1.31D+00

E= -1914.33295975259 Delta-E= -0.000001321734 Rises=F Damp=F

DIIS: error= 1.35D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33295975259 IErMin=10 ErrMin= 1.35D-05

ErrMax= 1.35D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.79D-07 BMatP= 8.84D-07

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

Coeff-Com: 0.232D-03-0.770D-02 0.281D-01 0.183D-01 0.857D-01 0.192D-01

Coeff-Com: -0.319D+00-0.163D+00 0.643D+00 0.695D+00

Coeff: 0.232D-03-0.770D-02 0.281D-01 0.183D-01 0.857D-01 0.192D-01

Coeff: -0.319D+00-0.163D+00 0.643D+00 0.695D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.33D-06 MaxDP=9.11D-05 DE=-1.32D-06 OVMax= 1.14D-03

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.00D-07 CP: 9.98D-01 1.24D+00 2.13D+00 1.35D+00 2.92D+00

CP: 3.00D+00 2.49D+00 2.01D+00 1.50D+00 1.29D+00

E= -1914.33296015309 Delta-E= -0.000000400506 Rises=F Damp=F

DIIS: error= 6.61D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33296015309 IErMin=11 ErrMin= 6.61D-06

ErrMax= 6.61D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-07 BMatP= 4.79D-07

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

Coeff-Com: 0.250D-03-0.500D-02 0.243D-02 0.281D-02 0.267D-01 0.344D-01

Coeff-Com: -0.104D+00-0.955D-01-0.782D-02 0.354D+00 0.792D+00

Coeff: 0.250D-03-0.500D-02 0.243D-02 0.281D-02 0.267D-01 0.344D-01

Coeff: -0.104D+00-0.955D-01-0.782D-02 0.354D+00 0.792D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=8.42D-07 MaxDP=6.78D-05 DE=-4.01D-07 OVMax= 8.26D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.66D-07 CP: 9.98D-01 1.24D+00 2.13D+00 1.36D+00 2.94D+00

CP: 3.00D+00 2.53D+00 2.10D+00 1.58D+00 1.53D+00

CP: 9.88D-01

E= -1914.33296025801 Delta-E= -0.000000104916 Rises=F Damp=F

DIIS: error= 3.07D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.33296025801 IErMin=12 ErrMin= 3.07D-06

ErrMax= 3.07D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.42D-08 BMatP= 1.03D-07

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

Coeff-Com: 0.101D-03-0.143D-02-0.395D-02-0.163D-02-0.933D-03 0.150D-01

Coeff-Com: -0.859D-03-0.196D-01-0.120D+00 0.646D-01 0.453D+00 0.616D+00

Coeff: 0.101D-03-0.143D-02-0.395D-02-0.163D-02-0.933D-03 0.150D-01

Coeff: -0.859D-03-0.196D-01-0.120D+00 0.646D-01 0.453D+00 0.616D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=3.35D-07 MaxDP=2.80D-05 DE=-1.05D-07 OVMax= 3.21D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.40D-07 CP: 9.98D-01 1.24D+00 2.13D+00 1.36D+00 2.95D+00

CP: 3.00D+00 2.55D+00 2.12D+00 1.62D+00 1.56D+00

CP: 1.16D+00 9.58D-01

E= -1914.33296028007 Delta-E= -0.000000022055 Rises=F Damp=F

DIIS: error= 2.16D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.33296028007 IErMin=13 ErrMin= 2.16D-06

ErrMax= 2.16D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.99D-09 BMatP= 3.42D-08

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

Coeff-Com: -0.420D-04 0.112D-02-0.245D-02-0.148D-02-0.985D-02-0.676D-02

Coeff-Com: 0.337D-01 0.270D-01-0.555D-01-0.101D+00-0.590D-01 0.340D+00

Coeff-Com: 0.835D+00

Coeff: -0.420D-04 0.112D-02-0.245D-02-0.148D-02-0.985D-02-0.676D-02

Coeff: 0.337D-01 0.270D-01-0.555D-01-0.101D+00-0.590D-01 0.340D+00

Coeff: 0.835D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=2.78D-07 MaxDP=2.30D-05 DE=-2.21D-08 OVMax= 2.89D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 6.95D-08 CP: 9.98D-01 1.24D+00 2.14D+00 1.36D+00 2.95D+00

CP: 3.00D+00 2.56D+00 2.14D+00 1.64D+00 1.60D+00

CP: 1.18D+00 1.22D+00 1.24D+00

E= -1914.33296028864 Delta-E= -0.000000008579 Rises=F Damp=F

DIIS: error= 8.26D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.33296028864 IErMin=14 ErrMin= 8.26D-07

ErrMax= 8.26D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.29D-09 BMatP= 7.99D-09

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

Coeff-Com: -0.312D-04 0.628D-03-0.190D-03-0.217D-03-0.336D-02-0.494D-02

Coeff-Com: 0.124D-01 0.138D-01-0.159D-02-0.524D-01-0.102D+00 0.352D-01

Coeff-Com: 0.324D+00 0.779D+00

Coeff: -0.312D-04 0.628D-03-0.190D-03-0.217D-03-0.336D-02-0.494D-02

Coeff: 0.124D-01 0.138D-01-0.159D-02-0.524D-01-0.102D+00 0.352D-01

Coeff: 0.324D+00 0.779D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=6.37D-08 MaxDP=5.21D-06 DE=-8.58D-09 OVMax= 5.24D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 2.88D-08 CP: 9.98D-01 1.24D+00 2.14D+00 1.36D+00 2.95D+00

CP: 3.00D+00 2.56D+00 2.15D+00 1.64D+00 1.61D+00

CP: 1.20D+00 1.27D+00 1.42D+00 1.17D+00

E= -1914.33296028976 Delta-E= -0.000000001114 Rises=F Damp=F

DIIS: error= 4.45D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.33296028976 IErMin=15 ErrMin= 4.45D-07

ErrMax= 4.45D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.76D-10 BMatP= 1.29D-09

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

Coeff-Com: -0.430D-05 0.191D-05 0.653D-03 0.334D-03 0.113D-02-0.544D-03

Coeff-Com: -0.325D-02-0.733D-03 0.151D-01 0.770D-03-0.399D-01-0.827D-01

Coeff-Com: -0.841D-01 0.472D+00 0.721D+00

Coeff: -0.430D-05 0.191D-05 0.653D-03 0.334D-03 0.113D-02-0.544D-03

Coeff: -0.325D-02-0.733D-03 0.151D-01 0.770D-03-0.399D-01-0.827D-01

Coeff: -0.841D-01 0.472D+00 0.721D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=2.96D-08 MaxDP=2.35D-06 DE=-1.11D-09 OVMax= 1.55D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.80D-08 CP: 9.98D-01 1.24D+00 2.14D+00 1.36D+00 2.95D+00

CP: 3.00D+00 2.56D+00 2.15D+00 1.64D+00 1.61D+00

CP: 1.21D+00 1.32D+00 1.48D+00 1.33D+00 1.10D+00

E= -1914.33296029018 Delta-E= -0.000000000423 Rises=F Damp=F

DIIS: error= 1.20D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1914.33296029018 IErMin=16 ErrMin= 1.20D-07

ErrMax= 1.20D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.26D-11 BMatP= 5.76D-10

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

Coeff-Com: 0.434D-05-0.108D-03 0.173D-03 0.970D-04 0.813D-03 0.708D-03

Coeff-Com: -0.292D-02-0.272D-02 0.484D-02 0.102D-01 0.817D-02-0.266D-01

Coeff-Com: -0.852D-01-0.358D-01 0.163D+00 0.965D+00

Coeff: 0.434D-05-0.108D-03 0.173D-03 0.970D-04 0.813D-03 0.708D-03

Coeff: -0.292D-02-0.272D-02 0.484D-02 0.102D-01 0.817D-02-0.266D-01

Coeff: -0.852D-01-0.358D-01 0.163D+00 0.965D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.42D-08 MaxDP=1.20D-06 DE=-4.23D-10 OVMax= 9.50D-06

Cycle 17 Pass 1 IDiag 1:

RMSU= 5.59D-09 CP: 9.98D-01 1.24D+00 2.14D+00 1.36D+00 2.95D+00

CP: 3.00D+00 2.56D+00 2.15D+00 1.64D+00 1.61D+00

CP: 1.21D+00 1.33D+00 1.51D+00 1.41D+00 1.31D+00

CP: 1.22D+00

E= -1914.33296029026 Delta-E= -0.000000000080 Rises=F Damp=F

DIIS: error= 6.03D-08 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1914.33296029026 IErMin=17 ErrMin= 6.03D-08

ErrMax= 6.03D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.26D-11 BMatP= 5.26D-11

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

Coeff-Com: 0.293D-05-0.572D-04-0.524D-05 0.409D-06 0.279D-03 0.478D-03

Coeff-Com: -0.108D-02-0.139D-02 0.217D-03 0.569D-02 0.111D-01 0.392D-03

Coeff-Com: -0.312D-01-0.102D+00-0.455D-01 0.515D+00 0.647D+00

Coeff: 0.293D-05-0.572D-04-0.524D-05 0.409D-06 0.279D-03 0.478D-03

Coeff: -0.108D-02-0.139D-02 0.217D-03 0.569D-02 0.111D-01 0.392D-03

Coeff: -0.312D-01-0.102D+00-0.455D-01 0.515D+00 0.647D+00

Gap= 0.053 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=5.12D-09 MaxDP=4.08D-07 DE=-8.00D-11 OVMax= 2.76D-06

Error on total polarization charges = 0.08280

SCF Done: E(UB3LYP) = -1914.33296029 A.U. after 17 cycles

NFock= 17 Conv=0.51D-08 -V/T= 2.0041

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0545 S= 1.0181

<L.S>= 0.000000000000E+00

KE= 1.906423103208D+03 PE=-1.516718511259D+04 EE= 5.987669807547D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.33

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0545, after 2.0017

Leave Link 502 at Mon Aug 26 09:02:16 2019, MaxMem= 4294967296 cpu: 7667.8

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

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

Range of M.O.s used for correlation: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.52821863D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.65492419D-01

Leave Link 801 at Mon Aug 26 09:02:16 2019, MaxMem= 4294967296 cpu: 0.9

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

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

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

Leave Link 1101 at Mon Aug 26 09:02:23 2019, MaxMem= 4294967296 cpu: 111.5

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

Symmetrizing basis deriv contribution to polar:

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

Leave Link 1102 at Mon Aug 26 09:02:23 2019, MaxMem= 4294967296 cpu: 2.0

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

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 198

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 Mon Aug 26 09:22:21 2019, MaxMem= 4294967296 cpu: 19151.5

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

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 580000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 4.81D+03 3.75D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 3.85D+02 3.02D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 8.13D+00 3.78D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 9.36D-02 3.30D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.03D-04 1.85D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 3.85D-06 1.12D-04.

190 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 1.74D-08 8.43D-06.

84 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 7.32D-11 4.87D-07.

34 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 4.29D-13 2.93D-08.

3 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 6.50D-15 2.23D-09.

3 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 5.95D-15 2.64D-09.

3 vectors produced by pass 11 Test12= 2.55D-13 1.00D-09 XBig12= 8.94D-15 2.82D-09.

3 vectors produced by pass 12 Test12= 2.55D-13 1.00D-09 XBig12= 9.06D-15 3.27D-09.

3 vectors produced by pass 13 Test12= 2.55D-13 1.00D-09 XBig12= 1.31D-14 3.20D-09.

3 vectors produced by pass 14 Test12= 2.55D-13 1.00D-09 XBig12= 7.40D-15 3.44D-09.

3 vectors produced by pass 15 Test12= 2.55D-13 1.00D-09 XBig12= 1.27D-14 2.78D-09.

3 vectors produced by pass 16 Test12= 2.55D-13 1.00D-09 XBig12= 8.52D-15 2.61D-09.

3 vectors produced by pass 17 Test12= 2.55D-13 1.00D-09 XBig12= 1.62D-14 3.86D-09.

2 vectors produced by pass 18 Test12= 2.55D-13 1.00D-09 XBig12= 2.42D-15 1.27D-09.

InvSVY: IOpt=1 It= 1 EMax= 1.28D-13

Solved reduced A of dimension 1744 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1112.64 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 Mon Aug 26 13:17:41 2019, MaxMem= 4294967296 cpu: 225865.0

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 198

Leave Link 701 at Mon Aug 26 13:19:11 2019, MaxMem= 4294967296 cpu: 1428.8

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

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

Leave Link 702 at Mon Aug 26 13:19:11 2019, MaxMem= 4294967296 cpu: 0.4

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

Leave Link 703 at Mon Aug 26 13:37:30 2019, MaxMem= 4294967296 cpu: 17576.8

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

Dipole =-2.80256599D-03 9.56496171D-03-4.75602534D-01

Polarizability= 1.28312348D+03-1.34695624D+02 1.60353018D+03

-7.32485848D-02 7.30225506D-02 4.51252730D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.002616733 -0.000581837 -0.003608601

2 6 -0.003293298 0.001636152 0.004859380

3 7 -0.001491902 0.000301673 -0.000434185

4 6 -0.003765886 0.001634484 -0.005017825

5 6 0.002564636 -0.000940275 0.003622359

6 6 0.006535626 -0.001509981 0.005253746

7 6 -0.005093192 0.001006509 -0.002619965

8 7 0.001813151 -0.001216652 0.000599195

9 6 0.003229735 0.001507408 -0.003780845

10 6 -0.001984975 0.000669118 0.001257031

11 6 0.001742441 -0.000474741 0.001126366

12 6 0.005929781 -0.001656094 -0.004844535

13 6 -0.003217320 0.001454774 0.003753512

14 6 0.001984572 0.000623914 -0.001230169

15 6 -0.001743647 -0.000473751 -0.001147825

16 6 0.005065005 0.001025452 0.002622305

17 7 -0.001804513 -0.001102556 -0.000574519

18 6 -0.006494547 -0.001506683 -0.005209616

19 6 0.003712592 0.001637172 0.004987400

20 6 -0.002548179 -0.000950796 -0.003614928

21 6 -0.002603402 -0.000581717 0.003613545

22 6 0.003268846 0.001679470 -0.004857848

23 7 0.001473642 0.000316838 0.000448345

24 6 -0.005964159 -0.001722963 0.004829384

25 6 -0.000119113 -0.000033630 0.000181167

26 6 0.000051575 0.000250390 -0.000069307

27 6 0.000245722 -0.000247309 -0.000233089

28 6 0.000151126 0.000101680 0.000040087

29 6 -0.000336001 -0.000191445 0.000074662

30 6 0.000022957 0.000152679 0.000098317

31 6 0.000080907 0.000212296 0.000064956

32 6 0.000166017 0.000014974 0.000116682

33 6 -0.000429921 -0.000093441 -0.000179521

34 6 0.000351407 -0.000374933 0.000061367

35 6 0.000140621 -0.000192375 0.000146939

36 6 -0.000133930 0.000045542 -0.000011729

37 6 -0.000340920 -0.000394949 -0.000052542

38 6 -0.000156331 -0.000191148 -0.000143463

39 6 0.000150183 0.000060467 0.000015221

40 6 -0.000093252 0.000211165 -0.000074458

41 6 -0.000152424 0.000027480 -0.000123000

42 6 0.000423264 -0.000103143 0.000187143

43 6 0.000133013 -0.000040052 -0.000168507

44 6 -0.000036179 0.000135741 -0.000096034

45 6 0.000353767 -0.000170632 -0.000051478

46 6 -0.000156589 0.000098020 -0.000056150

47 6 -0.000242603 -0.000232562 0.000239779

48 6 -0.000053717 0.000245947 0.000049809

49 1 0.000128355 -0.000015484 -0.000057898

50 1 0.000050479 0.000035963 0.000168381

51 1 0.000177640 -0.000100218 0.000021022

52 1 0.000040063 -0.000178199 -0.000009265

53 1 -0.000175600 -0.000099407 -0.000021187

54 1 -0.000041794 -0.000174839 0.000011213

55 1 -0.000050298 0.000021290 -0.000180959

56 1 -0.000132038 -0.000025208 0.000051205

57 1 -0.000050657 0.000111949 -0.000035288

58 1 -0.000006138 -0.000025860 0.000013465

59 1 -0.000055403 0.000025027 0.000005495

60 1 0.000016141 -0.000021876 0.000048955

61 1 0.000131622 0.000041527 -0.000161035

62 1 -0.000024453 0.000012940 -0.000040098

63 1 -0.000013390 -0.000042483 -0.000007797

64 1 -0.000025268 0.000004423 0.000100272

65 1 0.000011714 -0.000024630 0.000061544

66 1 -0.000007171 0.000001367 -0.000046796

67 1 -0.000001257 -0.000014117 -0.000064932

68 1 0.000008270 0.000002964 0.000044811

69 1 0.000024609 0.000019196 0.000041646

70 1 0.000011755 -0.000041072 0.000007288

71 1 0.000031897 0.000012701 -0.000095519

72 1 -0.000127492 0.000049471 0.000165107

73 1 -0.000018431 -0.000016976 -0.000049427

74 1 0.000060808 0.000029673 -0.000006551

75 1 0.000007467 -0.000027485 -0.000013961

76 1 0.000037144 0.000113264 0.000034254

77 1 -0.000133533 0.000261392 -0.000188872

78 1 0.000173635 -0.000000972 0.000156368

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

Cartesian Forces: Max 0.006535626 RMS 0.001687413

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

Leave Link 716 at Mon Aug 26 13:37:30 2019, MaxMem= 4294967296 cpu: 1.9

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.005005518 RMS 0.000749244

Search for a local minimum.

Step number 5 out of a maximum of 452

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

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -1.74D-03 DEPred=-1.70D-03 R= 1.02D+00

TightC=F SS= 1.41D+00 RLast= 4.32D-01 DXNew= 4.2426D-01 1.2954D+00

Trust test= 1.02D+00 RLast= 4.32D-01 DXMaxT set to 4.24D-01

ITU= 1 1 -1 1 0

Eigenvalues --- 0.00449 0.00493 0.00549 0.00604 0.00742

Eigenvalues --- 0.00814 0.00982 0.01022 0.01033 0.01130

Eigenvalues --- 0.01152 0.01192 0.01280 0.01289 0.01294

Eigenvalues --- 0.01300 0.01342 0.01443 0.01455 0.01589

Eigenvalues --- 0.01604 0.01610 0.01621 0.01665 0.01716

Eigenvalues --- 0.01722 0.01736 0.01742 0.01777 0.01780

Eigenvalues --- 0.01791 0.01793 0.01829 0.01835 0.01925

Eigenvalues --- 0.01973 0.02030 0.02073 0.02099 0.02253

Eigenvalues --- 0.02257 0.02266 0.02298 0.02320 0.02327

Eigenvalues --- 0.02341 0.02396 0.02498 0.02504 0.02534

Eigenvalues --- 0.02537 0.02581 0.02630 0.02633 0.02637

Eigenvalues --- 0.02638 0.02665 0.02773 0.02795 0.02795

Eigenvalues --- 0.02807 0.02853 0.02855 0.02859 0.02860

Eigenvalues --- 0.02955 0.02993 0.04085 0.04106 0.04190

Eigenvalues --- 0.04394 0.04478 0.04490 0.04594 0.04629

Eigenvalues --- 0.09601 0.09656 0.09657 0.09782 0.09809

Eigenvalues --- 0.10117 0.10387 0.10409 0.10621 0.10698

Eigenvalues --- 0.10698 0.10700 0.10702 0.10761 0.11368

Eigenvalues --- 0.11372 0.11389 0.11391 0.11943 0.11960

Eigenvalues --- 0.11963 0.11965 0.12288 0.12289 0.12290

Eigenvalues --- 0.12290 0.12606 0.12747 0.12751 0.12758

Eigenvalues --- 0.12765 0.15897 0.16028 0.16439 0.17236

Eigenvalues --- 0.17560 0.17648 0.17659 0.18139 0.18184

Eigenvalues --- 0.18258 0.18263 0.18556 0.19280 0.19321

Eigenvalues --- 0.19360 0.19371 0.19415 0.19445 0.19456

Eigenvalues --- 0.19509 0.19548 0.19550 0.19555 0.19556

Eigenvalues --- 0.20346 0.21501 0.22067 0.22882 0.23181

Eigenvalues --- 0.23443 0.23674 0.24203 0.24802 0.26069

Eigenvalues --- 0.26431 0.26472 0.26574 0.27223 0.28518

Eigenvalues --- 0.28562 0.28675 0.29040 0.29893 0.30977

Eigenvalues --- 0.31727 0.32548 0.33282 0.33310 0.33428

Eigenvalues --- 0.34160 0.34168 0.35285 0.35566 0.35613

Eigenvalues --- 0.35620 0.35635 0.35638 0.35646 0.35744

Eigenvalues --- 0.35769 0.35796 0.35816 0.35917 0.35921

Eigenvalues --- 0.35925 0.35926 0.35990 0.35994 0.36004

Eigenvalues --- 0.36015 0.36201 0.36234 0.36266 0.36368

Eigenvalues --- 0.37081 0.37141 0.37179 0.37433 0.37454

Eigenvalues --- 0.37517 0.38200 0.38631 0.38643 0.38907

Eigenvalues --- 0.39352 0.39976 0.40961 0.41118 0.41159

Eigenvalues --- 0.41184 0.41227 0.41250 0.41283 0.41436

Eigenvalues --- 0.41726 0.41886 0.41910 0.42514 0.44575

Eigenvalues --- 0.44786 0.45911 0.45924 0.45951 0.45971

Eigenvalues --- 0.46109 0.46263 0.46271 0.46314 0.46328

Eigenvalues --- 0.48078 0.49893 0.49986 0.50708 0.50740

Eigenvalues --- 0.50755 0.50769 0.50891 0.51379 0.52222

Eigenvalues --- 0.52755 0.57799 0.59104

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 1.03001 -0.59544 0.56543

Cosine: 0.917 > 0.840

Length: 1.743

GDIIS step was calculated using 3 of the last 5 vectors.

Iteration 1 RMS(Cart)= 0.03903020 RMS(Int)= 0.00032395

Iteration 2 RMS(Cart)= 0.00058180 RMS(Int)= 0.00023034

Iteration 3 RMS(Cart)= 0.00000072 RMS(Int)= 0.00023034

ITry= 1 IFail=0 DXMaxC= 1.68D-01 DCOld= 1.00D+10 DXMaxT= 4.24D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.64844 0.00292 0.01491 0.00466 0.01954 2.66797

R2 2.65130 -0.00289 -0.01278 -0.00666 -0.01967 2.63163

R3 2.03691 0.00007 -0.00001 0.00023 0.00022 2.03713

R4 2.59744 0.00154 0.00073 0.00175 0.00265 2.60009

R5 2.72695 -0.00330 -0.01894 -0.00528 -0.02419 2.70277

R6 2.59646 0.00091 0.00207 0.00270 0.00497 2.60143

R7 1.90986 0.00018 -0.00037 0.00034 -0.00003 1.90983

R8 2.64663 0.00290 0.01097 0.00564 0.01650 2.66313

R9 2.73377 -0.00406 -0.01455 -0.01287 -0.02746 2.70631

R10 2.03727 -0.00007 0.00016 -0.00030 -0.00014 2.03713

R11 2.62351 0.00499 0.00343 0.01551 0.01893 2.64243

R12 2.80481 0.00007 -0.00019 -0.00008 -0.00027 2.80453

R13 2.60178 -0.00032 0.00930 -0.00629 0.00329 2.60507

R14 2.76812 -0.00111 -0.01128 -0.00280 -0.01417 2.75395

R15 2.58514 0.00168 -0.01172 0.01095 -0.00056 2.58458

R16 2.76961 -0.00116 -0.00892 -0.00365 -0.01264 2.75696

R17 2.63423 0.00501 0.02994 0.00204 0.03203 2.66625

R18 2.54970 0.00174 0.00838 0.00201 0.01010 2.55981

R19 2.03933 -0.00014 0.00052 -0.00086 -0.00035 2.03898

R20 2.03902 -0.00001 0.00016 -0.00003 0.00013 2.03915

R21 2.63414 0.00497 0.02951 0.00225 0.03180 2.66594

R22 2.80226 0.00028 -0.00158 0.00146 -0.00012 2.80214

R23 2.76958 -0.00115 -0.00879 -0.00368 -0.01253 2.75706

R24 2.58525 0.00166 -0.01166 0.01095 -0.00053 2.58472

R25 2.54970 0.00175 0.00833 0.00204 0.01009 2.55980

R26 2.03932 -0.00014 0.00050 -0.00084 -0.00035 2.03898

R27 2.76812 -0.00111 -0.01128 -0.00278 -0.01416 2.75396

R28 2.03903 -0.00001 0.00017 -0.00004 0.00013 2.03916

R29 2.60171 -0.00035 0.00933 -0.00631 0.00327 2.60498

R30 2.62370 0.00498 0.00340 0.01535 0.01872 2.64241

R31 2.73380 -0.00397 -0.01450 -0.01291 -0.02746 2.70634

R32 2.80413 0.00007 -0.00021 0.00067 0.00047 2.80460

R33 2.64642 0.00291 0.01089 0.00591 0.01667 2.66309

R34 2.59611 0.00091 0.00207 0.00315 0.00542 2.60153

R35 2.65152 -0.00285 -0.01276 -0.00691 -0.01990 2.63162

R36 2.03736 -0.00008 0.00016 -0.00040 -0.00024 2.03712

R37 2.64827 0.00291 0.01487 0.00483 0.01967 2.66794

R38 2.03694 0.00008 -0.00005 0.00025 0.00020 2.03714

R39 2.59719 0.00150 0.00072 0.00209 0.00299 2.60018

R40 2.72711 -0.00328 -0.01883 -0.00550 -0.02429 2.70282

R41 1.90938 0.00017 -0.00042 0.00095 0.00053 1.90991

R42 2.80174 0.00025 -0.00187 0.00202 0.00016 2.80190

R43 2.65128 0.00030 -0.00000 0.00025 0.00025 2.65153

R44 2.64942 -0.00004 0.00036 0.00004 0.00040 2.64982

R45 2.62781 0.00031 0.00003 0.00106 0.00109 2.62890

R46 2.04829 0.00004 -0.00014 0.00019 0.00005 2.04835

R47 2.63673 -0.00010 -0.00030 -0.00042 -0.00073 2.63600

R48 2.05014 -0.00002 -0.00007 -0.00009 -0.00015 2.04999

R49 2.63370 0.00005 0.00029 0.00031 0.00060 2.63430

R50 2.05010 -0.00004 -0.00000 -0.00017 -0.00017 2.04993

R51 2.63177 -0.00029 -0.00042 -0.00072 -0.00114 2.63063

R52 2.05009 -0.00002 -0.00008 -0.00010 -0.00019 2.04991

R53 2.04850 -0.00011 -0.00026 -0.00010 -0.00036 2.04814

R54 2.63656 -0.00013 -0.00069 0.00001 -0.00069 2.63586

R55 2.63385 0.00014 0.00082 0.00019 0.00100 2.63485

R56 2.05010 -0.00005 -0.00002 -0.00012 -0.00015 2.04995

R57 2.62848 0.00011 0.00071 0.00002 0.00073 2.62921

R58 2.05017 -0.00004 0.00004 -0.00013 -0.00009 2.05008

R59 2.65233 -0.00025 0.00009 -0.00045 -0.00036 2.65197

R60 2.04837 -0.00007 -0.00004 -0.00024 -0.00027 2.04810

R61 2.65066 0.00021 0.00099 -0.00038 0.00062 2.65128

R62 2.63057 -0.00002 -0.00071 0.00030 -0.00041 2.63016

R63 2.04836 0.00001 0.00018 -0.00015 0.00003 2.04839

R64 2.05013 -0.00004 0.00005 -0.00013 -0.00008 2.05005

R65 2.65089 0.00019 0.00109 -0.00060 0.00051 2.65140

R66 2.65249 -0.00025 0.00020 -0.00067 -0.00046 2.65203

R67 2.63051 -0.00001 -0.00075 0.00034 -0.00040 2.63011

R68 2.04832 0.00001 0.00015 -0.00009 0.00006 2.04838

R69 2.63385 0.00015 0.00086 0.00017 0.00102 2.63487

R70 2.05013 -0.00004 0.00004 -0.00012 -0.00008 2.05005

R71 2.63659 -0.00013 -0.00068 -0.00003 -0.00072 2.63587

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R81 2.05010 -0.00003 -0.00008 -0.00011 -0.00019 2.04991

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A1 1.87975 0.00038 0.00148 0.00132 0.00290 1.88265

A2 2.18982 -0.00006 -0.00269 -0.00049 -0.00323 2.18659

A3 2.21361 -0.00032 0.00120 -0.00084 0.00031 2.21393

A4 1.86932 -0.00010 -0.00375 -0.00027 -0.00401 1.86531

A5 2.22726 -0.00090 0.00243 -0.00726 -0.00567 2.22159

A6 2.18560 0.00100 0.00134 0.00813 0.01022 2.19582

A7 1.92501 -0.00074 0.00247 -0.00110 0.00117 1.92618

A8 2.17444 0.00056 -0.00101 0.00433 0.00341 2.17785

A9 2.18239 0.00018 -0.00175 -0.00252 -0.00417 2.17822

A10 1.87019 0.00005 -0.00308 -0.00073 -0.00375 1.86645

A11 2.19212 0.00021 0.00160 0.00185 0.00402 2.19613

A12 2.22036 -0.00026 0.00148 -0.00105 -0.00005 2.22031

A13 1.88011 0.00042 0.00274 0.00089 0.00367 1.88379

A14 2.21397 -0.00037 0.00005 -0.00084 -0.00077 2.21320

A15 2.18908 -0.00005 -0.00292 -0.00002 -0.00291 2.18617

A16 2.18820 -0.00070 -0.00152 -0.00011 -0.00086 2.18734

A17 2.01565 0.00066 0.00489 0.00482 0.00934 2.02499

A18 2.07923 0.00004 -0.00333 -0.00471 -0.00842 2.07081

A19 2.19289 -0.00066 -0.00565 0.00019 -0.00485 2.18804

A20 2.16737 0.00063 0.00592 -0.00245 0.00288 2.17025

A21 1.92273 0.00003 -0.00059 0.00261 0.00212 1.92485

A22 1.84917 0.00023 -0.00154 -0.00100 -0.00278 1.84639

A23 1.92693 -0.00038 0.00475 -0.00186 0.00292 1.92985

A24 2.19429 -0.00026 -0.00430 -0.00093 -0.00431 2.18998

A25 2.16196 0.00064 -0.00064 0.00279 0.00138 2.16334

A26 1.86239 -0.00006 -0.00148 0.00011 -0.00135 1.86104

A27 2.19503 0.00015 0.00067 0.00263 0.00333 2.19836

A28 2.22504 -0.00008 0.00092 -0.00244 -0.00149 2.22356

A29 1.86212 0.00020 -0.00105 0.00073 -0.00033 1.86179

A30 2.19690 -0.00014 0.00127 -0.00052 0.00077 2.19766

A31 2.22393 -0.00006 -0.00018 -0.00040 -0.00056 2.22337

A32 2.18302 0.00004 -0.00508 0.00294 -0.00104 2.18198

A33 2.02396 -0.00009 0.01236 -0.00193 0.00991 2.03386

A34 2.07610 0.00005 -0.00728 -0.00096 -0.00876 2.06734

A35 2.16184 0.00069 -0.00062 0.00288 0.00152 2.16336

A36 2.19439 -0.00031 -0.00425 -0.00095 -0.00435 2.19004

A37 1.92695 -0.00038 0.00472 -0.00193 0.00282 1.92977

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A40 2.22497 -0.00007 0.00084 -0.00231 -0.00144 2.22353

A41 1.86211 0.00021 -0.00101 0.00072 -0.00031 1.86180

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A45 2.16732 0.00061 0.00574 -0.00228 0.00296 2.17028

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A48 2.18723 -0.00064 -0.00140 0.00092 0.00024 2.18747

A49 2.08054 -0.00004 -0.00336 -0.00607 -0.00980 2.07073

A50 2.01525 0.00068 0.00481 0.00525 0.00969 2.02494

A51 2.22047 -0.00021 0.00140 -0.00132 -0.00035 2.22012

A52 2.19212 0.00019 0.00167 0.00197 0.00423 2.19635

A53 1.87024 0.00002 -0.00311 -0.00076 -0.00379 1.86644

A54 1.88001 0.00042 0.00275 0.00103 0.00381 1.88382

A55 2.18873 -0.00004 -0.00293 0.00043 -0.00246 2.18627

A56 2.21441 -0.00038 0.00002 -0.00141 -0.00135 2.21306

A57 1.87971 0.00038 0.00153 0.00132 0.00295 1.88266

A58 2.21389 -0.00031 0.00107 -0.00105 -0.00002 2.21387

A59 2.18958 -0.00006 -0.00263 -0.00027 -0.00294 2.18663

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A61 2.22745 -0.00083 0.00263 -0.00767 -0.00585 2.22160

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A63 1.92518 -0.00070 0.00256 -0.00137 0.00096 1.92613

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A66 2.18223 0.00006 -0.00528 0.00373 -0.00040 2.18182

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A68 2.02339 -0.00004 0.01269 -0.00123 0.01087 2.03426

A69 2.09945 0.00082 0.00037 0.00531 0.00568 2.10513

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A87 2.08904 -0.00004 -0.00036 -0.00015 -0.00050 2.08854

A88 2.09686 -0.00000 0.00032 0.00008 0.00041 2.09726

A89 2.09728 0.00004 0.00004 0.00006 0.00010 2.09738

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A95 2.08492 -0.00005 0.00011 -0.00018 -0.00008 2.08484

A96 2.11120 -0.00062 0.00296 -0.00572 -0.00279 2.10841

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A99 2.10639 -0.00010 0.00033 -0.00079 -0.00043 2.10596

A100 2.08350 0.00012 0.00018 0.00049 0.00066 2.08415

A101 2.09311 -0.00001 -0.00052 0.00037 -0.00017 2.09294

A102 2.09697 0.00008 0.00031 0.00062 0.00095 2.09792

A103 2.09725 -0.00002 -0.00044 -0.00007 -0.00052 2.09672

A104 2.08896 -0.00006 0.00013 -0.00055 -0.00042 2.08854

A105 2.10160 0.00069 -0.00196 0.00507 0.00306 2.10467

A106 2.11108 -0.00067 0.00300 -0.00538 -0.00243 2.10865

A107 2.07042 -0.00001 -0.00104 0.00047 -0.00055 2.06986

A108 2.10644 -0.00011 0.00035 -0.00081 -0.00043 2.10601

A109 2.08359 0.00012 0.00022 0.00033 0.00053 2.08412

A110 2.09293 -0.00000 -0.00057 0.00058 -0.00002 2.09292

A111 2.09698 0.00009 0.00036 0.00058 0.00095 2.09794

A112 2.08894 -0.00006 0.00010 -0.00052 -0.00042 2.08852

A113 2.09726 -0.00002 -0.00046 -0.00007 -0.00053 2.09672

A114 2.08906 -0.00005 -0.00040 -0.00015 -0.00055 2.08851

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A116 2.09688 -0.00000 0.00034 0.00002 0.00037 2.09725

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A122 2.09323 -0.00008 -0.00068 -0.00044 -0.00113 2.09210

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A125 2.07204 -0.00016 0.00029 -0.00013 0.00017 2.07221

A126 2.10431 0.00024 -0.00041 0.00100 0.00060 2.10491

A127 2.08358 0.00006 0.00007 0.00115 0.00121 2.08479

A128 2.09515 -0.00030 0.00030 -0.00210 -0.00180 2.09334

A129 2.09784 0.00001 0.00009 -0.00051 -0.00041 2.09743

A130 2.08833 -0.00002 0.00001 0.00032 0.00033 2.08866

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A132 2.08925 -0.00003 0.00030 -0.00015 0.00015 2.08940

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D2 -3.07621 -0.00024 0.00341 -0.01872 -0.01511 -3.09132

D3 -3.12182 -0.00002 0.00583 -0.00131 0.00454 -3.11728

D4 0.06636 -0.00012 0.00456 -0.01539 -0.01078 0.05558

D5 -0.00392 0.00008 -0.00314 0.00318 -0.00014 -0.00406

D6 -3.13912 0.00007 0.00238 -0.00048 0.00177 -3.13735

D7 3.13668 -0.00004 -0.00436 -0.00020 -0.00455 3.13212

D8 0.00148 -0.00006 0.00116 -0.00387 -0.00265 -0.00117

D9 -0.02727 0.00017 -0.00453 0.00448 -0.00018 -0.02745

D10 3.06095 0.00008 -0.01003 0.01862 0.00853 3.06947

D11 3.06914 0.00020 -0.00328 0.01762 0.01433 3.08347

D12 -0.12583 0.00012 -0.00877 0.03176 0.02303 -0.10280

D13 -2.96407 0.00011 -0.03615 0.02339 -0.01316 -2.97723

D14 0.16187 0.00025 -0.02217 0.02724 0.00456 0.16643

D15 0.23204 0.00003 -0.03760 0.00722 -0.03078 0.20126

D16 -2.92520 0.00018 -0.02362 0.01108 -0.01306 -2.93826

D17 0.02485 -0.00011 0.00268 -0.00251 0.00013 0.02499

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D24 -0.05204 0.00008 0.00130 0.00523 0.00646 -0.04558

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D26 2.88953 0.00017 -0.00055 0.01931 0.01815 2.90768

D27 2.91354 0.00012 -0.00300 0.01735 0.01387 2.92741

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D29 -0.10353 -0.00028 -0.03814 0.00615 -0.03259 -0.13612

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D31 3.02245 -0.00028 -0.03308 0.00670 -0.02698 2.99547

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D35 2.16185 -0.00007 0.01751 -0.01542 0.00206 2.16391

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D37 -3.06943 -0.00038 0.00517 -0.02997 -0.02447 -3.09390

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D45 0.01958 0.00011 0.00184 0.00477 0.00679 0.02637

D46 -3.08355 -0.00007 -0.00676 -0.00327 -0.00998 -3.09353

D47 -3.12352 0.00011 0.01129 0.00301 0.01441 -3.10911

D48 0.05654 -0.00007 0.00269 -0.00502 -0.00237 0.05417

D49 0.12973 0.00036 0.08182 -0.02761 0.05391 0.18364

D50 -2.98952 0.00011 0.06801 -0.03803 0.02947 -2.96005

D51 -3.01013 0.00036 0.07115 -0.02559 0.04515 -2.96498

D52 0.15380 0.00011 0.05734 -0.03600 0.02071 0.17452

D53 0.01228 -0.00030 -0.00337 -0.01122 -0.01474 -0.00246

D54 -3.10661 -0.00006 -0.00705 -0.00240 -0.00948 -3.11609

D55 3.11454 -0.00011 0.00540 -0.00286 0.00249 3.11703

D56 -0.00435 0.00013 0.00172 0.00597 0.00775 0.00340

D57 -3.00738 0.00033 0.06785 -0.02794 0.03953 -2.96786

D58 0.13133 0.00037 0.07751 -0.02791 0.04932 0.18065

D59 0.15029 0.00019 0.05386 -0.03189 0.02134 0.17163

D60 -2.99418 0.00023 0.06351 -0.03186 0.03113 -2.96305

D61 0.97712 0.00009 -0.01489 0.00957 -0.00525 0.97186

D62 -2.15274 -0.00003 -0.01945 -0.00031 -0.01969 -2.17243

D63 -2.17911 0.00022 -0.00182 0.01320 0.01131 -2.16780

D64 0.97422 0.00011 -0.00638 0.00333 -0.00312 0.97110

D65 -3.12454 0.00013 0.01043 0.00485 0.01539 -3.10915

D66 0.05511 -0.00004 0.00223 -0.00308 -0.00088 0.05423

D67 0.01955 0.00009 0.00188 0.00482 0.00688 0.02643

D68 -3.08399 -0.00008 -0.00632 -0.00311 -0.00939 -3.09338

D69 3.10049 0.00009 -0.00815 0.00381 -0.00435 3.09614

D70 -0.04365 0.00012 0.00058 0.00384 0.00432 -0.03933

D71 0.01194 -0.00027 -0.00322 -0.01092 -0.01429 -0.00235

D72 -3.10615 -0.00006 -0.00717 -0.00289 -0.01009 -3.11625

D73 3.11463 -0.00009 0.00514 -0.00268 0.00241 3.11704

D74 -0.00347 0.00012 0.00119 0.00535 0.00661 0.00315

D75 -0.03999 0.00035 0.00388 0.01384 0.01787 -0.02212

D76 3.08190 0.00041 -0.00603 0.03247 0.02660 3.10850

D77 3.07857 0.00015 0.00775 0.00597 0.01373 3.09230

D78 -0.08272 0.00021 -0.00216 0.02460 0.02245 -0.06026

D79 0.05110 -0.00028 -0.00267 -0.01063 -0.01332 0.03778

D80 -3.07044 -0.00036 0.00695 -0.02956 -0.02226 -3.09271

D81 3.06024 -0.00029 -0.02823 -0.01360 -0.04227 3.01797

D82 -0.10201 -0.00022 -0.02414 -0.00716 -0.03177 -0.13379

D83 -0.10411 -0.00021 -0.03950 0.00794 -0.03214 -0.13624

D84 3.01683 -0.00014 -0.03540 0.01438 -0.02164 2.99519

D85 2.89306 0.00026 -0.00421 0.03971 0.03504 2.92811

D86 -0.28101 0.00030 0.00522 0.03478 0.03934 -0.24167

D87 -0.22856 0.00020 -0.00816 0.03360 0.02499 -0.20356

D88 2.88055 0.00024 0.00127 0.02867 0.02929 2.90984

D89 -0.97586 -0.00007 0.01996 -0.02555 -0.00561 -0.98146

D90 2.17185 -0.00008 0.01839 -0.02692 -0.00855 2.16329

D91 2.14707 -0.00002 0.02359 -0.01977 0.00384 2.15091

D92 -0.98842 -0.00002 0.02202 -0.02114 0.00089 -0.98752

D93 3.10212 -0.00003 0.00881 -0.00548 0.00338 3.10550

D94 -0.04822 0.00004 0.00288 0.00111 0.00393 -0.04429

D95 -0.01183 -0.00007 0.00085 -0.00132 -0.00038 -0.01220

D96 3.12101 -0.00000 -0.00508 0.00526 0.00018 3.12119

D97 -3.09063 -0.00003 -0.00606 0.00307 -0.00293 -3.09356

D98 0.08978 0.00003 -0.00197 0.00468 0.00272 0.09250

D99 0.02389 -0.00000 0.00177 -0.00106 0.00068 0.02456

D100 -3.07888 0.00006 0.00587 0.00055 0.00632 -3.07256

D101 -0.00403 0.00009 -0.00297 0.00313 -0.00002 -0.00405

D102 3.13425 0.00001 -0.00503 0.00269 -0.00234 3.13192

D103 -3.13670 0.00003 0.00314 -0.00359 -0.00058 -3.13728

D104 0.00158 -0.00006 0.00108 -0.00403 -0.00289 -0.00131

D105 0.01832 -0.00009 0.00397 -0.00372 0.00043 0.01875

D106 -3.08250 -0.00015 0.00102 -0.01026 -0.00908 -3.09158

D107 -3.12002 -0.00000 0.00593 -0.00328 0.00269 -3.11733

D108 0.06235 -0.00007 0.00299 -0.00982 -0.00682 0.05553

D109 -0.02637 0.00006 -0.00353 0.00300 -0.00065 -0.02702

D110 3.07660 -0.00000 -0.00762 0.00124 -0.00648 3.07012

D111 3.07568 0.00008 -0.00064 0.00889 0.00821 3.08390

D112 -0.10453 0.00001 -0.00473 0.00712 0.00238 -0.10215

D113 -2.94431 -0.00002 -0.03520 0.00157 -0.03405 -2.97837

D114 0.17556 0.00022 -0.02144 0.01168 -0.01027 0.16529

D115 0.24500 -0.00007 -0.03864 -0.00581 -0.04488 0.20012

D116 -2.91831 0.00017 -0.02488 0.00430 -0.02109 -2.93940

D117 0.96685 0.00013 -0.00933 0.01107 0.00167 0.96853

D118 -2.18913 0.00027 -0.00495 0.02406 0.01904 -2.17009

D119 -2.15440 -0.00010 -0.02219 0.00152 -0.02059 -2.17499

D120 0.97280 0.00005 -0.01781 0.01451 -0.00323 0.96957

D121 -3.12487 -0.00012 -0.00254 -0.00211 -0.00467 -3.12954

D122 -0.00342 -0.00009 -0.00372 -0.00280 -0.00653 -0.00995

D123 0.02051 -0.00010 -0.00447 -0.00119 -0.00566 0.01485

D124 -3.14122 -0.00007 -0.00564 -0.00189 -0.00752 3.13444

D125 3.13809 0.00008 0.00297 0.00042 0.00338 3.14147

D126 -0.02119 0.00005 0.00103 0.00173 0.00275 -0.01844

D127 -0.00732 0.00006 0.00488 -0.00048 0.00439 -0.00292

D128 3.11659 0.00003 0.00294 0.00083 0.00377 3.12036

D129 -0.01935 0.00007 0.00178 0.00144 0.00323 -0.01612

D130 3.12301 0.00004 0.00137 0.00010 0.00148 3.12449

D131 -3.14071 0.00005 0.00296 0.00213 0.00510 -3.13562

D132 0.00165 0.00001 0.00255 0.00080 0.00335 0.00500

D133 0.00468 -0.00001 0.00056 -0.00002 0.00055 0.00523

D134 -3.13315 -0.00004 -0.00014 -0.00166 -0.00180 -3.13496

D135 -3.13768 0.00002 0.00097 0.00133 0.00231 -3.13538

D136 0.00767 -0.00000 0.00027 -0.00032 -0.00005 0.00762

D137 0.00845 -0.00002 -0.00015 -0.00164 -0.00179 0.00666

D138 -3.13128 0.00001 -0.00021 -0.00047 -0.00069 -3.13197

D139 -3.13690 0.00001 0.00055 0.00000 0.00056 -3.13634

D140 0.00656 0.00003 0.00050 0.00117 0.00166 0.00822

D141 -0.00706 -0.00000 -0.00260 0.00189 -0.00072 -0.00778

D142 -3.13085 0.00002 -0.00065 0.00054 -0.00012 -3.13097

D143 3.13268 -0.00003 -0.00254 0.00073 -0.00182 3.13086

D144 0.00889 -0.00001 -0.00059 -0.00062 -0.00122 0.00767

D145 -0.00681 0.00004 -0.00166 0.00396 0.00229 -0.00452

D146 3.13474 0.00001 -0.00208 0.00196 -0.00011 3.13463

D147 3.13319 0.00002 0.00061 0.00186 0.00246 3.13564

D148 -0.00845 -0.00001 0.00019 -0.00014 0.00006 -0.00839

D149 -0.00541 -0.00002 0.00131 -0.00199 -0.00069 -0.00610

D150 3.13302 -0.00002 0.00181 -0.00229 -0.00048 3.13254

D151 3.13778 0.00001 -0.00096 0.00011 -0.00085 3.13693

D152 -0.00697 0.00000 -0.00046 -0.00019 -0.00064 -0.00762

D153 0.01598 -0.00003 -0.00210 -0.00113 -0.00321 0.01277

D154 3.13961 -0.00009 -0.00338 -0.00305 -0.00640 3.13321

D155 -3.12557 0.00000 -0.00168 0.00086 -0.00082 -3.12639

D156 -0.00194 -0.00006 -0.00297 -0.00106 -0.00401 -0.00595

D157 3.14045 -0.00013 0.00157 -0.01334 -0.01171 3.12874

D158 -0.01268 -0.00001 0.00606 -0.00360 0.00247 -0.01020

D159 0.01673 -0.00007 0.00285 -0.01143 -0.00852 0.00821

D160 -3.13639 0.00005 0.00735 -0.00169 0.00566 -3.13073

D161 3.13054 0.00014 -0.00201 0.01518 0.01324 -3.13940

D162 0.01014 0.00009 -0.00167 0.01153 0.00991 0.02005

D163 0.00041 0.00003 -0.00642 0.00557 -0.00086 -0.00045

D164 -3.11999 -0.00002 -0.00608 0.00192 -0.00419 -3.12418

D165 0.00860 -0.00002 0.00281 -0.00282 -0.00001 0.00858

D166 -3.12985 -0.00002 0.00232 -0.00253 -0.00022 -3.13007

D167 3.12888 0.00004 0.00248 0.00085 0.00334 3.13222

D168 -0.00956 0.00004 0.00198 0.00114 0.00313 -0.00643

D169 3.12823 0.00018 -0.00250 0.01814 0.01572 -3.13923

D170 0.00902 0.00010 -0.00199 0.01300 0.01107 0.02009

D171 0.00069 0.00004 -0.00673 0.00550 -0.00124 -0.00055

D172 -3.11851 -0.00004 -0.00622 0.00036 -0.00590 -3.12441

D173 -3.14051 -0.00016 0.00214 -0.01625 -0.01404 3.12864

D174 0.01842 -0.00009 0.00352 -0.01364 -0.01007 0.00835

D175 -0.01305 -0.00001 0.00645 -0.00345 0.00301 -0.01004

D176 -3.13731 0.00006 0.00783 -0.00084 0.00699 -3.13033

D177 0.00859 -0.00002 0.00281 -0.00286 -0.00005 0.00854

D178 -3.12947 -0.00002 0.00242 -0.00305 -0.00064 -3.13011

D179 3.12768 0.00005 0.00231 0.00231 0.00463 3.13231

D180 -0.01038 0.00005 0.00191 0.00212 0.00404 -0.00634

D181 -0.00560 -0.00001 0.00155 -0.00192 -0.00038 -0.00598

D182 3.13805 0.00001 -0.00090 -0.00026 -0.00117 3.13688

D183 3.13245 -0.00001 0.00195 -0.00173 0.00021 3.13266

D184 -0.00709 0.00000 -0.00051 -0.00007 -0.00057 -0.00767

D185 -0.00672 0.00004 -0.00182 0.00397 0.00215 -0.00457

D186 3.13503 0.00001 -0.00240 0.00186 -0.00052 3.13451

D187 3.13282 0.00002 0.00064 0.00231 0.00293 3.13575

D188 -0.00862 -0.00001 0.00005 0.00020 0.00026 -0.00835

D189 0.01617 -0.00003 -0.00226 -0.00125 -0.00349 0.01268

D190 3.14035 -0.00010 -0.00364 -0.00387 -0.00747 3.13288

D191 -3.12557 0.00001 -0.00169 0.00085 -0.00083 -3.12641

D192 -0.00140 -0.00006 -0.00306 -0.00177 -0.00481 -0.00621

D193 3.14032 0.00005 0.00347 -0.00205 0.00142 -3.14145

D194 -0.02018 0.00004 0.00145 0.00063 0.00207 -0.01811

D195 -0.00729 0.00005 0.00502 -0.00069 0.00433 -0.00296

D196 3.11539 0.00004 0.00300 0.00199 0.00498 3.12038

D197 -3.12677 -0.00009 -0.00307 0.00006 -0.00302 -3.12979

D198 -0.00514 -0.00007 -0.00419 -0.00084 -0.00503 -0.01017

D199 0.02080 -0.00010 -0.00463 -0.00126 -0.00589 0.01491

D200 -3.14076 -0.00007 -0.00575 -0.00216 -0.00790 3.13452

D201 -0.00738 0.00001 -0.00263 0.00229 -0.00035 -0.00773

D202 3.13216 -0.00002 -0.00255 0.00128 -0.00127 3.13089

D203 -3.12994 0.00001 -0.00059 -0.00045 -0.00104 -3.13098

D204 0.00960 -0.00002 -0.00051 -0.00145 -0.00196 0.00764

D205 0.00875 -0.00003 -0.00021 -0.00195 -0.00217 0.00659

D206 -3.13708 0.00001 0.00054 0.00020 0.00074 -3.13633

D207 -3.13078 0.00000 -0.00029 -0.00094 -0.00124 -3.13202

D208 0.00658 0.00004 0.00046 0.00121 0.00166 0.00824

D209 0.00470 -0.00001 0.00060 0.00002 0.00062 0.00532

D210 -3.13790 0.00003 0.00110 0.00139 0.00249 -3.13541

D211 -3.13266 -0.00004 -0.00016 -0.00213 -0.00228 -3.13494

D212 0.00793 -0.00001 0.00035 -0.00076 -0.00042 0.00751

D213 -0.01966 0.00007 0.00186 0.00159 0.00346 -0.01620

D214 -3.14120 0.00005 0.00298 0.00248 0.00547 -3.13573

D215 3.12293 0.00004 0.00136 0.00024 0.00160 3.12453

D216 0.00139 0.00001 0.00248 0.00113 0.00361 0.00501

Item Value Threshold Converged?

Maximum Force 0.005006 0.000450 NO

RMS Force 0.000749 0.000300 NO

Maximum Displacement 0.168413 0.001800 NO

RMS Displacement 0.039061 0.001200 NO

Predicted change in Energy=-8.722317D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Mon Aug 26 13:37:30 2019, MaxMem= 4294967296 cpu: 2.4

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

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=1 Diff= 4.45D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.751321 -4.160846 0.565740

2 6 0 1.172475 -2.859580 0.215589

3 7 0 0.034925 -2.114660 0.005354

4 6 0 -1.086546 -2.895316 0.172541

5 6 0 -0.640789 -4.182018 0.535494

6 6 0 -2.440261 -2.470722 -0.022726

7 6 0 -2.861689 -1.142933 -0.143821

8 7 0 -2.069077 -0.032876 0.055976

9 6 0 -2.893356 1.046708 -0.104235

10 6 0 -4.238842 0.614998 -0.467205

11 6 0 -4.218696 -0.739262 -0.489342

12 6 0 2.516726 -2.395772 0.062404

13 6 0 2.893565 -1.046477 -0.103802

14 6 0 4.239701 -0.614965 -0.464794

15 6 0 4.219524 0.739271 -0.488077

16 6 0 2.861932 1.143173 -0.145106

17 7 0 2.068961 0.033306 0.054004

18 6 0 2.440539 2.471006 -0.024497

19 6 0 1.086702 2.895951 0.169301

20 6 0 0.641091 4.183041 0.530970

21 6 0 -0.751001 4.161940 0.561832

22 6 0 -1.172348 2.860307 0.213366

23 7 0 -0.034892 2.115150 0.003154

24 6 0 -2.516715 2.396281 0.061578

25 6 0 -3.458154 -3.548886 -0.085924

26 6 0 -3.345623 -4.583564 -1.026958

27 6 0 -4.307730 -5.586071 -1.095110

28 6 0 -5.387822 -5.582951 -0.212403

29 6 0 -5.502889 -4.566957 0.735110

30 6 0 -4.548698 -3.555161 0.795499

31 6 0 5.604624 -5.375772 0.106802

32 6 0 4.553217 -5.470396 -0.804881

33 6 0 3.545992 -4.510615 -0.813681

34 6 0 3.580025 -3.429150 0.080020

35 6 0 4.644201 -3.343343 0.990277

36 6 0 5.644352 -4.311129 1.006270

37 6 0 -3.580468 3.428988 0.080226

38 6 0 -4.645286 3.340823 0.989605

39 6 0 -5.646155 4.307812 1.006623

40 6 0 -5.606600 5.374123 0.109111

41 6 0 -4.554667 5.471084 -0.801728

42 6 0 -3.546749 4.512050 -0.811602

43 6 0 3.458763 3.548976 -0.086425

44 6 0 4.547592 3.555558 0.797090

45 6 0 5.501937 4.567297 0.738156

46 6 0 5.388692 5.582945 -0.209939

47 6 0 4.310329 5.585734 -1.094745

48 6 0 3.348041 4.583295 -1.028046

49 1 0 1.405086 -4.980908 0.815099

50 1 0 -1.278876 -5.022457 0.755944

51 1 0 -5.072388 1.261806 -0.693138

52 1 0 -5.032127 -1.402678 -0.739549

53 1 0 5.073663 -1.261892 -0.688826

54 1 0 5.033396 1.402536 -0.737279

55 1 0 1.279171 5.023777 0.750267

56 1 0 -1.404589 4.982293 0.810715

57 1 0 -2.511148 -4.587305 -1.718739

58 1 0 -4.214608 -6.370228 -1.838905

59 1 0 -6.134233 -6.368522 -0.262304

60 1 0 -6.335096 -4.562445 1.430901

61 1 0 -4.636527 -2.772534 1.540120

62 1 0 6.386713 -6.127439 0.116827

63 1 0 4.518159 -6.292022 -1.512422

64 1 0 2.735660 -4.585066 -1.529544

65 1 0 4.674989 -2.522359 1.697392

66 1 0 6.454058 -4.234636 1.724186

67 1 0 -4.676030 2.518509 1.695168

68 1 0 -6.456314 4.229402 1.723823

69 1 0 -6.389264 6.125175 0.119872

70 1 0 -4.519781 6.293952 -1.507835

71 1 0 -2.736218 4.588228 -1.527038

72 1 0 4.633991 2.773194 1.542153

73 1 0 6.332812 4.563021 1.435539

74 1 0 6.135223 6.368475 -0.258713

75 1 0 4.218628 6.369643 -1.838977

76 1 0 2.514874 4.586874 -1.721407

77 1 0 0.023576 -1.125419 -0.201210

78 1 0 -0.023763 1.125756 -0.202887

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Rotational constants (GHZ): 0.0588633 0.0581878 0.0300945

Leave Link 202 at Mon Aug 26 13:37:30 2019, MaxMem= 4294967296 cpu: 0.3

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

Standard basis: 6-311G(d) (5D, 7F)

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

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5356.8941572018 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122248560 Hartrees.

Nuclear repulsion after empirical dispersion term = 5356.6819323459 Hartrees.

Force inversion solution in PCM.

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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 : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5735

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.47D-11

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 287

GePol: Fraction of low-weight points (<1% of avg) = 5.00%

GePol: Cavity surface area = 611.583 Ang\*\*2

GePol: Cavity volume = 628.371 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0021058867 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5356.6798264592 Hartrees.

Leave Link 301 at Mon Aug 26 13:37:30 2019, MaxMem= 4294967296 cpu: 2.1

(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.

NBasis= 954 RedAO= T EigKep= 1.30D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Mon Aug 26 13:37:32 2019, MaxMem= 4294967296 cpu: 27.5

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

DipDrv: MaxL=1.

Leave Link 303 at Mon Aug 26 13:37:32 2019, MaxMem= 4294967296 cpu: 2.4

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

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= 0.000000 -0.000000 -0.000000

Rot= 0.987554 0.000047 0.000036 0.157279 Ang= 18.10 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0550 S= 1.0182

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30442599480

Leave Link 401 at Mon Aug 26 13:37:37 2019, MaxMem= 4294967296 cpu: 81.3

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 580000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 98670675.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.11D-15 for 5714.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.52D-15 for 2070 1783.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.33D-15 for 5714.

Iteration 1 A^-1\*A deviation from orthogonality is 2.88D-07 for 4188 3906.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.44D-15 for 2509.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.42D-15 for 3939 446.

Iteration 2 A^-1\*A deviation from unit magnitude is 8.88D-16 for 377.

Iteration 2 A^-1\*A deviation from orthogonality is 3.09D-16 for 2297 1936.

E= -1914.32544442919

DIIS: error= 1.75D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.32544442919 IErMin= 1 ErrMin= 1.75D-03

ErrMax= 1.75D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.68D-02 BMatP= 1.68D-02

IDIUse=3 WtCom= 9.83D-01 WtEn= 1.75D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.639 Goal= None Shift= 0.000

Gap= 0.706 Goal= None Shift= 0.000

GapD= 0.639 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.25D-04 MaxDP=4.98D-03 OVMax= 2.15D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.25D-04 CP: 1.00D+00

E= -1914.33274708618 Delta-E= -0.007302656983 Rises=F Damp=F

DIIS: error= 2.36D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33274708618 IErMin= 2 ErrMin= 2.36D-04

ErrMax= 2.36D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.72D-04 BMatP= 1.68D-02

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.36D-03

Coeff-Com: -0.374D-01 0.104D+01

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

Coeff: -0.373D-01 0.104D+01

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.20D-05 MaxDP=1.09D-03 DE=-7.30D-03 OVMax= 1.01D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.05D-05 CP: 1.00D+00 1.06D+00

E= -1914.33282515043 Delta-E= -0.000078064250 Rises=F Damp=F

DIIS: error= 2.76D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33282515043 IErMin= 2 ErrMin= 2.36D-04

ErrMax= 2.76D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.24D-04 BMatP= 3.72D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.76D-03

Coeff-Com: -0.317D-01 0.515D+00 0.516D+00

Coeff-En: 0.000D+00 0.135D+00 0.865D+00

Coeff: -0.316D-01 0.514D+00 0.517D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.17D-05 MaxDP=8.64D-04 DE=-7.81D-05 OVMax= 2.92D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 9.67D-06 CP: 1.00D+00 1.07D+00 6.84D-01

E= -1914.33289538505 Delta-E= -0.000070234619 Rises=F Damp=F

DIIS: error= 1.36D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33289538505 IErMin= 4 ErrMin= 1.36D-04

ErrMax= 1.36D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.26D-05 BMatP= 3.24D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.36D-03

Coeff-Com: -0.115D-01 0.143D+00 0.301D+00 0.568D+00

Coeff-En: 0.000D+00 0.000D+00 0.112D+00 0.888D+00

Coeff: -0.114D-01 0.143D+00 0.300D+00 0.568D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=6.19D-06 MaxDP=4.52D-04 DE=-7.02D-05 OVMax= 4.94D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.84D-06 CP: 1.00D+00 1.08D+00 8.64D-01 8.86D-01

E= -1914.33291069242 Delta-E= -0.000015307372 Rises=F Damp=F

DIIS: error= 8.58D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33291069242 IErMin= 5 ErrMin= 8.58D-05

ErrMax= 8.58D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.32D-06 BMatP= 5.26D-05

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

Coeff-Com: -0.340D-02 0.278D-01 0.128D+00 0.356D+00 0.491D+00

Coeff: -0.340D-02 0.278D-01 0.128D+00 0.356D+00 0.491D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.80D-06 MaxDP=1.64D-04 DE=-1.53D-05 OVMax= 2.23D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.92D-06 CP: 1.00D+00 1.08D+00 9.03D-01 1.07D+00 1.07D+00

E= -1914.33291496308 Delta-E= -0.000004270664 Rises=F Damp=F

DIIS: error= 5.86D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33291496308 IErMin= 6 ErrMin= 5.86D-05

ErrMax= 5.86D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.16D-06 BMatP= 9.32D-06

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

Coeff-Com: 0.179D-02-0.312D-01-0.259D-01 0.164D-01 0.166D+00 0.873D+00

Coeff: 0.179D-02-0.312D-01-0.259D-01 0.164D-01 0.166D+00 0.873D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.04D-06 MaxDP=3.33D-04 DE=-4.27D-06 OVMax= 4.48D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.31D-06 CP: 1.00D+00 1.08D+00 9.87D-01 1.26D+00 1.59D+00

CP: 1.69D+00

E= -1914.33291786031 Delta-E= -0.000002897227 Rises=F Damp=F

DIIS: error= 4.10D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33291786031 IErMin= 7 ErrMin= 4.10D-05

ErrMax= 4.10D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.49D-07 BMatP= 1.16D-06

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

Coeff-Com: 0.181D-02-0.238D-01-0.452D-01-0.691D-01-0.799D-01 0.530D+00

Coeff-Com: 0.686D+00

Coeff: 0.181D-02-0.238D-01-0.452D-01-0.691D-01-0.799D-01 0.530D+00

Coeff: 0.686D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.04D-06 MaxDP=2.29D-04 DE=-2.90D-06 OVMax= 3.34D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 5.34D-07 CP: 1.00D+00 1.08D+00 1.04D+00 1.41D+00 1.95D+00

CP: 2.43D+00 1.47D+00

E= -1914.33291968788 Delta-E= -0.000001827570 Rises=F Damp=F

DIIS: error= 3.59D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33291968788 IErMin= 8 ErrMin= 3.59D-05

ErrMax= 3.59D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.16D-07 BMatP= 9.49D-07

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

Coeff-Com: -0.655D-03 0.174D-01-0.961D-03-0.364D-01-0.274D+00-0.411D+00

Coeff-Com: 0.294D+00 0.141D+01

Coeff: -0.655D-03 0.174D-01-0.961D-03-0.364D-01-0.274D+00-0.411D+00

Coeff: 0.294D+00 0.141D+01

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=6.16D-06 MaxDP=5.03D-04 DE=-1.83D-06 OVMax= 6.91D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.79D-06 CP: 1.00D+00 1.08D+00 1.15D+00 1.70D+00 2.72D+00

CP: 3.00D+00 2.78D+00 2.04D+00

E= -1914.33292207986 Delta-E= -0.000002391981 Rises=F Damp=F

DIIS: error= 1.88D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33292207986 IErMin= 9 ErrMin= 1.88D-05

ErrMax= 1.88D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.66D-07 BMatP= 4.16D-07

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

Coeff-Com: -0.804D-03 0.137D-01 0.130D-01 0.192D-01-0.907D-01-0.279D+00

Coeff-Com: -0.200D+00 0.523D+00 0.100D+01

Coeff: -0.804D-03 0.137D-01 0.130D-01 0.192D-01-0.907D-01-0.279D+00

Coeff: -0.200D+00 0.523D+00 0.100D+01

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.48D-06 MaxDP=2.86D-04 DE=-2.39D-06 OVMax= 3.91D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.07D-06 CP: 1.00D+00 1.09D+00 1.21D+00 1.86D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.96D+00 1.92D+00

E= -1914.33292281188 Delta-E= -0.000000732018 Rises=F Damp=F

DIIS: error= 9.49D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33292281188 IErMin=10 ErrMin= 9.49D-06

ErrMax= 9.49D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.57D-08 BMatP= 1.66D-07

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

Coeff-Com: -0.172D-03-0.719D-03 0.815D-02 0.376D-01 0.786D-01 0.723D-01

Coeff-Com: -0.313D+00-0.410D+00 0.692D+00 0.836D+00

Coeff: -0.172D-03-0.719D-03 0.815D-02 0.376D-01 0.786D-01 0.723D-01

Coeff: -0.313D+00-0.410D+00 0.692D+00 0.836D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.18D-06 MaxDP=1.84D-04 DE=-7.32D-07 OVMax= 2.44D-03

Cycle 11 Pass 1 IDiag 1:

RMSU= 7.38D-07 CP: 1.00D+00 1.09D+00 1.25D+00 1.96D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.52D+00 2.20D+00

E= -1914.33292306392 Delta-E= -0.000000252041 Rises=F Damp=F

DIIS: error= 4.28D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33292306392 IErMin=11 ErrMin= 4.28D-06

ErrMax= 4.28D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.03D-08 BMatP= 9.57D-08

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

Coeff-Com: 0.249D-03-0.630D-02-0.192D-02 0.122D-01 0.719D-01 0.169D+00

Coeff-Com: -0.977D-01-0.441D+00-0.241D-01 0.402D+00 0.916D+00

Coeff: 0.249D-03-0.630D-02-0.192D-02 0.122D-01 0.719D-01 0.169D+00

Coeff: -0.977D-01-0.441D+00-0.241D-01 0.402D+00 0.916D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.29D-06 MaxDP=1.08D-04 DE=-2.52D-07 OVMax= 1.44D-03

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.69D-07 CP: 1.00D+00 1.09D+00 1.27D+00 2.01D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.87D+00 2.92D+00

CP: 1.56D+00

E= -1914.33292312388 Delta-E= -0.000000059963 Rises=F Damp=F

DIIS: error= 1.64D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.33292312388 IErMin=12 ErrMin= 1.64D-06

ErrMax= 1.64D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.68D-09 BMatP= 2.03D-08

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

Coeff-Com: 0.185D-03-0.358D-02-0.271D-02 0.212D-03 0.261D-01 0.906D-01

Coeff-Com: 0.287D-02-0.173D+00-0.150D+00 0.497D-01 0.521D+00 0.639D+00

Coeff: 0.185D-03-0.358D-02-0.271D-02 0.212D-03 0.261D-01 0.906D-01

Coeff: 0.287D-02-0.173D+00-0.150D+00 0.497D-01 0.521D+00 0.639D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.64D-07 MaxDP=2.33D-05 DE=-6.00D-08 OVMax= 2.85D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 9.47D-08 CP: 1.00D+00 1.09D+00 1.27D+00 2.02D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.95D+00 3.00D+00

CP: 1.67D+00 9.70D-01

E= -1914.33292312905 Delta-E= -0.000000005166 Rises=F Damp=F

DIIS: error= 7.98D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.33292312905 IErMin=13 ErrMin= 7.98D-07

ErrMax= 7.98D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.38D-09 BMatP= 6.68D-09

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

Coeff-Com: 0.366D-04-0.359D-03-0.102D-02-0.286D-02-0.428D-02 0.704D-02

Coeff-Com: 0.216D-01 0.145D-01-0.734D-01-0.685D-01 0.707D-01 0.355D+00

Coeff-Com: 0.682D+00

Coeff: 0.366D-04-0.359D-03-0.102D-02-0.286D-02-0.428D-02 0.704D-02

Coeff: 0.216D-01 0.145D-01-0.734D-01-0.685D-01 0.707D-01 0.355D+00

Coeff: 0.682D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.18D-07 MaxDP=1.00D-05 DE=-5.17D-09 OVMax= 1.28D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 5.63D-08 CP: 1.00D+00 1.09D+00 1.27D+00 2.03D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.98D+00 3.00D+00

CP: 1.72D+00 1.10D+00 1.47D+00

E= -1914.33292313001 Delta-E= -0.000000000968 Rises=F Damp=F

DIIS: error= 3.29D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.33292313001 IErMin=14 ErrMin= 3.29D-07

ErrMax= 3.29D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.90D-10 BMatP= 1.38D-09

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

Coeff-Com: -0.208D-04 0.585D-03 0.991D-04-0.126D-02-0.750D-02-0.158D-01

Coeff-Com: 0.865D-02 0.450D-01-0.207D-02-0.447D-01-0.811D-01 0.235D-01

Coeff-Com: 0.339D+00 0.736D+00

Coeff: -0.208D-04 0.585D-03 0.991D-04-0.126D-02-0.750D-02-0.158D-01

Coeff: 0.865D-02 0.450D-01-0.207D-02-0.447D-01-0.811D-01 0.235D-01

Coeff: 0.339D+00 0.736D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.35D-08 MaxDP=2.49D-06 DE=-9.68D-10 OVMax= 3.12D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.40D-08 CP: 1.00D+00 1.09D+00 1.27D+00 2.03D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.99D+00 3.00D+00

CP: 1.74D+00 1.09D+00 1.69D+00 1.08D+00

E= -1914.33292313025 Delta-E= -0.000000000234 Rises=F Damp=F

DIIS: error= 2.23D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.33292313025 IErMin=15 ErrMin= 2.23D-07

ErrMax= 2.23D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.05D-11 BMatP= 2.90D-10

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

Coeff-Com: -0.223D-04 0.437D-03 0.325D-03 0.306D-04-0.335D-02-0.114D-01

Coeff-Com: -0.885D-03 0.228D-01 0.182D-01-0.753D-02-0.648D-01-0.792D-01

Coeff-Com: 0.195D-01 0.414D+00 0.692D+00

Coeff: -0.223D-04 0.437D-03 0.325D-03 0.306D-04-0.335D-02-0.114D-01

Coeff: -0.885D-03 0.228D-01 0.182D-01-0.753D-02-0.648D-01-0.792D-01

Coeff: 0.195D-01 0.414D+00 0.692D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.39D-08 MaxDP=1.25D-06 DE=-2.34D-10 OVMax= 1.17D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 7.49D-09 CP: 1.00D+00 1.09D+00 1.27D+00 2.03D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.99D+00 3.00D+00

CP: 1.74D+00 1.10D+00 1.74D+00 1.17D+00 1.23D+00

E= -1914.33292313025 Delta-E= -0.000000000005 Rises=F Damp=F

DIIS: error= 1.24D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1914.33292313025 IErMin=16 ErrMin= 1.24D-07

ErrMax= 1.24D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.98D-11 BMatP= 9.05D-11

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

Coeff-Com: -0.316D-05-0.869D-06 0.124D-03 0.473D-03 0.107D-02 0.177D-03

Coeff-Com: -0.320D-02-0.502D-02 0.909D-02 0.121D-01-0.294D-02-0.441D-01

Coeff-Com: -0.110D+00-0.611D-01 0.317D+00 0.886D+00

Coeff: -0.316D-05-0.869D-06 0.124D-03 0.473D-03 0.107D-02 0.177D-03

Coeff: -0.320D-02-0.502D-02 0.909D-02 0.121D-01-0.294D-02-0.441D-01

Coeff: -0.110D+00-0.611D-01 0.317D+00 0.886D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.07D-09 MaxDP=6.95D-07 DE=-4.55D-12 OVMax= 3.97D-06

Error on total polarization charges = 0.08258

SCF Done: E(UB3LYP) = -1914.33292313 A.U. after 16 cycles

NFock= 16 Conv=0.71D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0547 S= 1.0181

<L.S>= 0.000000000000E+00

KE= 1.906359172649D+03 PE=-1.516296795565D+04 EE= 5.985596033408D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0547, after 2.0017

Leave Link 502 at Mon Aug 26 13:45:05 2019, MaxMem= 4294967296 cpu: 7090.1

(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: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.44694152D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.63604160D-01

Leave Link 801 at Mon Aug 26 13:45:05 2019, MaxMem= 4294967296 cpu: 1.0

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

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

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

Leave Link 1101 at Mon Aug 26 13:45:12 2019, MaxMem= 4294967296 cpu: 110.4

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

Symmetrizing basis deriv contribution to polar:

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

Leave Link 1102 at Mon Aug 26 13:45:12 2019, MaxMem= 4294967296 cpu: 2.4

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

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 184

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 Mon Aug 26 14:04:57 2019, MaxMem= 4294967296 cpu: 18946.0

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

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 580000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.65D+03 4.71D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.78D+02 3.44D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.90D+00 4.73D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.09D-01 4.18D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.94D-04 2.24D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.84D-06 1.39D-04.

190 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 2.17D-08 1.01D-05.

78 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 9.03D-11 6.24D-07.

44 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.72D-13 3.89D-08.

3 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 9.54D-15 7.55D-09.

2 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 5.58D-15 2.21D-09.

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

Solved reduced A of dimension 1724 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1145.50 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 Mon Aug 26 17:55:08 2019, MaxMem= 4294967296 cpu: 220919.1

(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.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 184

Leave Link 701 at Mon Aug 26 17:56:37 2019, MaxMem= 4294967296 cpu: 1425.0

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

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

Leave Link 702 at Mon Aug 26 17:56:37 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

Leave Link 703 at Mon Aug 26 18:15:13 2019, MaxMem= 4294967296 cpu: 17849.8

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

Dipole =-1.01866318D-03 3.70295125D-04-5.04180077D-01

Polarizability= 1.28377763D+03-3.10583344D+01 1.70132671D+03

2.99859208D-02-1.96405672D-01 4.51393162D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.002480344 0.000612326 0.003326565

2 6 0.003339871 -0.001760467 -0.003920147

3 7 0.001264924 -0.000150908 -0.000146071

4 6 0.002914193 -0.001315757 0.005036631

5 6 -0.002008947 0.000668415 -0.003229045

6 6 -0.003846238 0.001105917 -0.004761682

7 6 0.002461161 -0.001007158 0.002301155

8 7 -0.000094664 0.001158710 0.000366734

9 6 -0.004888471 -0.001485001 0.002692881

10 6 0.001904022 -0.000700753 -0.001360499

11 6 -0.001865333 0.000567464 -0.001191288

12 6 -0.006018157 0.001626743 0.004485561

13 6 0.004836852 -0.001418413 -0.002654312

14 6 -0.001906674 -0.000663374 0.001333846

15 6 0.001872338 0.000554671 0.001202081

16 6 -0.002444853 -0.001053192 -0.002311732

17 7 0.000122338 0.001088096 -0.000356458

18 6 0.003828144 0.001169271 0.004737395

19 6 -0.002878578 -0.001323487 -0.005023030

20 6 0.001987781 0.000663502 0.003207326

21 6 0.002479638 0.000579857 -0.003316862

22 6 -0.003337127 -0.001752312 0.003904719

23 7 -0.001268748 -0.000152423 0.000138786

24 6 0.006083033 0.001650290 -0.004489157

25 6 0.000037803 0.000073210 0.000190549

26 6 0.000016642 -0.000147279 -0.000128839

27 6 -0.000205381 0.000122499 0.000209025

28 6 -0.000103175 -0.000115940 -0.000139223

29 6 0.000215450 0.000174186 0.000024318

30 6 0.000097745 -0.000047784 -0.000094850

31 6 -0.000110945 -0.000230234 -0.000002135

32 6 -0.000256980 0.000082007 -0.000109695

33 6 0.000356900 -0.000022258 0.000100808

34 6 -0.000121009 0.000498655 -0.000030634

35 6 -0.000061718 0.000060206 -0.000142934

36 6 0.000130488 0.000082994 0.000019997

37 6 0.000100460 0.000536299 0.000017784

38 6 0.000066553 0.000071749 0.000157178

39 6 -0.000136580 0.000076710 -0.000022823

40 6 0.000119193 -0.000222853 0.000010067

41 6 0.000254374 0.000081496 0.000110089

42 6 -0.000360156 -0.000012675 -0.000119992

43 6 -0.000049866 0.000079903 -0.000202942

44 6 -0.000088590 -0.000045565 0.000101174

45 6 -0.000215868 0.000172762 -0.000027345

46 6 0.000101173 -0.000110675 0.000148699

47 6 0.000198906 0.000117366 -0.000216458

48 6 -0.000017227 -0.000137327 0.000138617

49 1 -0.000090875 0.000024156 0.000031502

50 1 -0.000060229 -0.000036474 -0.000197068

51 1 -0.000142346 0.000132918 -0.000040523

52 1 -0.000042631 0.000179111 0.000021740

53 1 0.000142513 0.000128159 0.000042736

54 1 0.000043966 0.000175114 -0.000023148

55 1 0.000066044 -0.000045824 0.000203649

56 1 0.000098953 0.000016979 -0.000021716

57 1 0.000023811 -0.000066660 0.000078737

58 1 0.000040604 0.000041507 -0.000006695

59 1 0.000061869 -0.000020413 -0.000015887

60 1 -0.000007404 -0.000038888 -0.000056040

61 1 -0.000100643 -0.000048280 0.000076390

62 1 0.000032537 -0.000009802 0.000032938

63 1 0.000021929 0.000040199 0.000017954

64 1 -0.000018271 0.000042825 -0.000086515

65 1 -0.000077061 -0.000016792 -0.000088447

66 1 -0.000021119 -0.000022448 0.000043119

67 1 0.000066711 -0.000025827 0.000091602

68 1 0.000020254 -0.000022313 -0.000041743

69 1 -0.000032816 -0.000014976 -0.000033275

70 1 -0.000019707 0.000041531 -0.000018684

71 1 0.000014282 0.000043732 0.000085692

72 1 0.000104298 -0.000048808 -0.000079914

73 1 0.000008163 -0.000038853 0.000056385

74 1 -0.000062278 -0.000021395 0.000014841

75 1 -0.000040022 0.000043587 0.000007718

76 1 -0.000017868 -0.000070016 -0.000081027

77 1 0.000246572 -0.000071246 0.000152939

78 1 -0.000283590 -0.000090270 -0.000131094

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

Cartesian Forces: Max 0.006083033 RMS 0.001479409

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

Leave Link 716 at Mon Aug 26 18:15:13 2019, MaxMem= 4294967296 cpu: 1.8

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.005121376 RMS 0.000648651

Search for a local minimum.

Step number 6 out of a maximum of 452

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

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= 3.72D-05 DEPred=-8.72D-05 R=-4.26D-01

Trust test=-4.26D-01 RLast= 2.33D-01 DXMaxT set to 2.12D-01

ITU= -1 1 1 -1 1 0

Eigenvalues --- -0.00459 0.00046 0.00532 0.00628 0.00723

Eigenvalues --- 0.00883 0.00974 0.01027 0.01075 0.01107

Eigenvalues --- 0.01157 0.01216 0.01249 0.01296 0.01301

Eigenvalues --- 0.01308 0.01354 0.01390 0.01422 0.01446

Eigenvalues --- 0.01466 0.01517 0.01545 0.01639 0.01717

Eigenvalues --- 0.01718 0.01732 0.01742 0.01751 0.01763

Eigenvalues --- 0.01764 0.01787 0.01807 0.01819 0.01890

Eigenvalues --- 0.01892 0.01937 0.01972 0.02034 0.02147

Eigenvalues --- 0.02177 0.02245 0.02273 0.02277 0.02306

Eigenvalues --- 0.02332 0.02430 0.02466 0.02527 0.02551

Eigenvalues --- 0.02553 0.02558 0.02600 0.02603 0.02611

Eigenvalues --- 0.02614 0.02634 0.02734 0.02738 0.02763

Eigenvalues --- 0.02790 0.02861 0.02863 0.02868 0.02873

Eigenvalues --- 0.03055 0.03065 0.03817 0.04105 0.04222

Eigenvalues --- 0.04306 0.04340 0.04456 0.04527 0.04550

Eigenvalues --- 0.08056 0.08628 0.09703 0.09736 0.09789

Eigenvalues --- 0.09921 0.09955 0.10470 0.10495 0.10688

Eigenvalues --- 0.10689 0.10697 0.10718 0.10719 0.10743

Eigenvalues --- 0.11399 0.11400 0.11424 0.11426 0.12006

Eigenvalues --- 0.12007 0.12008 0.12009 0.12266 0.12267

Eigenvalues --- 0.12299 0.12300 0.12774 0.12775 0.12787

Eigenvalues --- 0.12789 0.15688 0.15946 0.16290 0.17114

Eigenvalues --- 0.17369 0.17374 0.17557 0.17983 0.18040

Eigenvalues --- 0.18149 0.18218 0.18476 0.19251 0.19278

Eigenvalues --- 0.19358 0.19364 0.19393 0.19409 0.19420

Eigenvalues --- 0.19460 0.19550 0.19550 0.19554 0.19555

Eigenvalues --- 0.20314 0.21481 0.22037 0.22581 0.22849

Eigenvalues --- 0.23454 0.23881 0.24357 0.24763 0.25391

Eigenvalues --- 0.26231 0.26745 0.26857 0.27171 0.28501

Eigenvalues --- 0.28645 0.28809 0.28909 0.29608 0.31005

Eigenvalues --- 0.31533 0.31721 0.32525 0.33079 0.33267

Eigenvalues --- 0.33467 0.34223 0.34927 0.35588 0.35604

Eigenvalues --- 0.35643 0.35651 0.35664 0.35669 0.35765

Eigenvalues --- 0.35770 0.35788 0.35833 0.35934 0.35935

Eigenvalues --- 0.35947 0.35949 0.36034 0.36038 0.36045

Eigenvalues --- 0.36049 0.36232 0.36260 0.36286 0.36291

Eigenvalues --- 0.37048 0.37055 0.37295 0.37351 0.37365

Eigenvalues --- 0.37546 0.38303 0.38325 0.38462 0.38864

Eigenvalues --- 0.39655 0.40493 0.40907 0.41006 0.41011

Eigenvalues --- 0.41087 0.41183 0.41192 0.41310 0.41420

Eigenvalues --- 0.41452 0.41796 0.42989 0.43466 0.45058

Eigenvalues --- 0.45739 0.45871 0.45915 0.45984 0.46069

Eigenvalues --- 0.46174 0.46202 0.46216 0.46294 0.46301

Eigenvalues --- 0.47113 0.47315 0.48389 0.49253 0.49864

Eigenvalues --- 0.50733 0.50736 0.50776 0.50777 0.51657

Eigenvalues --- 0.52300 0.56519 0.57798

Eigenvalue 1 is -4.59D-03 should be greater than 0.000000 Eigenvector:

D112 D12 D27 D20 D98

1 0.22945 -0.22935 0.22882 0.22866 -0.22835

D85 D113 D13 D100 D19

1 -0.22751 0.22206 -0.22074 -0.16946 0.16935

Cosine: 0.958 < 0.970

Cut down GDIIS temporarily because of the cosine check. E 9

DIIS coeff's: 0.60155 0.39845

Cosine: 0.958 > 0.500

Length: 1.021

GDIIS step was calculated using 2 of the last 6 vectors.

Iteration 1 RMS(Cart)= 0.32404246 RMS(Int)= 0.00543778

Iteration 2 RMS(Cart)= 0.02899503 RMS(Int)= 0.00039854

Iteration 3 RMS(Cart)= 0.00019066 RMS(Int)= 0.00039701

Iteration 4 RMS(Cart)= 0.00000010 RMS(Int)= 0.00039701

ITry= 1 IFail=0 DXMaxC= 1.68D+00 DCOld= 1.00D+10 DXMaxT= 2.12D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.66797 -0.00268 -0.00779 -0.00801 -0.01567 2.65231

R2 2.63163 0.00271 0.00784 0.00319 0.01157 2.64320

R3 2.03713 -0.00006 -0.00009 0.00047 0.00039 2.03752

R4 2.60009 -0.00097 -0.00106 -0.00110 -0.00262 2.59748

R5 2.70277 0.00294 0.00964 0.01274 0.02235 2.72511

R6 2.60143 -0.00113 -0.00198 -0.00012 -0.00254 2.59888

R7 1.90983 -0.00025 0.00001 -0.00053 -0.00051 1.90932

R8 2.66313 -0.00231 -0.00657 0.00166 -0.00472 2.65841

R9 2.70631 0.00401 0.01094 -0.00407 0.00688 2.71319

R10 2.03713 0.00008 0.00005 -0.00025 -0.00019 2.03694

R11 2.64243 -0.00229 -0.00754 0.02013 0.01259 2.65503

R12 2.80453 -0.00004 0.00011 -0.00262 -0.00251 2.80202

R13 2.60507 0.00011 -0.00131 -0.02432 -0.02609 2.57898

R14 2.75395 0.00141 0.00565 0.00498 0.01082 2.76477

R15 2.58458 0.00012 0.00022 0.02708 0.02684 2.61141

R16 2.75696 0.00111 0.00504 -0.00038 0.00479 2.76175

R17 2.66625 -0.00512 -0.01276 -0.02809 -0.04088 2.62537

R18 2.55981 -0.00166 -0.00403 -0.00217 -0.00562 2.55418

R19 2.03898 0.00015 0.00014 -0.00044 -0.00031 2.03868

R20 2.03915 -0.00000 -0.00005 0.00029 0.00023 2.03938

R21 2.66594 -0.00509 -0.01267 -0.02777 -0.04043 2.62551

R22 2.80214 -0.00027 0.00005 0.00388 0.00393 2.80607

R23 2.75706 0.00109 0.00499 -0.00056 0.00456 2.76162

R24 2.58472 0.00011 0.00021 0.02681 0.02661 2.61133

R25 2.55980 -0.00167 -0.00402 -0.00214 -0.00561 2.55418

R26 2.03898 0.00015 0.00014 -0.00039 -0.00026 2.03872

R27 2.75396 0.00142 0.00564 0.00507 0.01090 2.76486

R28 2.03916 -0.00000 -0.00005 0.00025 0.00020 2.03936

R29 2.60498 0.00012 -0.00130 -0.02426 -0.02598 2.57901

R30 2.64241 -0.00227 -0.00746 0.02004 0.01263 2.65504

R31 2.70634 0.00399 0.01094 -0.00404 0.00693 2.71327

R32 2.80460 -0.00004 -0.00019 -0.00227 -0.00246 2.80214

R33 2.66309 -0.00230 -0.00664 0.00191 -0.00453 2.65856

R34 2.60153 -0.00116 -0.00216 -0.00009 -0.00269 2.59884

R35 2.63162 0.00270 0.00793 0.00310 0.01156 2.64318

R36 2.03712 0.00008 0.00010 -0.00028 -0.00019 2.03693

R37 2.66794 -0.00267 -0.00784 -0.00784 -0.01556 2.65237

R38 2.03714 -0.00007 -0.00008 0.00046 0.00038 2.03752

R39 2.60018 -0.00098 -0.00119 -0.00114 -0.00277 2.59741

R40 2.70282 0.00295 0.00968 0.01270 0.02235 2.72517

R41 1.90991 -0.00029 -0.00021 -0.00039 -0.00061 1.90931

R42 2.80190 -0.00024 -0.00006 0.00440 0.00433 2.80623

R43 2.65153 -0.00016 -0.00010 0.00004 -0.00006 2.65146

R44 2.64982 0.00009 -0.00016 0.00119 0.00103 2.65085

R45 2.62890 -0.00016 -0.00043 0.00034 -0.00010 2.62881

R46 2.04835 0.00002 -0.00002 0.00011 0.00009 2.04844

R47 2.63600 0.00013 0.00029 0.00012 0.00041 2.63641

R48 2.04999 0.00006 0.00006 0.00018 0.00024 2.05023

R49 2.63430 -0.00009 -0.00024 0.00060 0.00036 2.63466

R50 2.04993 0.00005 0.00007 0.00007 0.00014 2.05007

R51 2.63063 0.00016 0.00045 -0.00062 -0.00017 2.63046

R52 2.04991 0.00007 0.00007 0.00021 0.00029 2.05020

R53 2.04814 0.00010 0.00014 0.00055 0.00069 2.04883

R54 2.63586 0.00017 0.00028 0.00064 0.00092 2.63679

R55 2.63485 -0.00014 -0.00040 -0.00054 -0.00093 2.63392

R56 2.04995 0.00005 0.00006 0.00007 0.00013 2.05008

R57 2.62921 -0.00014 -0.00029 -0.00100 -0.00129 2.62791

R58 2.05008 0.00004 0.00004 -0.00001 0.00003 2.05011

R59 2.65197 0.00010 0.00014 -0.00109 -0.00095 2.65102

R60 2.04810 0.00009 0.00011 0.00015 0.00026 2.04836

R61 2.65128 -0.00018 -0.00025 -0.00203 -0.00229 2.64899

R62 2.63016 -0.00001 0.00016 0.00148 0.00165 2.63181

R63 2.04839 0.00007 -0.00001 0.00013 0.00012 2.04851

R64 2.05005 0.00005 0.00003 -0.00002 0.00002 2.05007

R65 2.65140 -0.00019 -0.00020 -0.00228 -0.00249 2.64891

R66 2.65203 0.00011 0.00018 -0.00116 -0.00098 2.65105

R67 2.63011 -0.00001 0.00016 0.00157 0.00173 2.63184

R68 2.04838 0.00006 -0.00002 0.00015 0.00013 2.04851

R69 2.63487 -0.00015 -0.00041 -0.00055 -0.00095 2.63392

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R71 2.63587 0.00016 0.00029 0.00062 0.00092 2.63679

R72 2.04995 0.00005 0.00006 0.00007 0.00014 2.05008

R73 2.62919 -0.00014 -0.00032 -0.00098 -0.00129 2.62790

R74 2.05008 0.00004 0.00003 -0.00001 0.00003 2.05011

R75 2.04808 0.00009 0.00012 0.00017 0.00029 2.04836

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R78 2.63063 0.00016 0.00042 -0.00059 -0.00017 2.63047

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A2 2.18659 0.00008 0.00129 -0.00138 0.00000 2.18659

A3 2.21393 0.00025 -0.00013 0.00041 0.00038 2.21431

A4 1.86531 0.00004 0.00160 0.00218 0.00371 1.86901

A5 2.22159 0.00102 0.00226 -0.00918 -0.00531 2.21628

A6 2.19582 -0.00106 -0.00407 0.00746 0.00184 2.19766

A7 1.92618 0.00074 -0.00047 -0.00034 -0.00036 1.92582

A8 2.17785 -0.00052 -0.00136 0.00849 0.00690 2.18476

A9 2.17822 -0.00022 0.00166 -0.00772 -0.00629 2.17193

A10 1.86645 -0.00006 0.00149 -0.00071 0.00066 1.86710

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A12 2.22031 0.00023 0.00002 0.00804 0.00942 2.22973

A13 1.88379 -0.00038 -0.00146 -0.00199 -0.00359 1.88020

A14 2.21320 0.00038 0.00031 -0.00037 -0.00001 2.21319

A15 2.18617 -0.00000 0.00116 0.00242 0.00363 2.18980

A16 2.18734 0.00041 0.00034 -0.00553 -0.00726 2.18008

A17 2.02499 -0.00053 -0.00372 0.01100 0.00827 2.03326

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A22 1.84639 -0.00038 0.00111 0.00002 0.00163 1.84802

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A27 2.19836 -0.00011 -0.00133 0.00188 0.00063 2.19899

A28 2.22356 0.00003 0.00059 -0.00271 -0.00204 2.22152

A29 1.86179 0.00012 0.00013 0.00013 0.00017 1.86196

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A32 2.18198 0.00000 0.00042 0.00951 0.00782 2.18980

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A34 2.06734 -0.00026 0.00349 0.00865 0.01317 2.08052

A35 2.16336 -0.00065 -0.00061 0.00922 0.01015 2.17351

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A57 1.88266 -0.00033 -0.00118 0.00091 -0.00046 1.88220

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A90 2.09790 0.00004 0.00020 -0.00139 -0.00120 2.09670

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A97 2.10481 -0.00059 -0.00138 0.01374 0.01240 2.11720

A98 2.06997 0.00011 0.00024 0.00284 0.00306 2.07302

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A103 2.09672 0.00005 0.00021 -0.00027 -0.00006 2.09666

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A105 2.10467 -0.00061 -0.00122 0.01419 0.01301 2.11768

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A107 2.06986 0.00010 0.00022 0.00296 0.00316 2.07303

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A126 2.10491 -0.00006 -0.00024 0.00114 0.00090 2.10581

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D3 -3.11728 -0.00001 -0.00181 -0.00518 -0.00700 -3.12428

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D5 -0.00406 -0.00001 0.00006 0.01284 0.01294 0.00888

D6 -3.13735 0.00001 -0.00070 0.00426 0.00361 -3.13375

D7 3.13212 0.00001 0.00181 0.00695 0.00873 3.14086

D8 -0.00117 0.00003 0.00105 -0.00163 -0.00060 -0.00177

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D11 3.08347 -0.00004 -0.00571 0.01984 0.01434 3.09781

D12 -0.10280 -0.00001 -0.00918 0.02993 0.02080 -0.08199

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D15 0.20126 0.00010 0.01227 0.08264 0.09491 0.29617

D16 -2.93826 -0.00004 0.00520 0.07514 0.08048 -2.85778

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D18 -3.09206 0.00005 0.00315 0.02591 0.02867 -3.06338

D19 -3.07193 -0.00001 0.00353 -0.00767 -0.00396 -3.07589

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D85 2.92811 -0.00011 -0.01396 0.09843 0.08468 3.01279

D86 -0.24167 -0.00016 -0.01568 0.06579 0.05051 -0.19116

D87 -0.20356 -0.00008 -0.00996 0.07761 0.06790 -0.13566

D88 2.90984 -0.00012 -0.01167 0.04498 0.03373 2.94357

D89 -0.98146 0.00005 0.00223 -0.00831 -0.00610 -0.98756

D90 2.16329 0.00004 0.00341 -0.01273 -0.00935 2.15395

D91 2.15091 0.00002 -0.00153 0.01103 0.00953 2.16043

D92 -0.98752 0.00001 -0.00036 0.00661 0.00628 -0.98124

D93 3.10550 -0.00005 -0.00135 -0.03965 -0.04107 3.06444

D94 -0.04429 -0.00006 -0.00157 -0.02912 -0.03072 -0.07501

D95 -0.01220 -0.00000 0.00015 -0.01187 -0.01169 -0.02389

D96 3.12119 -0.00002 -0.00007 -0.00133 -0.00134 3.11984

D97 -3.09356 0.00006 0.00117 0.03337 0.03413 -3.05943

D98 0.09250 0.00003 -0.00108 0.02856 0.02729 0.11979

D99 0.02456 0.00003 -0.00027 0.00636 0.00606 0.03063

D100 -3.07256 -0.00001 -0.00252 0.00154 -0.00078 -3.07334

D101 -0.00405 -0.00001 0.00001 0.01288 0.01293 0.00889

D102 3.13192 0.00001 0.00093 0.00934 0.01024 -3.14103

D103 -3.13728 0.00000 0.00023 0.00211 0.00239 -3.13489

D104 -0.00131 0.00003 0.00115 -0.00142 -0.00031 -0.00162

D105 0.01875 0.00002 -0.00017 -0.00893 -0.00919 0.00956

D106 -3.09158 0.00008 0.00362 -0.02072 -0.01724 -3.10882

D107 -3.11733 -0.00000 -0.00107 -0.00546 -0.00654 -3.12387

D108 0.05553 0.00005 0.00272 -0.01726 -0.01460 0.04093

D109 -0.02702 -0.00004 0.00026 0.00149 0.00185 -0.02518

D110 3.07012 0.00000 0.00258 0.00581 0.00834 3.07846

D111 3.08390 -0.00005 -0.00327 0.01269 0.00963 3.09353

D112 -0.10215 -0.00001 -0.00095 0.01701 0.01613 -0.08602

D113 -2.97837 0.00007 0.01357 0.08955 0.10322 -2.87514

D114 0.16529 -0.00006 0.00409 0.08788 0.09215 0.25745

D115 0.20012 0.00011 0.01788 0.07580 0.09372 0.29384

D116 -2.93940 -0.00003 0.00840 0.07412 0.08265 -2.85676

D117 0.96853 -0.00002 -0.00067 0.02545 0.02485 0.99337

D118 -2.17009 -0.00004 -0.00758 0.03229 0.02476 -2.14533

D119 -2.17499 0.00011 0.00821 0.02702 0.03517 -2.13982

D120 0.96957 0.00009 0.00129 0.03386 0.03509 1.00466

D121 -3.12954 0.00006 0.00186 -0.00497 -0.00311 -3.13265

D122 -0.00995 0.00006 0.00260 -0.00377 -0.00116 -0.01111

D123 0.01485 0.00005 0.00225 -0.00781 -0.00555 0.00930

D124 3.13444 0.00006 0.00300 -0.00660 -0.00361 3.13083

D125 3.14147 -0.00003 -0.00135 0.00429 0.00295 -3.13877

D126 -0.01844 -0.00002 -0.00110 0.00386 0.00277 -0.01567

D127 -0.00292 -0.00003 -0.00175 0.00715 0.00540 0.00248

D128 3.12036 -0.00002 -0.00150 0.00672 0.00521 3.12557

D129 -0.01612 -0.00004 -0.00129 0.00384 0.00255 -0.01357

D130 3.12449 -0.00001 -0.00059 0.00218 0.00159 3.12608

D131 -3.13562 -0.00004 -0.00203 0.00265 0.00062 -3.13500

D132 0.00500 -0.00002 -0.00133 0.00099 -0.00034 0.00465

D133 0.00523 0.00000 -0.00022 0.00092 0.00070 0.00593

D134 -3.13496 0.00003 0.00072 -0.00051 0.00021 -3.13475

D135 -3.13538 -0.00002 -0.00092 0.00258 0.00167 -3.13371

D136 0.00762 0.00001 0.00002 0.00116 0.00118 0.00880

D137 0.00666 0.00002 0.00072 -0.00158 -0.00086 0.00580

D138 -3.13197 0.00001 0.00028 -0.00282 -0.00255 -3.13451

D139 -3.13634 -0.00001 -0.00022 -0.00015 -0.00037 -3.13671

D140 0.00822 -0.00002 -0.00066 -0.00140 -0.00206 0.00616

D141 -0.00778 -0.00000 0.00029 -0.00253 -0.00224 -0.01002

D142 -3.13097 -0.00001 0.00005 -0.00206 -0.00201 -3.13298

D143 3.13086 0.00001 0.00072 -0.00129 -0.00057 3.13030

D144 0.00767 -0.00000 0.00049 -0.00082 -0.00033 0.00734

D145 -0.00452 -0.00005 -0.00091 0.00274 0.00182 -0.00270

D146 3.13463 -0.00002 0.00004 0.00548 0.00551 3.14014

D147 3.13564 -0.00002 -0.00098 0.00020 -0.00078 3.13487

D148 -0.00839 0.00000 -0.00002 0.00294 0.00291 -0.00548

D149 -0.00610 0.00001 0.00027 -0.00430 -0.00402 -0.01012

D150 3.13254 0.00002 0.00019 -0.00485 -0.00465 3.12789

D151 3.13693 -0.00001 0.00034 -0.00176 -0.00142 3.13551

D152 -0.00762 -0.00000 0.00026 -0.00231 -0.00206 -0.00967

D153 0.01277 0.00006 0.00128 0.00745 0.00871 0.02148

D154 3.13321 0.00002 0.00255 0.00182 0.00435 3.13756

D155 -3.12639 0.00003 0.00033 0.00472 0.00504 -3.12135

D156 -0.00595 -0.00000 0.00160 -0.00091 0.00068 -0.00527

D157 3.12874 -0.00002 0.00466 -0.02056 -0.01591 3.11283

D158 -0.01020 -0.00004 -0.00098 -0.01579 -0.01679 -0.02699

D159 0.00821 0.00001 0.00340 -0.01499 -0.01162 -0.00340

D160 -3.13073 -0.00001 -0.00225 -0.01022 -0.01249 3.13996

D161 -3.13940 -0.00002 -0.00528 0.01903 0.01372 -3.12568

D162 0.02005 -0.00000 -0.00395 0.01253 0.00857 0.02862

D163 -0.00045 0.00001 0.00034 0.01422 0.01456 0.01411

D164 -3.12418 0.00002 0.00167 0.00772 0.00941 -3.11478

D165 0.00858 0.00001 0.00001 -0.00432 -0.00431 0.00427

D166 -3.13007 -0.00000 0.00009 -0.00378 -0.00368 -3.13375

D167 3.13222 -0.00000 -0.00133 0.00219 0.00085 3.13308

D168 -0.00643 -0.00001 -0.00125 0.00273 0.00148 -0.00495

D169 -3.13923 -0.00002 -0.00627 0.02115 0.01487 -3.12437

D170 0.02009 0.00000 -0.00441 0.01402 0.00960 0.02969

D171 -0.00055 0.00000 0.00050 0.01443 0.01492 0.01437

D172 -3.12441 0.00002 0.00235 0.00729 0.00965 -3.11475

D173 3.12864 -0.00002 0.00560 -0.02274 -0.01716 3.11147

D174 0.00835 0.00001 0.00401 -0.01660 -0.01261 -0.00426

D175 -0.01004 -0.00004 -0.00120 -0.01605 -0.01726 -0.02731

D176 -3.13033 -0.00001 -0.00278 -0.00991 -0.01271 3.14015

D177 0.00854 0.00001 0.00002 -0.00433 -0.00430 0.00424

D178 -3.13011 0.00000 0.00026 -0.00399 -0.00373 -3.13384

D179 3.13231 -0.00001 -0.00185 0.00282 0.00097 3.13328

D180 -0.00634 -0.00002 -0.00161 0.00315 0.00155 -0.00480

D181 -0.00598 0.00001 0.00015 -0.00444 -0.00427 -0.01025

D182 3.13688 -0.00001 0.00047 -0.00197 -0.00150 3.13538

D183 3.13266 0.00002 -0.00008 -0.00478 -0.00485 3.12781

D184 -0.00767 -0.00000 0.00023 -0.00231 -0.00208 -0.00974

D185 -0.00457 -0.00005 -0.00086 0.00282 0.00195 -0.00262

D186 3.13451 -0.00002 0.00021 0.00548 0.00567 3.14017

D187 3.13575 -0.00003 -0.00117 0.00034 -0.00082 3.13493

D188 -0.00835 0.00000 -0.00010 0.00301 0.00290 -0.00546

D189 0.01268 0.00006 0.00139 0.00758 0.00895 0.02163

D190 3.13288 0.00003 0.00298 0.00137 0.00432 3.13720

D191 -3.12641 0.00003 0.00033 0.00493 0.00525 -3.12116

D192 -0.00621 -0.00000 0.00192 -0.00128 0.00063 -0.00559

D193 -3.14145 -0.00004 -0.00056 0.00276 0.00220 -3.13925

D194 -0.01811 -0.00003 -0.00083 0.00276 0.00194 -0.01618

D195 -0.00296 -0.00003 -0.00172 0.00711 0.00538 0.00243

D196 3.12038 -0.00002 -0.00199 0.00711 0.00512 3.12550

D197 -3.12979 0.00006 0.00120 -0.00357 -0.00236 -3.13215

D198 -0.01017 0.00006 0.00200 -0.00272 -0.00071 -0.01088

D199 0.01491 0.00005 0.00235 -0.00789 -0.00554 0.00936

D200 3.13452 0.00005 0.00315 -0.00704 -0.00389 3.13063

D201 -0.00773 -0.00001 0.00014 -0.00243 -0.00229 -0.01003

D202 3.13089 0.00001 0.00051 -0.00109 -0.00059 3.13030

D203 -3.13098 -0.00001 0.00041 -0.00240 -0.00198 -3.13296

D204 0.00764 -0.00000 0.00078 -0.00106 -0.00028 0.00736

D205 0.00659 0.00002 0.00086 -0.00161 -0.00074 0.00584

D206 -3.13633 -0.00001 -0.00030 -0.00002 -0.00032 -3.13665

D207 -3.13202 0.00001 0.00050 -0.00295 -0.00246 -3.13447

D208 0.00824 -0.00002 -0.00066 -0.00137 -0.00203 0.00621

D209 0.00532 -0.00000 -0.00025 0.00082 0.00058 0.00590

D210 -3.13541 -0.00002 -0.00099 0.00273 0.00174 -3.13367

D211 -3.13494 0.00003 0.00091 -0.00076 0.00015 -3.13479

D212 0.00751 0.00001 0.00017 0.00114 0.00131 0.00882

D213 -0.01620 -0.00004 -0.00138 0.00399 0.00261 -0.01359

D214 -3.13573 -0.00004 -0.00218 0.00315 0.00098 -3.13475

D215 3.12453 -0.00001 -0.00064 0.00209 0.00145 3.12599

D216 0.00501 -0.00002 -0.00144 0.00126 -0.00018 0.00483

Item Value Threshold Converged?

Maximum Force 0.005121 0.000450 NO

RMS Force 0.000649 0.000300 NO

Maximum Displacement 1.684736 0.001800 NO

RMS Displacement 0.343800 0.001200 NO

Predicted change in Energy=-5.039420D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Mon Aug 26 18:15:14 2019, MaxMem= 4294967296 cpu: 2.4

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

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=1 Diff= 7.59D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -1.428402 -3.974532 0.540141

2 6 0 -0.441565 -3.051008 0.161746

3 7 0 -1.058206 -1.828743 0.038684

4 6 0 -2.404197 -1.944258 0.296229

5 6 0 -2.644366 -3.289288 0.631209

6 6 0 -3.364914 -0.884838 0.169545

7 6 0 -3.046925 0.470700 -0.018521

8 7 0 -1.800323 1.017161 0.080815

9 6 0 -1.960536 2.369682 -0.153001

10 6 0 -3.357079 2.662417 -0.468962

11 6 0 -4.030097 1.494112 -0.374222

12 6 0 0.953091 -3.323428 -0.083774

13 6 0 1.959999 -2.368994 -0.158003

14 6 0 3.356788 -2.661151 -0.473072

15 6 0 4.029727 -1.493045 -0.375371

16 6 0 3.046357 -0.470415 -0.017762

17 7 0 1.799611 -1.017072 0.078863

18 6 0 3.364055 0.884752 0.173500

19 6 0 2.403410 1.943901 0.303444

20 6 0 2.644355 3.289386 0.636367

21 6 0 1.428423 3.974790 0.546237

22 6 0 0.440822 3.050951 0.170487

23 7 0 1.056651 1.828040 0.050210

24 6 0 -0.953470 3.323701 -0.076909

25 6 0 -4.793581 -1.275469 0.239643

26 6 0 -5.323019 -2.234986 -0.636539

27 6 0 -6.666826 -2.588799 -0.571944

28 6 0 -7.502125 -2.002596 0.379385

29 6 0 -6.985323 -1.054469 1.261300

30 6 0 -5.644086 -0.689200 1.188691

31 6 0 1.965038 -7.458433 -0.620031

32 6 0 1.014696 -6.852111 -1.442321

33 6 0 0.675985 -5.517001 -1.250976

34 6 0 1.300419 -4.757503 -0.250345

35 6 0 2.248648 -5.377911 0.574860

36 6 0 2.575557 -6.719243 0.391689

37 6 0 -1.299511 4.757666 -0.247805

38 6 0 -2.248826 5.381354 0.573593

39 6 0 -2.575146 6.722075 0.384845

40 6 0 -1.962913 7.457345 -0.628692

41 6 0 -1.011307 6.847773 -1.447115

42 6 0 -0.673159 5.513345 -1.250148

43 6 0 4.792845 1.275613 0.241086

44 6 0 5.645807 0.687656 1.186861

45 6 0 6.987243 1.052754 1.256666

46 6 0 7.501812 2.002431 0.375121

47 6 0 6.664060 2.590377 -0.572953

48 6 0 5.320069 2.236733 -0.634701

49 1 0 -1.260179 -5.022072 0.732214

50 1 0 -3.600460 -3.704237 0.906114

51 1 0 -3.756099 3.625925 -0.745170

52 1 0 -5.079743 1.324972 -0.559421

53 1 0 3.755900 -3.624214 -0.750782

54 1 0 5.079504 -1.323625 -0.559484

55 1 0 3.601079 3.704780 0.908378

56 1 0 1.261014 5.022851 0.736168

57 1 0 -4.679160 -2.688545 -1.381358

58 1 0 -7.063236 -3.321982 -1.266480

59 1 0 -8.548501 -2.283866 0.433108

60 1 0 -7.626673 -0.598741 2.008312

61 1 0 -5.242656 0.042440 1.880811

62 1 0 2.224901 -8.501674 -0.765071

63 1 0 0.535993 -7.420293 -2.232862

64 1 0 -0.059853 -5.047385 -1.893579

65 1 0 2.719206 -4.807531 1.367546

66 1 0 3.305989 -7.187276 1.043081

67 1 0 -2.720868 4.813991 1.367565

68 1 0 -3.306523 7.192696 1.033307

69 1 0 -2.222408 8.500054 -0.778137

70 1 0 -0.531216 7.412865 -2.239031

71 1 0 0.063416 5.041034 -1.889930

72 1 0 5.246175 -0.045191 1.878735

73 1 0 7.630491 0.595664 2.001208

74 1 0 8.548342 2.283549 0.426590

75 1 0 7.058686 3.324763 -1.267236

76 1 0 4.674383 2.691522 -1.377175

77 1 0 -0.589848 -0.959384 -0.175092

78 1 0 0.587214 0.958208 -0.159201

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

Rotational constants (GHZ): 0.0588123 0.0581379 0.0302366

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

Standard basis: 6-311G(d) (5D, 7F)

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

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5358.1015697596 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2121431263 Hartrees.

Nuclear repulsion after empirical dispersion term = 5357.8894266334 Hartrees.

Force inversion solution in PCM.

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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 : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5758

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.44D-10

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 279

GePol: Fraction of low-weight points (<1% of avg) = 4.85%

GePol: Cavity surface area = 612.585 Ang\*\*2

GePol: Cavity volume = 628.507 Ang\*\*3

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

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

PCM non-electrostatic energy = -0.0020934253 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5357.8873332080 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.

NBasis= 954 RedAO= T EigKep= 1.30D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

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

DipDrv: MaxL=1.

Leave Link 303 at Mon Aug 26 18:15:16 2019, MaxMem= 4294967296 cpu: 2.4

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

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= -0.000000 0.000000 0.000000

Rot= 0.963480 0.000017 -0.000013 0.267781 Ang= 31.06 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0546 S= 1.0181

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30478484170

Leave Link 401 at Mon Aug 26 18:15:21 2019, MaxMem= 4294967296 cpu: 81.4

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 590000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 99463692.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.55D-15 for 5729.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.68D-15 for 4059 3002.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.44D-15 for 5729.

Iteration 1 A^-1\*A deviation from orthogonality is 2.96D-10 for 2300 2243.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.89D-15 for 27.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.27D-15 for 3767 268.

Iteration 2 A^-1\*A deviation from unit magnitude is 8.88D-16 for 885.

Iteration 2 A^-1\*A deviation from orthogonality is 4.00D-16 for 5125 5028.

E= -1914.15935874226

DIIS: error= 1.61D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.15935874226 IErMin= 1 ErrMin= 1.61D-02

ErrMax= 1.61D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.22D-01 BMatP= 4.22D-01

IDIUse=3 WtCom= 8.39D-01 WtEn= 1.61D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Recover alternate guess density for next cycle.

RMSDP=1.13D-03 MaxDP=5.57D-02 OVMax= 0.00D+00

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.13D-03 CP: 9.91D-01

E= -1913.37596010850 Delta-E= 0.783398633765 Rises=F Damp=F

Switch densities from cycles 1 and 2 for lowest energy.

DIIS: error= 3.06D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -1914.15935874226 IErMin= 1 ErrMin= 1.61D-02

ErrMax= 3.06D-02 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.03D+00 BMatP= 4.22D-01

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

Coeff-Com: 0.905D+00 0.949D-01

Coeff: 0.905D+00 0.949D-01

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.060 Goal= None Shift= 0.000

RMSDP=5.38D-03 MaxDP=3.31D-01 DE= 7.83D-01 OVMax= 1.52D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.86D-04 CP: 9.97D-01 7.04D-02

E= -1914.32326731584 Delta-E= -0.947307207341 Rises=F Damp=F

DIIS: error= 2.06D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.32326731584 IErMin= 3 ErrMin= 2.06D-03

ErrMax= 2.06D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.30D-02 BMatP= 4.22D-01

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

Coeff-Com: -0.333D-01 0.730D-01 0.960D+00

Coeff: -0.333D-01 0.730D-01 0.960D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.38D-04 MaxDP=7.61D-03 DE=-9.47D-01 OVMax= 4.18D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.03D-04 CP: 9.96D-01 1.51D-01 9.65D-01

E= -1914.32993693724 Delta-E= -0.006669621397 Rises=F Damp=F

DIIS: error= 1.79D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.32993693724 IErMin= 4 ErrMin= 1.79D-03

ErrMax= 1.79D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.09D-02 BMatP= 3.30D-02

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

Coeff-Com: -0.277D-01 0.277D-01 0.498D+00 0.502D+00

Coeff: -0.277D-01 0.277D-01 0.498D+00 0.502D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=6.27D-05 MaxDP=4.09D-03 DE=-6.67D-03 OVMax= 1.49D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.30D-05 CP: 9.97D-01 1.43D-01 9.98D-01 5.88D-01

E= -1914.33246110948 Delta-E= -0.002524172241 Rises=F Damp=F

DIIS: error= 6.11D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33246110948 IErMin= 5 ErrMin= 6.11D-04

ErrMax= 6.11D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.10D-03 BMatP= 1.09D-02

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

Coeff-Com: -0.897D-02 0.359D-02 0.133D+00 0.275D+00 0.597D+00

Coeff: -0.897D-02 0.359D-02 0.133D+00 0.275D+00 0.597D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.53D-05 MaxDP=1.62D-03 DE=-2.52D-03 OVMax= 1.31D-02

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.10D-05 CP: 9.96D-01 1.44D-01 1.00D+00 6.87D-01 7.88D-01

E= -1914.33276345923 Delta-E= -0.000302349752 Rises=F Damp=F

DIIS: error= 2.40D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33276345923 IErMin= 6 ErrMin= 2.40D-04

ErrMax= 2.40D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.35D-04 BMatP= 1.10D-03

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

Coeff-Com: -0.261D-02-0.370D-03 0.306D-01 0.108D+00 0.333D+00 0.532D+00

Coeff: -0.261D-02-0.370D-03 0.306D-01 0.108D+00 0.333D+00 0.532D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.14D-05 MaxDP=7.28D-04 DE=-3.02D-04 OVMax= 7.68D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 9.36D-06 CP: 9.96D-01 1.43D-01 1.00D+00 7.19D-01 9.09D-01

CP: 9.56D-01

E= -1914.33281777586 Delta-E= -0.000054316632 Rises=F Damp=F

DIIS: error= 1.72D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33281777586 IErMin= 7 ErrMin= 1.72D-04

ErrMax= 1.72D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.34D-05 BMatP= 1.35D-04

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

Coeff-Com: 0.209D-03-0.715D-03-0.812D-02 0.433D-02 0.623D-01 0.269D+00

Coeff-Com: 0.673D+00

Coeff: 0.209D-03-0.715D-03-0.812D-02 0.433D-02 0.623D-01 0.269D+00

Coeff: 0.673D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=9.57D-06 MaxDP=7.20D-04 DE=-5.43D-05 OVMax= 9.62D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 4.23D-06 CP: 9.96D-01 1.44D-01 1.01D+00 7.44D-01 9.93D-01

CP: 1.26D+00 1.33D+00

E= -1914.33284516860 Delta-E= -0.000027392742 Rises=F Damp=F

DIIS: error= 1.30D-04 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33284516860 IErMin= 8 ErrMin= 1.30D-04

ErrMax= 1.30D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 9.78D-06 BMatP= 2.34D-05

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

Coeff-Com: 0.912D-03-0.251D-03-0.137D-01-0.315D-01-0.700D-01-0.320D-01

Coeff-Com: 0.335D+00 0.811D+00

Coeff: 0.912D-03-0.251D-03-0.137D-01-0.315D-01-0.700D-01-0.320D-01

Coeff: 0.335D+00 0.811D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=9.95D-06 MaxDP=7.31D-04 DE=-2.74D-05 OVMax= 1.02D-02

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.43D-06 CP: 9.96D-01 1.45D-01 1.01D+00 7.68D-01 1.09D+00

CP: 1.53D+00 1.94D+00 1.49D+00

E= -1914.33286627969 Delta-E= -0.000021111084 Rises=F Damp=F

DIIS: error= 1.05D-04 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33286627969 IErMin= 9 ErrMin= 1.05D-04

ErrMax= 1.05D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.47D-06 BMatP= 9.78D-06

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

Coeff-Com: 0.472D-03 0.287D-03-0.326D-02-0.222D-01-0.816D-01-0.194D+00

Coeff-Com: -0.204D+00 0.462D+00 0.104D+01

Coeff: 0.472D-03 0.287D-03-0.326D-02-0.222D-01-0.816D-01-0.194D+00

Coeff: -0.204D+00 0.462D+00 0.104D+01

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.33D-05 MaxDP=1.03D-03 DE=-2.11D-05 OVMax= 1.43D-02

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.72D-06 CP: 9.96D-01 1.47D-01 1.01D+00 8.00D-01 1.20D+00

CP: 1.90D+00 2.71D+00 2.50D+00 1.59D+00

E= -1914.33288366411 Delta-E= -0.000017384422 Rises=F Damp=F

DIIS: error= 5.26D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33288366411 IErMin=10 ErrMin= 5.26D-05

ErrMax= 5.26D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.24D-06 BMatP= 4.47D-06

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

Coeff-Com: -0.117D-03 0.214D-03 0.368D-02 0.135D-02-0.100D-01-0.770D-01

Coeff-Com: -0.201D+00-0.133D+00 0.568D+00 0.848D+00

Coeff: -0.117D-03 0.214D-03 0.368D-02 0.135D-02-0.100D-01-0.770D-01

Coeff: -0.201D+00-0.133D+00 0.568D+00 0.848D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=7.46D-06 MaxDP=5.82D-04 DE=-1.74D-05 OVMax= 8.00D-03

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.92D-06 CP: 9.96D-01 1.47D-01 1.01D+00 8.17D-01 1.26D+00

CP: 2.10D+00 3.00D+00 3.00D+00 2.22D+00 1.39D+00

E= -1914.33288914429 Delta-E= -0.000005480183 Rises=F Damp=F

DIIS: error= 3.39D-05 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33288914429 IErMin=11 ErrMin= 3.39D-05

ErrMax= 3.39D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 9.73D-07 BMatP= 2.24D-06

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

Coeff-Com: -0.335D-03 0.438D-05 0.447D-02 0.124D-01 0.372D-01 0.474D-01

Coeff-Com: -0.219D-01-0.351D+00-0.719D-01 0.564D+00 0.779D+00

Coeff: -0.335D-03 0.438D-05 0.447D-02 0.124D-01 0.372D-01 0.474D-01

Coeff: -0.219D-01-0.351D+00-0.719D-01 0.564D+00 0.779D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=4.57D-06 MaxDP=3.96D-04 DE=-5.48D-06 OVMax= 5.08D-03

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.09D-06 CP: 9.96D-01 1.48D-01 1.01D+00 8.27D-01 1.30D+00

CP: 2.21D+00 3.00D+00 3.00D+00 2.68D+00 2.07D+00

CP: 2.20D+00

E= -1914.33289109107 Delta-E= -0.000001946776 Rises=F Damp=F

DIIS: error= 1.55D-05 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.33289109107 IErMin=12 ErrMin= 1.55D-05

ErrMax= 1.55D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.30D-07 BMatP= 9.73D-07

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

Coeff-Com: -0.139D-03-0.512D-04 0.111D-02 0.560D-02 0.227D-01 0.451D-01

Coeff-Com: 0.519D-01-0.155D+00-0.188D+00-0.114D-01 0.412D+00 0.816D+00

Coeff: -0.139D-03-0.512D-04 0.111D-02 0.560D-02 0.227D-01 0.451D-01

Coeff: 0.519D-01-0.155D+00-0.188D+00-0.114D-01 0.412D+00 0.816D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=2.55D-06 MaxDP=2.21D-04 DE=-1.95D-06 OVMax= 2.76D-03

Cycle 13 Pass 1 IDiag 1:

RMSU= 4.34D-07 CP: 9.96D-01 1.48D-01 1.01D+00 8.31D-01 1.32D+00

CP: 2.27D+00 3.00D+00 3.00D+00 2.97D+00 2.42D+00

CP: 2.97D+00 1.32D+00

E= -1914.33289167325 Delta-E= -0.000000582180 Rises=F Damp=F

DIIS: error= 8.38D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.33289167325 IErMin=13 ErrMin= 8.38D-06

ErrMax= 8.38D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.41D-07 BMatP= 3.30D-07

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

Coeff-Com: 0.705D-04-0.409D-04-0.160D-02-0.245D-02-0.220D-02 0.762D-02

Coeff-Com: 0.529D-01 0.675D-01-0.816D-01-0.320D+00-0.105D+00 0.590D+00

Coeff-Com: 0.794D+00

Coeff: 0.705D-04-0.409D-04-0.160D-02-0.245D-02-0.220D-02 0.762D-02

Coeff: 0.529D-01 0.675D-01-0.816D-01-0.320D+00-0.105D+00 0.590D+00

Coeff: 0.794D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.51D-06 MaxDP=1.39D-04 DE=-5.82D-07 OVMax= 1.65D-03

Cycle 14 Pass 1 IDiag 1:

RMSU= 9.13D-07 CP: 9.96D-01 1.48D-01 1.01D+00 8.34D-01 1.33D+00

CP: 2.30D+00 3.00D+00 3.00D+00 3.00D+00 2.71D+00

CP: 3.00D+00 1.58D+00 1.01D+00

E= -1914.33289184640 Delta-E= -0.000000173150 Rises=F Damp=F

DIIS: error= 2.64D-06 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.33289184640 IErMin=14 ErrMin= 2.64D-06

ErrMax= 2.64D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.27D-08 BMatP= 1.41D-07

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

Coeff-Com: 0.404D-04-0.605D-05-0.712D-03-0.156D-02-0.350D-02-0.302D-02

Coeff-Com: 0.143D-01 0.403D-01-0.652D-02-0.122D+00-0.862D-01 0.115D+00

Coeff-Com: 0.299D+00 0.755D+00

Coeff: 0.404D-04-0.605D-05-0.712D-03-0.156D-02-0.350D-02-0.302D-02

Coeff: 0.143D-01 0.403D-01-0.652D-02-0.122D+00-0.862D-01 0.115D+00

Coeff: 0.299D+00 0.755D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=4.03D-07 MaxDP=3.62D-05 DE=-1.73D-07 OVMax= 4.33D-04

Cycle 15 Pass 1 IDiag 1:

RMSU= 9.50D-08 CP: 9.96D-01 1.48D-01 1.01D+00 8.35D-01 1.33D+00

CP: 2.31D+00 3.00D+00 3.00D+00 3.00D+00 2.76D+00

CP: 3.00D+00 1.64D+00 1.12D+00 1.28D+00

E= -1914.33289186146 Delta-E= -0.000000015062 Rises=F Damp=F

DIIS: error= 1.15D-06 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.33289186146 IErMin=15 ErrMin= 1.15D-06

ErrMax= 1.15D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.19D-09 BMatP= 1.27D-08

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

Coeff-Com: 0.404D-05 0.726D-05 0.380D-04-0.231D-03-0.143D-02-0.402D-02

Coeff-Com: -0.628D-02 0.301D-02 0.198D-01 0.189D-01-0.169D-01-0.102D+00

Coeff-Com: -0.500D-01 0.446D+00 0.693D+00

Coeff: 0.404D-05 0.726D-05 0.380D-04-0.231D-03-0.143D-02-0.402D-02

Coeff: -0.628D-02 0.301D-02 0.198D-01 0.189D-01-0.169D-01-0.102D+00

Coeff: -0.500D-01 0.446D+00 0.693D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.68D-07 MaxDP=1.56D-05 DE=-1.51D-08 OVMax= 1.80D-04

Cycle 16 Pass 1 IDiag 1:

RMSU= 4.87D-08 CP: 9.96D-01 1.48D-01 1.01D+00 8.35D-01 1.33D+00

CP: 2.31D+00 3.00D+00 3.00D+00 3.00D+00 2.78D+00

CP: 3.00D+00 1.67D+00 1.16D+00 1.38D+00 1.00D+00

E= -1914.33289186552 Delta-E= -0.000000004061 Rises=F Damp=F

DIIS: error= 5.95D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1914.33289186552 IErMin=16 ErrMin= 5.95D-07

ErrMax= 5.95D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 7.29D-10 BMatP= 5.19D-09

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

Coeff-Com: -0.666D-05 0.285D-05 0.162D-03 0.251D-03 0.310D-03-0.604D-03

Coeff-Com: -0.524D-02-0.796D-02 0.782D-02 0.318D-01 0.138D-01-0.606D-01

Coeff-Com: -0.766D-01-0.134D-01 0.228D+00 0.882D+00

Coeff: -0.666D-05 0.285D-05 0.162D-03 0.251D-03 0.310D-03-0.604D-03

Coeff: -0.524D-02-0.796D-02 0.782D-02 0.318D-01 0.138D-01-0.606D-01

Coeff: -0.766D-01-0.134D-01 0.228D+00 0.882D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=7.52D-08 MaxDP=6.59D-06 DE=-4.06D-09 OVMax= 7.65D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 2.35D-08 CP: 9.96D-01 1.48D-01 1.01D+00 8.35D-01 1.33D+00

CP: 2.32D+00 3.00D+00 3.00D+00 3.00D+00 2.79D+00

CP: 3.00D+00 1.68D+00 1.18D+00 1.43D+00 1.16D+00

CP: 1.34D+00

E= -1914.33289186639 Delta-E= -0.000000000863 Rises=F Damp=F

DIIS: error= 4.13D-07 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1914.33289186639 IErMin=17 ErrMin= 4.13D-07

ErrMax= 4.13D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.69D-10 BMatP= 7.29D-10

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

Coeff-Com: -0.538D-05-0.636D-06 0.827D-04 0.224D-03 0.671D-03 0.105D-02

Coeff-Com: -0.994D-03-0.554D-02-0.234D-02 0.118D-01 0.139D-01-0.312D-02

Coeff-Com: -0.275D-01-0.156D+00-0.901D-01 0.548D+00 0.709D+00

Coeff: -0.538D-05-0.636D-06 0.827D-04 0.224D-03 0.671D-03 0.105D-02

Coeff: -0.994D-03-0.554D-02-0.234D-02 0.118D-01 0.139D-01-0.312D-02

Coeff: -0.275D-01-0.156D+00-0.901D-01 0.548D+00 0.709D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=3.90D-08 MaxDP=3.35D-06 DE=-8.63D-10 OVMax= 3.83D-05

Cycle 18 Pass 1 IDiag 1:

RMSU= 1.11D-08 CP: 9.96D-01 1.48D-01 1.01D+00 8.36D-01 1.33D+00

CP: 2.32D+00 3.00D+00 3.00D+00 3.00D+00 2.80D+00

CP: 3.00D+00 1.69D+00 1.19D+00 1.45D+00 1.23D+00

CP: 1.62D+00 1.08D+00

E= -1914.33289186663 Delta-E= -0.000000000246 Rises=F Damp=F

DIIS: error= 1.29D-07 at cycle 18 NSaved= 18.

NSaved=18 IEnMin=18 EnMin= -1914.33289186663 IErMin=18 ErrMin= 1.29D-07

ErrMax= 1.29D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.55D-11 BMatP= 3.69D-10

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

Coeff-Com: 0.558D-07-0.597D-06-0.145D-04 0.208D-05 0.917D-04 0.400D-03

Coeff-Com: 0.813D-03 0.570D-03-0.212D-02-0.412D-02 0.431D-03 0.125D-01

Coeff-Com: 0.105D-01-0.352D-01-0.735D-01-0.600D-01 0.174D+00 0.975D+00

Coeff: 0.558D-07-0.597D-06-0.145D-04 0.208D-05 0.917D-04 0.400D-03

Coeff: 0.813D-03 0.570D-03-0.212D-02-0.412D-02 0.431D-03 0.125D-01

Coeff: 0.105D-01-0.352D-01-0.735D-01-0.600D-01 0.174D+00 0.975D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.06D-08 MaxDP=7.62D-07 DE=-2.46D-10 OVMax= 6.85D-06

Cycle 19 Pass 1 IDiag 1:

RMSU= 5.83D-09 CP: 9.96D-01 1.48D-01 1.01D+00 8.36D-01 1.33D+00

CP: 2.32D+00 3.00D+00 3.00D+00 3.00D+00 2.80D+00

CP: 3.00D+00 1.69D+00 1.19D+00 1.45D+00 1.25D+00

CP: 1.73D+00 1.30D+00 1.30D+00

E= -1914.33289186669 Delta-E= -0.000000000057 Rises=F Damp=F

DIIS: error= 6.36D-08 at cycle 19 NSaved= 19.

NSaved=19 IEnMin=19 EnMin= -1914.33289186669 IErMin=19 ErrMin= 6.36D-08

ErrMax= 6.36D-08 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.43D-11 BMatP= 3.55D-11

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

Coeff-Com: 0.966D-06-0.205D-06-0.223D-04-0.382D-04-0.738D-04 0.241D-04

Coeff-Com: 0.584D-03 0.134D-02-0.703D-03-0.427D-02-0.219D-02 0.703D-02

Coeff-Com: 0.102D-01 0.950D-02-0.220D-01-0.133D+00-0.312D-01 0.517D+00

Coeff-Com: 0.647D+00

Coeff: 0.966D-06-0.205D-06-0.223D-04-0.382D-04-0.738D-04 0.241D-04

Coeff: 0.584D-03 0.134D-02-0.703D-03-0.427D-02-0.219D-02 0.703D-02

Coeff: 0.102D-01 0.950D-02-0.220D-01-0.133D+00-0.312D-01 0.517D+00

Coeff: 0.647D+00

Gap= 0.050 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=4.25D-09 MaxDP=2.58D-07 DE=-5.73D-11 OVMax= 3.44D-06

Error on total polarization charges = 0.08290

SCF Done: E(UB3LYP) = -1914.33289187 A.U. after 19 cycles

NFock= 19 Conv=0.42D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0540 S= 1.0179

<L.S>= 0.000000000000E+00

KE= 1.906380759760D+03 PE=-1.516537650504D+04 EE= 5.986775520201D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.31

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0540, after 2.0016

Leave Link 502 at Mon Aug 26 18:24:17 2019, MaxMem= 4294967296 cpu: 8500.5

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

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

Range of M.O.s used for correlation: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.49706170D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64856977D-01

Leave Link 801 at Mon Aug 26 18:24:17 2019, MaxMem= 4294967296 cpu: 1.1

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

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

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

Leave Link 1101 at Mon Aug 26 18:24:24 2019, MaxMem= 4294967296 cpu: 110.5

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

Symmetrizing basis deriv contribution to polar:

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

Leave Link 1102 at Mon Aug 26 18:24:24 2019, MaxMem= 4294967296 cpu: 1.9

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

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 187

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 Mon Aug 26 18:43:57 2019, MaxMem= 4294967296 cpu: 18756.4

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

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 590000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 4.38D+03 3.11D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 3.41D+02 2.99D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 7.18D+00 3.48D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 9.16D-02 3.13D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 5.73D-04 1.84D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 3.43D-06 1.18D-04.

185 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 1.61D-08 8.65D-06.

78 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 7.11D-11 4.13D-07.

40 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 4.02D-13 2.76D-08.

2 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 6.84D-15 2.46D-09.

InvSVY: IOpt=1 It= 1 EMax= 5.68D-14

Solved reduced A of dimension 1712 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1120.91 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 Mon Aug 26 22:39:55 2019, MaxMem= 4294967296 cpu: 226477.3

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 187

Leave Link 701 at Mon Aug 26 22:41:25 2019, MaxMem= 4294967296 cpu: 1433.5

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

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

Leave Link 702 at Mon Aug 26 22:41:25 2019, MaxMem= 4294967296 cpu: 0.4

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

Leave Link 703 at Mon Aug 26 23:00:05 2019, MaxMem= 4294967296 cpu: 17911.3

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

Dipole =-1.11523882D-03-2.00485790D-03-5.65883439D-01

Polarizability= 1.36303651D+03 1.82795867D+02 1.54024645D+03

9.82153278D-02 3.49761600D-01 4.59443171D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000829827 -0.000476325 -0.000890438

2 6 -0.001343792 0.000726285 0.000372957

3 7 -0.000298801 -0.000161751 0.000825465

4 6 -0.000183153 0.000348191 -0.001572703

5 6 0.000210654 0.000216562 0.000644756

6 6 -0.000059619 -0.000168430 0.000811712

7 6 0.001144079 0.000220023 -0.000709603

8 7 -0.001493079 -0.000370001 -0.000097624

9 6 0.002911101 0.000199851 -0.000042469

10 6 -0.000109303 0.000016351 0.000227717

11 6 0.000228127 0.000019150 0.000158422

12 6 0.002699423 -0.000702640 -0.000966593

13 6 -0.002854977 0.000080946 0.000016970

14 6 0.000111612 0.000012841 -0.000214880

15 6 -0.000233890 0.000017733 -0.000146666

16 6 -0.001146278 0.000314971 0.000677465

17 7 0.001468547 -0.000366697 0.000077772

18 6 0.000040037 -0.000177228 -0.000793836

19 6 0.000223457 0.000184970 0.001563840

20 6 -0.000217984 0.000255637 -0.000630215

21 6 -0.000833054 -0.000405032 0.000895815

22 6 0.001380747 0.000571466 -0.000397283

23 7 0.000254217 0.000085451 -0.000798251

24 6 -0.002764512 -0.000696409 0.000991494

25 6 -0.000064533 -0.000166802 -0.000001689

26 6 -0.000000011 -0.000007181 0.000250055

27 6 0.000006660 0.000005055 -0.000136620

28 6 -0.000016418 0.000041857 0.000118262

29 6 -0.000085440 0.000100001 -0.000078049

30 6 -0.000085599 0.000050069 0.000085751

31 6 0.000055789 -0.000002366 -0.000085258

32 6 0.000213758 -0.000293773 0.000073601

33 6 -0.000031066 0.000415150 0.000224845

34 6 -0.000361504 -0.000066900 0.000017581

35 6 -0.000333333 0.000440447 -0.000068389

36 6 0.000003695 -0.000370341 -0.000119846

37 6 0.000368167 -0.000119914 -0.000011268

38 6 0.000334335 0.000430873 0.000077969

39 6 -0.000007356 -0.000375667 0.000116278

40 6 -0.000059615 -0.000001068 0.000094077

41 6 -0.000218065 -0.000308349 -0.000074721

42 6 0.000055271 0.000428860 -0.000241752

43 6 0.000048619 -0.000200306 -0.000003342

44 6 0.000065495 0.000027866 -0.000097478

45 6 0.000085685 0.000099025 0.000077181

46 6 0.000011417 0.000041076 -0.000119203

47 6 -0.000006241 0.000005299 0.000130968

48 6 0.000025675 0.000007153 -0.000229035

49 1 -0.000051551 -0.000044120 -0.000002411

50 1 -0.000069371 -0.000009791 -0.000080856

51 1 -0.000151683 -0.000038668 0.000031549

52 1 0.000085091 -0.000128670 0.000024425

53 1 0.000138073 -0.000023847 -0.000035828

54 1 -0.000083777 -0.000132891 -0.000021973

55 1 0.000070387 -0.000005729 0.000076742

56 1 0.000053139 -0.000035238 -0.000001738

57 1 0.000153096 0.000020200 -0.000072498

58 1 -0.000016658 -0.000003139 -0.000017813

59 1 -0.000025111 -0.000004758 0.000018631

60 1 -0.000000339 -0.000021615 0.000048615

61 1 0.000102036 0.000002317 -0.000137469

62 1 -0.000003938 -0.000014430 -0.000028792

63 1 -0.000023395 0.000002222 0.000040107

64 1 0.000164078 0.000152129 0.000041816

65 1 0.000104513 0.000028711 0.000092795

66 1 -0.000008374 -0.000000997 0.000019165

67 1 -0.000106725 0.000027098 -0.000097032

68 1 0.000010369 -0.000000828 -0.000020891

69 1 0.000004674 -0.000018083 0.000027554

70 1 0.000024035 0.000000774 -0.000039293

71 1 -0.000177893 0.000154030 -0.000045684

72 1 -0.000098179 0.000000809 0.000136056

73 1 0.000001091 -0.000022075 -0.000047507

74 1 0.000026436 -0.000006911 -0.000018309

75 1 0.000016482 -0.000004925 0.000018196

76 1 -0.000154444 0.000020106 0.000074061

77 1 -0.000703908 0.000034257 -0.000073411

78 1 0.000753074 0.000148085 0.000088056

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

Cartesian Forces: Max 0.002911101 RMS 0.000524111

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

Leave Link 716 at Mon Aug 26 23:00:05 2019, MaxMem= 4294967296 cpu: 2.1

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.001790521 RMS 0.000308272

Search for a local minimum.

Step number 7 out of a maximum of 452

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

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= 3.13D-05 DEPred=-5.04D-04 R=-6.20D-02

Trust test=-6.20D-02 RLast= 5.04D-01 DXMaxT set to 1.06D-01

ITU= -1 -1 1 1 -1 1 0

Eigenvalues --- 0.00312 0.00470 0.00515 0.00604 0.00738

Eigenvalues --- 0.00745 0.00881 0.01065 0.01069 0.01142

Eigenvalues --- 0.01145 0.01167 0.01265 0.01281 0.01291

Eigenvalues --- 0.01310 0.01313 0.01423 0.01433 0.01553

Eigenvalues --- 0.01568 0.01606 0.01619 0.01660 0.01711

Eigenvalues --- 0.01721 0.01729 0.01739 0.01763 0.01774

Eigenvalues --- 0.01785 0.01786 0.01793 0.01795 0.01883

Eigenvalues --- 0.01943 0.01982 0.02072 0.02082 0.02219

Eigenvalues --- 0.02228 0.02238 0.02280 0.02310 0.02322

Eigenvalues --- 0.02332 0.02397 0.02503 0.02512 0.02546

Eigenvalues --- 0.02555 0.02566 0.02615 0.02631 0.02631

Eigenvalues --- 0.02633 0.02649 0.02724 0.02731 0.02776

Eigenvalues --- 0.02779 0.02808 0.02812 0.02862 0.02863

Eigenvalues --- 0.02864 0.02868 0.04074 0.04128 0.04188

Eigenvalues --- 0.04333 0.04438 0.04450 0.04538 0.04563

Eigenvalues --- 0.09263 0.09672 0.09676 0.09844 0.09863

Eigenvalues --- 0.09889 0.10398 0.10451 0.10612 0.10703

Eigenvalues --- 0.10705 0.10715 0.10724 0.10725 0.11378

Eigenvalues --- 0.11386 0.11393 0.11394 0.11546 0.11967

Eigenvalues --- 0.11981 0.11998 0.12006 0.12289 0.12290

Eigenvalues --- 0.12309 0.12310 0.12758 0.12760 0.12781

Eigenvalues --- 0.12785 0.15784 0.15926 0.16312 0.17160

Eigenvalues --- 0.17376 0.17524 0.17591 0.18088 0.18095

Eigenvalues --- 0.18103 0.18133 0.18572 0.19265 0.19293

Eigenvalues --- 0.19333 0.19362 0.19389 0.19391 0.19436

Eigenvalues --- 0.19509 0.19542 0.19544 0.19546 0.19548

Eigenvalues --- 0.20288 0.21496 0.22039 0.22855 0.22939

Eigenvalues --- 0.23464 0.23706 0.24315 0.24742 0.25791

Eigenvalues --- 0.26156 0.26226 0.26496 0.27099 0.28513

Eigenvalues --- 0.28530 0.28641 0.28841 0.29715 0.30986

Eigenvalues --- 0.31714 0.32077 0.32847 0.33074 0.33081

Eigenvalues --- 0.34074 0.34212 0.35117 0.35561 0.35606

Eigenvalues --- 0.35613 0.35630 0.35633 0.35693 0.35744

Eigenvalues --- 0.35764 0.35806 0.35816 0.35912 0.35915

Eigenvalues --- 0.35930 0.35932 0.35976 0.35985 0.35993

Eigenvalues --- 0.35994 0.36180 0.36228 0.36240 0.36275

Eigenvalues --- 0.37066 0.37068 0.37211 0.37403 0.37404

Eigenvalues --- 0.37567 0.38119 0.38513 0.38586 0.38776

Eigenvalues --- 0.39493 0.40328 0.41034 0.41058 0.41132

Eigenvalues --- 0.41137 0.41140 0.41156 0.41195 0.41452

Eigenvalues --- 0.41603 0.41862 0.42029 0.42569 0.44749

Eigenvalues --- 0.45050 0.45887 0.45896 0.45981 0.45983

Eigenvalues --- 0.46081 0.46259 0.46264 0.46309 0.46320

Eigenvalues --- 0.48012 0.48439 0.49041 0.50368 0.50729

Eigenvalues --- 0.50737 0.50769 0.50795 0.51237 0.51861

Eigenvalues --- 0.52590 0.57109 0.58923

Cosine: 0.963 < 0.970

Cut down GDIIS temporarily because of the cosine check. E 6

Eigenvalues --- 0.00312 0.00470 0.00515 0.00604 0.00738

Eigenvalues --- 0.00745 0.00881 0.01065 0.01069 0.01142

Eigenvalues --- 0.01145 0.01167 0.01265 0.01281 0.01291

Eigenvalues --- 0.01310 0.01313 0.01423 0.01433 0.01553

Eigenvalues --- 0.01568 0.01606 0.01619 0.01660 0.01711

Eigenvalues --- 0.01721 0.01729 0.01739 0.01763 0.01774

Eigenvalues --- 0.01785 0.01786 0.01793 0.01795 0.01883

Eigenvalues --- 0.01943 0.01982 0.02072 0.02082 0.02219

Eigenvalues --- 0.02228 0.02238 0.02280 0.02310 0.02322

Eigenvalues --- 0.02332 0.02397 0.02503 0.02512 0.02546

Eigenvalues --- 0.02555 0.02566 0.02615 0.02631 0.02631

Eigenvalues --- 0.02633 0.02649 0.02724 0.02731 0.02776

Eigenvalues --- 0.02779 0.02808 0.02812 0.02862 0.02863

Eigenvalues --- 0.02864 0.02868 0.04074 0.04128 0.04188

Eigenvalues --- 0.04333 0.04438 0.04450 0.04538 0.04563

Eigenvalues --- 0.09263 0.09672 0.09676 0.09844 0.09863

Eigenvalues --- 0.09889 0.10398 0.10451 0.10612 0.10703

Eigenvalues --- 0.10705 0.10715 0.10724 0.10725 0.11378

Eigenvalues --- 0.11386 0.11393 0.11394 0.11546 0.11967

Eigenvalues --- 0.11981 0.11998 0.12006 0.12289 0.12290

Eigenvalues --- 0.12309 0.12310 0.12758 0.12760 0.12781

Eigenvalues --- 0.12785 0.15784 0.15926 0.16312 0.17160

Eigenvalues --- 0.17376 0.17524 0.17591 0.18088 0.18095

Eigenvalues --- 0.18103 0.18133 0.18572 0.19265 0.19293

Eigenvalues --- 0.19333 0.19362 0.19389 0.19391 0.19436

Eigenvalues --- 0.19509 0.19542 0.19544 0.19546 0.19548

Eigenvalues --- 0.20288 0.21496 0.22039 0.22855 0.22939

Eigenvalues --- 0.23464 0.23706 0.24315 0.24742 0.25791

Eigenvalues --- 0.26156 0.26226 0.26496 0.27099 0.28513

Eigenvalues --- 0.28530 0.28641 0.28841 0.29715 0.30986

Eigenvalues --- 0.31714 0.32077 0.32847 0.33074 0.33081

Eigenvalues --- 0.34074 0.34212 0.35117 0.35561 0.35606

Eigenvalues --- 0.35613 0.35630 0.35633 0.35693 0.35744

Eigenvalues --- 0.35764 0.35806 0.35816 0.35912 0.35915

Eigenvalues --- 0.35930 0.35932 0.35976 0.35985 0.35993

Eigenvalues --- 0.35994 0.36180 0.36228 0.36240 0.36275

Eigenvalues --- 0.37066 0.37068 0.37211 0.37403 0.37404

Eigenvalues --- 0.37567 0.38119 0.38513 0.38586 0.38776

Eigenvalues --- 0.39493 0.40328 0.41034 0.41058 0.41132

Eigenvalues --- 0.41137 0.41140 0.41156 0.41195 0.41452

Eigenvalues --- 0.41603 0.41862 0.42029 0.42569 0.44749

Eigenvalues --- 0.45050 0.45887 0.45896 0.45981 0.45983

Eigenvalues --- 0.46081 0.46259 0.46264 0.46309 0.46320

Eigenvalues --- 0.48012 0.48439 0.49041 0.50368 0.50729

Eigenvalues --- 0.50737 0.50769 0.50795 0.51237 0.51861

Eigenvalues --- 0.52590 0.57109 0.58923

Quadratic step=4.028D-01 exceeds max=1.061D-01 adjusted using Lamda=-1.525D-02.

Angle between NR and scaled steps= 22.87 degrees.

Angle between quadratic step and forces= 54.70 degrees.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.07513176 RMS(Int)= 0.00044605

Iteration 2 RMS(Cart)= 0.00146586 RMS(Int)= 0.00001372

Iteration 3 RMS(Cart)= 0.00000042 RMS(Int)= 0.00001372

ITry= 1 IFail=0 DXMaxC= 4.28D-01 DCOld= 1.00D+10 DXMaxT= 1.06D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.65231 0.00089 0.00000 0.00298 0.00299 2.65529

R2 2.64320 -0.00074 0.00000 -0.00206 -0.00204 2.64116

R3 2.03752 -0.00003 0.00000 -0.00022 -0.00022 2.03730

R4 2.59748 0.00011 0.00000 0.00038 0.00036 2.59784

R5 2.72511 -0.00052 0.00000 -0.00383 -0.00383 2.72128

R6 2.59888 0.00099 0.00000 0.00195 0.00194 2.60082

R7 1.90932 0.00070 0.00000 0.00123 0.00123 1.91055

R8 2.65841 0.00003 0.00000 -0.00083 -0.00082 2.65759

R9 2.71319 -0.00125 0.00000 -0.00071 -0.00071 2.71248

R10 2.03694 -0.00000 0.00000 -0.00003 -0.00003 2.03691

R11 2.65503 -0.00093 0.00000 -0.00644 -0.00644 2.64858

R12 2.80202 -0.00008 0.00000 0.00045 0.00045 2.80248

R13 2.57898 0.00062 0.00000 0.00786 0.00784 2.58682

R14 2.76477 -0.00040 0.00000 -0.00194 -0.00193 2.76283

R15 2.61141 -0.00122 0.00000 -0.00882 -0.00883 2.60258

R16 2.76175 -0.00011 0.00000 -0.00014 -0.00013 2.76162

R17 2.62537 0.00179 0.00000 0.00898 0.00898 2.63436

R18 2.55418 0.00017 0.00000 0.00051 0.00053 2.55471

R19 2.03868 0.00006 0.00000 0.00021 0.00021 2.03889

R20 2.03938 0.00001 0.00000 -0.00009 -0.00009 2.03930

R21 2.62551 0.00177 0.00000 0.00892 0.00892 2.63442

R22 2.80607 0.00002 0.00000 -0.00091 -0.00091 2.80516

R23 2.76162 -0.00008 0.00000 -0.00001 -0.00000 2.76161

R24 2.61133 -0.00120 0.00000 -0.00879 -0.00880 2.60253

R25 2.55418 0.00016 0.00000 0.00051 0.00053 2.55471

R26 2.03872 0.00005 0.00000 0.00018 0.00018 2.03890

R27 2.76486 -0.00040 0.00000 -0.00203 -0.00203 2.76284

R28 2.03936 0.00001 0.00000 -0.00007 -0.00007 2.03929

R29 2.57901 0.00063 0.00000 0.00787 0.00785 2.58686

R30 2.65504 -0.00094 0.00000 -0.00650 -0.00650 2.64855

R31 2.71327 -0.00128 0.00000 -0.00081 -0.00080 2.71246

R32 2.80214 -0.00007 0.00000 0.00041 0.00041 2.80255

R33 2.65856 0.00002 0.00000 -0.00093 -0.00093 2.65763

R34 2.59884 0.00103 0.00000 0.00202 0.00201 2.60086

R35 2.64318 -0.00077 0.00000 -0.00207 -0.00206 2.64112

R36 2.03693 -0.00001 0.00000 -0.00003 -0.00003 2.03690

R37 2.65237 0.00087 0.00000 0.00293 0.00293 2.65531

R38 2.03752 -0.00003 0.00000 -0.00022 -0.00022 2.03729

R39 2.59741 0.00017 0.00000 0.00046 0.00045 2.59786

R40 2.72517 -0.00055 0.00000 -0.00391 -0.00391 2.72126

R41 1.90931 0.00077 0.00000 0.00132 0.00132 1.91063

R42 2.80623 0.00001 0.00000 -0.00099 -0.00099 2.80524

R43 2.65146 0.00017 0.00000 0.00033 0.00033 2.65179

R44 2.65085 -0.00002 0.00000 -0.00036 -0.00036 2.65049

R45 2.62881 0.00002 0.00000 0.00003 0.00003 2.62884

R46 2.04844 -0.00003 0.00000 -0.00008 -0.00008 2.04836

R47 2.63641 -0.00013 0.00000 -0.00024 -0.00024 2.63617

R48 2.05023 -0.00002 0.00000 -0.00005 -0.00005 2.05018

R49 2.63466 -0.00006 0.00000 -0.00026 -0.00026 2.63440

R50 2.05007 -0.00003 0.00000 -0.00009 -0.00009 2.04999

R51 2.63046 -0.00009 0.00000 -0.00003 -0.00003 2.63043

R52 2.05020 -0.00002 0.00000 -0.00007 -0.00007 2.05013

R53 2.04883 -0.00008 0.00000 -0.00029 -0.00029 2.04854

R54 2.63679 -0.00007 0.00000 -0.00026 -0.00026 2.63652

R55 2.63392 -0.00007 0.00000 0.00004 0.00004 2.63396

R56 2.05008 -0.00002 0.00000 -0.00005 -0.00005 2.05004

R57 2.62791 0.00020 0.00000 0.00068 0.00068 2.62859

R58 2.05011 -0.00002 0.00000 -0.00002 -0.00002 2.05009

R59 2.65102 0.00048 0.00000 0.00049 0.00049 2.65151

R60 2.04836 0.00005 0.00000 0.00009 0.00009 2.04844

R61 2.64899 -0.00014 0.00000 0.00046 0.00046 2.64945

R62 2.63181 -0.00020 0.00000 -0.00071 -0.00071 2.63110

R63 2.04851 -0.00008 0.00000 -0.00018 -0.00018 2.04833

R64 2.05007 0.00002 0.00000 0.00002 0.00002 2.05009

R65 2.64891 -0.00013 0.00000 0.00050 0.00050 2.64940

R66 2.65105 0.00048 0.00000 0.00045 0.00045 2.65150

R67 2.63184 -0.00020 0.00000 -0.00072 -0.00072 2.63112

R68 2.04851 -0.00008 0.00000 -0.00018 -0.00018 2.04834

R69 2.63392 -0.00008 0.00000 0.00004 0.00004 2.63396

R70 2.05007 0.00002 0.00000 0.00002 0.00002 2.05009

R71 2.63679 -0.00008 0.00000 -0.00027 -0.00027 2.63652

R72 2.05008 -0.00002 0.00000 -0.00004 -0.00004 2.05004

R73 2.62790 0.00021 0.00000 0.00070 0.00070 2.62860

R74 2.05011 -0.00002 0.00000 -0.00002 -0.00002 2.05009

R75 2.04836 0.00005 0.00000 0.00009 0.00009 2.04845

R76 2.65083 -0.00001 0.00000 -0.00036 -0.00036 2.65047

R77 2.65150 0.00016 0.00000 0.00028 0.00028 2.65177

R78 2.63047 -0.00010 0.00000 -0.00003 -0.00003 2.63044

R79 2.04881 -0.00007 0.00000 -0.00027 -0.00027 2.04854

R80 2.63465 -0.00006 0.00000 -0.00026 -0.00026 2.63439

R81 2.05019 -0.00002 0.00000 -0.00007 -0.00007 2.05013

R82 2.63639 -0.00013 0.00000 -0.00023 -0.00023 2.63616

R83 2.05007 -0.00003 0.00000 -0.00009 -0.00009 2.04998

R84 2.62882 0.00002 0.00000 0.00003 0.00003 2.62885

R85 2.05023 -0.00002 0.00000 -0.00005 -0.00005 2.05018

R86 2.04842 -0.00003 0.00000 -0.00007 -0.00007 2.04835

A1 1.88224 0.00011 0.00000 -0.00012 -0.00013 1.88211

A2 2.18659 -0.00007 0.00000 -0.00047 -0.00047 2.18612

A3 2.21431 -0.00003 0.00000 0.00061 0.00061 2.21492

A4 1.86901 0.00005 0.00000 -0.00016 -0.00016 1.86886

A5 2.21628 -0.00038 0.00000 -0.00161 -0.00156 2.21472

A6 2.19766 0.00034 0.00000 0.00180 0.00175 2.19941

A7 1.92582 -0.00048 0.00000 -0.00107 -0.00106 1.92476

A8 2.18476 0.00029 0.00000 0.00044 0.00043 2.18519

A9 2.17193 0.00018 0.00000 0.00049 0.00048 2.17241

A10 1.86710 0.00017 0.00000 0.00057 0.00057 1.86767

A11 2.18510 0.00045 0.00000 0.00357 0.00351 2.18861

A12 2.22973 -0.00061 0.00000 -0.00379 -0.00375 2.22598

A13 1.88020 0.00015 0.00000 0.00083 0.00082 1.88101

A14 2.21319 0.00003 0.00000 0.00066 0.00065 2.21384

A15 2.18980 -0.00018 0.00000 -0.00148 -0.00148 2.18832

A16 2.18008 -0.00021 0.00000 0.00122 0.00114 2.18122

A17 2.03326 0.00025 0.00000 -0.00161 -0.00158 2.03169

A18 2.06983 -0.00004 0.00000 0.00041 0.00045 2.07028

A19 2.19361 -0.00038 0.00000 -0.00182 -0.00188 2.19172

A20 2.15957 0.00030 0.00000 0.00328 0.00333 2.16290

A21 1.92990 0.00008 0.00000 -0.00137 -0.00138 1.92852

A22 1.84802 -0.00011 0.00000 -0.00060 -0.00059 1.84743

A23 1.92134 0.00029 0.00000 0.00268 0.00267 1.92402

A24 2.18804 -0.00027 0.00000 0.00097 0.00093 2.18896

A25 2.17363 -0.00002 0.00000 -0.00362 -0.00357 2.17006

A26 1.86244 0.00003 0.00000 -0.00027 -0.00028 1.86217

A27 2.19899 -0.00016 0.00000 -0.00125 -0.00125 2.19774

A28 2.22152 0.00013 0.00000 0.00148 0.00148 2.22299

A29 1.86196 -0.00029 0.00000 -0.00032 -0.00032 1.86163

A30 2.19653 0.00004 0.00000 -0.00041 -0.00041 2.19611

A31 2.22401 0.00026 0.00000 0.00089 0.00089 2.22490

A32 2.18980 -0.00042 0.00000 -0.00170 -0.00177 2.18803

A33 2.01280 0.00074 0.00000 0.00465 0.00468 2.01748

A34 2.08052 -0.00033 0.00000 -0.00299 -0.00296 2.07756

A35 2.17351 -0.00006 0.00000 -0.00360 -0.00356 2.16995

A36 2.18806 -0.00021 0.00000 0.00104 0.00100 2.18905

A37 1.92142 0.00027 0.00000 0.00261 0.00261 1.92402

A38 1.86242 0.00004 0.00000 -0.00025 -0.00025 1.86217

A39 2.19883 -0.00016 0.00000 -0.00114 -0.00114 2.19768

A40 2.22170 0.00011 0.00000 0.00134 0.00134 2.22304

A41 1.86198 -0.00030 0.00000 -0.00035 -0.00036 1.86162

A42 2.22390 0.00026 0.00000 0.00097 0.00097 2.22487

A43 2.19663 0.00004 0.00000 -0.00047 -0.00047 2.19615

A44 1.92979 0.00010 0.00000 -0.00128 -0.00129 1.92851

A45 2.15971 0.00031 0.00000 0.00323 0.00327 2.16297

A46 2.19356 -0.00041 0.00000 -0.00185 -0.00190 2.19166

A47 1.84804 -0.00012 0.00000 -0.00062 -0.00061 1.84744

A48 2.18040 -0.00027 0.00000 0.00096 0.00089 2.18129

A49 2.06955 0.00002 0.00000 0.00059 0.00062 2.07017

A50 2.03322 0.00025 0.00000 -0.00151 -0.00149 2.03173

A51 2.22979 -0.00065 0.00000 -0.00389 -0.00386 2.22594

A52 2.18511 0.00047 0.00000 0.00357 0.00352 2.18862

A53 1.86697 0.00019 0.00000 0.00069 0.00069 1.86766

A54 1.88023 0.00016 0.00000 0.00080 0.00080 1.88102

A55 2.18989 -0.00018 0.00000 -0.00151 -0.00152 2.18837

A56 2.21307 0.00003 0.00000 0.00072 0.00071 2.21378

A57 1.88220 0.00012 0.00000 -0.00009 -0.00010 1.88211

A58 2.21423 -0.00004 0.00000 0.00066 0.00066 2.21490

A59 2.18672 -0.00009 0.00000 -0.00056 -0.00056 2.18615

A60 1.86898 0.00006 0.00000 -0.00010 -0.00011 1.86887

A61 2.21648 -0.00045 0.00000 -0.00185 -0.00180 2.21468

A62 2.19747 0.00039 0.00000 0.00199 0.00195 2.19941

A63 1.92590 -0.00053 0.00000 -0.00118 -0.00117 1.92473

A64 2.17207 0.00020 0.00000 0.00042 0.00040 2.17247

A65 2.18454 0.00032 0.00000 0.00058 0.00057 2.18512

A66 2.18998 -0.00045 0.00000 -0.00181 -0.00188 2.18810

A67 2.08046 -0.00031 0.00000 -0.00298 -0.00295 2.07751

A68 2.01272 0.00076 0.00000 0.00474 0.00477 2.01748

A69 2.11088 -0.00001 0.00000 -0.00091 -0.00091 2.10997

A70 2.10141 0.00003 0.00000 0.00087 0.00087 2.10228

A71 2.07089 -0.00002 0.00000 0.00005 0.00005 2.07094

A72 2.10533 -0.00006 0.00000 -0.00020 -0.00020 2.10513

A73 2.08413 0.00020 0.00000 0.00135 0.00135 2.08548

A74 2.09355 -0.00014 0.00000 -0.00116 -0.00116 2.09238

A75 2.09805 0.00001 0.00000 0.00007 0.00007 2.09813

A76 2.08876 0.00001 0.00000 -0.00003 -0.00003 2.08873

A77 2.09638 -0.00001 0.00000 -0.00005 -0.00005 2.09633

A78 2.08880 0.00005 0.00000 0.00001 0.00001 2.08881

A79 2.09708 -0.00002 0.00000 0.00003 0.00003 2.09711

A80 2.09731 -0.00003 0.00000 -0.00004 -0.00004 2.09727

A81 2.09743 0.00003 0.00000 0.00009 0.00009 2.09752

A82 2.09679 0.00001 0.00000 0.00025 0.00025 2.09705

A83 2.08897 -0.00004 0.00000 -0.00035 -0.00035 2.08862

A84 2.10577 -0.00000 0.00000 -0.00003 -0.00003 2.10575

A85 2.08224 0.00016 0.00000 0.00114 0.00114 2.08338

A86 2.09502 -0.00015 0.00000 -0.00110 -0.00110 2.09392

A87 2.08937 0.00001 0.00000 -0.00008 -0.00008 2.08930

A88 2.09697 -0.00001 0.00000 -0.00028 -0.00028 2.09668

A89 2.09684 -0.00000 0.00000 0.00036 0.00036 2.09720

A90 2.09670 0.00013 0.00000 0.00103 0.00103 2.09773

A91 2.09715 -0.00009 0.00000 -0.00062 -0.00062 2.09653

A92 2.08934 -0.00004 0.00000 -0.00041 -0.00041 2.08892

A93 2.10541 -0.00021 0.00000 -0.00085 -0.00086 2.10455

A94 2.09407 -0.00012 0.00000 -0.00081 -0.00081 2.09326

A95 2.08342 0.00033 0.00000 0.00176 0.00175 2.08518

A96 2.09296 0.00134 0.00000 0.00830 0.00830 2.10126

A97 2.11720 -0.00117 0.00000 -0.00759 -0.00759 2.10961

A98 2.07302 -0.00017 0.00000 -0.00071 -0.00071 2.07231

A99 2.10322 0.00031 0.00000 0.00160 0.00160 2.10481

A100 2.08430 -0.00004 0.00000 -0.00010 -0.00010 2.08420

A101 2.09560 -0.00028 0.00000 -0.00155 -0.00156 2.09405

A102 2.09836 -0.00007 0.00000 -0.00090 -0.00090 2.09746

A103 2.09666 0.00004 0.00000 0.00042 0.00042 2.09708

A104 2.08816 0.00004 0.00000 0.00048 0.00048 2.08864

A105 2.11768 -0.00122 0.00000 -0.00799 -0.00800 2.10968

A106 2.09248 0.00140 0.00000 0.00868 0.00867 2.10115

A107 2.07303 -0.00018 0.00000 -0.00067 -0.00068 2.07235

A108 2.10319 0.00032 0.00000 0.00162 0.00162 2.10480

A109 2.08429 -0.00004 0.00000 -0.00013 -0.00014 2.08415

A110 2.09564 -0.00029 0.00000 -0.00154 -0.00154 2.09410

A111 2.09840 -0.00008 0.00000 -0.00095 -0.00096 2.09744

A112 2.08814 0.00004 0.00000 0.00053 0.00053 2.08867

A113 2.09664 0.00004 0.00000 0.00043 0.00043 2.09707

A114 2.08935 0.00001 0.00000 -0.00004 -0.00004 2.08931

A115 2.09686 -0.00000 0.00000 0.00033 0.00033 2.09719

A116 2.09697 -0.00000 0.00000 -0.00029 -0.00028 2.09668

A117 2.09667 0.00014 0.00000 0.00106 0.00106 2.09773

A118 2.09717 -0.00010 0.00000 -0.00065 -0.00065 2.09652

A119 2.08934 -0.00005 0.00000 -0.00040 -0.00040 2.08894

A120 2.10543 -0.00021 0.00000 -0.00091 -0.00091 2.10452

A121 2.08334 0.00035 0.00000 0.00182 0.00181 2.08516

A122 2.09412 -0.00013 0.00000 -0.00080 -0.00081 2.09331

A123 2.10151 0.00001 0.00000 0.00075 0.00075 2.10226

A124 2.11083 0.00000 0.00000 -0.00085 -0.00085 2.10998

A125 2.07084 -0.00002 0.00000 0.00010 0.00010 2.07094

A126 2.10581 -0.00000 0.00000 -0.00006 -0.00006 2.10576

A127 2.08225 0.00015 0.00000 0.00113 0.00113 2.08338

A128 2.09498 -0.00015 0.00000 -0.00106 -0.00106 2.09391

A129 2.09743 0.00002 0.00000 0.00008 0.00008 2.09751

A130 2.08895 -0.00004 0.00000 -0.00033 -0.00033 2.08862

A131 2.09680 0.00002 0.00000 0.00026 0.00026 2.09705

A132 2.08877 0.00004 0.00000 0.00003 0.00003 2.08880

A133 2.09735 -0.00003 0.00000 -0.00006 -0.00006 2.09728

A134 2.09707 -0.00001 0.00000 0.00004 0.00004 2.09710

A135 2.09807 0.00001 0.00000 0.00007 0.00007 2.09814

A136 2.09639 -0.00002 0.00000 -0.00006 -0.00006 2.09633

A137 2.08873 0.00001 0.00000 -0.00001 -0.00001 2.08872

A138 2.10535 -0.00006 0.00000 -0.00023 -0.00023 2.10512

A139 2.08415 0.00020 0.00000 0.00135 0.00135 2.08550

A140 2.09351 -0.00014 0.00000 -0.00114 -0.00114 2.09237

D1 0.00789 0.00015 0.00000 0.00319 0.00319 0.01108

D2 -3.11201 0.00003 0.00000 0.00179 0.00179 -3.11021

D3 -3.12428 0.00009 0.00000 0.00187 0.00187 -3.12241

D4 0.03901 -0.00003 0.00000 0.00047 0.00047 0.03948

D5 0.00888 -0.00017 0.00000 -0.00417 -0.00417 0.00470

D6 -3.13375 0.00002 0.00000 0.00108 0.00108 -3.13267

D7 3.14086 -0.00011 0.00000 -0.00283 -0.00283 3.13802

D8 -0.00177 0.00008 0.00000 0.00242 0.00242 0.00065

D9 -0.02238 -0.00005 0.00000 -0.00094 -0.00094 -0.02333

D10 3.08100 -0.00016 0.00000 -0.00482 -0.00483 3.07617

D11 3.09781 0.00005 0.00000 0.00037 0.00038 3.09819

D12 -0.08199 -0.00005 0.00000 -0.00350 -0.00350 -0.08549

D13 -2.87103 -0.00017 0.00000 -0.01663 -0.01663 -2.88766

D14 0.25820 -0.00037 0.00000 -0.02082 -0.02082 0.23738

D15 0.29617 -0.00030 0.00000 -0.01824 -0.01825 0.27792

D16 -2.85778 -0.00051 0.00000 -0.02242 -0.02244 -2.88022

D17 0.02783 -0.00005 0.00000 -0.00162 -0.00162 0.02621

D18 -3.06338 -0.00019 0.00000 -0.00868 -0.00871 -3.07209

D19 -3.07589 0.00005 0.00000 0.00222 0.00223 -3.07366

D20 0.11608 -0.00009 0.00000 -0.00484 -0.00486 0.11122

D21 -0.02221 0.00014 0.00000 0.00355 0.00356 -0.01866

D22 3.12039 -0.00006 0.00000 -0.00161 -0.00160 3.11880

D23 3.06731 0.00032 0.00000 0.01113 0.01112 3.07844

D24 -0.07327 0.00013 0.00000 0.00598 0.00597 -0.06730

D25 -0.19466 -0.00004 0.00000 -0.00647 -0.00647 -0.20112

D26 2.94205 0.00009 0.00000 -0.00130 -0.00130 2.94075

D27 3.00789 -0.00024 0.00000 -0.01520 -0.01520 2.99268

D28 -0.13859 -0.00011 0.00000 -0.01004 -0.01004 -0.14863

D29 -0.17423 0.00023 0.00000 0.01198 0.01199 -0.16225

D30 2.94964 0.00042 0.00000 0.01862 0.01862 2.96826

D31 2.97234 0.00010 0.00000 0.00672 0.00672 2.97906

D32 -0.18697 0.00029 0.00000 0.01336 0.01336 -0.17362

D33 -0.98175 0.00004 0.00000 -0.00149 -0.00148 -0.98324

D34 2.15948 0.00011 0.00000 -0.00048 -0.00047 2.15901

D35 2.15528 0.00016 0.00000 0.00334 0.00334 2.15862

D36 -0.98667 0.00023 0.00000 0.00435 0.00435 -0.98232

D37 -3.12064 0.00013 0.00000 0.00618 0.00617 -3.11447

D38 0.03669 -0.00004 0.00000 0.00024 0.00024 0.03694

D39 -3.13983 -0.00020 0.00000 -0.00863 -0.00863 3.13473

D40 -0.03573 -0.00005 0.00000 -0.00428 -0.00429 -0.04002

D41 -0.01361 -0.00004 0.00000 -0.00288 -0.00288 -0.01649

D42 3.09049 0.00011 0.00000 0.00146 0.00146 3.09195

D43 -0.04566 0.00010 0.00000 0.00234 0.00234 -0.04333

D44 3.07641 0.00004 0.00000 0.00391 0.00391 3.08032

D45 0.03817 -0.00012 0.00000 -0.00416 -0.00416 0.03401

D46 -3.08133 -0.00008 0.00000 -0.00189 -0.00189 -3.08322

D47 -3.08410 -0.00005 0.00000 -0.00577 -0.00577 -3.08987

D48 0.07959 -0.00001 0.00000 -0.00350 -0.00351 0.07608

D49 0.07656 0.00033 0.00000 0.01368 0.01369 0.09025

D50 -3.05571 0.00060 0.00000 0.01986 0.01984 -3.03587

D51 -3.08729 0.00025 0.00000 0.01555 0.01555 -3.07174

D52 0.06362 0.00053 0.00000 0.02172 0.02171 0.08533

D53 -0.01443 0.00011 0.00000 0.00420 0.00419 -0.01024

D54 -3.11775 -0.00004 0.00000 -0.00020 -0.00020 -3.11796

D55 3.10470 0.00006 0.00000 0.00184 0.00183 3.10653

D56 0.00137 -0.00009 0.00000 -0.00255 -0.00256 -0.00119

D57 -3.08645 0.00023 0.00000 0.01513 0.01512 -3.07132

D58 0.07903 0.00026 0.00000 0.01218 0.01217 0.09121

D59 0.06794 0.00044 0.00000 0.01941 0.01940 0.08734

D60 -3.04976 0.00046 0.00000 0.01646 0.01645 -3.03331

D61 1.00482 0.00005 0.00000 -0.00003 -0.00003 1.00479

D62 -2.13859 0.00021 0.00000 0.00612 0.00612 -2.13247

D63 -2.14830 -0.00015 0.00000 -0.00393 -0.00394 -2.15224

D64 0.99147 0.00001 0.00000 0.00222 0.00222 0.99369

D65 -3.08315 -0.00007 0.00000 -0.00632 -0.00632 -3.08947

D66 0.08061 -0.00004 0.00000 -0.00410 -0.00410 0.07651

D67 0.03770 -0.00009 0.00000 -0.00376 -0.00376 0.03394

D68 -3.08173 -0.00006 0.00000 -0.00154 -0.00154 -3.08327

D69 3.07499 0.00007 0.00000 0.00481 0.00482 3.07981

D70 -0.04565 0.00009 0.00000 0.00230 0.00230 -0.04335

D71 -0.01374 0.00007 0.00000 0.00364 0.00363 -0.01011

D72 -3.11738 -0.00005 0.00000 -0.00044 -0.00045 -3.11783

D73 3.10531 0.00003 0.00000 0.00134 0.00133 3.10664

D74 0.00167 -0.00009 0.00000 -0.00274 -0.00275 -0.00108

D75 -0.01433 -0.00001 0.00000 -0.00231 -0.00231 -0.01664

D76 -3.13977 -0.00020 0.00000 -0.00865 -0.00865 3.13476

D77 3.09008 0.00012 0.00000 0.00173 0.00172 3.09180

D78 -0.03537 -0.00007 0.00000 -0.00461 -0.00462 -0.03998

D79 0.03710 -0.00005 0.00000 -0.00006 -0.00006 0.03704

D80 -3.12102 0.00015 0.00000 0.00648 0.00646 -3.11456

D81 2.95069 0.00038 0.00000 0.01783 0.01783 2.96852

D82 -0.18391 0.00021 0.00000 0.01151 0.01150 -0.17241

D83 -0.17229 0.00016 0.00000 0.01051 0.01051 -0.16178

D84 2.97629 -0.00001 0.00000 0.00419 0.00419 2.98048

D85 3.01279 -0.00030 0.00000 -0.01712 -0.01712 2.99566

D86 -0.19116 -0.00012 0.00000 -0.00819 -0.00819 -0.19935

D87 -0.13566 -0.00014 0.00000 -0.01091 -0.01092 -0.14658

D88 2.94357 0.00004 0.00000 -0.00198 -0.00198 2.94159

D89 -0.98756 0.00021 0.00000 0.00423 0.00423 -0.98334

D90 2.15395 0.00014 0.00000 0.00337 0.00337 2.15731

D91 2.16043 0.00006 0.00000 -0.00157 -0.00157 2.15886

D92 -0.98124 -0.00001 0.00000 -0.00243 -0.00243 -0.98367

D93 3.06444 0.00038 0.00000 0.01263 0.01262 3.07706

D94 -0.07501 0.00014 0.00000 0.00667 0.00666 -0.06835

D95 -0.02389 0.00021 0.00000 0.00488 0.00488 -0.01901

D96 3.11984 -0.00002 0.00000 -0.00109 -0.00108 3.11877

D97 -3.05943 -0.00030 0.00000 -0.01105 -0.01107 -3.07051

D98 0.11979 -0.00011 0.00000 -0.00597 -0.00599 0.11380

D99 0.03063 -0.00018 0.00000 -0.00383 -0.00383 0.02680

D100 -3.07334 0.00000 0.00000 0.00125 0.00126 -3.07208

D101 0.00889 -0.00017 0.00000 -0.00417 -0.00418 0.00471

D102 -3.14103 -0.00016 0.00000 -0.00370 -0.00370 3.13845

D103 -3.13489 0.00007 0.00000 0.00189 0.00189 -3.13300

D104 -0.00162 0.00008 0.00000 0.00236 0.00237 0.00075

D105 0.00956 0.00007 0.00000 0.00186 0.00187 0.01143

D106 -3.10882 -0.00003 0.00000 0.00012 0.00012 -3.10870

D107 -3.12387 0.00006 0.00000 0.00139 0.00139 -3.12248

D108 0.04093 -0.00005 0.00000 -0.00035 -0.00035 0.04058

D109 -0.02518 0.00008 0.00000 0.00127 0.00127 -0.02391

D110 3.07846 -0.00011 0.00000 -0.00386 -0.00387 3.07459

D111 3.09353 0.00017 0.00000 0.00292 0.00293 3.09646

D112 -0.08602 -0.00002 0.00000 -0.00220 -0.00220 -0.08822

D113 -2.87514 -0.00013 0.00000 -0.01511 -0.01511 -2.89025

D114 0.25745 -0.00040 0.00000 -0.02110 -0.02111 0.23633

D115 0.29384 -0.00025 0.00000 -0.01713 -0.01713 0.27671

D116 -2.85676 -0.00052 0.00000 -0.02312 -0.02314 -2.87989

D117 0.99337 -0.00000 0.00000 0.00180 0.00180 0.99517

D118 -2.14533 -0.00017 0.00000 -0.00486 -0.00487 -2.15020

D119 -2.13982 0.00025 0.00000 0.00739 0.00739 -2.13243

D120 1.00466 0.00008 0.00000 0.00073 0.00073 1.00539

D121 -3.13265 0.00010 0.00000 0.00249 0.00249 -3.13016

D122 -0.01111 0.00007 0.00000 0.00174 0.00174 -0.00937

D123 0.00930 0.00003 0.00000 0.00150 0.00150 0.01080

D124 3.13083 -0.00001 0.00000 0.00075 0.00075 3.13158

D125 -3.13877 -0.00010 0.00000 -0.00222 -0.00222 -3.14099

D126 -0.01567 -0.00006 0.00000 -0.00167 -0.00167 -0.01735

D127 0.00248 -0.00003 0.00000 -0.00123 -0.00123 0.00125

D128 3.12557 0.00002 0.00000 -0.00069 -0.00069 3.12489

D129 -0.01357 -0.00002 0.00000 -0.00103 -0.00103 -0.01459

D130 3.12608 -0.00002 0.00000 -0.00078 -0.00078 3.12531

D131 -3.13500 0.00001 0.00000 -0.00030 -0.00030 -3.13529

D132 0.00465 0.00001 0.00000 -0.00005 -0.00005 0.00461

D133 0.00593 0.00001 0.00000 0.00025 0.00025 0.00618

D134 -3.13475 0.00001 0.00000 0.00035 0.00035 -3.13440

D135 -3.13371 0.00001 0.00000 0.00000 0.00000 -3.13371

D136 0.00880 0.00001 0.00000 0.00010 0.00010 0.00890

D137 0.00580 -0.00001 0.00000 0.00002 0.00002 0.00582

D138 -3.13451 0.00001 0.00000 0.00074 0.00074 -3.13378

D139 -3.13671 -0.00000 0.00000 -0.00008 -0.00008 -3.13679

D140 0.00616 0.00002 0.00000 0.00064 0.00064 0.00680

D141 -0.01002 0.00002 0.00000 0.00048 0.00048 -0.00954

D142 -3.13298 -0.00003 0.00000 -0.00009 -0.00009 -3.13307

D143 3.13030 -0.00000 0.00000 -0.00023 -0.00023 3.13007

D144 0.00734 -0.00005 0.00000 -0.00080 -0.00080 0.00654

D145 -0.00270 -0.00005 0.00000 -0.00146 -0.00146 -0.00415

D146 3.14014 -0.00004 0.00000 -0.00160 -0.00160 3.13854

D147 3.13487 -0.00002 0.00000 -0.00067 -0.00067 3.13420

D148 -0.00548 -0.00001 0.00000 -0.00081 -0.00081 -0.00630

D149 -0.01012 0.00003 0.00000 0.00112 0.00112 -0.00900

D150 3.12789 0.00003 0.00000 0.00135 0.00136 3.12925

D151 3.13551 0.00000 0.00000 0.00033 0.00033 3.13584

D152 -0.00967 0.00000 0.00000 0.00057 0.00057 -0.00911

D153 0.02148 -0.00007 0.00000 -0.00197 -0.00196 0.01951

D154 3.13756 0.00010 0.00000 0.00239 0.00240 3.13995

D155 -3.12135 -0.00008 0.00000 -0.00182 -0.00182 -3.12317

D156 -0.00527 0.00009 0.00000 0.00254 0.00254 -0.00273

D157 3.11283 0.00036 0.00000 0.01163 0.01166 3.12449

D158 -0.02699 0.00021 0.00000 0.00565 0.00564 -0.02135

D159 -0.00340 0.00019 0.00000 0.00734 0.00735 0.00395

D160 3.13996 0.00004 0.00000 0.00135 0.00134 3.14130

D161 -3.12568 -0.00037 0.00000 -0.01204 -0.01202 -3.13770

D162 0.02862 -0.00018 0.00000 -0.00757 -0.00755 0.02106

D163 0.01411 -0.00021 0.00000 -0.00595 -0.00596 0.00816

D164 -3.11478 -0.00002 0.00000 -0.00148 -0.00149 -3.11627

D165 0.00427 0.00010 0.00000 0.00263 0.00264 0.00691

D166 -3.13375 0.00010 0.00000 0.00240 0.00241 -3.13135

D167 3.13308 -0.00010 0.00000 -0.00185 -0.00184 3.13124

D168 -0.00495 -0.00009 0.00000 -0.00208 -0.00207 -0.00702

D169 -3.12437 -0.00039 0.00000 -0.01273 -0.01270 -3.13707

D170 0.02969 -0.00019 0.00000 -0.00811 -0.00809 0.02161

D171 0.01437 -0.00022 0.00000 -0.00613 -0.00613 0.00824

D172 -3.11475 -0.00002 0.00000 -0.00151 -0.00152 -3.11627

D173 3.11147 0.00038 0.00000 0.01234 0.01237 3.12384

D174 -0.00426 0.00020 0.00000 0.00772 0.00774 0.00349

D175 -0.02731 0.00021 0.00000 0.00586 0.00586 -0.02145

D176 3.14015 0.00004 0.00000 0.00125 0.00123 3.14138

D177 0.00424 0.00010 0.00000 0.00266 0.00266 0.00690

D178 -3.13384 0.00010 0.00000 0.00246 0.00246 -3.13138

D179 3.13328 -0.00010 0.00000 -0.00198 -0.00197 3.13132

D180 -0.00480 -0.00010 0.00000 -0.00218 -0.00217 -0.00697

D181 -0.01025 0.00003 0.00000 0.00122 0.00122 -0.00904

D182 3.13538 0.00001 0.00000 0.00039 0.00039 3.13577

D183 3.12781 0.00003 0.00000 0.00142 0.00142 3.12923

D184 -0.00974 0.00000 0.00000 0.00060 0.00060 -0.00915

D185 -0.00262 -0.00005 0.00000 -0.00151 -0.00152 -0.00414

D186 3.14017 -0.00004 0.00000 -0.00160 -0.00160 3.13857

D187 3.13493 -0.00002 0.00000 -0.00069 -0.00069 3.13424

D188 -0.00546 -0.00001 0.00000 -0.00078 -0.00078 -0.00624

D189 0.02163 -0.00008 0.00000 -0.00206 -0.00206 0.01957

D190 3.13720 0.00011 0.00000 0.00262 0.00262 3.13982

D191 -3.12116 -0.00009 0.00000 -0.00198 -0.00198 -3.12313

D192 -0.00559 0.00010 0.00000 0.00271 0.00271 -0.00288

D193 -3.13925 -0.00009 0.00000 -0.00201 -0.00201 -3.14126

D194 -0.01618 -0.00005 0.00000 -0.00144 -0.00144 -0.01762

D195 0.00243 -0.00002 0.00000 -0.00117 -0.00117 0.00125

D196 3.12550 0.00002 0.00000 -0.00060 -0.00060 3.12489

D197 -3.13215 0.00009 0.00000 0.00226 0.00226 -3.12989

D198 -0.01088 0.00006 0.00000 0.00166 0.00166 -0.00922

D199 0.00936 0.00002 0.00000 0.00142 0.00142 0.01078

D200 3.13063 -0.00001 0.00000 0.00082 0.00082 3.13145

D201 -0.01003 0.00002 0.00000 0.00049 0.00049 -0.00954

D202 3.13030 -0.00000 0.00000 -0.00022 -0.00022 3.13008

D203 -3.13296 -0.00003 0.00000 -0.00011 -0.00011 -3.13307

D204 0.00736 -0.00005 0.00000 -0.00082 -0.00082 0.00655

D205 0.00584 -0.00001 0.00000 -0.00002 -0.00002 0.00582

D206 -3.13665 -0.00001 0.00000 -0.00010 -0.00010 -3.13676

D207 -3.13447 0.00001 0.00000 0.00069 0.00069 -3.13379

D208 0.00621 0.00002 0.00000 0.00061 0.00061 0.00682

D209 0.00590 0.00001 0.00000 0.00027 0.00027 0.00617

D210 -3.13367 0.00001 0.00000 -0.00001 -0.00001 -3.13369

D211 -3.13479 0.00001 0.00000 0.00035 0.00035 -3.13444

D212 0.00882 0.00000 0.00000 0.00006 0.00006 0.00889

D213 -0.01359 -0.00002 0.00000 -0.00098 -0.00098 -0.01458

D214 -3.13475 0.00001 0.00000 -0.00041 -0.00041 -3.13516

D215 3.12599 -0.00002 0.00000 -0.00070 -0.00070 3.12529

D216 0.00483 0.00001 0.00000 -0.00012 -0.00012 0.00470

Item Value Threshold Converged?

Maximum Force 0.001791 0.000450 NO

RMS Force 0.000308 0.000300 NO

Maximum Displacement 0.428184 0.001800 NO

RMS Displacement 0.075640 0.001200 NO

Predicted change in Energy=-2.866067D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Mon Aug 26 23:00:06 2019, MaxMem= 4294967296 cpu: 3.5

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

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=1 Diff= 1.85D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.911592 -4.122046 0.529580

2 6 0 -0.044947 -3.081009 0.156038

3 7 0 -0.811267 -1.948268 0.016404

4 6 0 -2.135486 -2.235433 0.257587

5 6 0 -2.205748 -3.598515 0.596475

6 6 0 -3.224804 -1.310516 0.122561

7 6 0 -3.086858 0.073398 -0.051093

8 7 0 -1.918064 0.777340 0.059533

9 6 0 -2.251835 2.096438 -0.153371

10 6 0 -3.674788 2.213907 -0.464906

11 6 0 -4.192232 0.967013 -0.393331

12 6 0 1.374377 -3.176102 -0.068005

13 6 0 2.251568 -2.096135 -0.155500

14 6 0 3.674564 -2.213337 -0.466927

15 6 0 4.192048 -0.966536 -0.394025

16 6 0 3.086680 -0.073251 -0.050895

17 7 0 1.917822 -0.777278 0.058755

18 6 0 3.224539 1.310469 0.124195

19 6 0 2.135239 2.235217 0.260455

20 6 0 2.205882 3.598747 0.597563

21 6 0 0.911731 4.122294 0.531076

22 6 0 0.044691 3.080848 0.159571

23 7 0 0.810722 1.947747 0.021176

24 6 0 -1.374508 3.176187 -0.065082

25 6 0 -4.590063 -1.887314 0.174318

26 6 0 -4.977098 -2.903239 -0.712960

27 6 0 -6.263551 -3.430739 -0.668267

28 6 0 -7.180675 -2.965541 0.274338

29 6 0 -6.804393 -1.963471 1.167468

30 6 0 -5.522075 -1.424537 1.114756

31 6 0 2.937409 -7.154657 -0.442776

32 6 0 1.933475 -6.710258 -1.303692

33 6 0 1.417236 -5.425339 -1.172039

34 6 0 1.913307 -4.553790 -0.190686

35 6 0 2.920369 -5.011684 0.670618

36 6 0 3.424961 -6.303493 0.547467

37 6 0 -1.912923 4.553960 -0.189560

38 6 0 -2.920073 5.013305 0.670827

39 6 0 -3.424626 6.304924 0.545430

40 6 0 -2.936900 7.154394 -0.446181

41 6 0 -1.932817 6.708544 -1.306171

42 6 0 -1.416607 5.423841 -1.172261

43 6 0 4.589840 1.887358 0.175015

44 6 0 5.522588 1.424420 1.114625

45 6 0 6.805030 1.963176 1.166271

46 6 0 7.180684 2.965232 0.272865

47 6 0 6.262812 3.430587 -0.668927

48 6 0 4.976245 2.903255 -0.712551

49 1 0 -0.612807 -5.137751 0.732929

50 1 0 -3.105009 -4.129961 0.862429

51 1 0 -4.192874 3.123983 -0.724608

52 1 0 -5.211541 0.667264 -0.582338

53 1 0 4.192612 -3.123201 -0.727469

54 1 0 5.211380 -0.666656 -0.582681

55 1 0 3.105411 4.130573 0.861832

56 1 0 0.613279 5.138372 0.733034

57 1 0 -4.270597 -3.264493 -1.451395

58 1 0 -6.551245 -4.205191 -1.371459

59 1 0 -8.181512 -3.382261 0.312709

60 1 0 -7.509159 -1.601097 1.908383

61 1 0 -5.230464 -0.651018 1.816022

62 1 0 3.334507 -8.159319 -0.541927

63 1 0 1.551064 -7.366133 -2.078618

64 1 0 0.638359 -5.083815 -1.844160

65 1 0 3.294984 -4.355678 1.447938

66 1 0 4.197416 -6.645451 1.228127

67 1 0 -3.294829 4.358546 1.449134

68 1 0 -4.197189 6.648059 1.225374

69 1 0 -3.334006 8.158878 -0.547121

70 1 0 -1.550268 7.363126 -2.082122

71 1 0 -0.637699 5.081090 -1.843724

72 1 0 5.231471 0.650908 1.816106

73 1 0 7.510377 1.600662 1.906565

74 1 0 8.181617 3.381799 0.310370

75 1 0 6.550006 4.205016 -1.372349

76 1 0 4.269212 3.264559 -1.450447

77 1 0 -0.454953 -1.025871 -0.194284

78 1 0 0.453908 1.024858 -0.186673

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

Rotational constants (GHZ): 0.0588122 0.0581818 0.0301662

Leave Link 202 at Mon Aug 26 23:00:06 2019, MaxMem= 4294967296 cpu: 0.0

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

Standard basis: 6-311G(d) (5D, 7F)

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

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5357.6102676684 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2121761632 Hartrees.

Nuclear repulsion after empirical dispersion term = 5357.3980915052 Hartrees.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5759

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.28D-10

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 331

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

GePol: Cavity surface area = 612.529 Ang\*\*2

GePol: Cavity volume = 628.710 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0020993624 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5357.3959921428 Hartrees.

Leave Link 301 at Mon Aug 26 23:00:06 2019, MaxMem= 4294967296 cpu: 2.1

(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.

NBasis= 954 RedAO= T EigKep= 1.30D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Mon Aug 26 23:00:08 2019, MaxMem= 4294967296 cpu: 28.0

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

DipDrv: MaxL=1.

Leave Link 303 at Mon Aug 26 23:00:08 2019, MaxMem= 4294967296 cpu: 2.5

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

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= 0.000000 -0.000000 0.000000

Rot= 0.997858 -0.000005 -0.000005 -0.065420 Ang= -7.50 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0540 S= 1.0179

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30487261170

Leave Link 401 at Mon Aug 26 23:00:13 2019, MaxMem= 4294967296 cpu: 85.8

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 580000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 99498243.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.53D-14 for 5748.

Iteration 1 A\*A^-1 deviation from orthogonality is 6.07D-15 for 5746 5488.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.47D-14 for 5748.

Iteration 1 A^-1\*A deviation from orthogonality is 1.57D-10 for 1542 1477.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.78D-15 for 3062.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.14D-15 for 2507 147.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.22D-15 for 1063.

Iteration 2 A^-1\*A deviation from orthogonality is 3.34D-16 for 4229 514.

E= -1914.32330676852

DIIS: error= 4.07D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.32330676852 IErMin= 1 ErrMin= 4.07D-03

ErrMax= 4.07D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.45D-02 BMatP= 2.45D-02

IDIUse=3 WtCom= 9.59D-01 WtEn= 4.07D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.640 Goal= None Shift= 0.000

Gap= 0.705 Goal= None Shift= 0.000

GapD= 0.640 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=9.03D-05 MaxDP=3.49D-03 OVMax= 1.45D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 9.03D-05 CP: 1.00D+00

E= -1914.33317773814 Delta-E= -0.009870969623 Rises=F Damp=F

DIIS: error= 3.26D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33317773814 IErMin= 2 ErrMin= 3.26D-04

ErrMax= 3.26D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.31D-04 BMatP= 2.45D-02

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.26D-03

Coeff-Com: -0.599D-01 0.106D+01

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

Coeff: -0.597D-01 0.106D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.88D-05 MaxDP=9.80D-04 DE=-9.87D-03 OVMax= 9.35D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.75D-05 CP: 1.00D+00 1.08D+00

E= -1914.33325940858 Delta-E= -0.000081670436 Rises=F Damp=F

DIIS: error= 2.69D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33325940858 IErMin= 3 ErrMin= 2.69D-04

ErrMax= 2.69D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.84D-04 BMatP= 2.31D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.69D-03

Coeff-Com: -0.360D-01 0.562D+00 0.474D+00

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

Coeff: -0.359D-01 0.560D+00 0.475D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=8.58D-06 MaxDP=5.72D-04 DE=-8.17D-05 OVMax= 2.55D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 7.21D-06 CP: 1.00D+00 1.09D+00 7.45D-01

E= -1914.33330474664 Delta-E= -0.000045338056 Rises=F Damp=F

DIIS: error= 9.42D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33330474664 IErMin= 4 ErrMin= 9.42D-05

ErrMax= 9.42D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.10D-05 BMatP= 1.84D-04

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

Coeff-Com: -0.700D-02 0.872D-01 0.250D+00 0.670D+00

Coeff: -0.700D-02 0.872D-01 0.250D+00 0.670D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.09D-06 MaxDP=4.08D-04 DE=-4.53D-05 OVMax= 4.31D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.91D-06 CP: 1.00D+00 1.10D+00 9.27D-01 9.36D-01

E= -1914.33331275940 Delta-E= -0.000008012762 Rises=F Damp=F

DIIS: error= 7.34D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33331275940 IErMin= 5 ErrMin= 7.34D-05

ErrMax= 7.34D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.58D-06 BMatP= 2.10D-05

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

Coeff-Com: -0.641D-03-0.449D-02 0.106D+00 0.439D+00 0.459D+00

Coeff: -0.641D-03-0.449D-02 0.106D+00 0.439D+00 0.459D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.29D-06 MaxDP=1.33D-04 DE=-8.01D-06 OVMax= 1.77D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.54D-06 CP: 1.00D+00 1.10D+00 9.69D-01 1.13D+00 1.11D+00

E= -1914.33331592984 Delta-E= -0.000003170439 Rises=F Damp=F

DIIS: error= 4.53D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33331592984 IErMin= 6 ErrMin= 4.53D-05

ErrMax= 4.53D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.22D-07 BMatP= 6.58D-06

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

Coeff-Com: 0.166D-02-0.268D-01-0.265D-01 0.334D-01 0.145D+00 0.874D+00

Coeff: 0.166D-02-0.268D-01-0.265D-01 0.334D-01 0.145D+00 0.874D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.17D-06 MaxDP=2.51D-04 DE=-3.17D-06 OVMax= 3.31D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 7.94D-07 CP: 1.00D+00 1.10D+00 1.05D+00 1.31D+00 1.64D+00

CP: 1.67D+00

E= -1914.33331813013 Delta-E= -0.000002200288 Rises=F Damp=F

DIIS: error= 3.32D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33331813013 IErMin= 7 ErrMin= 3.32D-05

ErrMax= 3.32D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.80D-07 BMatP= 8.22D-07

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

Coeff-Com: 0.863D-03-0.867D-02-0.509D-01-0.109D+00-0.140D+00 0.382D+00

Coeff-Com: 0.926D+00

Coeff: 0.863D-03-0.867D-02-0.509D-01-0.109D+00-0.140D+00 0.382D+00

Coeff: 0.926D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.15D-06 MaxDP=2.50D-04 DE=-2.20D-06 OVMax= 3.28D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 4.47D-07 CP: 1.00D+00 1.11D+00 1.13D+00 1.50D+00 2.13D+00

CP: 2.58D+00 1.64D+00

E= -1914.33331975788 Delta-E= -0.000001627750 Rises=F Damp=F

DIIS: error= 2.48D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33331975788 IErMin= 8 ErrMin= 2.48D-05

ErrMax= 2.48D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.92D-07 BMatP= 5.80D-07

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

Coeff-Com: -0.987D-03 0.211D-01-0.213D-01-0.106D+00-0.306D+00-0.583D+00

Coeff-Com: 0.702D+00 0.129D+01

Coeff: -0.987D-03 0.211D-01-0.213D-01-0.106D+00-0.306D+00-0.583D+00

Coeff: 0.702D+00 0.129D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.54D-06 MaxDP=4.40D-04 DE=-1.63D-06 OVMax= 5.96D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.81D-06 CP: 1.00D+00 1.11D+00 1.26D+00 1.81D+00 3.00D+00

CP: 3.00D+00 3.00D+00 1.88D+00

E= -1914.33332118243 Delta-E= -0.000001424550 Rises=F Damp=F

DIIS: error= 6.97D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33332118243 IErMin= 9 ErrMin= 6.97D-06

ErrMax= 6.97D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.51D-08 BMatP= 2.92D-07

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

Coeff-Com: -0.390D-03 0.633D-02 0.325D-02 0.791D-02-0.359D-01-0.187D+00

Coeff-Com: -0.102D+00 0.407D+00 0.901D+00

Coeff: -0.390D-03 0.633D-02 0.325D-02 0.791D-02-0.359D-01-0.187D+00

Coeff: -0.102D+00 0.407D+00 0.901D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.21D-06 MaxDP=1.01D-04 DE=-1.42D-06 OVMax= 1.34D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 7.37D-07 CP: 1.00D+00 1.11D+00 1.29D+00 1.87D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.49D+00 1.37D+00

E= -1914.33332128896 Delta-E= -0.000000106539 Rises=F Damp=F

DIIS: error= 5.06D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33332128896 IErMin=10 ErrMin= 5.06D-06

ErrMax= 5.06D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.89D-08 BMatP= 5.51D-08

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

Coeff-Com: 0.183D-04-0.175D-02 0.681D-02 0.357D-01 0.627D-01 0.443D-01

Coeff-Com: -0.294D+00-0.519D-01 0.562D+00 0.637D+00

Coeff: 0.183D-04-0.175D-02 0.681D-02 0.357D-01 0.627D-01 0.443D-01

Coeff: -0.294D+00-0.519D-01 0.562D+00 0.637D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.86D-07 MaxDP=3.82D-05 DE=-1.07D-07 OVMax= 5.22D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.69D-07 CP: 1.00D+00 1.11D+00 1.30D+00 1.89D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.77D+00 1.53D+00 1.35D+00

E= -1914.33332131874 Delta-E= -0.000000029780 Rises=F Damp=F

DIIS: error= 2.93D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33332131874 IErMin=11 ErrMin= 2.93D-06

ErrMax= 2.93D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.01D-09 BMatP= 2.89D-08

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

Coeff-Com: 0.155D-03-0.312D-02 0.534D-03 0.125D-01 0.415D-01 0.966D-01

Coeff-Com: -0.111D+00-0.145D+00-0.152D+00 0.294D+00 0.966D+00

Coeff: 0.155D-03-0.312D-02 0.534D-03 0.125D-01 0.415D-01 0.966D-01

Coeff: -0.111D+00-0.145D+00-0.152D+00 0.294D+00 0.966D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.27D-07 MaxDP=2.57D-05 DE=-2.98D-08 OVMax= 3.21D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.27D-07 CP: 1.00D+00 1.11D+00 1.30D+00 1.89D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.63D+00 1.58D+00

CP: 1.39D+00

E= -1914.33332133080 Delta-E= -0.000000012060 Rises=F Damp=F

DIIS: error= 1.07D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.33332133080 IErMin=12 ErrMin= 1.07D-06

ErrMax= 1.07D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.41D-09 BMatP= 7.01D-09

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

Coeff-Com: 0.823D-04-0.132D-02-0.159D-02-0.953D-03 0.879D-02 0.459D-01

Coeff-Com: 0.407D-02-0.593D-01-0.230D+00 0.815D-02 0.548D+00 0.678D+00

Coeff: 0.823D-04-0.132D-02-0.159D-02-0.953D-03 0.879D-02 0.459D-01

Coeff: 0.407D-02-0.593D-01-0.230D+00 0.815D-02 0.548D+00 0.678D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.01D-07 MaxDP=6.63D-06 DE=-1.21D-08 OVMax= 9.34D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 5.23D-08 CP: 1.00D+00 1.11D+00 1.30D+00 1.89D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.66D+00 1.63D+00

CP: 1.70D+00 1.33D+00

E= -1914.33332133298 Delta-E= -0.000000002171 Rises=F Damp=F

DIIS: error= 5.31D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.33332133298 IErMin=13 ErrMin= 5.31D-07

ErrMax= 5.31D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.28D-10 BMatP= 2.41D-09

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

Coeff-Com: -0.102D-04 0.392D-03-0.116D-02-0.469D-02-0.996D-02-0.104D-01

Coeff-Com: 0.365D-01 0.227D-01-0.658D-01-0.967D-01-0.532D-01 0.366D+00

Coeff-Com: 0.817D+00

Coeff: -0.102D-04 0.392D-03-0.116D-02-0.469D-02-0.996D-02-0.104D-01

Coeff: 0.365D-01 0.227D-01-0.658D-01-0.967D-01-0.532D-01 0.366D+00

Coeff: 0.817D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.32D-08 MaxDP=6.12D-06 DE=-2.17D-09 OVMax= 7.21D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 2.38D-08 CP: 1.00D+00 1.11D+00 1.30D+00 1.90D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.68D+00 1.68D+00

CP: 1.79D+00 1.57D+00 1.21D+00

E= -1914.33332133367 Delta-E= -0.000000000689 Rises=F Damp=F

DIIS: error= 2.59D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.33332133367 IErMin=14 ErrMin= 2.59D-07

ErrMax= 2.59D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.58D-10 BMatP= 6.28D-10

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

Coeff-Com: -0.244D-04 0.513D-03-0.224D-03-0.216D-02-0.751D-02-0.168D-01

Coeff-Com: 0.174D-01 0.259D-01 0.222D-01-0.542D-01-0.163D+00 0.454D-01

Coeff-Com: 0.432D+00 0.700D+00

Coeff: -0.244D-04 0.513D-03-0.224D-03-0.216D-02-0.751D-02-0.168D-01

Coeff: 0.174D-01 0.259D-01 0.222D-01-0.542D-01-0.163D+00 0.454D-01

Coeff: 0.432D+00 0.700D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.58D-08 MaxDP=3.23D-06 DE=-6.89D-10 OVMax= 3.80D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.12D-08 CP: 1.00D+00 1.11D+00 1.31D+00 1.90D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.69D+00 1.71D+00

CP: 1.83D+00 1.60D+00 1.33D+00 1.28D+00

E= -1914.33332133383 Delta-E= -0.000000000162 Rises=F Damp=F

DIIS: error= 1.26D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.33332133383 IErMin=15 ErrMin= 1.26D-07

ErrMax= 1.26D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.57D-11 BMatP= 1.58D-10

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

Coeff-Com: -0.788D-05 0.101D-03 0.332D-03 0.711D-03-0.204D-03-0.446D-02

Coeff-Com: -0.484D-02 0.415D-02 0.367D-01 0.855D-02-0.617D-01-0.994D-01

Coeff-Com: -0.782D-01 0.337D+00 0.861D+00

Coeff: -0.788D-05 0.101D-03 0.332D-03 0.711D-03-0.204D-03-0.446D-02

Coeff: -0.484D-02 0.415D-02 0.367D-01 0.855D-02-0.617D-01-0.994D-01

Coeff: -0.782D-01 0.337D+00 0.861D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.66D-08 MaxDP=1.46D-06 DE=-1.62D-10 OVMax= 1.64D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 5.33D-09 CP: 1.00D+00 1.11D+00 1.31D+00 1.90D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.69D+00 1.72D+00

CP: 1.83D+00 1.60D+00 1.35D+00 1.53D+00 1.30D+00

E= -1914.33332133387 Delta-E= -0.000000000042 Rises=F Damp=F

DIIS: error= 5.46D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1914.33332133387 IErMin=16 ErrMin= 5.46D-08

ErrMax= 5.46D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.89D-12 BMatP= 3.57D-11

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

Coeff-Com: -0.532D-06-0.202D-04 0.199D-03 0.619D-03 0.877D-03 0.102D-03

Coeff-Com: -0.464D-02-0.176D-02 0.143D-01 0.116D-01-0.682D-02-0.516D-01

Coeff-Com: -0.960D-01 0.571D-01 0.387D+00 0.689D+00

Coeff: -0.532D-06-0.202D-04 0.199D-03 0.619D-03 0.877D-03 0.102D-03

Coeff: -0.464D-02-0.176D-02 0.143D-01 0.116D-01-0.682D-02-0.516D-01

Coeff: -0.960D-01 0.571D-01 0.387D+00 0.689D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.61D-09 MaxDP=4.39D-07 DE=-4.18D-11 OVMax= 5.35D-06

Error on total polarization charges = 0.08280

SCF Done: E(UB3LYP) = -1914.33332133 A.U. after 16 cycles

NFock= 16 Conv=0.56D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0548 S= 1.0182

<L.S>= 0.000000000000E+00

KE= 1.906381899069D+03 PE=-1.516441800951D+04 EE= 5.986306796968D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0548, after 2.0017

Leave Link 502 at Mon Aug 26 23:07:41 2019, MaxMem= 4294967296 cpu: 7079.1

(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: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48876146D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64477556D-01

Leave Link 801 at Mon Aug 26 23:07:41 2019, MaxMem= 4294967296 cpu: 0.9

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

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

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

Leave Link 1101 at Mon Aug 26 23:07:48 2019, MaxMem= 4294967296 cpu: 112.4

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

Symmetrizing basis deriv contribution to polar:

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

Leave Link 1102 at Mon Aug 26 23:07:48 2019, MaxMem= 4294967296 cpu: 2.1

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

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 196

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 Mon Aug 26 23:27:33 2019, MaxMem= 4294967296 cpu: 18947.0

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

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 580000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 4.81D+03 3.70D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 3.88D+02 3.10D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 8.20D+00 3.91D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 9.83D-02 3.49D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.16D-04 1.96D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 3.90D-06 1.16D-04.

188 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 1.80D-08 8.78D-06.

88 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 7.82D-11 4.93D-07.

32 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 4.57D-13 2.89D-08.

2 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 6.46D-15 2.75D-09.

InvSVY: IOpt=1 It= 1 EMax= 5.68D-14

Solved reduced A of dimension 1717 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1124.78 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 27 03:18:08 2019, MaxMem= 4294967296 cpu: 221301.8

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 196

Leave Link 701 at Tue Aug 27 03:19:38 2019, MaxMem= 4294967296 cpu: 1431.5

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

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

Leave Link 702 at Tue Aug 27 03:19:38 2019, MaxMem= 4294967296 cpu: 0.5

(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=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

Leave Link 703 at Tue Aug 27 03:38:24 2019, MaxMem= 4294967296 cpu: 18021.5

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

Dipole =-4.79754756D-04-1.30153641D-03-5.10204487D-01

Polarizability= 1.31789002D+03 1.50826956D+02 1.59880139D+03

-5.35534008D-03 1.38529309D-01 4.57649910D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000085032 0.000134140 -0.000027274

2 6 -0.000099099 0.000187832 0.000181873

3 7 -0.000083758 -0.000043552 0.000099395

4 6 -0.000031535 0.000229568 -0.000120030

5 6 0.000050190 -0.000163445 0.000079367

6 6 -0.000176093 -0.000092490 -0.000040521

7 6 0.000346530 0.000046121 -0.000136510

8 7 -0.000421171 -0.000158638 0.000141274

9 6 0.000361125 -0.000024809 0.000000343

10 6 -0.000044823 0.000205395 0.000015051

11 6 0.000024992 -0.000026721 0.000091215

12 6 0.000430134 0.000078388 -0.000377592

13 6 -0.000352288 -0.000048771 0.000004700

14 6 0.000045760 0.000194751 -0.000012184

15 6 -0.000026387 -0.000017194 -0.000091079

16 6 -0.000344084 0.000060924 0.000125729

17 7 0.000424215 -0.000151017 -0.000157457

18 6 0.000177001 -0.000088115 0.000038708

19 6 0.000032661 0.000219069 0.000115352

20 6 -0.000048801 -0.000173566 -0.000078689

21 6 -0.000086440 0.000138641 0.000027954

22 6 0.000100670 0.000184103 -0.000182839

23 7 0.000075782 -0.000006124 -0.000097512

24 6 -0.000435438 0.000095935 0.000391755

25 6 0.000101116 0.000303541 0.000094539

26 6 -0.000071731 -0.000062375 0.000139300

27 6 0.000076240 0.000005316 -0.000003046

28 6 -0.000030973 -0.000067032 -0.000013210

29 6 -0.000010079 0.000023494 -0.000071722

30 6 -0.000038930 0.000024428 -0.000044356

31 6 0.000044679 -0.000029167 0.000080580

32 6 0.000059580 -0.000137767 -0.000041989

33 6 -0.000080540 -0.000082827 0.000193048

34 6 -0.000173425 -0.000189572 0.000058756

35 6 -0.000076564 0.000136544 -0.000077805

36 6 0.000036238 -0.000029933 -0.000058549

37 6 0.000180415 -0.000210991 -0.000070565

38 6 0.000072978 0.000129569 0.000080488

39 6 -0.000040149 -0.000030641 0.000064151

40 6 -0.000045127 -0.000032039 -0.000084964

41 6 -0.000063253 -0.000144203 0.000044983

42 6 0.000092646 -0.000078814 -0.000199519

43 6 -0.000100903 0.000288377 -0.000090008

44 6 0.000035258 0.000014891 0.000038873

45 6 0.000008622 0.000022078 0.000070359

46 6 0.000031746 -0.000066924 0.000012393

47 6 -0.000076964 0.000005013 0.000002105

48 6 0.000076355 -0.000054089 -0.000131032

49 1 0.000032055 -0.000035194 -0.000068228

50 1 0.000091451 0.000043105 -0.000048036

51 1 -0.000055636 -0.000105595 -0.000018429

52 1 -0.000053723 -0.000003970 0.000006196

53 1 0.000052533 -0.000101290 0.000018125

54 1 0.000052188 -0.000007907 -0.000005385

55 1 -0.000090093 0.000046543 0.000049245

56 1 -0.000032777 -0.000030759 0.000066614

57 1 -0.000011878 -0.000050744 0.000000194

58 1 -0.000029271 -0.000030576 0.000021846

59 1 -0.000018129 0.000007500 -0.000006583

60 1 -0.000000164 -0.000002563 0.000008116

61 1 0.000027216 -0.000054119 -0.000063717

62 1 0.000009986 -0.000018070 -0.000027138

63 1 -0.000001880 0.000022086 0.000001754

64 1 -0.000042485 0.000019106 -0.000025574

65 1 -0.000010991 -0.000006303 0.000095528

66 1 -0.000010293 0.000010312 0.000000565

67 1 0.000012317 -0.000005612 -0.000101811

68 1 0.000012210 0.000009650 -0.000000780

69 1 -0.000009952 -0.000018695 0.000028628

70 1 0.000003455 0.000023477 -0.000000743

71 1 0.000037602 0.000017469 0.000023239

72 1 -0.000024885 -0.000051321 0.000065547

73 1 0.000000514 -0.000002325 -0.000007604

74 1 0.000017609 0.000006673 0.000006773

75 1 0.000029068 -0.000030715 -0.000022028

76 1 0.000011411 -0.000051338 -0.000000480

77 1 0.000027528 -0.000063823 0.000351793

78 1 -0.000036395 -0.000052306 -0.000331467

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

Cartesian Forces: Max 0.000435438 RMS 0.000120238

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

Leave Link 716 at Tue Aug 27 03:38:24 2019, MaxMem= 4294967296 cpu: 2.0

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000612255 RMS 0.000141088

Search for a local minimum.

Step number 8 out of a maximum of 452

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

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -4.29D-04 DEPred=-2.87D-04 R= 1.50D+00

TightC=F SS= 1.41D+00 RLast= 1.07D-01 DXNew= 1.7838D-01 3.2009D-01

Trust test= 1.50D+00 RLast= 1.07D-01 DXMaxT set to 1.78D-01

ITU= 1 -1 -1 1 1 -1 1 0

Eigenvalues --- 0.00272 0.00396 0.00609 0.00709 0.00795

Eigenvalues --- 0.00823 0.00947 0.01089 0.01096 0.01138

Eigenvalues --- 0.01181 0.01189 0.01282 0.01288 0.01309

Eigenvalues --- 0.01318 0.01354 0.01436 0.01458 0.01582

Eigenvalues --- 0.01597 0.01620 0.01643 0.01674 0.01706

Eigenvalues --- 0.01711 0.01726 0.01733 0.01766 0.01766

Eigenvalues --- 0.01781 0.01786 0.01810 0.01819 0.01921

Eigenvalues --- 0.01990 0.02050 0.02058 0.02074 0.02198

Eigenvalues --- 0.02243 0.02252 0.02292 0.02297 0.02325

Eigenvalues --- 0.02329 0.02381 0.02450 0.02525 0.02532

Eigenvalues --- 0.02549 0.02557 0.02621 0.02621 0.02637

Eigenvalues --- 0.02638 0.02758 0.02769 0.02785 0.02795

Eigenvalues --- 0.02845 0.02858 0.02862 0.02863 0.02886

Eigenvalues --- 0.02942 0.03028 0.03961 0.04110 0.04235

Eigenvalues --- 0.04390 0.04491 0.04519 0.04588 0.04625

Eigenvalues --- 0.08396 0.09691 0.09699 0.09877 0.09898

Eigenvalues --- 0.09933 0.10353 0.10445 0.10617 0.10699

Eigenvalues --- 0.10699 0.10721 0.10721 0.10756 0.11180

Eigenvalues --- 0.11379 0.11382 0.11389 0.11391 0.11933

Eigenvalues --- 0.11939 0.11964 0.11974 0.12289 0.12289

Eigenvalues --- 0.12315 0.12316 0.12734 0.12735 0.12755

Eigenvalues --- 0.12755 0.15710 0.15997 0.16437 0.17206

Eigenvalues --- 0.17582 0.17696 0.17777 0.18221 0.18251

Eigenvalues --- 0.18291 0.18355 0.18625 0.19241 0.19293

Eigenvalues --- 0.19373 0.19409 0.19417 0.19439 0.19453

Eigenvalues --- 0.19480 0.19558 0.19560 0.19560 0.19561

Eigenvalues --- 0.20361 0.21527 0.22056 0.22918 0.22947

Eigenvalues --- 0.23469 0.23798 0.24421 0.24779 0.26092

Eigenvalues --- 0.26243 0.26586 0.26606 0.27183 0.28526

Eigenvalues --- 0.28554 0.28676 0.28954 0.29748 0.31025

Eigenvalues --- 0.31727 0.32098 0.32869 0.33181 0.33340

Eigenvalues --- 0.33924 0.34305 0.35226 0.35599 0.35617

Eigenvalues --- 0.35627 0.35641 0.35649 0.35677 0.35754

Eigenvalues --- 0.35779 0.35821 0.35841 0.35925 0.35929

Eigenvalues --- 0.35933 0.35935 0.35994 0.36002 0.36013

Eigenvalues --- 0.36018 0.36198 0.36244 0.36281 0.36307

Eigenvalues --- 0.37056 0.37100 0.37259 0.37413 0.37432

Eigenvalues --- 0.37586 0.38260 0.38619 0.38640 0.38806

Eigenvalues --- 0.39579 0.40461 0.40691 0.41131 0.41164

Eigenvalues --- 0.41243 0.41261 0.41272 0.41366 0.41499

Eigenvalues --- 0.41575 0.41912 0.42114 0.42875 0.44581

Eigenvalues --- 0.45160 0.45930 0.45937 0.45949 0.45966

Eigenvalues --- 0.46179 0.46272 0.46273 0.46299 0.46310

Eigenvalues --- 0.48157 0.48651 0.49175 0.50020 0.50746

Eigenvalues --- 0.50754 0.50757 0.50782 0.51153 0.51833

Eigenvalues --- 0.52485 0.57151 0.59130

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 1.10828 -0.10828

Cosine: 1.000 > 0.970

Length: 1.041

GDIIS step was calculated using 2 of the last 8 vectors.

Iteration 1 RMS(Cart)= 0.16570254 RMS(Int)= 0.00157372

Iteration 2 RMS(Cart)= 0.00539529 RMS(Int)= 0.00010717

Iteration 3 RMS(Cart)= 0.00000450 RMS(Int)= 0.00010716

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00010716

ITry= 1 IFail=0 DXMaxC= 7.99D-01 DCOld= 1.00D+10 DXMaxT= 1.78D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.65529 0.00006 0.00032 0.00024 0.00061 2.65590

R2 2.64116 -0.00001 -0.00022 0.00003 -0.00005 2.64111

R3 2.03730 -0.00001 -0.00002 -0.00024 -0.00026 2.03703

R4 2.59784 -0.00022 0.00004 0.00105 0.00097 2.59881

R5 2.72128 -0.00040 -0.00041 -0.00323 -0.00364 2.71764

R6 2.60082 0.00015 0.00021 -0.00093 -0.00083 2.59999

R7 1.91055 -0.00005 0.00013 -0.00036 -0.00023 1.91033

R8 2.65759 0.00021 -0.00009 -0.00033 -0.00038 2.65721

R9 2.71248 0.00010 -0.00008 0.00403 0.00395 2.71643

R10 2.03691 0.00009 -0.00000 0.00029 0.00029 2.03720

R11 2.64858 -0.00003 -0.00070 -0.00487 -0.00558 2.64301

R12 2.80248 -0.00005 0.00005 0.00043 0.00048 2.80296

R13 2.58682 0.00029 0.00085 0.00562 0.00635 2.59317

R14 2.76283 0.00001 -0.00021 -0.00056 -0.00072 2.76211

R15 2.60258 -0.00006 -0.00096 -0.00503 -0.00611 2.59647

R16 2.76162 -0.00012 -0.00001 0.00014 0.00016 2.76178

R17 2.63436 0.00006 0.00097 0.00570 0.00668 2.64103

R18 2.55471 -0.00002 0.00006 -0.00005 0.00016 2.55487

R19 2.03889 0.00002 0.00002 0.00026 0.00028 2.03917

R20 2.03930 -0.00004 -0.00001 -0.00029 -0.00030 2.03899

R21 2.63442 0.00006 0.00097 0.00564 0.00661 2.64103

R22 2.80516 -0.00006 -0.00010 -0.00280 -0.00289 2.80226

R23 2.76161 -0.00011 -0.00000 0.00012 0.00016 2.76177

R24 2.60253 -0.00005 -0.00095 -0.00499 -0.00606 2.59647

R25 2.55471 -0.00002 0.00006 -0.00004 0.00017 2.55488

R26 2.03890 0.00002 0.00002 0.00026 0.00028 2.03918

R27 2.76284 0.00001 -0.00022 -0.00056 -0.00073 2.76211

R28 2.03929 -0.00004 -0.00001 -0.00029 -0.00030 2.03899

R29 2.58686 0.00030 0.00085 0.00557 0.00631 2.59317

R30 2.64855 -0.00003 -0.00070 -0.00482 -0.00552 2.64302

R31 2.71246 0.00009 -0.00009 0.00407 0.00398 2.71644

R32 2.80255 -0.00005 0.00004 0.00032 0.00037 2.80292

R33 2.65763 0.00021 -0.00010 -0.00038 -0.00044 2.65720

R34 2.60086 0.00014 0.00022 -0.00096 -0.00086 2.59999

R35 2.64112 -0.00001 -0.00022 0.00008 -0.00000 2.64112

R36 2.03690 0.00009 -0.00000 0.00030 0.00030 2.03720

R37 2.65531 0.00006 0.00032 0.00022 0.00058 2.65589

R38 2.03729 -0.00001 -0.00002 -0.00024 -0.00026 2.03703

R39 2.59786 -0.00021 0.00005 0.00101 0.00094 2.59879

R40 2.72126 -0.00039 -0.00042 -0.00317 -0.00359 2.71767

R41 1.91063 -0.00005 0.00014 -0.00045 -0.00031 1.91032

R42 2.80524 -0.00006 -0.00011 -0.00290 -0.00301 2.80223

R43 2.65179 -0.00014 0.00004 -0.00022 -0.00018 2.65161

R44 2.65049 0.00014 -0.00004 0.00064 0.00060 2.65109

R45 2.62884 0.00005 0.00000 -0.00007 -0.00006 2.62877

R46 2.04836 -0.00004 -0.00001 -0.00013 -0.00014 2.04821

R47 2.63617 0.00006 -0.00003 0.00027 0.00025 2.63642

R48 2.05018 -0.00004 -0.00001 -0.00016 -0.00016 2.05002

R49 2.63440 -0.00005 -0.00003 -0.00018 -0.00021 2.63419

R50 2.04999 -0.00001 -0.00001 -0.00001 -0.00002 2.04996

R51 2.63043 -0.00001 -0.00000 0.00001 0.00001 2.63044

R52 2.05013 -0.00000 -0.00001 -0.00002 -0.00003 2.05010

R53 2.04854 0.00002 -0.00003 -0.00011 -0.00014 2.04839

R54 2.63652 -0.00001 -0.00003 -0.00008 -0.00011 2.63642

R55 2.63396 -0.00005 0.00000 0.00013 0.00013 2.63409

R56 2.05004 -0.00001 -0.00000 -0.00009 -0.00009 2.04994

R57 2.62859 0.00005 0.00007 -0.00029 -0.00021 2.62838

R58 2.05009 0.00001 -0.00000 0.00005 0.00005 2.05014

R59 2.65151 -0.00013 0.00005 0.00058 0.00063 2.65214

R60 2.04844 0.00003 0.00001 -0.00008 -0.00007 2.04837

R61 2.64945 -0.00002 0.00005 0.00104 0.00109 2.65054

R62 2.63110 0.00000 -0.00008 -0.00041 -0.00049 2.63061

R63 2.04833 0.00002 -0.00002 -0.00011 -0.00013 2.04820

R64 2.05009 -0.00001 0.00000 -0.00008 -0.00008 2.05001

R65 2.64940 -0.00002 0.00005 0.00111 0.00116 2.65056

R66 2.65150 -0.00013 0.00005 0.00060 0.00065 2.65214

R67 2.63112 0.00000 -0.00008 -0.00044 -0.00052 2.63060

R68 2.04834 0.00002 -0.00002 -0.00012 -0.00014 2.04820

R69 2.63396 -0.00006 0.00000 0.00012 0.00013 2.63409

R70 2.05009 -0.00001 0.00000 -0.00008 -0.00008 2.05001

R71 2.63652 -0.00001 -0.00003 -0.00007 -0.00010 2.63642

R72 2.05004 -0.00001 -0.00000 -0.00009 -0.00010 2.04994

R73 2.62860 0.00005 0.00008 -0.00030 -0.00022 2.62838

R74 2.05009 0.00001 -0.00000 0.00005 0.00005 2.05014

R75 2.04845 0.00003 0.00001 -0.00008 -0.00007 2.04837

R76 2.65047 0.00014 -0.00004 0.00068 0.00064 2.65111

R77 2.65177 -0.00014 0.00003 -0.00018 -0.00015 2.65162

R78 2.63044 -0.00001 -0.00000 -0.00000 -0.00000 2.63044

R79 2.04854 0.00002 -0.00003 -0.00012 -0.00015 2.04839

R80 2.63439 -0.00005 -0.00003 -0.00018 -0.00020 2.63419

R81 2.05013 -0.00000 -0.00001 -0.00002 -0.00003 2.05010

R82 2.63616 0.00006 -0.00002 0.00028 0.00026 2.63642

R83 2.04998 -0.00001 -0.00001 -0.00001 -0.00002 2.04996

R84 2.62885 0.00005 0.00000 -0.00009 -0.00009 2.62876

R85 2.05018 -0.00004 -0.00001 -0.00015 -0.00016 2.05002

R86 2.04835 -0.00004 -0.00001 -0.00013 -0.00014 2.04821

A1 1.88211 -0.00009 -0.00001 -0.00068 -0.00073 1.88138

A2 2.18612 0.00012 -0.00005 0.00167 0.00163 2.18776

A3 2.21492 -0.00004 0.00007 -0.00097 -0.00089 2.21403

A4 1.86886 0.00013 -0.00002 -0.00017 -0.00022 1.86864

A5 2.21472 0.00048 -0.00017 0.00777 0.00796 2.22268

A6 2.19941 -0.00061 0.00019 -0.00785 -0.00807 2.19135

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A8 2.18519 -0.00035 0.00005 -0.01090 -0.01092 2.17427

A9 2.17241 0.00032 0.00005 0.01036 0.01034 2.18275

A10 1.86767 -0.00011 0.00006 -0.00034 -0.00030 1.86737

A11 2.18861 0.00040 0.00038 0.00556 0.00552 2.19413

A12 2.22598 -0.00028 -0.00041 -0.00493 -0.00493 2.22105

A13 1.88101 0.00005 0.00009 0.00089 0.00094 1.88195

A14 2.21384 -0.00003 0.00007 -0.00040 -0.00031 2.21354

A15 2.18832 -0.00002 -0.00016 -0.00049 -0.00063 2.18769

A16 2.18122 0.00055 0.00012 0.00435 0.00387 2.18509

A17 2.03169 -0.00033 -0.00017 -0.00606 -0.00597 2.02572

A18 2.07028 -0.00022 0.00005 0.00170 0.00201 2.07229

A19 2.19172 0.00024 -0.00020 0.00002 -0.00066 2.19106

A20 2.16290 -0.00015 0.00036 0.00180 0.00254 2.16543

A21 1.92852 -0.00009 -0.00015 -0.00165 -0.00188 1.92665

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A24 2.18896 -0.00011 0.00010 0.00021 -0.00010 2.18887

A25 2.17006 -0.00005 -0.00039 -0.00178 -0.00175 2.16831

A26 1.86217 -0.00005 -0.00003 -0.00032 -0.00040 1.86177

A27 2.19774 -0.00002 -0.00014 -0.00015 -0.00026 2.19747

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A34 2.07756 0.00008 -0.00032 -0.00157 -0.00162 2.07593

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A53 1.86766 -0.00011 0.00007 -0.00035 -0.00030 1.86736

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A70 2.10228 0.00006 0.00009 0.00170 0.00179 2.10407

A71 2.07094 0.00002 0.00001 -0.00015 -0.00015 2.07079

A72 2.10513 -0.00002 -0.00002 0.00011 0.00009 2.10522

A73 2.08548 -0.00002 0.00015 -0.00065 -0.00051 2.08498

A74 2.09238 0.00004 -0.00013 0.00056 0.00044 2.09282

A75 2.09813 0.00002 0.00001 -0.00002 -0.00001 2.09811

A76 2.08873 -0.00002 -0.00000 -0.00015 -0.00015 2.08858

A77 2.09633 0.00001 -0.00001 0.00017 0.00016 2.09649

A78 2.08881 0.00001 0.00000 0.00009 0.00009 2.08890

A79 2.09711 0.00000 0.00000 -0.00013 -0.00013 2.09698

A80 2.09727 -0.00001 -0.00000 0.00004 0.00003 2.09731

A81 2.09752 -0.00003 0.00001 -0.00009 -0.00008 2.09744

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A87 2.08930 -0.00008 -0.00001 -0.00066 -0.00067 2.08863

A88 2.09668 0.00004 -0.00003 0.00018 0.00015 2.09683

A89 2.09720 0.00005 0.00004 0.00048 0.00052 2.09772

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A93 2.10455 0.00005 -0.00009 0.00120 0.00111 2.10566

A94 2.09326 0.00001 -0.00009 -0.00063 -0.00072 2.09254

A95 2.08518 -0.00006 0.00019 -0.00056 -0.00037 2.08481

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A97 2.10961 -0.00016 -0.00082 -0.00234 -0.00316 2.10645

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A102 2.09746 0.00002 -0.00010 0.00043 0.00033 2.09779

A103 2.09708 -0.00001 0.00005 -0.00009 -0.00004 2.09704

A104 2.08864 -0.00001 0.00005 -0.00035 -0.00029 2.08835

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A107 2.07235 -0.00008 -0.00007 -0.00191 -0.00198 2.07037

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A114 2.08931 -0.00008 -0.00000 -0.00069 -0.00070 2.08862

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D2 -3.11021 0.00003 0.00019 0.01653 0.01678 -3.09343

D3 -3.12241 0.00002 0.00020 0.00132 0.00151 -3.12090

D4 0.03948 -0.00001 0.00005 0.01448 0.01457 0.05405

D5 0.00470 -0.00008 -0.00045 -0.00318 -0.00365 0.00105

D6 -3.13267 -0.00002 0.00012 -0.00360 -0.00348 -3.13615

D7 3.13802 -0.00005 -0.00031 -0.00107 -0.00138 3.13664

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D10 3.07617 -0.00007 -0.00052 -0.00850 -0.00902 3.06715

D11 3.09819 0.00004 0.00004 -0.01510 -0.01494 3.08325

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D13 -2.88766 -0.00034 -0.00180 -0.04080 -0.04265 -2.93031

D14 0.23738 -0.00043 -0.00225 -0.03681 -0.03911 0.19827

D15 0.27792 -0.00038 -0.00198 -0.02538 -0.02744 0.25048

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D18 -3.07209 -0.00011 -0.00094 -0.00612 -0.00716 -3.07926

D19 -3.07366 0.00003 0.00024 0.00709 0.00742 -3.06623

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D21 -0.01866 0.00008 0.00039 0.00176 0.00218 -0.01648

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D23 3.07844 0.00016 0.00120 0.00876 0.00999 3.08842

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D27 2.99268 -0.00029 -0.00165 -0.04896 -0.05063 2.94205

D28 -0.14863 -0.00020 -0.00109 -0.03569 -0.03682 -0.18545

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D31 2.97906 -0.00004 0.00073 -0.00028 0.00042 2.97948

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D97 -3.07051 -0.00013 -0.00120 -0.00782 -0.00912 -3.07963

D98 0.11380 -0.00003 -0.00065 -0.00275 -0.00341 0.11040

D99 0.02680 -0.00007 -0.00041 -0.00006 -0.00050 0.02630

D100 -3.07208 0.00003 0.00014 0.00500 0.00522 -3.06686

D101 0.00471 -0.00008 -0.00045 -0.00322 -0.00369 0.00102

D102 3.13845 -0.00005 -0.00040 -0.00158 -0.00199 3.13646

D103 -3.13300 -0.00001 0.00020 -0.00322 -0.00302 -3.13602

D104 0.00075 0.00002 0.00026 -0.00159 -0.00132 -0.00057

D105 0.01143 0.00004 0.00020 0.00315 0.00335 0.01478

D106 -3.10870 0.00001 0.00001 0.01487 0.01492 -3.09378

D107 -3.12248 0.00001 0.00015 0.00157 0.00170 -3.12078

D108 0.04058 -0.00002 -0.00004 0.01328 0.01327 0.05384

D109 -0.02391 0.00002 0.00014 -0.00193 -0.00178 -0.02569

D110 3.07459 -0.00007 -0.00042 -0.00640 -0.00683 3.06776

D111 3.09646 0.00006 0.00032 -0.01326 -0.01283 3.08364

D112 -0.08822 -0.00002 -0.00024 -0.01773 -0.01788 -0.10610

D113 -2.89025 -0.00033 -0.00164 -0.03739 -0.03907 -2.92932

D114 0.23633 -0.00045 -0.00229 -0.03524 -0.03756 0.19877

D115 0.27671 -0.00037 -0.00186 -0.02369 -0.02562 0.25109

D116 -2.87989 -0.00049 -0.00251 -0.02154 -0.02412 -2.90401

D117 0.99517 -0.00007 0.00019 -0.03266 -0.03246 0.96271

D118 -2.15020 -0.00017 -0.00053 -0.03418 -0.03471 -2.18491

D119 -2.13243 0.00004 0.00080 -0.03462 -0.03382 -2.16625

D120 1.00539 -0.00005 0.00008 -0.03614 -0.03607 0.96932

D121 -3.13016 -0.00001 0.00027 -0.00430 -0.00402 -3.13417

D122 -0.00937 0.00001 0.00019 -0.00324 -0.00304 -0.01242

D123 0.01080 0.00000 0.00016 0.00192 0.00209 0.01288

D124 3.13158 0.00002 0.00008 0.00298 0.00306 3.13464

D125 -3.14099 -0.00002 -0.00024 0.00364 0.00340 -3.13758

D126 -0.01735 0.00000 -0.00018 0.00184 0.00167 -0.01568

D127 0.00125 -0.00003 -0.00013 -0.00255 -0.00268 -0.00144

D128 3.12489 -0.00001 -0.00007 -0.00434 -0.00442 3.12046

D129 -0.01459 0.00002 -0.00011 -0.00017 -0.00028 -0.01488

D130 3.12531 0.00001 -0.00008 0.00060 0.00051 3.12582

D131 -3.13529 -0.00000 -0.00003 -0.00122 -0.00125 -3.13655

D132 0.00461 -0.00001 -0.00001 -0.00045 -0.00046 0.00415

D133 0.00618 -0.00002 0.00003 -0.00099 -0.00096 0.00522

D134 -3.13440 -0.00002 0.00004 -0.00036 -0.00032 -3.13472

D135 -3.13371 -0.00001 0.00000 -0.00176 -0.00176 -3.13547

D136 0.00890 -0.00001 0.00001 -0.00113 -0.00112 0.00778

D137 0.00582 -0.00001 0.00000 0.00036 0.00037 0.00618

D138 -3.13378 0.00001 0.00008 0.00169 0.00177 -3.13201

D139 -3.13679 -0.00001 -0.00001 -0.00027 -0.00028 -3.13707

D140 0.00680 0.00001 0.00007 0.00106 0.00113 0.00793

D141 -0.00954 0.00003 0.00005 0.00143 0.00148 -0.00805

D142 -3.13307 0.00001 -0.00001 0.00321 0.00321 -3.12986

D143 3.13007 0.00001 -0.00002 0.00011 0.00008 3.13015

D144 0.00654 -0.00000 -0.00009 0.00189 0.00181 0.00834

D145 -0.00415 -0.00001 -0.00016 -0.00063 -0.00079 -0.00495

D146 3.13854 -0.00002 -0.00017 -0.00208 -0.00226 3.13628

D147 3.13420 -0.00001 -0.00007 -0.00004 -0.00012 3.13408

D148 -0.00630 -0.00001 -0.00009 -0.00149 -0.00158 -0.00788

D149 -0.00900 0.00003 0.00012 0.00237 0.00250 -0.00650

D150 3.12925 0.00002 0.00015 0.00183 0.00198 3.13122

D151 3.13584 0.00002 0.00004 0.00178 0.00182 3.13766

D152 -0.00911 0.00001 0.00006 0.00124 0.00130 -0.00780

D153 0.01951 -0.00005 -0.00021 -0.00342 -0.00363 0.01588

D154 3.13995 0.00003 0.00026 -0.00298 -0.00272 3.13724

D155 -3.12317 -0.00004 -0.00020 -0.00198 -0.00218 -3.12535

D156 -0.00273 0.00004 0.00028 -0.00153 -0.00126 -0.00399

D157 3.12449 0.00017 0.00126 0.00640 0.00767 3.13215

D158 -0.02135 0.00008 0.00061 0.00567 0.00628 -0.01507

D159 0.00395 0.00009 0.00080 0.00596 0.00676 0.01071

D160 3.14130 0.00001 0.00014 0.00523 0.00537 -3.13652

D161 -3.13770 -0.00015 -0.00130 -0.00465 -0.00595 3.13954

D162 0.02106 -0.00011 -0.00082 -0.00279 -0.00360 0.01746

D163 0.00816 -0.00007 -0.00064 -0.00393 -0.00458 0.00358

D164 -3.11627 -0.00003 -0.00016 -0.00207 -0.00223 -3.11850

D165 0.00691 0.00001 0.00029 -0.00006 0.00023 0.00714

D166 -3.13135 0.00002 0.00026 0.00048 0.00074 -3.13060

D167 3.13124 -0.00003 -0.00020 -0.00191 -0.00210 3.12914

D168 -0.00702 -0.00002 -0.00022 -0.00137 -0.00159 -0.00861

D169 -3.13707 -0.00016 -0.00138 -0.00545 -0.00682 3.13929

D170 0.02161 -0.00012 -0.00088 -0.00345 -0.00432 0.01729

D171 0.00824 -0.00007 -0.00066 -0.00397 -0.00464 0.00360

D172 -3.11627 -0.00003 -0.00016 -0.00197 -0.00213 -3.11841

D173 3.12384 0.00018 0.00134 0.00723 0.00857 3.13241

D174 0.00349 0.00010 0.00084 0.00661 0.00745 0.01094

D175 -0.02145 0.00009 0.00063 0.00574 0.00637 -0.01508

D176 3.14138 0.00001 0.00013 0.00512 0.00525 -3.13655

D177 0.00690 0.00001 0.00029 -0.00008 0.00021 0.00712

D178 -3.13138 0.00002 0.00027 0.00053 0.00080 -3.13058

D179 3.13132 -0.00003 -0.00021 -0.00207 -0.00228 3.12904

D180 -0.00697 -0.00002 -0.00024 -0.00146 -0.00169 -0.00866

D181 -0.00904 0.00003 0.00013 0.00243 0.00256 -0.00648

D182 3.13577 0.00003 0.00004 0.00185 0.00189 3.13766

D183 3.12923 0.00002 0.00015 0.00181 0.00197 3.13120

D184 -0.00915 0.00001 0.00006 0.00124 0.00130 -0.00784

D185 -0.00414 -0.00001 -0.00016 -0.00066 -0.00083 -0.00496

D186 3.13857 -0.00002 -0.00017 -0.00212 -0.00230 3.13627

D187 3.13424 -0.00001 -0.00007 -0.00008 -0.00016 3.13408

D188 -0.00624 -0.00001 -0.00008 -0.00155 -0.00163 -0.00787

D189 0.01957 -0.00005 -0.00022 -0.00345 -0.00368 0.01589

D190 3.13982 0.00003 0.00028 -0.00283 -0.00255 3.13727

D191 -3.12313 -0.00004 -0.00021 -0.00200 -0.00221 -3.12535

D192 -0.00288 0.00004 0.00029 -0.00138 -0.00108 -0.00396

D193 -3.14126 -0.00001 -0.00022 0.00393 0.00372 -3.13754

D194 -0.01762 0.00000 -0.00016 0.00210 0.00195 -0.01567

D195 0.00125 -0.00003 -0.00013 -0.00257 -0.00270 -0.00145

D196 3.12489 -0.00001 -0.00007 -0.00441 -0.00447 3.12042

D197 -3.12989 -0.00001 0.00024 -0.00457 -0.00432 -3.13421

D198 -0.00922 0.00001 0.00018 -0.00341 -0.00323 -0.01245

D199 0.01078 -0.00000 0.00015 0.00197 0.00212 0.01290

D200 3.13145 0.00003 0.00009 0.00313 0.00322 3.13466

D201 -0.00954 0.00003 0.00005 0.00142 0.00148 -0.00806

D202 3.13008 0.00001 -0.00002 0.00008 0.00006 3.13014

D203 -3.13307 0.00001 -0.00001 0.00325 0.00324 -3.12983

D204 0.00655 -0.00000 -0.00009 0.00191 0.00182 0.00837

D205 0.00582 -0.00001 -0.00000 0.00038 0.00037 0.00619

D206 -3.13676 -0.00001 -0.00001 -0.00031 -0.00032 -3.13708

D207 -3.13379 0.00001 0.00007 0.00172 0.00180 -3.13199

D208 0.00682 0.00001 0.00007 0.00104 0.00110 0.00793

D209 0.00617 -0.00002 0.00003 -0.00098 -0.00095 0.00522

D210 -3.13369 -0.00001 -0.00000 -0.00180 -0.00180 -3.13549

D211 -3.13444 -0.00002 0.00004 -0.00029 -0.00026 -3.13470

D212 0.00889 -0.00001 0.00001 -0.00111 -0.00111 0.00778

D213 -0.01458 0.00002 -0.00011 -0.00021 -0.00032 -0.01489

D214 -3.13516 -0.00000 -0.00004 -0.00136 -0.00140 -3.13657

D215 3.12529 0.00001 -0.00008 0.00060 0.00053 3.12582

D216 0.00470 -0.00001 -0.00001 -0.00055 -0.00056 0.00414

Item Value Threshold Converged?

Maximum Force 0.000612 0.000450 NO

RMS Force 0.000141 0.000300 YES

Maximum Displacement 0.798758 0.001800 NO

RMS Displacement 0.166954 0.001200 NO

Predicted change in Energy=-2.159437D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Aug 27 03:38:25 2019, MaxMem= 4294967296 cpu: 2.3

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

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=2 Diff= 7.69D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 1.347098 -3.995864 0.577551

2 6 0 1.570408 -2.661209 0.197951

3 7 0 0.336936 -2.085864 0.001024

4 6 0 -0.659918 -3.011174 0.208539

5 6 0 -0.033604 -4.212512 0.585012

6 6 0 -2.067127 -2.784686 0.022011

7 6 0 -2.668619 -1.531290 -0.130772

8 7 0 -2.043473 -0.321031 0.035147

9 6 0 -3.017863 0.631566 -0.140848

10 6 0 -4.289169 0.000002 -0.488421

11 6 0 -4.073913 -1.334712 -0.481368

12 6 0 2.837686 -2.010194 0.002086

13 6 0 3.017911 -0.631605 -0.140128

14 6 0 4.289268 -0.000156 -0.487703

15 6 0 4.074016 1.334564 -0.481061

16 6 0 2.668687 1.531254 -0.130679

17 7 0 2.043517 0.321049 0.035533

18 6 0 2.067156 2.784689 0.021703

19 6 0 0.659903 3.011144 0.207988

20 6 0 0.033590 4.212221 0.585276

21 6 0 -1.347116 3.995582 0.577682

22 6 0 -1.570427 2.661199 0.197147

23 7 0 -0.336963 2.086003 -0.000221

24 6 0 -2.837710 2.010180 0.001217

25 6 0 -2.926185 -3.993814 0.012197

26 6 0 -2.678919 -5.043512 -0.885512

27 6 0 -3.492270 -6.171979 -0.897504

28 6 0 -4.556089 -6.280184 -0.001416

29 6 0 -4.804665 -5.248830 0.902807

30 6 0 -4.000070 -4.112964 0.907013

31 6 0 6.278301 -4.572642 -0.096040

32 6 0 5.216385 -4.790606 -0.974232

33 6 0 4.096509 -3.966608 -0.936253

34 6 0 4.026129 -2.896469 -0.030978

35 6 0 5.100139 -2.686833 0.846436

36 6 0 6.214340 -3.520791 0.816363

37 6 0 -4.026165 2.896424 -0.031429

38 6 0 -5.100141 2.686273 0.845925

39 6 0 -6.214276 3.520330 0.816518

40 6 0 -6.278226 4.572840 -0.095124

41 6 0 -5.216358 4.791334 -0.973245

42 6 0 -4.096546 3.967219 -0.935934

43 6 0 2.926181 3.993818 0.012018

44 6 0 4.000160 4.112856 0.906750

45 6 0 4.804691 5.248765 0.902685

46 6 0 4.555973 6.280283 -0.001314

47 6 0 3.492063 6.172201 -0.897311

48 6 0 2.678767 5.043698 -0.885450

49 1 0 2.115176 -4.711513 0.822255

50 1 0 -0.542511 -5.129055 0.836265

51 1 0 -5.206289 0.514700 -0.730078

52 1 0 -4.782240 -2.114206 -0.715634

53 1 0 5.206427 -0.514930 -0.729064

54 1 0 4.782371 2.113989 -0.715472

55 1 0 0.542509 5.128554 0.837279

56 1 0 -2.115181 4.711026 0.823021

57 1 0 -1.856659 -4.962475 -1.587005

58 1 0 -3.295906 -6.967855 -1.608039

59 1 0 -5.185785 -7.163486 -0.007404

60 1 0 -5.624313 -5.328740 1.609011

61 1 0 -4.190528 -3.318390 1.619301

62 1 0 7.148189 -5.220241 -0.121881

63 1 0 5.260548 -5.604062 -1.690692

64 1 0 3.276095 -4.138033 -1.623631

65 1 0 5.050492 -1.877543 1.565699

66 1 0 7.031373 -3.350089 1.509291

67 1 0 -5.050494 1.876530 1.564679

68 1 0 -7.031259 3.349215 1.509406

69 1 0 -7.148063 5.220528 -0.120446

70 1 0 -5.260494 5.605297 -1.689131

71 1 0 -3.276159 4.139081 -1.623234

72 1 0 4.190722 3.318173 1.618888

73 1 0 5.624400 5.328587 1.608829

74 1 0 5.185617 7.163623 -0.007184

75 1 0 3.295577 6.968210 -1.607664

76 1 0 1.856427 4.962768 -1.586861

77 1 0 0.187383 -1.110754 -0.219693

78 1 0 -0.187477 1.111159 -0.222127

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

Rotational constants (GHZ): 0.0588269 0.0583397 0.0300987

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

Standard basis: 6-311G(d) (5D, 7F)

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

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5358.3591606316 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2123081876 Hartrees.

Nuclear repulsion after empirical dispersion term = 5358.1468524440 Hartrees.

Force inversion solution in PCM.

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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 : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5738

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.33D-09

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 311

GePol: Fraction of low-weight points (<1% of avg) = 5.42%

GePol: Cavity surface area = 611.553 Ang\*\*2

GePol: Cavity volume = 629.011 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021275177 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5358.1447249263 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.

NBasis= 954 RedAO= T EigKep= 1.30D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Aug 27 03:38:27 2019, MaxMem= 4294967296 cpu: 2.5

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

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= 0.000000 -0.000000 -0.000000

Rot= 0.962403 -0.000017 0.000001 -0.271624 Ang= -31.52 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0549 S= 1.0182

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30558787236

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 580000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 98773932.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.22D-15 for 5729.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.57D-15 for 3794 3497.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.77D-15 for 5729.

Iteration 1 A^-1\*A deviation from orthogonality is 2.53D-11 for 4065 4064.

E= -1914.28505168937

DIIS: error= 7.73D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.28505168937 IErMin= 1 ErrMin= 7.73D-03

ErrMax= 7.73D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.11D-01 BMatP= 1.11D-01

IDIUse=3 WtCom= 9.23D-01 WtEn= 7.73D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.642 Goal= None Shift= 0.000

Gap= 0.707 Goal= None Shift= 0.000

GapD= 0.642 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=2.02D-04 MaxDP=7.17D-03 OVMax= 2.47D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.02D-04 CP: 9.99D-01

E= -1914.33247249889 Delta-E= -0.047420809526 Rises=F Damp=F

DIIS: error= 5.94D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33247249889 IErMin= 2 ErrMin= 5.94D-04

ErrMax= 5.94D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-03 BMatP= 1.11D-01

IDIUse=3 WtCom= 9.94D-01 WtEn= 5.94D-03

Coeff-Com: -0.636D-01 0.106D+01

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

Coeff: -0.632D-01 0.106D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.73D-05 MaxDP=1.55D-03 DE=-4.74D-02 OVMax= 9.01D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.31D-05 CP: 9.99D-01 1.09D+00

E= -1914.33297825328 Delta-E= -0.000505754384 Rises=F Damp=F

DIIS: error= 3.63D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33297825328 IErMin= 3 ErrMin= 3.63D-04

ErrMax= 3.63D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.63D-04 BMatP= 1.04D-03

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.63D-03

Coeff-Com: -0.323D-01 0.476D+00 0.556D+00

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

Coeff: -0.321D-01 0.475D+00 0.557D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.37D-05 MaxDP=1.09D-03 DE=-5.06D-04 OVMax= 3.64D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.18D-05 CP: 9.99D-01 1.10D+00 7.98D-01

E= -1914.33307856439 Delta-E= -0.000100311114 Rises=F Damp=F

DIIS: error= 1.79D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33307856439 IErMin= 4 ErrMin= 1.79D-04

ErrMax= 1.79D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.57D-05 BMatP= 4.63D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.79D-03

Coeff-Com: -0.493D-02 0.491D-01 0.310D+00 0.646D+00

Coeff-En: 0.000D+00 0.000D+00 0.154D+00 0.846D+00

Coeff: -0.492D-02 0.490D-01 0.310D+00 0.646D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=6.10D-06 MaxDP=3.73D-04 DE=-1.00D-04 OVMax= 3.46D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.71D-06 CP: 9.99D-01 1.10D+00 9.00D-01 8.56D-01

E= -1914.33310630822 Delta-E= -0.000027743829 Rises=F Damp=F

DIIS: error= 5.29D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33310630822 IErMin= 5 ErrMin= 5.29D-05

ErrMax= 5.29D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.17D-06 BMatP= 9.57D-05

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

Coeff-Com: 0.192D-03-0.144D-01 0.941D-01 0.282D+00 0.638D+00

Coeff: 0.192D-03-0.144D-01 0.941D-01 0.282D+00 0.638D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=3.05D-06 MaxDP=1.86D-04 DE=-2.77D-05 OVMax= 2.56D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.46D-06 CP: 9.99D-01 1.10D+00 9.24D-01 9.71D-01 1.18D+00

E= -1914.33310942808 Delta-E= -0.000003119863 Rises=F Damp=F

DIIS: error= 4.02D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33310942808 IErMin= 6 ErrMin= 4.02D-05

ErrMax= 4.02D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.23D-06 BMatP= 6.17D-06

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

Coeff-Com: 0.942D-03-0.171D-01 0.233D-02 0.588D-01 0.383D+00 0.572D+00

Coeff: 0.942D-03-0.171D-01 0.233D-02 0.588D-01 0.383D+00 0.572D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=2.19D-06 MaxDP=1.51D-04 DE=-3.12D-06 OVMax= 1.95D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.18D-06 CP: 9.99D-01 1.10D+00 9.47D-01 1.01D+00 1.50D+00

CP: 1.23D+00

E= -1914.33311123839 Delta-E= -0.000001810303 Rises=F Damp=F

DIIS: error= 3.51D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33311123839 IErMin= 7 ErrMin= 3.51D-05

ErrMax= 3.51D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.05D-07 BMatP= 2.23D-06

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

Coeff-Com: 0.210D-03-0.158D-02-0.184D-01-0.346D-01-0.203D-01 0.142D+00

Coeff-Com: 0.933D+00

Coeff: 0.210D-03-0.158D-02-0.184D-01-0.346D-01-0.203D-01 0.142D+00

Coeff: 0.933D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=2.59D-06 MaxDP=1.94D-04 DE=-1.81D-06 OVMax= 2.61D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 5.59D-07 CP: 9.99D-01 1.10D+00 9.64D-01 1.08D+00 1.85D+00

CP: 1.86D+00 1.48D+00

E= -1914.33311262717 Delta-E= -0.000001388786 Rises=F Damp=F

DIIS: error= 2.74D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33311262717 IErMin= 8 ErrMin= 2.74D-05

ErrMax= 2.74D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.05D-07 BMatP= 5.05D-07

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

Coeff-Com: -0.663D-03 0.143D-01-0.199D-01-0.818D-01-0.370D+00-0.423D+00

Coeff-Com: 0.867D+00 0.101D+01

Coeff: -0.663D-03 0.143D-01-0.199D-01-0.818D-01-0.370D+00-0.423D+00

Coeff: 0.867D+00 0.101D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=4.20D-06 MaxDP=3.04D-04 DE=-1.39D-06 OVMax= 4.38D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 5.66D-07 CP: 9.99D-01 1.10D+00 9.93D-01 1.17D+00 2.44D+00

CP: 2.77D+00 2.70D+00 1.57D+00

E= -1914.33311407637 Delta-E= -0.000001449195 Rises=F Damp=F

DIIS: error= 1.44D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33311407637 IErMin= 9 ErrMin= 1.44D-05

ErrMax= 1.44D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.52D-08 BMatP= 4.05D-07

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

Coeff-Com: -0.229D-03 0.359D-02 0.321D-02 0.235D-02-0.594D-01-0.189D+00

Coeff-Com: -0.198D+00 0.331D+00 0.111D+01

Coeff: -0.229D-03 0.359D-02 0.321D-02 0.235D-02-0.594D-01-0.189D+00

Coeff: -0.198D+00 0.331D+00 0.111D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=2.50D-06 MaxDP=1.97D-04 DE=-1.45D-06 OVMax= 2.71D-03

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.01D-06 CP: 9.99D-01 1.10D+00 1.01D+00 1.23D+00 2.77D+00

CP: 3.00D+00 3.00D+00 2.45D+00 1.73D+00

E= -1914.33311444742 Delta-E= -0.000000371052 Rises=F Damp=F

DIIS: error= 5.82D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33311444742 IErMin=10 ErrMin= 5.82D-06

ErrMax= 5.82D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.69D-08 BMatP= 9.52D-08

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

Coeff-Com: 0.284D-04-0.137D-02 0.606D-02 0.212D-01 0.575D-01-0.236D-01

Coeff-Com: -0.315D+00-0.305D-01 0.577D+00 0.709D+00

Coeff: 0.284D-04-0.137D-02 0.606D-02 0.212D-01 0.575D-01-0.236D-01

Coeff: -0.315D+00-0.305D-01 0.577D+00 0.709D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=9.07D-07 MaxDP=7.20D-05 DE=-3.71D-07 OVMax= 1.00D-03

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.73D-07 CP: 9.99D-01 1.10D+00 1.01D+00 1.24D+00 2.88D+00

CP: 3.00D+00 3.00D+00 2.83D+00 2.23D+00 1.56D+00

E= -1914.33311451193 Delta-E= -0.000000064510 Rises=F Damp=F

DIIS: error= 3.81D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33311451193 IErMin=11 ErrMin= 3.81D-06

ErrMax= 3.81D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.06D-08 BMatP= 3.69D-08

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

Coeff-Com: 0.919D-04-0.181D-02 0.869D-03 0.825D-02 0.491D-01 0.453D-01

Coeff-Com: -0.418D-01-0.105D+00-0.214D+00 0.295D+00 0.964D+00

Coeff: 0.919D-04-0.181D-02 0.869D-03 0.825D-02 0.491D-01 0.453D-01

Coeff: -0.418D-01-0.105D+00-0.214D+00 0.295D+00 0.964D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=4.60D-07 MaxDP=3.84D-05 DE=-6.45D-08 OVMax= 4.94D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.31D-07 CP: 9.99D-01 1.10D+00 1.02D+00 1.25D+00 2.93D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.62D+00 1.83D+00

CP: 1.17D+00

E= -1914.33311453376 Delta-E= -0.000000021828 Rises=F Damp=F

DIIS: error= 1.69D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.33311453376 IErMin=12 ErrMin= 1.69D-06

ErrMax= 1.69D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.66D-09 BMatP= 1.06D-08

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

Coeff-Com: 0.357D-04-0.458D-03-0.160D-02-0.208D-02 0.797D-02 0.227D-01

Coeff-Com: 0.755D-01-0.310D-01-0.289D+00-0.635D-01 0.491D+00 0.791D+00

Coeff: 0.357D-04-0.458D-03-0.160D-02-0.208D-02 0.797D-02 0.227D-01

Coeff: 0.755D-01-0.310D-01-0.289D+00-0.635D-01 0.491D+00 0.791D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=2.17D-07 MaxDP=1.76D-05 DE=-2.18D-08 OVMax= 2.19D-04

Cycle 13 Pass 1 IDiag 1:

RMSU= 6.00D-08 CP: 9.99D-01 1.10D+00 1.02D+00 1.25D+00 2.94D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.82D+00 1.95D+00

CP: 1.30D+00 1.65D+00

E= -1914.33311453967 Delta-E= -0.000000005909 Rises=F Damp=F

DIIS: error= 7.16D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.33311453967 IErMin=13 ErrMin= 7.16D-07

ErrMax= 7.16D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.44D-10 BMatP= 3.66D-09

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

Coeff-Com: -0.163D-04 0.444D-03-0.113D-02-0.377D-02-0.137D-01-0.822D-02

Coeff-Com: 0.495D-01 0.276D-01-0.564D-01-0.140D+00-0.126D+00 0.337D+00

Coeff-Com: 0.934D+00

Coeff: -0.163D-04 0.444D-03-0.113D-02-0.377D-02-0.137D-01-0.822D-02

Coeff: 0.495D-01 0.276D-01-0.564D-01-0.140D+00-0.126D+00 0.337D+00

Coeff: 0.934D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.30D-07 MaxDP=1.12D-05 DE=-5.91D-09 OVMax= 1.31D-04

Cycle 14 Pass 1 IDiag 1:

RMSU= 2.26D-08 CP: 9.99D-01 1.10D+00 1.02D+00 1.25D+00 2.95D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.94D+00 2.02D+00

CP: 1.40D+00 2.14D+00 1.29D+00

E= -1914.33311454123 Delta-E= -0.000000001562 Rises=F Damp=F

DIIS: error= 3.33D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.33311454123 IErMin=14 ErrMin= 3.33D-07

ErrMax= 3.33D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.69D-10 BMatP= 8.44D-10

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

Coeff-Com: -0.126D-04 0.248D-03-0.110D-03-0.976D-03-0.671D-02-0.754D-02

Coeff-Com: 0.259D-02 0.159D-01 0.350D-01-0.430D-01-0.137D+00-0.195D-01

Coeff-Com: 0.365D+00 0.796D+00

Coeff: -0.126D-04 0.248D-03-0.110D-03-0.976D-03-0.671D-02-0.754D-02

Coeff: 0.259D-02 0.159D-01 0.350D-01-0.430D-01-0.137D+00-0.195D-01

Coeff: 0.365D+00 0.796D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=4.82D-08 MaxDP=4.16D-06 DE=-1.56D-09 OVMax= 5.04D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.31D-08 CP: 9.99D-01 1.10D+00 1.02D+00 1.25D+00 2.96D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.96D+00 2.05D+00

CP: 1.45D+00 2.25D+00 1.42D+00 1.12D+00

E= -1914.33311454142 Delta-E= -0.000000000195 Rises=F Damp=F

DIIS: error= 2.39D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.33311454142 IErMin=15 ErrMin= 2.39D-07

ErrMax= 2.39D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.82D-11 BMatP= 1.69D-10

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

Coeff-Com: -0.377D-05 0.370D-04 0.269D-03 0.467D-03-0.569D-03-0.264D-02

Coeff-Com: -0.135D-01 0.302D-02 0.421D-01 0.110D-01-0.550D-01-0.107D+00

Coeff-Com: -0.130D-01 0.536D+00 0.598D+00

Coeff: -0.377D-05 0.370D-04 0.269D-03 0.467D-03-0.569D-03-0.264D-02

Coeff: -0.135D-01 0.302D-02 0.421D-01 0.110D-01-0.550D-01-0.107D+00

Coeff: -0.130D-01 0.536D+00 0.598D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.53D-08 MaxDP=1.37D-06 DE=-1.95D-10 OVMax= 1.47D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 7.55D-09 CP: 9.99D-01 1.10D+00 1.02D+00 1.25D+00 2.96D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.97D+00 2.06D+00

CP: 1.45D+00 2.26D+00 1.43D+00 1.35D+00 1.01D+00

E= -1914.33311454145 Delta-E= -0.000000000027 Rises=F Damp=F

DIIS: error= 1.25D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1914.33311454145 IErMin=16 ErrMin= 1.25D-07

ErrMax= 1.25D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.74D-11 BMatP= 9.82D-11

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

Coeff-Com: 0.779D-06-0.376D-04 0.189D-03 0.490D-03 0.121D-02 0.495D-03

Coeff-Com: -0.883D-02-0.251D-02 0.156D-01 0.157D-01 0.501D-03-0.556D-01

Coeff-Com: -0.965D-01 0.938D-01 0.330D+00 0.705D+00

Coeff: 0.779D-06-0.376D-04 0.189D-03 0.490D-03 0.121D-02 0.495D-03

Coeff: -0.883D-02-0.251D-02 0.156D-01 0.157D-01 0.501D-03-0.556D-01

Coeff: -0.965D-01 0.938D-01 0.330D+00 0.705D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.35D-08 MaxDP=1.03D-06 DE=-2.73D-11 OVMax= 1.33D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 2.44D-09 CP: 9.99D-01 1.10D+00 1.02D+00 1.25D+00 2.96D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.97D+00 2.07D+00

CP: 1.46D+00 2.27D+00 1.46D+00 1.44D+00 1.27D+00

CP: 9.83D-01

E= -1914.33311454147 Delta-E= -0.000000000015 Rises=F Damp=F

DIIS: error= 4.36D-08 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1914.33311454147 IErMin=17 ErrMin= 4.36D-08

ErrMax= 4.36D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.99D-12 BMatP= 1.74D-11

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

Coeff-Com: 0.118D-05-0.263D-04 0.363D-04 0.137D-03 0.697D-03 0.939D-03

Coeff-Com: -0.130D-02-0.184D-02-0.125D-02 0.496D-02 0.119D-01-0.249D-02

Coeff-Com: -0.414D-01-0.706D-01 0.314D-01 0.382D+00 0.687D+00

Coeff: 0.118D-05-0.263D-04 0.363D-04 0.137D-03 0.697D-03 0.939D-03

Coeff: -0.130D-02-0.184D-02-0.125D-02 0.496D-02 0.119D-01-0.249D-02

Coeff: -0.414D-01-0.706D-01 0.314D-01 0.382D+00 0.687D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=2.59D-09 MaxDP=1.28D-07 DE=-1.46D-11 OVMax= 2.05D-06

Error on total polarization charges = 0.08280

SCF Done: E(UB3LYP) = -1914.33311454 A.U. after 17 cycles

NFock= 17 Conv=0.26D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0552 S= 1.0183

<L.S>= 0.000000000000E+00

KE= 1.906385082948D+03 PE=-1.516594113905D+04 EE= 5.987078216631D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.34

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0552, after 2.0017

Leave Link 502 at Tue Aug 27 03:46:13 2019, MaxMem= 4294967296 cpu: 7293.0

(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: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48545387D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64555514D-01

Leave Link 801 at Tue Aug 27 03:46:13 2019, MaxMem= 4294967296 cpu: 0.8

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

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

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

Leave Link 1101 at Tue Aug 27 03:46:20 2019, MaxMem= 4294967296 cpu: 110.5

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

Symmetrizing basis deriv contribution to polar:

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

Leave Link 1102 at Tue Aug 27 03:46:20 2019, MaxMem= 4294967296 cpu: 2.3

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

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 187

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 27 04:06:02 2019, MaxMem= 4294967296 cpu: 18908.5

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

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 580000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.40D+03 4.44D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.50D+02 3.27D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.47D+00 4.51D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.04D-01 3.92D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.74D-04 2.13D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.57D-06 1.34D-04.

192 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 1.99D-08 9.45D-06.

72 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.24D-11 6.10D-07.

3 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.13D-13 3.80D-08.

2 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 7.80D-15 2.97D-09.

InvSVY: IOpt=1 It= 1 EMax= 1.42D-14

Solved reduced A of dimension 1676 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1132.42 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 27 07:57:37 2019, MaxMem= 4294967296 cpu: 222258.5

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 187

Leave Link 701 at Tue Aug 27 07:59:06 2019, MaxMem= 4294967296 cpu: 1421.3

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

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

Leave Link 702 at Tue Aug 27 07:59:06 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

Leave Link 703 at Tue Aug 27 08:17:43 2019, MaxMem= 4294967296 cpu: 17880.3

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

Dipole =-1.96594516D-04 5.50890836D-04-4.88635291D-01

Polarizability= 1.27234754D+03-6.87165709D+01 1.67697080D+03

1.38687199D-02-1.19959951D-02 4.47954581D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000004350 -0.000056521 -0.000126772

2 6 -0.000057597 0.000055742 0.000059075

3 7 0.000065369 -0.000084278 -0.000051198

4 6 0.000011294 -0.000036164 0.000016065

5 6 -0.000019870 0.000044638 0.000079845

6 6 0.000100070 -0.000050321 -0.000071683

7 6 0.000077799 -0.000003429 0.000031100

8 7 -0.000184292 0.000161690 -0.000010531

9 6 0.000214631 0.000101251 0.000091688

10 6 0.000042688 0.000016490 0.000042758

11 6 -0.000137950 -0.000047568 -0.000029390

12 6 0.000222030 -0.000169751 0.000070329

13 6 -0.000205558 0.000097397 -0.000095582

14 6 -0.000045664 0.000018441 -0.000040202

15 6 0.000139830 -0.000049611 0.000031735

16 6 -0.000075030 -0.000005469 -0.000037713

17 7 0.000179968 0.000166237 0.000004371

18 6 -0.000098649 -0.000049539 0.000077294

19 6 -0.000012869 -0.000036721 -0.000020490

20 6 0.000020832 0.000043922 -0.000078967

21 6 0.000005163 -0.000055171 0.000129215

22 6 0.000056693 0.000054673 -0.000063055

23 7 -0.000062386 -0.000085329 0.000052774

24 6 -0.000232178 -0.000173097 -0.000064761

25 6 -0.000069811 -0.000107661 -0.000036212

26 6 0.000034911 -0.000005492 -0.000081520

27 6 -0.000089897 0.000011523 -0.000008372

28 6 -0.000041067 0.000082459 0.000007444

29 6 0.000006359 0.000042590 0.000053352

30 6 0.000090169 0.000025054 0.000111534

31 6 0.000001628 0.000019823 -0.000067786

32 6 -0.000025011 -0.000009503 0.000003192

33 6 -0.000020470 0.000103997 -0.000063814

34 6 -0.000003704 0.000054088 0.000045668

35 6 0.000079720 -0.000021686 0.000117085

36 6 -0.000023031 -0.000005290 -0.000017354

37 6 0.000006607 0.000045906 -0.000048967

38 6 -0.000078763 -0.000022842 -0.000119219

39 6 0.000020911 -0.000006484 0.000014506

40 6 -0.000000256 0.000024501 0.000069084

41 6 0.000027282 -0.000007404 -0.000001666

42 6 0.000022651 0.000107465 0.000068625

43 6 0.000069311 -0.000106240 0.000035001

44 6 -0.000090789 0.000024714 -0.000111400

45 6 -0.000005861 0.000043789 -0.000053081

46 6 0.000040671 0.000082149 -0.000007866

47 6 0.000088825 0.000011455 0.000008507

48 6 -0.000034809 -0.000006631 0.000079302

49 1 -0.000016694 0.000023560 -0.000015979

50 1 -0.000068829 -0.000020101 -0.000007649

51 1 -0.000015480 -0.000022200 0.000028669

52 1 0.000039794 -0.000062995 0.000011275

53 1 0.000013096 -0.000021380 -0.000030565

54 1 -0.000039165 -0.000062550 -0.000011311

55 1 0.000069049 -0.000019396 0.000010014

56 1 0.000016587 0.000023940 0.000014384

57 1 0.000043996 0.000041263 0.000003329

58 1 0.000009328 0.000029918 -0.000034661

59 1 0.000033174 -0.000011952 -0.000005016

60 1 0.000017819 -0.000000379 -0.000012853

61 1 0.000011321 -0.000033238 -0.000001940

62 1 0.000009889 -0.000027086 0.000032866

63 1 0.000002308 0.000016479 0.000016656

64 1 0.000014924 0.000060647 0.000065236

65 1 -0.000050216 -0.000043803 -0.000040291

66 1 0.000013543 -0.000033095 0.000004341

67 1 0.000049483 -0.000041718 0.000041405

68 1 -0.000013279 -0.000032724 -0.000004225

69 1 -0.000009810 -0.000027821 -0.000032756

70 1 -0.000002474 0.000015218 -0.000017487

71 1 -0.000016499 0.000060952 -0.000066066

72 1 -0.000011948 -0.000033132 0.000001667

73 1 -0.000017643 -0.000000569 0.000012638

74 1 -0.000032847 -0.000011586 0.000004901

75 1 -0.000009163 0.000029838 0.000034933

76 1 -0.000043912 0.000041015 -0.000003498

77 1 0.000048222 -0.000036567 -0.000440466

78 1 -0.000050123 -0.000038329 0.000450494

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

Cartesian Forces: Max 0.000450494 RMS 0.000075835

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

Leave Link 716 at Tue Aug 27 08:17:44 2019, MaxMem= 4294967296 cpu: 1.8

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000513606 RMS 0.000119846

Search for a local minimum.

Step number 9 out of a maximum of 452

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

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= 2.07D-04 DEPred=-2.16D-04 R=-9.58D-01

Trust test=-9.58D-01 RLast= 2.62D-01 DXMaxT set to 8.92D-02

ITU= -1 1 -1 -1 1 1 -1 1 0

Eigenvalues --- -0.00055 0.00042 0.00427 0.00545 0.00588

Eigenvalues --- 0.00665 0.00756 0.01014 0.01031 0.01096

Eigenvalues --- 0.01107 0.01123 0.01240 0.01258 0.01280

Eigenvalues --- 0.01286 0.01304 0.01371 0.01419 0.01574

Eigenvalues --- 0.01593 0.01625 0.01637 0.01665 0.01702

Eigenvalues --- 0.01702 0.01711 0.01729 0.01750 0.01760

Eigenvalues --- 0.01769 0.01770 0.01776 0.01776 0.01879

Eigenvalues --- 0.01936 0.01966 0.01990 0.02018 0.02105

Eigenvalues --- 0.02180 0.02219 0.02270 0.02293 0.02302

Eigenvalues --- 0.02319 0.02366 0.02411 0.02459 0.02498

Eigenvalues --- 0.02543 0.02544 0.02564 0.02631 0.02637

Eigenvalues --- 0.02643 0.02650 0.02730 0.02766 0.02778

Eigenvalues --- 0.02783 0.02792 0.02803 0.02853 0.02853

Eigenvalues --- 0.02861 0.02861 0.03925 0.04095 0.04173

Eigenvalues --- 0.04236 0.04338 0.04456 0.04537 0.04568

Eigenvalues --- 0.08473 0.09583 0.09713 0.09734 0.09849

Eigenvalues --- 0.09861 0.10354 0.10463 0.10594 0.10695

Eigenvalues --- 0.10733 0.10733 0.10738 0.10739 0.11174

Eigenvalues --- 0.11406 0.11409 0.11419 0.11421 0.11970

Eigenvalues --- 0.11975 0.11996 0.12004 0.12320 0.12320

Eigenvalues --- 0.12323 0.12324 0.12763 0.12765 0.12783

Eigenvalues --- 0.12784 0.15414 0.15864 0.15971 0.16320

Eigenvalues --- 0.17279 0.17414 0.17612 0.18008 0.18255

Eigenvalues --- 0.18306 0.18327 0.18473 0.19250 0.19297

Eigenvalues --- 0.19371 0.19411 0.19421 0.19425 0.19432

Eigenvalues --- 0.19434 0.19546 0.19546 0.19552 0.19552

Eigenvalues --- 0.20314 0.21530 0.22032 0.22803 0.22875

Eigenvalues --- 0.23025 0.23763 0.24184 0.24773 0.25388

Eigenvalues --- 0.26348 0.26600 0.26726 0.27055 0.28586

Eigenvalues --- 0.28667 0.28791 0.29020 0.29777 0.30952

Eigenvalues --- 0.31642 0.32055 0.32709 0.32869 0.33171

Eigenvalues --- 0.33409 0.33695 0.34087 0.35218 0.35595

Eigenvalues --- 0.35641 0.35643 0.35655 0.35655 0.35761

Eigenvalues --- 0.35762 0.35784 0.35834 0.35935 0.35935

Eigenvalues --- 0.35943 0.35944 0.36008 0.36013 0.36023

Eigenvalues --- 0.36033 0.36214 0.36216 0.36267 0.36302

Eigenvalues --- 0.36919 0.37066 0.37237 0.37414 0.37428

Eigenvalues --- 0.37497 0.38156 0.38364 0.38679 0.38680

Eigenvalues --- 0.39471 0.40216 0.40727 0.41064 0.41122

Eigenvalues --- 0.41160 0.41253 0.41262 0.41287 0.41359

Eigenvalues --- 0.41549 0.41932 0.42514 0.42688 0.44621

Eigenvalues --- 0.45017 0.45531 0.45898 0.45921 0.45942

Eigenvalues --- 0.45975 0.46045 0.46273 0.46273 0.46291

Eigenvalues --- 0.46306 0.48656 0.49096 0.49670 0.49689

Eigenvalues --- 0.50742 0.50743 0.50781 0.50784 0.51812

Eigenvalues --- 0.52114 0.57066 0.57426

Eigenvalue 1 is -5.50D-04 should be greater than 0.000000 Eigenvector:

D90 D92 D35 D89 D33

1 0.17877 0.17621 0.17613 0.17585 0.17431

D36 D91 D120 D34 D116

1 0.17359 0.17329 -0.17219 0.17177 0.17111

Cosine: 0.939 < 0.970

Cut down GDIIS temporarily because of the cosine check. E 6

Eigenvalues --- -0.00055 0.00042 0.00427 0.00545 0.00588

Eigenvalues --- 0.00665 0.00756 0.01014 0.01031 0.01096

Eigenvalues --- 0.01107 0.01123 0.01240 0.01258 0.01280

Eigenvalues --- 0.01286 0.01304 0.01371 0.01419 0.01574

Eigenvalues --- 0.01593 0.01625 0.01637 0.01665 0.01702

Eigenvalues --- 0.01702 0.01711 0.01729 0.01750 0.01760

Eigenvalues --- 0.01769 0.01770 0.01776 0.01776 0.01879

Eigenvalues --- 0.01936 0.01966 0.01990 0.02018 0.02105

Eigenvalues --- 0.02180 0.02219 0.02270 0.02293 0.02302

Eigenvalues --- 0.02319 0.02366 0.02411 0.02459 0.02498

Eigenvalues --- 0.02543 0.02544 0.02564 0.02631 0.02637

Eigenvalues --- 0.02643 0.02650 0.02730 0.02766 0.02778

Eigenvalues --- 0.02783 0.02792 0.02803 0.02853 0.02853

Eigenvalues --- 0.02861 0.02861 0.03925 0.04095 0.04173

Eigenvalues --- 0.04236 0.04338 0.04456 0.04537 0.04568

Eigenvalues --- 0.08473 0.09583 0.09713 0.09734 0.09849

Eigenvalues --- 0.09861 0.10354 0.10463 0.10594 0.10695

Eigenvalues --- 0.10733 0.10733 0.10738 0.10739 0.11174

Eigenvalues --- 0.11406 0.11409 0.11419 0.11421 0.11970

Eigenvalues --- 0.11975 0.11996 0.12004 0.12320 0.12320

Eigenvalues --- 0.12323 0.12324 0.12763 0.12765 0.12783

Eigenvalues --- 0.12784 0.15414 0.15864 0.15971 0.16320

Eigenvalues --- 0.17279 0.17414 0.17612 0.18008 0.18255

Eigenvalues --- 0.18306 0.18327 0.18473 0.19250 0.19297

Eigenvalues --- 0.19371 0.19411 0.19421 0.19425 0.19432

Eigenvalues --- 0.19434 0.19546 0.19546 0.19552 0.19552

Eigenvalues --- 0.20314 0.21530 0.22032 0.22803 0.22875

Eigenvalues --- 0.23025 0.23763 0.24184 0.24773 0.25388

Eigenvalues --- 0.26348 0.26600 0.26726 0.27055 0.28586

Eigenvalues --- 0.28667 0.28791 0.29020 0.29777 0.30952

Eigenvalues --- 0.31642 0.32055 0.32709 0.32869 0.33171

Eigenvalues --- 0.33409 0.33695 0.34087 0.35218 0.35595

Eigenvalues --- 0.35641 0.35643 0.35655 0.35655 0.35761

Eigenvalues --- 0.35762 0.35784 0.35834 0.35935 0.35935

Eigenvalues --- 0.35943 0.35944 0.36008 0.36013 0.36023

Eigenvalues --- 0.36033 0.36214 0.36216 0.36267 0.36302

Eigenvalues --- 0.36919 0.37066 0.37237 0.37414 0.37428

Eigenvalues --- 0.37497 0.38156 0.38364 0.38679 0.38680

Eigenvalues --- 0.39471 0.40216 0.40727 0.41064 0.41122

Eigenvalues --- 0.41160 0.41253 0.41262 0.41287 0.41359

Eigenvalues --- 0.41549 0.41932 0.42514 0.42688 0.44621

Eigenvalues --- 0.45017 0.45531 0.45898 0.45921 0.45942

Eigenvalues --- 0.45975 0.46045 0.46273 0.46273 0.46291

Eigenvalues --- 0.46306 0.48656 0.49096 0.49670 0.49689

Eigenvalues --- 0.50742 0.50743 0.50781 0.50784 0.51812

Eigenvalues --- 0.52114 0.57066 0.57426

Eigenvalue 1 is -5.50D-04 should be greater than 0.000000 Eigenvector:

D90 D92 D35 D89 D33

1 0.17877 0.17621 0.17613 0.17585 0.17431

D36 D91 D120 D34 D116

1 0.17359 0.17329 -0.17219 0.17177 0.17111

Quadratic step=1.474D+00 exceeds max=8.919D-02 adjusted using Lamda=-9.122D-03.

Angle between NR and scaled steps= 18.81 degrees.

Angle between quadratic step and forces= 59.31 degrees.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.02986831 RMS(Int)= 0.00020555

Iteration 2 RMS(Cart)= 0.00036841 RMS(Int)= 0.00001411

Iteration 3 RMS(Cart)= 0.00000006 RMS(Int)= 0.00001411

ITry= 1 IFail=0 DXMaxC= 1.08D-01 DCOld= 1.00D+10 DXMaxT= 8.92D-02 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.65590 0.00010 0.00000 0.00060 0.00061 2.65651

R2 2.64111 -0.00005 0.00000 -0.00040 -0.00038 2.64073

R3 2.03703 -0.00003 0.00000 -0.00013 -0.00013 2.03690

R4 2.59881 0.00020 0.00000 0.00080 0.00079 2.59960

R5 2.71764 0.00025 0.00000 -0.00055 -0.00055 2.71710

R6 2.59999 -0.00029 0.00000 -0.00032 -0.00033 2.59966

R7 1.91033 -0.00006 0.00000 0.00047 0.00047 1.91080

R8 2.65721 -0.00016 0.00000 -0.00074 -0.00074 2.65647

R9 2.71643 -0.00019 0.00000 -0.00045 -0.00045 2.71598

R10 2.03720 -0.00004 0.00000 -0.00008 -0.00008 2.03712

R11 2.64301 0.00007 0.00000 -0.00092 -0.00092 2.64209

R12 2.80296 0.00004 0.00000 0.00046 0.00046 2.80342

R13 2.59317 0.00024 0.00000 0.00134 0.00132 2.59450

R14 2.76211 -0.00007 0.00000 -0.00020 -0.00020 2.76191

R15 2.59647 -0.00009 0.00000 -0.00090 -0.00091 2.59555

R16 2.76178 -0.00002 0.00000 0.00031 0.00031 2.76210

R17 2.64103 0.00021 0.00000 0.00022 0.00022 2.64126

R18 2.55487 -0.00008 0.00000 -0.00046 -0.00044 2.55443

R19 2.03917 -0.00002 0.00000 -0.00012 -0.00012 2.03906

R20 2.03899 0.00000 0.00000 -0.00001 -0.00001 2.03899

R21 2.64103 0.00021 0.00000 0.00020 0.00021 2.64124

R22 2.80226 0.00007 0.00000 0.00135 0.00135 2.80361

R23 2.76177 -0.00002 0.00000 0.00031 0.00032 2.76209

R24 2.59647 -0.00008 0.00000 -0.00088 -0.00090 2.59557

R25 2.55488 -0.00008 0.00000 -0.00046 -0.00045 2.55443

R26 2.03918 -0.00002 0.00000 -0.00012 -0.00012 2.03906

R27 2.76211 -0.00007 0.00000 -0.00020 -0.00019 2.76192

R28 2.03899 0.00000 0.00000 -0.00001 -0.00001 2.03899

R29 2.59317 0.00024 0.00000 0.00134 0.00132 2.59449

R30 2.64302 0.00007 0.00000 -0.00092 -0.00092 2.64211

R31 2.71644 -0.00019 0.00000 -0.00044 -0.00044 2.71600

R32 2.80292 0.00004 0.00000 0.00045 0.00045 2.80337

R33 2.65720 -0.00017 0.00000 -0.00075 -0.00074 2.65645

R34 2.59999 -0.00030 0.00000 -0.00034 -0.00035 2.59964

R35 2.64112 -0.00004 0.00000 -0.00039 -0.00038 2.64074

R36 2.03720 -0.00004 0.00000 -0.00008 -0.00008 2.03712

R37 2.65589 0.00010 0.00000 0.00060 0.00061 2.65650

R38 2.03703 -0.00003 0.00000 -0.00012 -0.00012 2.03691

R39 2.59879 0.00021 0.00000 0.00081 0.00080 2.59959

R40 2.71767 0.00026 0.00000 -0.00055 -0.00055 2.71713

R41 1.91032 -0.00006 0.00000 0.00045 0.00045 1.91077

R42 2.80223 0.00007 0.00000 0.00134 0.00134 2.80357

R43 2.65161 0.00011 0.00000 -0.00001 -0.00001 2.65160

R44 2.65109 -0.00009 0.00000 -0.00077 -0.00077 2.65032

R45 2.62877 -0.00007 0.00000 -0.00007 -0.00007 2.62870

R46 2.04821 0.00003 0.00000 0.00019 0.00019 2.04840

R47 2.63642 -0.00010 0.00000 -0.00014 -0.00014 2.63628

R48 2.05002 0.00003 0.00000 0.00008 0.00008 2.05009

R49 2.63419 -0.00001 0.00000 -0.00013 -0.00013 2.63406

R50 2.04996 0.00003 0.00000 0.00007 0.00007 2.05003

R51 2.63044 0.00003 0.00000 0.00023 0.00023 2.63068

R52 2.05010 0.00001 0.00000 0.00003 0.00003 2.05013

R53 2.04839 0.00001 0.00000 0.00014 0.00014 2.04854

R54 2.63642 0.00002 0.00000 -0.00010 -0.00010 2.63632

R55 2.63409 -0.00000 0.00000 0.00004 0.00004 2.63413

R56 2.04994 0.00003 0.00000 0.00009 0.00009 2.05003

R57 2.62838 0.00002 0.00000 0.00031 0.00031 2.62869

R58 2.05014 0.00001 0.00000 0.00005 0.00005 2.05018

R59 2.65214 0.00009 0.00000 -0.00042 -0.00042 2.65172

R60 2.04837 -0.00001 0.00000 0.00011 0.00011 2.04848

R61 2.65054 0.00008 0.00000 -0.00028 -0.00028 2.65026

R62 2.63061 -0.00006 0.00000 -0.00002 -0.00002 2.63060

R63 2.04820 0.00007 0.00000 0.00027 0.00027 2.04847

R64 2.05001 0.00003 0.00000 0.00008 0.00008 2.05009

R65 2.65056 0.00008 0.00000 -0.00029 -0.00029 2.65027

R66 2.65214 0.00009 0.00000 -0.00041 -0.00041 2.65173

R67 2.63060 -0.00006 0.00000 -0.00001 -0.00001 2.63059

R68 2.04820 0.00006 0.00000 0.00027 0.00027 2.04847

R69 2.63409 0.00000 0.00000 0.00004 0.00004 2.63413

R70 2.05001 0.00003 0.00000 0.00008 0.00008 2.05009

R71 2.63642 0.00002 0.00000 -0.00010 -0.00010 2.63632

R72 2.04994 0.00003 0.00000 0.00009 0.00009 2.05003

R73 2.62838 0.00002 0.00000 0.00031 0.00031 2.62868

R74 2.05014 0.00001 0.00000 0.00004 0.00004 2.05018

R75 2.04837 -0.00001 0.00000 0.00011 0.00011 2.04848

R76 2.65111 -0.00010 0.00000 -0.00077 -0.00077 2.65034

R77 2.65162 0.00011 0.00000 -0.00000 -0.00000 2.65162

R78 2.63044 0.00003 0.00000 0.00023 0.00023 2.63067

R79 2.04839 0.00001 0.00000 0.00014 0.00014 2.04854

R80 2.63419 -0.00001 0.00000 -0.00013 -0.00013 2.63406

R81 2.05010 0.00001 0.00000 0.00003 0.00003 2.05013

R82 2.63642 -0.00010 0.00000 -0.00014 -0.00014 2.63628

R83 2.04996 0.00003 0.00000 0.00007 0.00007 2.05003

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A2 2.18776 -0.00005 0.00000 -0.00050 -0.00050 2.18725

A3 2.21403 -0.00004 0.00000 -0.00008 -0.00008 2.21395

A4 1.86864 -0.00023 0.00000 -0.00054 -0.00055 1.86809

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A6 2.19135 0.00041 0.00000 0.00420 0.00417 2.19551

A7 1.92505 0.00008 0.00000 -0.00050 -0.00049 1.92456

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A11 2.19413 -0.00046 0.00000 -0.00108 -0.00113 2.19300

A12 2.22105 0.00035 0.00000 0.00016 0.00021 2.22126

A13 1.88195 -0.00004 0.00000 -0.00054 -0.00055 1.88141

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A15 2.18769 -0.00002 0.00000 -0.00020 -0.00020 2.18749

A16 2.18509 -0.00051 0.00000 -0.00092 -0.00099 2.18410

A17 2.02572 0.00025 0.00000 0.00007 0.00010 2.02582

A18 2.07229 0.00027 0.00000 0.00090 0.00093 2.07322

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A29 1.86200 -0.00001 0.00000 -0.00003 -0.00003 1.86196

A30 2.19701 -0.00005 0.00000 -0.00052 -0.00052 2.19649

A31 2.22377 0.00005 0.00000 0.00054 0.00054 2.22431

A32 2.18222 0.00033 0.00000 0.00327 0.00322 2.18544

A33 2.02496 0.00007 0.00000 -0.00106 -0.00103 2.02393

A34 2.07593 -0.00040 0.00000 -0.00221 -0.00219 2.07374

A35 2.16830 -0.00032 0.00000 -0.00256 -0.00253 2.16577

A36 2.18887 0.00036 0.00000 0.00239 0.00236 2.19123

A37 1.92597 -0.00004 0.00000 0.00020 0.00019 1.92616

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A69 2.10831 -0.00015 0.00000 -0.00156 -0.00156 2.10675

A70 2.10407 0.00021 0.00000 0.00130 0.00129 2.10536

A71 2.07079 -0.00006 0.00000 0.00028 0.00028 2.07107

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A73 2.08498 0.00002 0.00000 0.00027 0.00027 2.08525

A74 2.09282 -0.00008 0.00000 -0.00024 -0.00024 2.09258

A75 2.09811 -0.00001 0.00000 -0.00008 -0.00008 2.09803

A76 2.08858 0.00003 0.00000 0.00023 0.00023 2.08881

A77 2.09649 -0.00001 0.00000 -0.00015 -0.00015 2.09634

A78 2.08890 -0.00002 0.00000 -0.00007 -0.00007 2.08883

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A88 2.09683 0.00002 0.00000 0.00017 0.00017 2.09701

A89 2.09772 -0.00005 0.00000 -0.00033 -0.00033 2.09739

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A91 2.09655 -0.00003 0.00000 -0.00019 -0.00019 2.09636

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A94 2.09254 -0.00002 0.00000 0.00004 0.00004 2.09258

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A99 2.10578 0.00002 0.00000 -0.00014 -0.00014 2.10564

A100 2.08478 -0.00005 0.00000 -0.00047 -0.00047 2.08432

A101 2.09245 0.00003 0.00000 0.00060 0.00060 2.09305

A102 2.09779 -0.00002 0.00000 -0.00022 -0.00022 2.09757

A103 2.09704 0.00001 0.00000 0.00000 0.00000 2.09704

A104 2.08835 0.00001 0.00000 0.00022 0.00022 2.08857

A105 2.10639 -0.00013 0.00000 -0.00088 -0.00088 2.10550

A106 2.10641 0.00011 0.00000 0.00022 0.00022 2.10664

A107 2.07037 0.00002 0.00000 0.00066 0.00066 2.07103

A108 2.10580 0.00002 0.00000 -0.00015 -0.00015 2.10565

A109 2.08480 -0.00005 0.00000 -0.00048 -0.00047 2.08432

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A117 2.09799 0.00003 0.00000 0.00010 0.00010 2.09809

A118 2.09656 -0.00003 0.00000 -0.00020 -0.00020 2.09636

A119 2.08864 -0.00000 0.00000 0.00010 0.00010 2.08874

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D98 0.11040 -0.00004 0.00000 -0.00224 -0.00226 0.10814

D99 0.02630 -0.00000 0.00000 -0.00187 -0.00188 0.02442

D100 -3.06686 0.00003 0.00000 0.00160 0.00159 -3.06528

D101 0.00102 0.00001 0.00000 -0.00040 -0.00041 0.00061

D102 3.13646 -0.00002 0.00000 -0.00071 -0.00071 3.13575

D103 -3.13602 0.00004 0.00000 0.00108 0.00108 -3.13494

D104 -0.00057 0.00001 0.00000 0.00077 0.00078 0.00020

D105 0.01478 -0.00002 0.00000 -0.00074 -0.00073 0.01405

D106 -3.09378 -0.00007 0.00000 -0.00510 -0.00510 -3.09888

D107 -3.12078 0.00001 0.00000 -0.00043 -0.00043 -3.12121

D108 0.05384 -0.00004 0.00000 -0.00480 -0.00480 0.04905

D109 -0.02569 0.00001 0.00000 0.00165 0.00165 -0.02404

D110 3.06776 -0.00004 0.00000 -0.00221 -0.00223 3.06553

D111 3.08364 0.00005 0.00000 0.00573 0.00575 3.08939

D112 -0.10610 -0.00001 0.00000 0.00188 0.00188 -0.10423

D113 -2.92932 0.00002 0.00000 -0.00686 -0.00688 -2.93620

D114 0.19877 0.00003 0.00000 -0.00680 -0.00682 0.19194

D115 0.25109 -0.00003 0.00000 -0.01187 -0.01191 0.23918

D116 -2.90401 -0.00001 0.00000 -0.01181 -0.01185 -2.91586

D117 0.96271 0.00017 0.00000 0.01736 0.01736 0.98007

D118 -2.18491 0.00019 0.00000 0.01761 0.01761 -2.16730

D119 -2.16625 0.00015 0.00000 0.01726 0.01726 -2.14899

D120 0.96932 0.00017 0.00000 0.01751 0.01751 0.98683

D121 -3.13417 0.00010 0.00000 0.00376 0.00376 -3.13042

D122 -0.01242 0.00005 0.00000 0.00250 0.00250 -0.00991

D123 0.01288 0.00005 0.00000 0.00167 0.00167 0.01455

D124 3.13464 -0.00001 0.00000 0.00042 0.00042 3.13506

D125 -3.13758 -0.00007 0.00000 -0.00274 -0.00274 -3.14032

D126 -0.01568 -0.00007 0.00000 -0.00223 -0.00223 -0.01791

D127 -0.00144 -0.00002 0.00000 -0.00067 -0.00067 -0.00211

D128 3.12046 -0.00001 0.00000 -0.00016 -0.00016 3.12031

D129 -0.01488 -0.00004 0.00000 -0.00127 -0.00127 -0.01615

D130 3.12582 -0.00004 0.00000 -0.00127 -0.00127 3.12455

D131 -3.13655 0.00002 0.00000 -0.00002 -0.00002 -3.13656

D132 0.00415 0.00002 0.00000 -0.00002 -0.00002 0.00413

D133 0.00522 0.00000 0.00000 -0.00016 -0.00016 0.00506

D134 -3.13472 0.00002 0.00000 0.00060 0.00060 -3.13412

D135 -3.13547 0.00001 0.00000 -0.00016 -0.00016 -3.13563

D136 0.00778 0.00002 0.00000 0.00060 0.00060 0.00838

D137 0.00618 0.00003 0.00000 0.00116 0.00116 0.00734

D138 -3.13201 0.00001 0.00000 0.00046 0.00046 -3.13155

D139 -3.13707 0.00001 0.00000 0.00040 0.00040 -3.13666

D140 0.00793 -0.00001 0.00000 -0.00030 -0.00030 0.00763

D141 -0.00805 -0.00002 0.00000 -0.00074 -0.00074 -0.00879

D142 -3.12986 -0.00002 0.00000 -0.00125 -0.00125 -3.13112

D143 3.13015 -0.00000 0.00000 -0.00004 -0.00004 3.13011

D144 0.00834 -0.00001 0.00000 -0.00056 -0.00056 0.00779

D145 -0.00495 -0.00003 0.00000 -0.00113 -0.00113 -0.00608

D146 3.13628 -0.00003 0.00000 -0.00096 -0.00096 3.13532

D147 3.13408 -0.00001 0.00000 -0.00055 -0.00055 3.13354

D148 -0.00788 -0.00001 0.00000 -0.00038 -0.00038 -0.00825

D149 -0.00650 0.00000 0.00000 0.00031 0.00031 -0.00619

D150 3.13122 -0.00000 0.00000 0.00036 0.00036 3.13159

D151 3.13766 -0.00001 0.00000 -0.00027 -0.00027 3.13738

D152 -0.00780 -0.00001 0.00000 -0.00022 -0.00022 -0.00803

D153 0.01588 0.00002 0.00000 0.00068 0.00068 0.01657

D154 3.13724 -0.00002 0.00000 -0.00002 -0.00002 3.13722

D155 -3.12535 0.00002 0.00000 0.00052 0.00052 -3.12483

D156 -0.00399 -0.00002 0.00000 -0.00019 -0.00019 -0.00418

D157 3.13215 -0.00000 0.00000 0.00044 0.00044 3.13260

D158 -0.01507 0.00001 0.00000 0.00057 0.00057 -0.01450

D159 0.01071 0.00003 0.00000 0.00115 0.00115 0.01186

D160 -3.13652 0.00005 0.00000 0.00127 0.00127 -3.13524

D161 3.13954 -0.00002 0.00000 -0.00126 -0.00126 3.13828

D162 0.01746 0.00002 0.00000 -0.00062 -0.00062 0.01684

D163 0.00358 -0.00004 0.00000 -0.00139 -0.00139 0.00219

D164 -3.11850 0.00000 0.00000 -0.00075 -0.00075 -3.11925

D165 0.00714 0.00003 0.00000 0.00096 0.00096 0.00810

D166 -3.13060 0.00003 0.00000 0.00091 0.00091 -3.12969

D167 3.12914 -0.00001 0.00000 0.00031 0.00031 3.12944

D168 -0.00861 -0.00001 0.00000 0.00026 0.00026 -0.00835

D169 3.13929 -0.00001 0.00000 -0.00113 -0.00113 3.13816

D170 0.01729 0.00002 0.00000 -0.00052 -0.00052 0.01676

D171 0.00360 -0.00004 0.00000 -0.00138 -0.00138 0.00222

D172 -3.11841 0.00000 0.00000 -0.00076 -0.00076 -3.11917

D173 3.13241 -0.00001 0.00000 0.00031 0.00031 3.13272

D174 0.01094 0.00003 0.00000 0.00105 0.00105 0.01199

D175 -0.01508 0.00001 0.00000 0.00055 0.00055 -0.01453

D176 -3.13655 0.00005 0.00000 0.00128 0.00128 -3.13527

D177 0.00712 0.00003 0.00000 0.00097 0.00097 0.00808

D178 -3.13058 0.00003 0.00000 0.00090 0.00090 -3.12968

D179 3.12904 -0.00001 0.00000 0.00034 0.00034 3.12938

D180 -0.00866 -0.00001 0.00000 0.00028 0.00028 -0.00838

D181 -0.00648 0.00000 0.00000 0.00029 0.00029 -0.00618

D182 3.13766 -0.00001 0.00000 -0.00027 -0.00027 3.13739

D183 3.13120 -0.00000 0.00000 0.00036 0.00036 3.13156

D184 -0.00784 -0.00001 0.00000 -0.00021 -0.00021 -0.00805

D185 -0.00496 -0.00002 0.00000 -0.00112 -0.00112 -0.00608

D186 3.13627 -0.00002 0.00000 -0.00095 -0.00095 3.13533

D187 3.13408 -0.00001 0.00000 -0.00056 -0.00056 3.13353

D188 -0.00787 -0.00001 0.00000 -0.00038 -0.00038 -0.00825

D189 0.01589 0.00002 0.00000 0.00069 0.00069 0.01658

D190 3.13727 -0.00002 0.00000 -0.00004 -0.00004 3.13723

D191 -3.12535 0.00002 0.00000 0.00052 0.00052 -3.12483

D192 -0.00396 -0.00002 0.00000 -0.00022 -0.00022 -0.00418

D193 -3.13754 -0.00007 0.00000 -0.00273 -0.00274 -3.14027

D194 -0.01567 -0.00007 0.00000 -0.00223 -0.00223 -0.01790

D195 -0.00145 -0.00002 0.00000 -0.00068 -0.00068 -0.00213

D196 3.12042 -0.00001 0.00000 -0.00018 -0.00018 3.12024

D197 -3.13421 0.00010 0.00000 0.00374 0.00374 -3.13047

D198 -0.01245 0.00005 0.00000 0.00249 0.00249 -0.00996

D199 0.01290 0.00005 0.00000 0.00168 0.00168 0.01458

D200 3.13466 -0.00001 0.00000 0.00042 0.00042 3.13509

D201 -0.00806 -0.00002 0.00000 -0.00072 -0.00072 -0.00879

D202 3.13014 -0.00000 0.00000 -0.00004 -0.00004 3.13010

D203 -3.12983 -0.00002 0.00000 -0.00124 -0.00124 -3.13107

D204 0.00837 -0.00001 0.00000 -0.00055 -0.00055 0.00781

D205 0.00619 0.00003 0.00000 0.00115 0.00115 0.00735

D206 -3.13708 0.00001 0.00000 0.00040 0.00040 -3.13667

D207 -3.13199 0.00001 0.00000 0.00046 0.00046 -3.13152

D208 0.00793 -0.00001 0.00000 -0.00029 -0.00029 0.00764

D209 0.00522 0.00000 0.00000 -0.00016 -0.00016 0.00506

D210 -3.13549 0.00001 0.00000 -0.00016 -0.00016 -3.13564

D211 -3.13470 0.00002 0.00000 0.00059 0.00059 -3.13411

D212 0.00778 0.00002 0.00000 0.00059 0.00059 0.00838

D213 -0.01489 -0.00004 0.00000 -0.00127 -0.00127 -0.01616

D214 -3.13657 0.00002 0.00000 -0.00001 -0.00001 -3.13658

D215 3.12582 -0.00004 0.00000 -0.00127 -0.00127 3.12454

D216 0.00414 0.00002 0.00000 -0.00002 -0.00002 0.00413

Item Value Threshold Converged?

Maximum Force 0.000514 0.000450 NO

RMS Force 0.000120 0.000300 YES

Maximum Displacement 0.108407 0.001800 NO

RMS Displacement 0.029926 0.001200 NO

Predicted change in Energy=-9.805267D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Aug 27 08:17:44 2019, MaxMem= 4294967296 cpu: 2.8

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

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=2 Diff= 3.38D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.356182 -4.208016 0.547608

2 6 0 0.887893 -2.957294 0.188229

3 7 0 -0.176148 -2.105422 0.002389

4 6 0 -1.362093 -2.774112 0.199582

5 6 0 -1.036602 -4.094616 0.555165

6 6 0 -2.676059 -2.218241 0.025955

7 6 0 -2.961950 -0.856702 -0.112792

8 7 0 -2.061998 0.168297 0.043574

9 6 0 -2.780795 1.326706 -0.123589

10 6 0 -4.171606 1.019353 -0.451555

11 6 0 -4.283604 -0.327722 -0.443725

12 6 0 2.274457 -2.623057 0.006368

13 6 0 2.780782 -1.326771 -0.123225

14 6 0 4.171603 -1.019502 -0.451215

15 6 0 4.283602 0.327574 -0.443702

16 6 0 2.961951 0.856638 -0.112889

17 7 0 2.061985 -0.168316 0.043686

18 6 0 2.676078 2.218213 0.025644

19 6 0 1.362083 2.774051 0.199232

20 6 0 1.036550 4.094261 0.555836

21 6 0 -0.356241 4.207652 0.548229

22 6 0 -0.887903 2.957220 0.187795

23 7 0 0.176170 2.105523 0.001351

24 6 0 -2.274484 2.623022 0.005875

25 6 0 -3.797642 -3.189085 0.008767

26 6 0 -3.815750 -4.246758 -0.913123

27 6 0 -4.874880 -5.148271 -0.936335

28 6 0 -5.925052 -5.020982 -0.026874

29 6 0 -5.911447 -3.981922 0.902146

30 6 0 -4.859609 -3.070144 0.917092

31 6 0 5.009551 -5.928479 -0.087193

32 6 0 3.947039 -5.872228 -0.989497

33 6 0 3.053893 -4.806396 -0.953567

34 6 0 3.219316 -3.766416 -0.026136

35 6 0 4.292340 -3.832607 0.874485

36 6 0 5.176717 -4.907278 0.846733

37 6 0 -3.219306 3.766389 -0.026402

38 6 0 -4.292585 3.832241 0.873956

39 6 0 -5.176844 4.907012 0.846500

40 6 0 -5.009305 5.928681 -0.086848

41 6 0 -3.946536 5.872790 -0.988873

42 6 0 -3.053511 4.806852 -0.953237

43 6 0 3.797610 3.189084 0.008582

44 6 0 4.859792 3.069882 0.916635

45 6 0 5.911549 3.981751 0.901819

46 6 0 5.924869 5.021181 -0.026792

47 6 0 4.874482 5.148751 -0.935968

48 6 0 3.815432 4.247147 -0.912879

49 1 0 0.934405 -5.087634 0.779476

50 1 0 -1.747293 -4.869129 0.794172

51 1 0 -4.941247 1.739731 -0.681766

52 1 0 -5.161620 -0.914291 -0.665608

53 1 0 4.941255 -1.739937 -0.681212

54 1 0 5.161621 0.914088 -0.665719

55 1 0 1.747223 4.868545 0.795645

56 1 0 -0.934509 5.087038 0.780865

57 1 0 -3.004697 -4.347622 -1.625166

58 1 0 -4.881092 -5.951057 -1.666008

59 1 0 -6.747131 -5.728678 -0.041284

60 1 0 -6.719529 -3.881261 1.618972

61 1 0 -4.848606 -2.269494 1.647832

62 1 0 5.701138 -6.763936 -0.111222

63 1 0 3.813688 -6.660262 -1.723151

64 1 0 2.232465 -4.765769 -1.659743

65 1 0 4.419608 -3.046429 1.609870

66 1 0 5.994837 -4.947919 1.558039

67 1 0 -4.420122 3.045735 1.608939

68 1 0 -5.995151 4.947379 1.557606

69 1 0 -5.700797 6.764223 -0.110641

70 1 0 -3.812887 6.661195 -1.722074

71 1 0 -2.231878 4.766521 -1.659190

72 1 0 4.849006 2.268974 1.647093

73 1 0 6.719788 3.880880 1.618439

74 1 0 6.746883 5.728954 -0.041094

75 1 0 4.880462 5.951834 -1.665315

76 1 0 3.004207 4.348241 -1.624693

77 1 0 -0.098524 -1.118044 -0.201281

78 1 0 0.098620 1.118438 -0.203698

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

Rotational constants (GHZ): 0.0587829 0.0582868 0.0300905

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

Standard basis: 6-311G(d) (5D, 7F)

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

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5357.2539505755 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122428373 Hartrees.

Nuclear repulsion after empirical dispersion term = 5357.0417077382 Hartrees.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5780

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.61D-09

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 310

GePol: Fraction of low-weight points (<1% of avg) = 5.36%

GePol: Cavity surface area = 610.189 Ang\*\*2

GePol: Cavity volume = 627.946 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021095583 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5357.0395981799 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.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Aug 27 08:17:46 2019, MaxMem= 4294967296 cpu: 2.3

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

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= 0.000000 0.000000 -0.000000

Rot= 0.992814 -0.000000 0.000000 0.119671 Ang= -13.75 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0183

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30525531226

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 590000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 100225200.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.13D-14 for 5779.

Iteration 1 A\*A^-1 deviation from orthogonality is 8.10D-15 for 5770 2067.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.13D-14 for 5779.

Iteration 1 A^-1\*A deviation from orthogonality is 5.28D-11 for 5776 5755.

E= -1914.32692761776

DIIS: error= 2.28D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.32692761776 IErMin= 1 ErrMin= 2.28D-03

ErrMax= 2.28D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.19D-02 BMatP= 1.19D-02

IDIUse=3 WtCom= 9.77D-01 WtEn= 2.28D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.641 Goal= None Shift= 0.000

Gap= 0.706 Goal= None Shift= 0.000

GapD= 0.641 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=7.58D-05 MaxDP=2.43D-03 OVMax= 1.34D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 7.58D-05 CP: 1.00D+00

E= -1914.33318469200 Delta-E= -0.006257074233 Rises=F Damp=F

DIIS: error= 3.34D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33318469200 IErMin= 2 ErrMin= 3.34D-04

ErrMax= 3.34D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.68D-04 BMatP= 1.19D-02

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.34D-03

Coeff-Com: -0.697D-01 0.107D+01

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

Coeff: -0.694D-01 0.107D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.44D-05 MaxDP=3.39D-04 DE=-6.26D-03 OVMax= 2.01D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.30D-05 CP: 1.00D+00 1.08D+00

E= -1914.33328330285 Delta-E= -0.000098610856 Rises=F Damp=F

DIIS: error= 8.67D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33328330285 IErMin= 3 ErrMin= 8.67D-05

ErrMax= 8.67D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.14D-05 BMatP= 1.68D-04

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

Coeff-Com: -0.294D-01 0.361D+00 0.669D+00

Coeff: -0.294D-01 0.361D+00 0.669D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.93D-06 MaxDP=2.32D-04 DE=-9.86D-05 OVMax= 1.14D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.97D-06 CP: 1.00D+00 1.10D+00 7.75D-01

E= -1914.33328811593 Delta-E= -0.000004813083 Rises=F Damp=F

DIIS: error= 8.96D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33328811593 IErMin= 3 ErrMin= 8.67D-05

ErrMax= 8.96D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.43D-05 BMatP= 4.14D-05

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

Coeff-Com: -0.989D-02 0.965D-01 0.431D+00 0.482D+00

Coeff: -0.989D-02 0.965D-01 0.431D+00 0.482D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.10D-06 MaxDP=1.82D-04 DE=-4.81D-06 OVMax= 9.29D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.82D-06 CP: 1.00D+00 1.10D+00 8.58D-01 5.48D-01

E= -1914.33329426635 Delta-E= -0.000006150412 Rises=F Damp=F

DIIS: error= 2.88D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33329426635 IErMin= 5 ErrMin= 2.88D-05

ErrMax= 2.88D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.52D-06 BMatP= 2.43D-05

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

Coeff-Com: -0.926D-03-0.361D-02 0.117D+00 0.240D+00 0.647D+00

Coeff: -0.926D-03-0.361D-02 0.117D+00 0.240D+00 0.647D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=9.90D-07 MaxDP=5.71D-05 DE=-6.15D-06 OVMax= 2.87D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.60D-07 CP: 1.00D+00 1.10D+00 8.68D-01 6.54D-01 7.29D-01

E= -1914.33329461384 Delta-E= -0.000000347491 Rises=F Damp=F

DIIS: error= 1.20D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33329461384 IErMin= 6 ErrMin= 1.20D-05

ErrMax= 1.20D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.46D-07 BMatP= 1.52D-06

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

Coeff-Com: 0.910D-03-0.175D-01 0.810D-02 0.805D-01 0.412D+00 0.516D+00

Coeff: 0.910D-03-0.175D-01 0.810D-02 0.805D-01 0.412D+00 0.516D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.23D-07 MaxDP=3.01D-05 DE=-3.47D-07 OVMax= 2.18D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.91D-07 CP: 1.00D+00 1.10D+00 8.78D-01 6.46D-01 8.36D-01

CP: 6.94D-01

E= -1914.33329474536 Delta-E= -0.000000131527 Rises=F Damp=F

DIIS: error= 3.41D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33329474536 IErMin= 7 ErrMin= 3.41D-06

ErrMax= 3.41D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.72D-08 BMatP= 4.46D-07

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

Coeff-Com: 0.482D-03-0.799D-02-0.339D-02 0.248D-01 0.154D+00 0.255D+00

Coeff-Com: 0.578D+00

Coeff: 0.482D-03-0.799D-02-0.339D-02 0.248D-01 0.154D+00 0.255D+00

Coeff: 0.578D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.53D-07 MaxDP=6.45D-06 DE=-1.32D-07 OVMax= 9.71D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.28D-07 CP: 1.00D+00 1.10D+00 8.79D-01 6.52D-01 8.52D-01

CP: 7.75D-01 1.16D+00

E= -1914.33329476063 Delta-E= -0.000000015266 Rises=F Damp=F

DIIS: error= 2.24D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33329476063 IErMin= 8 ErrMin= 2.24D-06

ErrMax= 2.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.39D-09 BMatP= 2.72D-08

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

Coeff-Com: -0.270D-03 0.592D-02-0.613D-02-0.310D-01-0.159D+00-0.152D+00

Coeff-Com: 0.266D+00 0.108D+01

Coeff: -0.270D-03 0.592D-02-0.613D-02-0.310D-01-0.159D+00-0.152D+00

Coeff: 0.266D+00 0.108D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.33D-07 MaxDP=1.24D-05 DE=-1.53D-08 OVMax= 1.77D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 8.32D-08 CP: 1.00D+00 1.10D+00 8.80D-01 6.57D-01 8.88D-01

CP: 9.02D-01 1.78D+00 1.42D+00

E= -1914.33329477442 Delta-E= -0.000000013788 Rises=F Damp=F

DIIS: error= 1.39D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33329477442 IErMin= 9 ErrMin= 1.39D-06

ErrMax= 1.39D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.11D-09 BMatP= 8.39D-09

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

Coeff-Com: -0.245D-03 0.483D-02-0.250D-02-0.213D-01-0.120D+00-0.130D+00

Coeff-Com: 0.247D-01 0.589D+00 0.655D+00

Coeff: -0.245D-03 0.483D-02-0.250D-02-0.213D-01-0.120D+00-0.130D+00

Coeff: 0.247D-01 0.589D+00 0.655D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.09D-07 MaxDP=6.24D-06 DE=-1.38D-08 OVMax= 8.95D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 5.14D-08 CP: 1.00D+00 1.10D+00 8.81D-01 6.57D-01 9.01D-01

CP: 9.55D-01 2.01D+00 1.79D+00 1.25D+00

E= -1914.33329477782 Delta-E= -0.000000003402 Rises=F Damp=F

DIIS: error= 1.00D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33329477782 IErMin=10 ErrMin= 1.00D-06

ErrMax= 1.00D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.18D-09 BMatP= 3.11D-09

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

Coeff-Com: 0.688D-05-0.486D-03 0.206D-02 0.527D-02 0.159D-01 0.150D-01

Coeff-Com: -0.137D+00-0.247D+00 0.396D+00 0.949D+00

Coeff: 0.688D-05-0.486D-03 0.206D-02 0.527D-02 0.159D-01 0.150D-01

Coeff: -0.137D+00-0.247D+00 0.396D+00 0.949D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.19D-07 MaxDP=8.47D-06 DE=-3.40D-09 OVMax= 1.17D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.77D-08 CP: 1.00D+00 1.10D+00 8.81D-01 6.59D-01 9.14D-01

CP: 9.96D-01 2.27D+00 2.12D+00 2.05D+00 1.38D+00

E= -1914.33329477998 Delta-E= -0.000000002156 Rises=F Damp=F

DIIS: error= 5.85D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33329477998 IErMin=11 ErrMin= 5.85D-07

ErrMax= 5.85D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.39D-10 BMatP= 1.18D-09

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

Coeff-Com: 0.588D-04-0.137D-02 0.172D-02 0.792D-02 0.355D-01 0.416D-01

Coeff-Com: -0.901D-01-0.275D+00 0.893D-01 0.569D+00 0.621D+00

Coeff: 0.588D-04-0.137D-02 0.172D-02 0.792D-02 0.355D-01 0.416D-01

Coeff: -0.901D-01-0.275D+00 0.893D-01 0.569D+00 0.621D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.98D-08 MaxDP=3.66D-06 DE=-2.16D-09 OVMax= 5.13D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.30D-08 CP: 1.00D+00 1.10D+00 8.81D-01 6.59D-01 9.19D-01

CP: 1.00D+00 2.35D+00 2.29D+00 2.35D+00 1.79D+00

CP: 1.29D+00

E= -1914.33329478050 Delta-E= -0.000000000523 Rises=F Damp=F

DIIS: error= 4.98D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.33329478050 IErMin=12 ErrMin= 4.98D-07

ErrMax= 4.98D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D-10 BMatP= 4.39D-10

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

Coeff-Com: 0.229D-04-0.360D-03-0.385D-03 0.823D-03 0.698D-02 0.157D-01

Coeff-Com: 0.236D-01 0.516D-02-0.169D+00-0.206D+00 0.191D+00 0.113D+01

Coeff: 0.229D-04-0.360D-03-0.385D-03 0.823D-03 0.698D-02 0.157D-01

Coeff: 0.236D-01 0.516D-02-0.169D+00-0.206D+00 0.191D+00 0.113D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=6.00D-08 MaxDP=4.72D-06 DE=-5.23D-10 OVMax= 6.56D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 9.22D-09 CP: 1.00D+00 1.10D+00 8.81D-01 6.59D-01 9.24D-01

CP: 1.01D+00 2.45D+00 2.44D+00 2.77D+00 2.23D+00

CP: 2.07D+00 1.56D+00

E= -1914.33329478085 Delta-E= -0.000000000350 Rises=F Damp=F

DIIS: error= 2.79D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.33329478085 IErMin=13 ErrMin= 2.79D-07

ErrMax= 2.79D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.83D-11 BMatP= 1.13D-10

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

Coeff-Com: -0.689D-05 0.238D-03-0.667D-03-0.182D-02-0.736D-02-0.334D-02

Coeff-Com: 0.315D-01 0.801D-01-0.908D-01-0.220D+00-0.165D+00 0.503D+00

Coeff-Com: 0.874D+00

Coeff: -0.689D-05 0.238D-03-0.667D-03-0.182D-02-0.736D-02-0.334D-02

Coeff: 0.315D-01 0.801D-01-0.908D-01-0.220D+00-0.165D+00 0.503D+00

Coeff: 0.874D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.20D-08 MaxDP=2.62D-06 DE=-3.50D-10 OVMax= 3.55D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 5.38D-09 CP: 1.00D+00 1.10D+00 8.81D-01 6.59D-01 9.26D-01

CP: 1.02D+00 2.49D+00 2.52D+00 2.98D+00 2.49D+00

CP: 2.50D+00 2.16D+00 1.35D+00

E= -1914.33329478097 Delta-E= -0.000000000120 Rises=F Damp=F

DIIS: error= 1.70D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.33329478097 IErMin=14 ErrMin= 1.70D-07

ErrMax= 1.70D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.46D-11 BMatP= 4.83D-11

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

Coeff-Com: -0.124D-04 0.277D-03-0.277D-03-0.140D-02-0.733D-02-0.689D-02

Coeff-Com: 0.949D-02 0.478D-01 0.453D-02-0.563D-01-0.203D+00-0.710D-01

Coeff-Com: 0.564D+00 0.720D+00

Coeff: -0.124D-04 0.277D-03-0.277D-03-0.140D-02-0.733D-02-0.689D-02

Coeff: 0.949D-02 0.478D-01 0.453D-02-0.563D-01-0.203D+00-0.710D-01

Coeff: 0.564D+00 0.720D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.01D-08 MaxDP=1.67D-06 DE=-1.20D-10 OVMax= 2.23D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 8.82D-09 CP: 1.00D+00 1.10D+00 8.81D-01 6.59D-01 9.28D-01

CP: 1.02D+00 2.52D+00 2.57D+00 3.00D+00 2.65D+00

CP: 2.78D+00 2.50D+00 1.81D+00 1.39D+00

E= -1914.33329478103 Delta-E= -0.000000000056 Rises=F Damp=F

DIIS: error= 1.06D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.33329478103 IErMin=15 ErrMin= 1.06D-07

ErrMax= 1.06D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.50D-12 BMatP= 2.46D-11

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

Coeff-Com: 0.142D-05-0.940D-04 0.402D-03 0.960D-03 0.280D-02 0.145D-02

Coeff-Com: -0.217D-01-0.436D-01 0.684D-01 0.145D+00 0.230D-01-0.349D+00

Coeff-Com: -0.381D+00 0.141D+00 0.141D+01

Coeff: 0.142D-05-0.940D-04 0.402D-03 0.960D-03 0.280D-02 0.145D-02

Coeff: -0.217D-01-0.436D-01 0.684D-01 0.145D+00 0.230D-01-0.349D+00

Coeff: -0.381D+00 0.141D+00 0.141D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.28D-08 MaxDP=1.91D-06 DE=-5.64D-11 OVMax= 2.54D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 3.30D-09 CP: 1.00D+00 1.10D+00 8.81D-01 6.59D-01 9.30D-01

CP: 1.02D+00 2.56D+00 2.63D+00 3.00D+00 2.81D+00

CP: 3.00D+00 2.91D+00 2.42D+00 2.29D+00 2.26D+00

E= -1914.33329478102 Delta-E= 0.000000000008 Rises=F Damp=F

DIIS: error= 3.29D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=15 EnMin= -1914.33329478103 IErMin=16 ErrMin= 3.29D-08

ErrMax= 3.29D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.18D-12 BMatP= 6.50D-12

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

Coeff-Com: 0.339D-05-0.110D-03 0.285D-03 0.843D-03 0.304D-02 0.243D-02

Coeff-Com: -0.142D-01-0.344D-01 0.385D-01 0.924D-01 0.513D-01-0.179D+00

Coeff-Com: -0.321D+00-0.740D-01 0.787D+00 0.646D+00

Coeff: 0.339D-05-0.110D-03 0.285D-03 0.843D-03 0.304D-02 0.243D-02

Coeff: -0.142D-01-0.344D-01 0.385D-01 0.924D-01 0.513D-01-0.179D+00

Coeff: -0.321D+00-0.740D-01 0.787D+00 0.646D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.78D-09 MaxDP=4.72D-07 DE= 8.19D-12 OVMax= 6.35D-06

Error on total polarization charges = 0.08257

SCF Done: E(UB3LYP) = -1914.33329478 A.U. after 16 cycles

NFock= 16 Conv=0.58D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0550 S= 1.0182

<L.S>= 0.000000000000E+00

KE= 1.906384384743D+03 PE=-1.516371631986D+04 EE= 5.985959042156D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0550, after 2.0017

Leave Link 502 at Tue Aug 27 08:24:51 2019, MaxMem= 4294967296 cpu: 6646.0

(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: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48591172D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64322730D-01

Leave Link 801 at Tue Aug 27 08:24:52 2019, MaxMem= 4294967296 cpu: 0.8

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

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

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

Leave Link 1101 at Tue Aug 27 08:24:58 2019, MaxMem= 4294967296 cpu: 110.3

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

Symmetrizing basis deriv contribution to polar:

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

Leave Link 1102 at Tue Aug 27 08:24:59 2019, MaxMem= 4294967296 cpu: 1.8

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

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 188

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 27 08:44:39 2019, MaxMem= 4294967296 cpu: 18879.0

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

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 590000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.42D+03 4.50D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.53D+02 3.68D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.56D+00 4.64D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.03D-01 3.96D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.66D-04 2.09D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.60D-06 1.35D-04.

189 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 2.00D-08 1.00D-05.

83 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.31D-11 6.21D-07.

38 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.16D-13 3.83D-08.

4 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 8.25D-15 4.64D-09.

4 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 5.31D-15 2.44D-09.

4 vectors produced by pass 11 Test12= 2.55D-13 1.00D-09 XBig12= 1.24D-14 3.65D-09.

4 vectors produced by pass 12 Test12= 2.55D-13 1.00D-09 XBig12= 1.05D-14 2.78D-09.

4 vectors produced by pass 13 Test12= 2.55D-13 1.00D-09 XBig12= 9.04D-15 4.24D-09.

4 vectors produced by pass 14 Test12= 2.55D-13 1.00D-09 XBig12= 7.00D-15 2.77D-09.

4 vectors produced by pass 15 Test12= 2.55D-13 1.00D-09 XBig12= 5.31D-15 2.95D-09.

4 vectors produced by pass 16 Test12= 2.55D-13 1.00D-09 XBig12= 5.74D-15 2.51D-09.

4 vectors produced by pass 17 Test12= 2.55D-13 1.00D-09 XBig12= 7.95D-15 2.79D-09.

4 vectors produced by pass 18 Test12= 2.55D-13 1.00D-09 XBig12= 6.72D-15 2.51D-09.

4 vectors produced by pass 19 Test12= 2.55D-13 1.00D-09 XBig12= 1.01D-14 3.83D-09.

4 vectors produced by pass 20 Test12= 2.55D-13 1.00D-09 XBig12= 6.73D-15 2.38D-09.

4 vectors produced by pass 21 Test12= 2.55D-13 1.00D-09 XBig12= 7.54D-15 2.67D-09.

3 vectors produced by pass 22 Test12= 2.55D-13 1.00D-09 XBig12= 6.02D-15 2.34D-09.

3 vectors produced by pass 23 Test12= 2.55D-13 1.00D-09 XBig12= 7.84D-15 2.38D-09.

3 vectors produced by pass 24 Test12= 2.55D-13 1.00D-09 XBig12= 6.49D-15 2.03D-09.

3 vectors produced by pass 25 Test12= 2.55D-13 1.00D-09 XBig12= 6.57D-15 2.41D-09.

3 vectors produced by pass 26 Test12= 2.55D-13 1.00D-09 XBig12= 6.51D-15 2.06D-09.

3 vectors produced by pass 27 Test12= 2.55D-13 1.00D-09 XBig12= 5.93D-15 1.98D-09.

3 vectors produced by pass 28 Test12= 2.55D-13 1.00D-09 XBig12= 7.54D-15 2.73D-09.

3 vectors produced by pass 29 Test12= 2.55D-13 1.00D-09 XBig12= 4.24D-15 1.70D-09.

3 vectors produced by pass 30 Test12= 2.55D-13 1.00D-09 XBig12= 6.64D-15 2.13D-09.

3 vectors produced by pass 31 Test12= 2.55D-13 1.00D-09 XBig12= 6.78D-15 2.76D-09.

3 vectors produced by pass 32 Test12= 2.55D-13 1.00D-09 XBig12= 6.73D-15 2.87D-09.

2 vectors produced by pass 33 Test12= 2.55D-13 1.00D-09 XBig12= 2.13D-15 1.41D-09.

InvSVY: IOpt=1 It= 1 EMax= 1.42D-13

Solved reduced A of dimension 1804 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1128.06 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 27 12:41:46 2019, MaxMem= 4294967296 cpu: 227567.8

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 188

Leave Link 701 at Tue Aug 27 12:43:16 2019, MaxMem= 4294967296 cpu: 1425.3

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

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

Leave Link 702 at Tue Aug 27 12:43:16 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

Leave Link 703 at Tue Aug 27 13:02:15 2019, MaxMem= 4294967296 cpu: 18221.5

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

Dipole = 9.94545634D-05 6.16549378D-04-4.74787702D-01

Polarizability= 1.25904369D+03 3.46191860D+01 1.67203054D+03

5.34679716D-03 3.64341918D-03 4.53109690D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000017710 0.000010837 -0.000018247

2 6 0.000094923 -0.000072952 0.000027989

3 7 -0.000051140 -0.000214840 0.000043549

4 6 0.000049472 0.000052469 0.000001169

5 6 -0.000040493 0.000008476 -0.000012523

6 6 -0.000065440 -0.000086672 0.000016111

7 6 -0.000002477 0.000030026 -0.000063162

8 7 -0.000067678 0.000021167 0.000033890

9 6 0.000014735 0.000133813 -0.000016616

10 6 -0.000000043 0.000040962 -0.000029066

11 6 -0.000050433 0.000007727 0.000042081

12 6 -0.000020804 0.000040284 -0.000112782

13 6 -0.000014555 0.000134001 0.000016363

14 6 -0.000000122 0.000041100 0.000029233

15 6 0.000050510 0.000006832 -0.000041560

16 6 0.000002580 0.000030394 0.000062582

17 7 0.000066216 0.000023858 -0.000028463

18 6 0.000065597 -0.000087320 -0.000015595

19 6 -0.000049405 0.000051777 -0.000001450

20 6 0.000041194 0.000009573 0.000013011

21 6 -0.000018109 0.000009556 0.000018226

22 6 -0.000094012 -0.000073528 -0.000028115

23 7 0.000050618 -0.000215974 -0.000044823

24 6 0.000021615 0.000038313 0.000112082

25 6 0.000021350 0.000053181 -0.000052008

26 6 0.000054745 0.000011114 0.000042800

27 6 -0.000028913 0.000027947 -0.000090219

28 6 0.000086265 -0.000053395 0.000050764

29 6 -0.000109278 0.000061549 -0.000047776

30 6 0.000114835 -0.000124289 0.000067207

31 6 -0.000104393 0.000086319 0.000029748

32 6 0.000032625 -0.000002416 -0.000071500

33 6 -0.000182836 0.000085924 0.000141815

34 6 0.000060225 -0.000077074 -0.000034432

35 6 0.000000881 -0.000073164 -0.000017075

36 6 0.000152092 -0.000027263 -0.000023888

37 6 -0.000062959 -0.000077808 0.000038005

38 6 0.000000254 -0.000072461 0.000016258

39 6 -0.000152146 -0.000027810 0.000024741

40 6 0.000104352 0.000087397 -0.000030824

41 6 -0.000032609 -0.000002235 0.000071494

42 6 0.000182826 0.000088338 -0.000143365

43 6 -0.000020422 0.000054693 0.000052911

44 6 -0.000115136 -0.000124397 -0.000067291

45 6 0.000109054 0.000061605 0.000047905

46 6 -0.000086216 -0.000053507 -0.000050714

47 6 0.000029429 0.000028528 0.000090052

48 6 -0.000055299 0.000010194 -0.000043370

49 1 0.000039240 -0.000084916 -0.000011044

50 1 0.000027105 0.000061045 0.000044480

51 1 -0.000029323 -0.000070757 0.000002796

52 1 -0.000009043 0.000034432 -0.000082142

53 1 0.000029512 -0.000070375 -0.000003045

54 1 0.000009170 0.000034799 0.000082195

55 1 -0.000027726 0.000061120 -0.000045161

56 1 -0.000038296 -0.000084815 0.000011129

57 1 -0.000045500 -0.000014513 0.000042743

58 1 0.000020572 0.000022285 0.000020919

59 1 -0.000006299 0.000008445 -0.000019007

60 1 -0.000002652 -0.000007412 -0.000002659

61 1 -0.000034600 0.000035203 0.000068870

62 1 0.000011649 -0.000007952 -0.000007076

63 1 -0.000010479 0.000000747 0.000011898

64 1 0.000017937 -0.000026176 0.000002701

65 1 -0.000041475 0.000004315 0.000009711

66 1 -0.000018459 -0.000000164 0.000021401

67 1 0.000041002 0.000004318 -0.000009366

68 1 0.000018561 -0.000000060 -0.000021592

69 1 -0.000011711 -0.000008143 0.000007158

70 1 0.000010631 0.000000901 -0.000012140

71 1 -0.000017805 -0.000025942 -0.000002553

72 1 0.000034028 0.000034826 -0.000069130

73 1 0.000002444 -0.000007473 0.000002470

74 1 0.000006361 0.000008591 0.000019072

75 1 -0.000020723 0.000022190 -0.000020892

76 1 0.000045496 -0.000013911 -0.000042523

77 1 0.000208021 0.000105235 0.000038742

78 1 -0.000206824 0.000103308 -0.000043076

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

Cartesian Forces: Max 0.000215974 RMS 0.000062143

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

Leave Link 716 at Tue Aug 27 13:02:15 2019, MaxMem= 4294967296 cpu: 2.0

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000302471 RMS 0.000062320

Search for a local minimum.

Step number 10 out of a maximum of 452

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

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -1.80D-04 DEPred=-9.81D-05 R= 1.84D+00

TightC=F SS= 1.41D+00 RLast= 8.96D-02 DXNew= 1.5000D-01 2.6875D-01

Trust test= 1.84D+00 RLast= 8.96D-02 DXMaxT set to 1.50D-01

ITU= 1 -1 1 -1 -1 1 1 -1 1 0

Eigenvalues --- 0.00108 0.00199 0.00353 0.00590 0.00715

Eigenvalues --- 0.00784 0.00905 0.01035 0.01048 0.01111

Eigenvalues --- 0.01131 0.01149 0.01258 0.01279 0.01298

Eigenvalues --- 0.01299 0.01320 0.01421 0.01427 0.01559

Eigenvalues --- 0.01565 0.01571 0.01605 0.01675 0.01713

Eigenvalues --- 0.01719 0.01727 0.01740 0.01757 0.01765

Eigenvalues --- 0.01765 0.01780 0.01795 0.01798 0.01884

Eigenvalues --- 0.01936 0.01995 0.02002 0.02006 0.02159

Eigenvalues --- 0.02159 0.02245 0.02288 0.02295 0.02303

Eigenvalues --- 0.02330 0.02398 0.02463 0.02476 0.02527

Eigenvalues --- 0.02551 0.02553 0.02588 0.02634 0.02634

Eigenvalues --- 0.02648 0.02651 0.02765 0.02777 0.02797

Eigenvalues --- 0.02805 0.02863 0.02867 0.02872 0.02873

Eigenvalues --- 0.02915 0.02944 0.03926 0.04088 0.04187

Eigenvalues --- 0.04303 0.04361 0.04470 0.04545 0.04576

Eigenvalues --- 0.08299 0.09643 0.09663 0.09738 0.09841

Eigenvalues --- 0.09860 0.10306 0.10418 0.10564 0.10691

Eigenvalues --- 0.10713 0.10714 0.10744 0.10744 0.11040

Eigenvalues --- 0.11407 0.11408 0.11420 0.11422 0.11997

Eigenvalues --- 0.11998 0.12000 0.12008 0.12293 0.12293

Eigenvalues --- 0.12331 0.12331 0.12775 0.12777 0.12782

Eigenvalues --- 0.12784 0.15705 0.15937 0.16305 0.16404

Eigenvalues --- 0.17223 0.17384 0.17613 0.17863 0.18034

Eigenvalues --- 0.18046 0.18309 0.18365 0.19240 0.19284

Eigenvalues --- 0.19360 0.19364 0.19376 0.19411 0.19416

Eigenvalues --- 0.19423 0.19552 0.19552 0.19554 0.19555

Eigenvalues --- 0.20319 0.21490 0.22033 0.22807 0.22920

Eigenvalues --- 0.23188 0.23781 0.24256 0.24756 0.25467

Eigenvalues --- 0.26253 0.26433 0.26678 0.27067 0.28539

Eigenvalues --- 0.28570 0.28764 0.29020 0.29792 0.31017

Eigenvalues --- 0.31693 0.32009 0.32866 0.33093 0.33283

Eigenvalues --- 0.33345 0.34132 0.34188 0.35029 0.35568

Eigenvalues --- 0.35634 0.35635 0.35642 0.35647 0.35765

Eigenvalues --- 0.35768 0.35774 0.35819 0.35934 0.35935

Eigenvalues --- 0.35940 0.35943 0.35997 0.35999 0.36014

Eigenvalues --- 0.36016 0.36200 0.36207 0.36260 0.36264

Eigenvalues --- 0.36957 0.37063 0.37248 0.37392 0.37398

Eigenvalues --- 0.37473 0.38164 0.38417 0.38493 0.38496

Eigenvalues --- 0.39497 0.40341 0.40721 0.41065 0.41088

Eigenvalues --- 0.41097 0.41204 0.41237 0.41341 0.41369

Eigenvalues --- 0.41550 0.41824 0.42288 0.42563 0.44554

Eigenvalues --- 0.45241 0.45469 0.45912 0.45926 0.45969

Eigenvalues --- 0.45987 0.46059 0.46266 0.46268 0.46304

Eigenvalues --- 0.46316 0.48545 0.49020 0.49350 0.49558

Eigenvalues --- 0.50748 0.50751 0.50778 0.50780 0.51856

Eigenvalues --- 0.52164 0.57147 0.57654

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.40331 -0.09882 -0.01757 0.14687 0.33080

DIIS coeff's: 0.24172 0.03038 -0.03669

Cosine: 0.776 > 0.500

Length: 0.842

GDIIS step was calculated using 8 of the last 10 vectors.

Iteration 1 RMS(Cart)= 0.03235334 RMS(Int)= 0.00006521

Iteration 2 RMS(Cart)= 0.00019665 RMS(Int)= 0.00003194

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00003194

ITry= 1 IFail=0 DXMaxC= 1.47D-01 DCOld= 1.00D+10 DXMaxT= 1.50D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.65651 0.00004 0.00023 -0.00023 -0.00002 2.65649

R2 2.64073 0.00004 0.00072 0.00018 0.00085 2.64158

R3 2.03690 0.00004 0.00015 0.00009 0.00024 2.03714

R4 2.59960 -0.00012 -0.00054 -0.00003 -0.00053 2.59907

R5 2.71710 -0.00000 0.00004 -0.00009 -0.00006 2.71704

R6 2.59966 -0.00010 -0.00056 -0.00024 -0.00077 2.59889

R7 1.91080 -0.00018 -0.00069 -0.00020 -0.00089 1.90990

R8 2.65647 0.00005 -0.00064 0.00022 -0.00042 2.65605

R9 2.71598 0.00010 0.00161 0.00031 0.00193 2.71791

R10 2.03712 -0.00002 -0.00000 -0.00000 -0.00000 2.03711

R11 2.64209 0.00023 -0.00250 0.00138 -0.00112 2.64096

R12 2.80342 -0.00001 0.00052 -0.00037 0.00015 2.80357

R13 2.59450 0.00012 0.00216 -0.00052 0.00167 2.59617

R14 2.76191 0.00011 0.00007 0.00052 0.00058 2.76249

R15 2.59555 0.00006 -0.00279 0.00139 -0.00136 2.59419

R16 2.76210 -0.00004 0.00062 -0.00012 0.00049 2.76258

R17 2.64126 0.00006 0.00198 -0.00102 0.00097 2.64223

R18 2.55443 -0.00000 0.00001 -0.00020 -0.00023 2.55420

R19 2.03906 0.00000 -0.00006 0.00009 0.00004 2.03909

R20 2.03899 0.00006 0.00010 0.00005 0.00016 2.03914

R21 2.64124 0.00006 0.00192 -0.00075 0.00117 2.64241

R22 2.80361 -0.00002 -0.00022 0.00016 -0.00006 2.80355

R23 2.76209 -0.00004 0.00062 -0.00010 0.00051 2.76260

R24 2.59557 0.00005 -0.00274 0.00129 -0.00142 2.59415

R25 2.55443 -0.00000 0.00001 -0.00022 -0.00024 2.55419

R26 2.03906 0.00000 -0.00005 0.00008 0.00003 2.03908

R27 2.76192 0.00011 0.00009 0.00047 0.00055 2.76247

R28 2.03899 0.00006 0.00011 0.00005 0.00016 2.03914

R29 2.59449 0.00012 0.00212 -0.00038 0.00176 2.59626

R30 2.64211 0.00023 -0.00247 0.00116 -0.00131 2.64079

R31 2.71600 0.00010 0.00163 0.00008 0.00171 2.71771

R32 2.80337 -0.00001 0.00043 0.00020 0.00063 2.80400

R33 2.65645 0.00005 -0.00067 0.00041 -0.00027 2.65619

R34 2.59964 -0.00010 -0.00061 -0.00007 -0.00065 2.59900

R35 2.64074 0.00004 0.00076 -0.00001 0.00071 2.64145

R36 2.03712 -0.00002 0.00001 -0.00007 -0.00005 2.03707

R37 2.65650 0.00004 0.00020 0.00003 0.00021 2.65671

R38 2.03691 0.00004 0.00016 0.00004 0.00021 2.03711

R39 2.59959 -0.00012 -0.00058 0.00017 -0.00037 2.59922

R40 2.71713 -0.00001 0.00008 -0.00041 -0.00033 2.71680

R41 1.91077 -0.00018 -0.00076 0.00015 -0.00061 1.91016

R42 2.80357 -0.00001 -0.00035 0.00085 0.00050 2.80406

R43 2.65160 0.00000 -0.00011 0.00014 0.00003 2.65164

R44 2.65032 -0.00008 -0.00038 0.00016 -0.00022 2.65010

R45 2.62870 0.00006 -0.00015 0.00009 -0.00005 2.62865

R46 2.04840 0.00002 -0.00001 0.00006 0.00005 2.04845

R47 2.63628 0.00004 0.00004 0.00003 0.00007 2.63635

R48 2.05009 0.00003 0.00001 0.00006 0.00007 2.05016

R49 2.63406 0.00006 0.00005 0.00004 0.00009 2.63415

R50 2.05003 0.00001 -0.00000 0.00001 0.00000 2.05004

R51 2.63068 -0.00002 0.00027 -0.00018 0.00009 2.63077

R52 2.05013 0.00001 -0.00006 0.00005 -0.00002 2.05011

R53 2.04854 -0.00000 -0.00007 -0.00005 -0.00011 2.04843

R54 2.63632 -0.00002 0.00001 0.00001 0.00002 2.63634

R55 2.63413 -0.00001 0.00009 -0.00005 0.00004 2.63417

R56 2.05003 0.00000 0.00001 0.00000 0.00001 2.05004

R57 2.62869 -0.00006 -0.00002 0.00003 0.00001 2.62870

R58 2.05018 -0.00001 -0.00005 0.00001 -0.00004 2.05014

R59 2.65172 -0.00008 0.00008 -0.00026 -0.00018 2.65154

R60 2.04848 -0.00002 -0.00016 0.00011 -0.00005 2.04843

R61 2.65026 0.00004 0.00015 -0.00018 -0.00002 2.65023

R62 2.63060 0.00008 0.00007 0.00009 0.00016 2.63076

R63 2.04847 0.00003 -0.00003 0.00008 0.00005 2.04852

R64 2.05009 0.00002 -0.00001 0.00004 0.00003 2.05013

R65 2.65027 0.00004 0.00021 -0.00047 -0.00026 2.65002

R66 2.65173 -0.00008 0.00012 -0.00054 -0.00042 2.65132

R67 2.63059 0.00008 0.00006 0.00019 0.00025 2.63084

R68 2.04847 0.00003 -0.00004 0.00015 0.00010 2.04857

R69 2.63413 -0.00001 0.00009 -0.00006 0.00003 2.63416

R70 2.05009 0.00002 -0.00001 0.00004 0.00004 2.05013

R71 2.63632 -0.00002 0.00003 -0.00005 -0.00002 2.63630

R72 2.05003 0.00000 0.00000 0.00001 0.00001 2.05004

R73 2.62868 -0.00006 -0.00004 0.00014 0.00010 2.62879

R74 2.05018 -0.00001 -0.00004 0.00002 -0.00003 2.05015

R75 2.04848 -0.00002 -0.00017 0.00014 -0.00003 2.04845

R76 2.65034 -0.00008 -0.00036 -0.00006 -0.00042 2.64992

R77 2.65162 0.00000 -0.00009 -0.00005 -0.00014 2.65148

R78 2.63067 -0.00002 0.00026 -0.00010 0.00015 2.63082

R79 2.04854 -0.00000 -0.00007 -0.00000 -0.00008 2.04846

R80 2.63406 0.00006 0.00005 0.00003 0.00008 2.63414

R81 2.05013 0.00001 -0.00006 0.00005 -0.00001 2.05012

R82 2.63628 0.00004 0.00005 -0.00001 0.00004 2.63632

R83 2.05003 0.00001 0.00000 0.00000 0.00001 2.05004

R84 2.62870 0.00006 -0.00016 0.00019 0.00003 2.62873

R85 2.05009 0.00003 0.00001 0.00007 0.00008 2.05017

R86 2.04840 0.00002 -0.00001 0.00007 0.00006 2.04846

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A2 2.18725 0.00008 0.00046 -0.00000 0.00045 2.18770

A3 2.21395 -0.00001 -0.00016 0.00020 0.00004 2.21399

A4 1.86809 -0.00001 -0.00029 0.00016 -0.00010 1.86798

A5 2.21919 0.00030 0.00185 0.00062 0.00238 2.22157

A6 2.19551 -0.00029 -0.00170 -0.00072 -0.00231 2.19320

A7 1.92456 0.00012 0.00060 0.00012 0.00067 1.92524

A8 2.18038 -0.00010 -0.00099 -0.00069 -0.00169 2.17869

A9 2.17694 -0.00002 0.00059 0.00103 0.00161 2.17855

A10 1.86843 -0.00008 -0.00009 -0.00019 -0.00027 1.86816

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A12 2.22126 0.00007 0.00057 -0.00059 -0.00016 2.22110

A13 1.88141 0.00004 0.00005 0.00012 0.00018 1.88159

A14 2.21427 -0.00006 -0.00050 0.00015 -0.00036 2.21392

A15 2.18749 0.00002 0.00046 -0.00028 0.00017 2.18765

A16 2.18410 0.00021 0.00138 -0.00014 0.00142 2.18552

A17 2.02582 -0.00017 -0.00198 -0.00026 -0.00232 2.02350

A18 2.07322 -0.00004 0.00059 0.00037 0.00088 2.07410

A19 2.19160 0.00007 -0.00017 0.00005 0.00001 2.19161

A20 2.16499 0.00001 0.00105 -0.00030 0.00063 2.16562

A21 1.92659 -0.00008 -0.00093 0.00024 -0.00066 1.92592

A22 1.84705 0.00001 0.00053 -0.00030 0.00019 1.84724

A23 1.92616 0.00002 0.00033 -0.00004 0.00031 1.92647

A24 2.19121 0.00011 0.00042 0.00072 0.00125 2.19246

A25 2.16579 -0.00012 -0.00075 -0.00067 -0.00155 2.16424

A26 1.86199 0.00002 -0.00003 0.00009 0.00008 1.86207

A27 2.19715 -0.00005 0.00006 -0.00052 -0.00047 2.19669

A28 2.22365 0.00003 -0.00004 0.00043 0.00039 2.22403

A29 1.86196 0.00003 0.00005 0.00002 0.00009 1.86205

A30 2.19649 0.00005 0.00035 0.00013 0.00047 2.19696

A31 2.22431 -0.00008 -0.00038 -0.00011 -0.00050 2.22381

A32 2.18544 0.00001 -0.00040 0.00044 0.00019 2.18563

A33 2.02393 0.00014 0.00070 -0.00018 0.00047 2.02439

A34 2.07374 -0.00015 -0.00029 -0.00028 -0.00063 2.07311

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A46 2.19159 0.00007 -0.00020 0.00039 0.00031 2.19190

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A48 2.18404 0.00021 0.00127 0.00067 0.00212 2.18616

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A50 2.02580 -0.00017 -0.00209 0.00011 -0.00206 2.02375

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A67 2.07381 -0.00015 -0.00011 -0.00145 -0.00163 2.07218

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D3 -3.12133 0.00003 0.00029 0.00172 0.00202 -3.11931

D4 0.04922 0.00003 0.00413 -0.00061 0.00350 0.05272

D5 0.00062 -0.00004 -0.00131 -0.00017 -0.00146 -0.00084

D6 -3.13507 -0.00003 -0.00171 0.00191 0.00022 -3.13486

D7 3.13590 -0.00003 -0.00006 -0.00209 -0.00215 3.13375

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D10 3.06483 0.00004 0.00320 0.00978 0.01298 3.07781

D11 3.08906 -0.00001 -0.00482 0.00277 -0.00208 3.08697

D12 -0.10522 0.00005 -0.00044 0.01210 0.01163 -0.09359

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D15 0.23844 -0.00002 -0.00404 0.00059 -0.00341 0.23503

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D33 -0.98839 -0.00003 -0.00225 0.00120 -0.00105 -0.98945

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D40 -0.05852 -0.00001 -0.00224 -0.00161 -0.00385 -0.06237

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D57 -3.02081 -0.00001 0.00673 -0.00073 0.00603 -3.01478

D58 0.12839 -0.00002 0.00510 -0.00107 0.00406 0.13245

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D61 0.98734 0.00014 -0.00266 0.00572 0.00306 0.99041

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D102 3.13575 -0.00003 -0.00036 0.00008 -0.00027 3.13548

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D128 3.12031 -0.00000 -0.00045 -0.00022 -0.00067 3.11964

D129 -0.01615 -0.00002 -0.00065 0.00003 -0.00062 -0.01677

D130 3.12455 -0.00001 -0.00039 0.00028 -0.00011 3.12444

D131 -3.13656 -0.00000 -0.00068 -0.00021 -0.00089 -3.13746

D132 0.00413 0.00001 -0.00043 0.00005 -0.00038 0.00375

D133 0.00506 0.00002 -0.00001 0.00014 0.00014 0.00520

D134 -3.13412 -0.00001 -0.00006 -0.00017 -0.00023 -3.13435

D135 -3.13563 0.00001 -0.00026 -0.00011 -0.00038 -3.13601

D136 0.00838 -0.00002 -0.00032 -0.00043 -0.00075 0.00763

D137 0.00734 -0.00003 -0.00003 -0.00044 -0.00047 0.00687

D138 -3.13155 -0.00001 -0.00039 0.00033 -0.00005 -3.13160

D139 -3.13666 -0.00000 0.00003 -0.00013 -0.00010 -3.13677

D140 0.00763 0.00002 -0.00033 0.00064 0.00031 0.00795

D141 -0.00879 0.00004 0.00072 0.00058 0.00130 -0.00750

D142 -3.13112 0.00001 -0.00017 0.00039 0.00022 -3.13090

D143 3.13011 0.00002 0.00108 -0.00019 0.00088 3.13099

D144 0.00779 -0.00002 0.00019 -0.00038 -0.00019 0.00759

D145 -0.00608 0.00002 0.00080 -0.00003 0.00077 -0.00531

D146 3.13532 0.00001 0.00035 -0.00001 0.00035 3.13566

D147 3.13354 0.00000 0.00068 -0.00036 0.00033 3.13387

D148 -0.00825 -0.00002 0.00024 -0.00033 -0.00009 -0.00835

D149 -0.00619 -0.00003 -0.00037 -0.00031 -0.00067 -0.00686

D150 3.13159 0.00001 0.00005 0.00037 0.00042 3.13201

D151 3.13738 -0.00001 -0.00025 0.00002 -0.00023 3.13715

D152 -0.00803 0.00003 0.00016 0.00069 0.00086 -0.00717

D153 0.01657 -0.00001 -0.00046 -0.00008 -0.00055 0.01602

D154 3.13722 -0.00001 -0.00050 0.00083 0.00032 3.13754

D155 -3.12483 0.00000 -0.00002 -0.00011 -0.00013 -3.12496

D156 -0.00418 0.00001 -0.00006 0.00080 0.00075 -0.00343

D157 3.13260 -0.00005 -0.00228 0.00130 -0.00100 3.13160

D158 -0.01450 0.00001 -0.00030 0.00052 0.00022 -0.01428

D159 0.01186 -0.00005 -0.00225 0.00039 -0.00187 0.00998

D160 -3.13524 0.00001 -0.00027 -0.00039 -0.00065 -3.13590

D161 3.13828 0.00004 0.00273 -0.00163 0.00109 3.13937

D162 0.01684 0.00003 0.00123 -0.00162 -0.00040 0.01644

D163 0.00219 -0.00002 0.00073 -0.00086 -0.00013 0.00206

D164 -3.11925 -0.00003 -0.00078 -0.00085 -0.00162 -3.12087

D165 0.00810 0.00003 -0.00040 0.00076 0.00036 0.00846

D166 -3.12969 -0.00001 -0.00082 0.00009 -0.00073 -3.13042

D167 3.12944 0.00004 0.00110 0.00075 0.00185 3.13129

D168 -0.00835 0.00000 0.00069 0.00008 0.00076 -0.00759

D169 3.13816 0.00004 0.00254 -0.00080 0.00173 3.13989

D170 0.01676 0.00003 0.00120 -0.00151 -0.00032 0.01644

D171 0.00222 -0.00002 0.00079 -0.00126 -0.00047 0.00176

D172 -3.11917 -0.00003 -0.00054 -0.00198 -0.00252 -3.12169

D173 3.13272 -0.00005 -0.00210 0.00055 -0.00157 3.13116

D174 0.01199 -0.00006 -0.00206 -0.00047 -0.00254 0.00945

D175 -0.01453 0.00001 -0.00038 0.00101 0.00063 -0.01390

D176 -3.13527 0.00001 -0.00034 -0.00001 -0.00034 -3.13561

D177 0.00808 0.00003 -0.00041 0.00082 0.00042 0.00850

D178 -3.12968 -0.00001 -0.00076 -0.00010 -0.00086 -3.13054

D179 3.12938 0.00004 0.00093 0.00154 0.00246 3.13184

D180 -0.00838 0.00000 0.00057 0.00062 0.00118 -0.00720

D181 -0.00618 -0.00003 -0.00041 -0.00010 -0.00051 -0.00670

D182 3.13739 -0.00001 -0.00023 -0.00003 -0.00026 3.13713

D183 3.13156 0.00001 -0.00005 0.00082 0.00077 3.13233

D184 -0.00805 0.00003 0.00013 0.00090 0.00103 -0.00702

D185 -0.00608 0.00003 0.00082 -0.00015 0.00067 -0.00541

D186 3.13533 0.00001 0.00040 -0.00020 0.00020 3.13552

D187 3.13353 0.00000 0.00064 -0.00022 0.00042 3.13395

D188 -0.00825 -0.00002 0.00022 -0.00027 -0.00005 -0.00830

D189 0.01658 -0.00001 -0.00042 -0.00032 -0.00074 0.01584

D190 3.13723 -0.00001 -0.00048 0.00071 0.00023 3.13746

D191 -3.12483 0.00000 -0.00000 -0.00027 -0.00027 -3.12510

D192 -0.00418 0.00001 -0.00006 0.00076 0.00070 -0.00348

D193 -3.14027 -0.00003 -0.00139 -0.00081 -0.00221 3.14070

D194 -0.01790 0.00000 -0.00074 0.00024 -0.00050 -0.01840

D195 -0.00213 -0.00004 -0.00136 -0.00000 -0.00136 -0.00349

D196 3.12024 -0.00000 -0.00071 0.00105 0.00035 3.12059

D197 -3.13047 0.00002 0.00146 0.00032 0.00178 -3.12868

D198 -0.00996 0.00001 0.00151 0.00058 0.00208 -0.00788

D199 0.01458 0.00003 0.00141 -0.00049 0.00093 0.01551

D200 3.13509 0.00001 0.00146 -0.00023 0.00123 3.13631

D201 -0.00879 0.00004 0.00065 0.00056 0.00122 -0.00757

D202 3.13010 0.00002 0.00097 0.00013 0.00110 3.13120

D203 -3.13107 0.00001 0.00001 -0.00049 -0.00048 -3.13155

D204 0.00781 -0.00001 0.00032 -0.00093 -0.00060 0.00721

D205 0.00735 -0.00003 0.00003 -0.00064 -0.00061 0.00673

D206 -3.13667 -0.00000 0.00000 -0.00003 -0.00002 -3.13670

D207 -3.13152 -0.00001 -0.00029 -0.00021 -0.00049 -3.13202

D208 0.00764 0.00002 -0.00031 0.00041 0.00010 0.00774

D209 0.00506 0.00002 0.00003 0.00016 0.00018 0.00524

D210 -3.13564 0.00001 -0.00032 0.00023 -0.00009 -3.13573

D211 -3.13411 -0.00001 0.00005 -0.00046 -0.00041 -3.13451

D212 0.00838 -0.00002 -0.00030 -0.00038 -0.00068 0.00770

D213 -0.01616 -0.00002 -0.00075 0.00041 -0.00034 -0.01651

D214 -3.13658 -0.00000 -0.00080 0.00016 -0.00064 -3.13722

D215 3.12454 -0.00001 -0.00041 0.00034 -0.00007 3.12447

D216 0.00413 0.00001 -0.00045 0.00008 -0.00037 0.00376

Item Value Threshold Converged?

Maximum Force 0.000302 0.000450 YES

RMS Force 0.000062 0.000300 YES

Maximum Displacement 0.147378 0.001800 NO

RMS Displacement 0.032385 0.001200 NO

Predicted change in Energy=-1.125355D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Aug 27 13:02:15 2019, MaxMem= 4294967296 cpu: 2.0

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

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=1 Diff= 1.12D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.681158 -4.168920 0.556914

2 6 0 1.117164 -2.881576 0.198049

3 7 0 -0.008060 -2.115808 0.000304

4 6 0 -1.140224 -2.873593 0.188299

5 6 0 -0.716682 -4.164003 0.550157

6 6 0 -2.493019 -2.419803 0.007740

7 6 0 -2.884804 -1.084522 -0.121269

8 7 0 -2.067773 0.007566 0.043732

9 6 0 -2.875826 1.106653 -0.109904

10 6 0 -4.239729 0.694085 -0.436544

11 6 0 -4.244913 -0.657505 -0.444937

12 6 0 2.473884 -2.438280 0.024664

13 6 0 2.876012 -1.105909 -0.110708

14 6 0 4.239684 -0.692450 -0.437215

15 6 0 4.244786 0.659149 -0.442361

16 6 0 2.884734 1.085287 -0.117356

17 7 0 2.067920 -0.007290 0.045839

18 6 0 2.492811 2.420325 0.012755

19 6 0 1.140213 2.874727 0.192416

20 6 0 0.716392 4.168715 0.541217

21 6 0 -0.681380 4.173645 0.547162

22 6 0 -1.117245 2.882667 0.200936

23 7 0 0.008172 2.114882 0.011712

24 6 0 -2.473610 2.438676 0.027636

25 6 0 -3.533334 -3.477042 -0.024021

26 6 0 -3.459398 -4.525186 -0.953997

27 6 0 -4.442621 -5.508402 -0.992773

28 6 0 -5.506130 -5.473301 -0.090549

29 6 0 -5.582698 -4.444380 0.846734

30 6 0 -4.607227 -3.451622 0.877506

31 6 0 5.468171 -5.511305 -0.032170

32 6 0 4.412682 -5.544354 -0.943835

33 6 0 3.435824 -4.554316 -0.919615

34 6 0 3.507945 -3.501931 0.005625

35 6 0 4.574451 -3.478016 0.916030

36 6 0 5.543344 -4.477534 0.899892

37 6 0 -3.508510 3.501868 0.007621

38 6 0 -4.571751 3.480762 0.921732

39 6 0 -5.541771 4.479226 0.904535

40 6 0 -5.470859 5.508929 -0.032342

41 6 0 -4.418668 5.538910 -0.947884

42 6 0 -3.440727 4.549902 -0.922692

43 6 0 3.533764 3.477190 -0.021247

44 6 0 4.605578 3.454717 0.882682

45 6 0 5.582322 4.446178 0.849301

46 6 0 5.509029 5.470661 -0.093088

47 6 0 4.447650 5.502581 -0.997908

48 6 0 3.463215 4.520624 -0.956641

49 1 0 1.323622 -5.000184 0.798463

50 1 0 -1.367207 -4.990816 0.785251

51 1 0 -5.064754 1.354419 -0.654769

52 1 0 -5.075081 -1.308557 -0.671521

53 1 0 5.064553 -1.352176 -0.657838

54 1 0 5.074832 1.310781 -0.667721

55 1 0 1.366616 4.998286 0.767138

56 1 0 -1.323739 5.007812 0.778699

57 1 0 -2.637153 -4.554839 -1.659740

58 1 0 -4.378878 -6.303093 -1.728576

59 1 0 -6.268852 -6.244279 -0.117175

60 1 0 -6.401410 -4.414847 1.557922

61 1 0 -4.664934 -2.658687 1.614347

62 1 0 6.225566 -6.287832 -0.047243

63 1 0 4.350392 -6.342680 -1.675804

64 1 0 2.619778 -4.582423 -1.632564

65 1 0 4.631080 -2.680981 1.648591

66 1 0 6.355982 -4.449324 1.618078

67 1 0 -4.625188 2.686548 1.657631

68 1 0 -6.351996 4.453287 1.625531

69 1 0 -6.229106 6.284608 -0.048260

70 1 0 -4.359772 6.333978 -1.683679

71 1 0 -2.627262 4.575509 -1.638695

72 1 0 4.660913 2.664843 1.623012

73 1 0 6.399579 4.418971 1.562256

74 1 0 6.272751 6.240574 -0.121793

75 1 0 4.386587 6.293647 -1.737840

76 1 0 2.642723 4.547614 -1.664540

77 1 0 -0.003727 -1.128621 -0.216293

78 1 0 0.004141 1.123850 -0.187256

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

Rotational constants (GHZ): 0.0587905 0.0582552 0.0300893

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

Standard basis: 6-311G(d) (5D, 7F)

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

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5356.8133262747 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122152959 Hartrees.

Nuclear repulsion after empirical dispersion term = 5356.6011109789 Hartrees.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5786

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.33D-11

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 313

GePol: Fraction of low-weight points (<1% of avg) = 5.41%

GePol: Cavity surface area = 611.280 Ang\*\*2

GePol: Cavity volume = 627.649 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021017442 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5356.5990092347 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.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Aug 27 13:02:17 2019, MaxMem= 4294967296 cpu: 2.3

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

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 0.999215 0.000068 -0.000010 -0.039604 Ang= 4.54 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0550 S= 1.0182

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30459244453

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 580000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 100433388.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.10D-15 for 5778.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.90D-15 for 4246 3903.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.33D-15 for 5778.

Iteration 1 A^-1\*A deviation from orthogonality is 7.24D-09 for 4965 4838.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.89D-15 for 10.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.19D-15 for 3044 2811.

Iteration 2 A^-1\*A deviation from unit magnitude is 8.88D-16 for 684.

Iteration 2 A^-1\*A deviation from orthogonality is 4.03D-16 for 3367 941.

E= -1914.33141721477

DIIS: error= 1.51D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.33141721477 IErMin= 1 ErrMin= 1.51D-03

ErrMax= 1.51D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.39D-03 BMatP= 4.39D-03

IDIUse=3 WtCom= 9.85D-01 WtEn= 1.51D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.640 Goal= None Shift= 0.000

Gap= 0.706 Goal= None Shift= 0.000

GapD= 0.640 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=4.72D-05 MaxDP=1.35D-03 OVMax= 5.29D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.72D-05 CP: 1.00D+00

E= -1914.33330695246 Delta-E= -0.001889737694 Rises=F Damp=F

DIIS: error= 1.16D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33330695246 IErMin= 2 ErrMin= 1.16D-04

ErrMax= 1.16D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.27D-05 BMatP= 4.39D-03

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.16D-03

Coeff-Com: -0.630D-01 0.106D+01

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

Coeff: -0.629D-01 0.106D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.69D-06 MaxDP=2.75D-04 DE=-1.89D-03 OVMax= 2.03D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 6.84D-06 CP: 1.00D+00 1.07D+00

E= -1914.33332747971 Delta-E= -0.000020527245 Rises=F Damp=F

DIIS: error= 6.32D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33332747971 IErMin= 3 ErrMin= 6.32D-05

ErrMax= 6.32D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.04D-05 BMatP= 4.27D-05

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

Coeff-Com: -0.328D-01 0.484D+00 0.549D+00

Coeff: -0.328D-01 0.484D+00 0.549D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.87D-06 MaxDP=1.86D-04 DE=-2.05D-05 OVMax= 7.64D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.54D-06 CP: 1.00D+00 1.08D+00 8.10D-01

E= -1914.33333181086 Delta-E= -0.000004331152 Rises=F Damp=F

DIIS: error= 2.84D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33333181086 IErMin= 4 ErrMin= 2.84D-05

ErrMax= 2.84D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.05D-06 BMatP= 2.04D-05

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

Coeff-Com: -0.561D-02 0.583D-01 0.306D+00 0.641D+00

Coeff: -0.561D-02 0.583D-01 0.306D+00 0.641D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.35D-06 MaxDP=9.09D-05 DE=-4.33D-06 OVMax= 8.75D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.07D-06 CP: 1.00D+00 1.08D+00 9.12D-01 8.39D-01

E= -1914.33333294539 Delta-E= -0.000001134527 Rises=F Damp=F

DIIS: error= 1.36D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33333294539 IErMin= 5 ErrMin= 1.36D-05

ErrMax= 1.36D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.89D-07 BMatP= 4.05D-06

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

Coeff-Com: -0.248D-03-0.983D-02 0.110D+00 0.323D+00 0.577D+00

Coeff: -0.248D-03-0.983D-02 0.110D+00 0.323D+00 0.577D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=6.06D-07 MaxDP=4.13D-05 DE=-1.13D-06 OVMax= 4.14D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 5.08D-07 CP: 1.00D+00 1.08D+00 9.34D-01 9.46D-01 1.09D+00

E= -1914.33333310495 Delta-E= -0.000000159564 Rises=F Damp=F

DIIS: error= 9.72D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33333310495 IErMin= 6 ErrMin= 9.72D-06

ErrMax= 9.72D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-07 BMatP= 3.89D-07

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

Coeff-Com: 0.100D-02-0.183D-01 0.241D-02 0.655D-01 0.341D+00 0.609D+00

Coeff: 0.100D-02-0.183D-01 0.241D-02 0.655D-01 0.341D+00 0.609D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.23D-07 MaxDP=4.00D-05 DE=-1.60D-07 OVMax= 5.06D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.80D-07 CP: 1.00D+00 1.08D+00 9.60D-01 9.84D-01 1.43D+00

CP: 1.27D+00

E= -1914.33333319724 Delta-E= -0.000000092284 Rises=F Damp=F

DIIS: error= 6.85D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33333319724 IErMin= 7 ErrMin= 6.85D-06

ErrMax= 6.85D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.26D-08 BMatP= 1.05D-07

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

Coeff-Com: 0.486D-03-0.652D-02-0.168D-01-0.167D-01 0.461D-01 0.307D+00

Coeff-Com: 0.687D+00

Coeff: 0.486D-03-0.652D-02-0.168D-01-0.167D-01 0.461D-01 0.307D+00

Coeff: 0.687D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.19D-07 MaxDP=2.99D-05 DE=-9.23D-08 OVMax= 4.07D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.09D-07 CP: 1.00D+00 1.09D+00 9.75D-01 1.03D+00 1.67D+00

CP: 1.76D+00 1.36D+00

E= -1914.33333325116 Delta-E= -0.000000053928 Rises=F Damp=F

DIIS: error= 6.27D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33333325116 IErMin= 8 ErrMin= 6.27D-06

ErrMax= 6.27D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.60D-08 BMatP= 3.26D-08

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

Coeff-Com: -0.654D-03 0.144D-01-0.193D-01-0.803D-01-0.355D+00-0.355D+00

Coeff-Com: 0.486D+00 0.131D+01

Coeff: -0.654D-03 0.144D-01-0.193D-01-0.803D-01-0.355D+00-0.355D+00

Coeff: 0.486D+00 0.131D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=9.86D-07 MaxDP=7.59D-05 DE=-5.39D-08 OVMax= 1.04D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.29D-07 CP: 1.00D+00 1.09D+00 1.01D+00 1.12D+00 2.29D+00

CP: 2.81D+00 2.61D+00 1.79D+00

E= -1914.33333332749 Delta-E= -0.000000076328 Rises=F Damp=F

DIIS: error= 2.84D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33333332749 IErMin= 9 ErrMin= 2.84D-06

ErrMax= 2.84D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.93D-09 BMatP= 1.60D-08

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

Coeff-Com: -0.359D-03 0.651D-02-0.105D-02-0.139D-01-0.128D+00-0.205D+00

Coeff-Com: -0.176D+00 0.580D+00 0.937D+00

Coeff: -0.359D-03 0.651D-02-0.105D-02-0.139D-01-0.128D+00-0.205D+00

Coeff: -0.176D+00 0.580D+00 0.937D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.73D-07 MaxDP=3.70D-05 DE=-7.63D-08 OVMax= 5.08D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.85D-07 CP: 1.00D+00 1.09D+00 1.02D+00 1.16D+00 2.56D+00

CP: 3.00D+00 3.00D+00 2.62D+00 1.61D+00

E= -1914.33333334391 Delta-E= -0.000000016422 Rises=F Damp=F

DIIS: error= 1.59D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33333334391 IErMin=10 ErrMin= 1.59D-06

ErrMax= 1.59D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.46D-09 BMatP= 5.93D-09

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

Coeff-Com: -0.168D-05-0.909D-03 0.559D-02 0.212D-01 0.434D-01-0.675D-02

Coeff-Com: -0.321D+00-0.139D-01 0.569D+00 0.704D+00

Coeff: -0.168D-05-0.909D-03 0.559D-02 0.212D-01 0.434D-01-0.675D-02

Coeff: -0.321D+00-0.139D-01 0.569D+00 0.704D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.12D-07 MaxDP=1.76D-05 DE=-1.64D-08 OVMax= 2.36D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.03D-08 CP: 1.00D+00 1.09D+00 1.03D+00 1.17D+00 2.68D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.15D+00 1.69D+00

E= -1914.33333334787 Delta-E= -0.000000003954 Rises=F Damp=F

DIIS: error= 7.84D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33333334787 IErMin=11 ErrMin= 7.84D-07

ErrMax= 7.84D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.05D-10 BMatP= 2.46D-09

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

Coeff-Com: 0.108D-03-0.238D-02 0.231D-02 0.147D-01 0.595D-01 0.583D-01

Coeff-Com: -0.117D+00-0.139D+00-0.854D-01 0.325D+00 0.883D+00

Coeff: 0.108D-03-0.238D-02 0.231D-02 0.147D-01 0.595D-01 0.583D-01

Coeff: -0.117D+00-0.139D+00-0.854D-01 0.325D+00 0.883D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.21D-07 MaxDP=1.05D-05 DE=-3.95D-09 OVMax= 1.33D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 4.21D-08 CP: 1.00D+00 1.09D+00 1.03D+00 1.18D+00 2.74D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.55D+00 2.08D+00

CP: 1.32D+00

E= -1914.33333334922 Delta-E= -0.000000001353 Rises=F Damp=F

DIIS: error= 3.94D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.33333334922 IErMin=12 ErrMin= 3.94D-07

ErrMax= 3.94D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.96D-10 BMatP= 7.05D-10

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

Coeff-Com: 0.599D-04-0.950D-03-0.119D-02 0.459D-03 0.167D-01 0.352D-01

Coeff-Com: 0.476D-01-0.423D-01-0.289D+00-0.915D-01 0.523D+00 0.801D+00

Coeff: 0.599D-04-0.950D-03-0.119D-02 0.459D-03 0.167D-01 0.352D-01

Coeff: 0.476D-01-0.423D-01-0.289D+00-0.915D-01 0.523D+00 0.801D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.99D-08 MaxDP=4.95D-06 DE=-1.35D-09 OVMax= 6.20D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.84D-08 CP: 1.00D+00 1.09D+00 1.03D+00 1.18D+00 2.76D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.80D+00 2.26D+00

CP: 1.56D+00 1.43D+00

E= -1914.33333334967 Delta-E= -0.000000000446 Rises=F Damp=F

DIIS: error= 1.78D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.33333334967 IErMin=13 ErrMin= 1.78D-07

ErrMax= 1.78D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.19D-11 BMatP= 2.96D-10

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

Coeff-Com: -0.481D-06 0.228D-03-0.155D-02-0.430D-02-0.994D-02 0.476D-03

Coeff-Com: 0.581D-01 0.287D-01-0.143D+00-0.153D+00 0.236D-01 0.442D+00

Coeff-Com: 0.758D+00

Coeff: -0.481D-06 0.228D-03-0.155D-02-0.430D-02-0.994D-02 0.476D-03

Coeff: 0.581D-01 0.287D-01-0.143D+00-0.153D+00 0.236D-01 0.442D+00

Coeff: 0.758D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.27D-08 MaxDP=3.13D-06 DE=-4.46D-10 OVMax= 3.42D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 7.28D-09 CP: 1.00D+00 1.09D+00 1.03D+00 1.18D+00 2.77D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.92D+00 2.36D+00

CP: 1.65D+00 1.74D+00 1.18D+00

E= -1914.33333334977 Delta-E= -0.000000000104 Rises=F Damp=F

DIIS: error= 8.31D-08 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.33333334977 IErMin=14 ErrMin= 8.31D-08

ErrMax= 8.31D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.72D-11 BMatP= 8.19D-11

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

Coeff-Com: -0.191D-04 0.439D-03-0.562D-03-0.264D-02-0.115D-01-0.109D-01

Coeff-Com: 0.181D-01 0.332D-01 0.722D-02-0.635D-01-0.160D+00 0.140D-01

Coeff-Com: 0.467D+00 0.709D+00

Coeff: -0.191D-04 0.439D-03-0.562D-03-0.264D-02-0.115D-01-0.109D-01

Coeff: 0.181D-01 0.332D-01 0.722D-02-0.635D-01-0.160D+00 0.140D-01

Coeff: 0.467D+00 0.709D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.44D-08 MaxDP=1.26D-06 DE=-1.04D-10 OVMax= 1.49D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 3.74D-09 CP: 1.00D+00 1.09D+00 1.04D+00 1.18D+00 2.77D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.96D+00 2.40D+00

CP: 1.72D+00 1.85D+00 1.39D+00 1.07D+00

E= -1914.33333334986 Delta-E= -0.000000000086 Rises=F Damp=F

DIIS: error= 4.30D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.33333334986 IErMin=15 ErrMin= 4.30D-08

ErrMax= 4.30D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.67D-12 BMatP= 2.72D-11

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

Coeff-Com: -0.767D-05 0.117D-03 0.199D-03 0.846D-04-0.224D-02-0.446D-02

Coeff-Com: -0.903D-02 0.591D-02 0.419D-01 0.154D-01-0.760D-01-0.106D+00

Coeff-Com: -0.554D-02 0.307D+00 0.833D+00

Coeff: -0.767D-05 0.117D-03 0.199D-03 0.846D-04-0.224D-02-0.446D-02

Coeff: -0.903D-02 0.591D-02 0.419D-01 0.154D-01-0.760D-01-0.106D+00

Coeff: -0.554D-02 0.307D+00 0.833D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=6.41D-09 MaxDP=5.87D-07 DE=-8.64D-11 OVMax= 6.59D-06

Error on total polarization charges = 0.08259

SCF Done: E(UB3LYP) = -1914.33333335 A.U. after 15 cycles

NFock= 15 Conv=0.64D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0183

<L.S>= 0.000000000000E+00

KE= 1.906378594746D+03 PE=-1.516281817684D+04 EE= 5.985507239506D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0551, after 2.0017

Leave Link 502 at Tue Aug 27 13:09:08 2019, MaxMem= 4294967296 cpu: 6411.5

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

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

Range of M.O.s used for correlation: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48783308D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64353144D-01

Leave Link 801 at Tue Aug 27 13:09:08 2019, MaxMem= 4294967296 cpu: 1.0

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

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

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

Leave Link 1101 at Tue Aug 27 13:09:15 2019, MaxMem= 4294967296 cpu: 111.3

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

Symmetrizing basis deriv contribution to polar:

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

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

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 191

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 27 13:29:04 2019, MaxMem= 4294967296 cpu: 19012.0

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

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 580000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.42D+03 4.53D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.55D+02 3.68D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.60D+00 4.69D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.03D-01 3.93D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.62D-04 2.10D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.62D-06 1.35D-04.

190 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 2.00D-08 1.02D-05.

86 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.28D-11 6.20D-07.

47 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.15D-13 3.93D-08.

6 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 8.99D-15 5.99D-09.

5 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 4.04D-15 1.98D-09.

5 vectors produced by pass 11 Test12= 2.55D-13 1.00D-09 XBig12= 7.90D-15 3.02D-09.

4 vectors produced by pass 12 Test12= 2.55D-13 1.00D-09 XBig12= 5.13D-15 2.98D-09.

4 vectors produced by pass 13 Test12= 2.55D-13 1.00D-09 XBig12= 8.07D-15 2.56D-09.

4 vectors produced by pass 14 Test12= 2.55D-13 1.00D-09 XBig12= 5.11D-15 2.03D-09.

3 vectors produced by pass 15 Test12= 2.55D-13 1.00D-09 XBig12= 3.69D-15 1.97D-09.

3 vectors produced by pass 16 Test12= 2.55D-13 1.00D-09 XBig12= 8.17D-15 2.82D-09.

3 vectors produced by pass 17 Test12= 2.55D-13 1.00D-09 XBig12= 5.56D-15 3.26D-09.

3 vectors produced by pass 18 Test12= 2.55D-13 1.00D-09 XBig12= 7.60D-15 3.19D-09.

3 vectors produced by pass 19 Test12= 2.55D-13 1.00D-09 XBig12= 5.36D-15 2.51D-09.

3 vectors produced by pass 20 Test12= 2.55D-13 1.00D-09 XBig12= 6.21D-15 2.91D-09.

3 vectors produced by pass 21 Test12= 2.55D-13 1.00D-09 XBig12= 5.71D-15 3.15D-09.

3 vectors produced by pass 22 Test12= 2.55D-13 1.00D-09 XBig12= 6.87D-15 2.78D-09.

3 vectors produced by pass 23 Test12= 2.55D-13 1.00D-09 XBig12= 7.34D-15 2.58D-09.

2 vectors produced by pass 24 Test12= 2.55D-13 1.00D-09 XBig12= 5.04D-15 2.07D-09.

InvSVY: IOpt=1 It= 1 EMax= 7.11D-14

Solved reduced A of dimension 1787 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1125.72 Bohr\*\*3.

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

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

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

Leave Link 1002 at Tue Aug 27 17:21:41 2019, MaxMem= 4294967296 cpu: 223255.0

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 191

Leave Link 701 at Tue Aug 27 17:23:10 2019, MaxMem= 4294967296 cpu: 1421.3

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

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

Leave Link 702 at Tue Aug 27 17:23:11 2019, MaxMem= 4294967296 cpu: 0.5

(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=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

Leave Link 703 at Tue Aug 27 17:40:44 2019, MaxMem= 4294967296 cpu: 16849.5

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

Dipole = 7.84497952D-04-7.11144424D-03-4.78769157D-01

Polarizability= 1.25360674D+03 1.64918338D+00 1.66953064D+03

4.98699627D-02-1.22909804D-01 4.54011876D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000078228 0.000000708 -0.000186209

2 6 -0.000097354 0.000080873 0.000218144

3 7 -0.000001240 0.000006006 -0.000037649

4 6 -0.000190075 0.000069182 -0.000220738

5 6 0.000134562 -0.000069069 0.000223961

6 6 0.000224119 -0.000018267 0.000282108

7 6 -0.000251276 0.000049650 -0.000074422

8 7 0.000156295 0.000091474 0.000039671

9 6 0.000024338 0.000045311 -0.000161894

10 6 -0.000076872 0.000005614 0.000092549

11 6 0.000081920 -0.000053692 0.000069173

12 6 0.000102347 -0.000025679 -0.000211056

13 6 -0.000026898 0.000046423 0.000166011

14 6 0.000076025 0.000012297 -0.000093234

15 6 -0.000081359 -0.000058198 -0.000070057

16 6 0.000252691 0.000058559 0.000087834

17 7 -0.000156820 0.000120437 -0.000033602

18 6 -0.000234616 -0.000023662 -0.000287820

19 6 0.000197658 0.000070011 0.000215760

20 6 -0.000132510 -0.000062564 -0.000234025

21 6 -0.000084222 -0.000003428 0.000192162

22 6 0.000097338 0.000080569 -0.000194440

23 7 0.000014616 0.000006911 0.000033769

24 6 -0.000095138 -0.000021813 0.000197687

25 6 0.000062432 0.000009533 -0.000030744

26 6 -0.000032824 -0.000050615 0.000019229

27 6 -0.000013058 0.000015910 0.000010556

28 6 -0.000014183 0.000024809 -0.000003205

29 6 0.000030804 0.000013062 0.000013848

30 6 0.000038157 -0.000031510 -0.000073588

31 6 0.000016367 0.000004362 -0.000020071

32 6 -0.000028318 0.000022831 0.000012804

33 6 -0.000015600 -0.000083306 -0.000055114

34 6 0.000086079 -0.000063049 0.000064948

35 6 0.000033028 -0.000034797 0.000047645

36 6 0.000003220 0.000039340 -0.000009603

37 6 -0.000098893 -0.000067226 -0.000062709

38 6 -0.000028315 -0.000041669 -0.000053430

39 6 0.000002317 0.000040867 0.000007867

40 6 -0.000016827 0.000002891 0.000022191

41 6 0.000021196 0.000023531 -0.000012778

42 6 0.000005305 -0.000076138 0.000059204

43 6 -0.000053305 0.000013504 0.000042240

44 6 -0.000042054 -0.000037424 0.000074158

45 6 -0.000025893 0.000015254 -0.000004479

46 6 0.000011332 0.000020513 -0.000003475

47 6 0.000016446 0.000020957 -0.000008633

48 6 0.000024079 -0.000058466 -0.000030189

49 1 -0.000005701 0.000033018 0.000038619

50 1 -0.000005780 -0.000008206 -0.000049726

51 1 0.000000283 0.000033941 -0.000017584

52 1 -0.000000599 0.000012168 0.000013585

53 1 0.000003275 0.000029875 0.000018324

54 1 0.000000832 0.000009461 -0.000014346

55 1 0.000000160 -0.000010890 0.000048232

56 1 0.000014599 0.000024039 -0.000044207

57 1 -0.000036890 -0.000020196 0.000013196

58 1 0.000008482 0.000003238 0.000002300

59 1 0.000016811 -0.000000182 -0.000009059

60 1 0.000001566 -0.000004051 -0.000014203

61 1 -0.000044562 0.000000063 0.000030634

62 1 0.000009132 0.000008184 0.000017810

63 1 0.000013487 0.000010512 -0.000005628

64 1 -0.000030764 -0.000013268 -0.000027986

65 1 -0.000036885 0.000015545 -0.000043855

66 1 -0.000005628 -0.000003647 0.000009522

67 1 0.000039138 0.000022754 0.000042789

68 1 0.000007342 -0.000003568 -0.000009930

69 1 -0.000008255 0.000008122 -0.000019098

70 1 -0.000011371 0.000008646 0.000005111

71 1 0.000030101 -0.000018676 0.000029507

72 1 0.000046186 -0.000000973 -0.000027995

73 1 -0.000002054 -0.000005654 0.000013166

74 1 -0.000015655 -0.000001033 0.000010029

75 1 -0.000009147 -0.000000711 -0.000003860

76 1 0.000034306 -0.000024634 -0.000012492

77 1 0.000290611 -0.000068361 0.000000062

78 1 -0.000296268 -0.000166332 -0.000013272

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

Cartesian Forces: Max 0.000296268 RMS 0.000082679

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

Leave Link 716 at Tue Aug 27 17:40:44 2019, MaxMem= 4294967296 cpu: 1.8

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000340511 RMS 0.000068251

Search for a local minimum.

Step number 11 out of a maximum of 452

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

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -3.86D-05 DEPred=-1.13D-05 R= 3.43D+00

TightC=F SS= 1.41D+00 RLast= 6.69D-02 DXNew= 2.5227D-01 2.0081D-01

Trust test= 3.43D+00 RLast= 6.69D-02 DXMaxT set to 2.01D-01

ITU= 1 1 -1 1 -1 -1 1 1 -1 1 0

Eigenvalues --- -0.00210 -0.00030 0.00516 0.00617 0.00732

Eigenvalues --- 0.00867 0.00988 0.01018 0.01019 0.01077

Eigenvalues --- 0.01113 0.01214 0.01236 0.01286 0.01297

Eigenvalues --- 0.01302 0.01336 0.01390 0.01421 0.01438

Eigenvalues --- 0.01461 0.01485 0.01514 0.01636 0.01711

Eigenvalues --- 0.01716 0.01724 0.01738 0.01745 0.01749

Eigenvalues --- 0.01756 0.01782 0.01801 0.01821 0.01880

Eigenvalues --- 0.01910 0.01928 0.01945 0.01953 0.02145

Eigenvalues --- 0.02182 0.02241 0.02259 0.02267 0.02305

Eigenvalues --- 0.02327 0.02421 0.02433 0.02515 0.02530

Eigenvalues --- 0.02544 0.02547 0.02592 0.02594 0.02599

Eigenvalues --- 0.02601 0.02608 0.02734 0.02740 0.02764

Eigenvalues --- 0.02785 0.02868 0.02871 0.02873 0.02876

Eigenvalues --- 0.03036 0.03047 0.03864 0.04087 0.04188

Eigenvalues --- 0.04314 0.04354 0.04426 0.04516 0.04528

Eigenvalues --- 0.08031 0.09697 0.09708 0.09860 0.09914

Eigenvalues --- 0.09940 0.10331 0.10453 0.10598 0.10688

Eigenvalues --- 0.10688 0.10694 0.10695 0.10740 0.11085

Eigenvalues --- 0.11388 0.11391 0.11395 0.11398 0.11996

Eigenvalues --- 0.12000 0.12002 0.12008 0.12267 0.12267

Eigenvalues --- 0.12274 0.12274 0.12764 0.12767 0.12769

Eigenvalues --- 0.12771 0.15633 0.15954 0.16249 0.16950

Eigenvalues --- 0.17166 0.17278 0.17389 0.17605 0.17970

Eigenvalues --- 0.18004 0.18057 0.18575 0.19244 0.19279

Eigenvalues --- 0.19331 0.19340 0.19360 0.19374 0.19395

Eigenvalues --- 0.19447 0.19550 0.19550 0.19554 0.19555

Eigenvalues --- 0.20275 0.21507 0.22033 0.22798 0.22883

Eigenvalues --- 0.23369 0.23705 0.24278 0.24693 0.25625

Eigenvalues --- 0.26176 0.26533 0.26571 0.27145 0.28460

Eigenvalues --- 0.28493 0.28575 0.28797 0.29672 0.30979

Eigenvalues --- 0.31674 0.31984 0.32764 0.33111 0.33307

Eigenvalues --- 0.33448 0.34213 0.35086 0.35589 0.35619

Eigenvalues --- 0.35625 0.35631 0.35640 0.35697 0.35752

Eigenvalues --- 0.35764 0.35815 0.35828 0.35921 0.35925

Eigenvalues --- 0.35928 0.35930 0.36005 0.36012 0.36017

Eigenvalues --- 0.36018 0.36205 0.36250 0.36267 0.36271

Eigenvalues --- 0.37078 0.37082 0.37248 0.37407 0.37420

Eigenvalues --- 0.37554 0.38126 0.38542 0.38597 0.38711

Eigenvalues --- 0.39515 0.40501 0.40622 0.41006 0.41012

Eigenvalues --- 0.41032 0.41033 0.41074 0.41125 0.41354

Eigenvalues --- 0.41527 0.41818 0.42279 0.42907 0.44774

Eigenvalues --- 0.45510 0.45896 0.45909 0.45933 0.45964

Eigenvalues --- 0.46216 0.46232 0.46242 0.46254 0.46267

Eigenvalues --- 0.48304 0.48760 0.49024 0.49336 0.50551

Eigenvalues --- 0.50756 0.50757 0.50782 0.50819 0.51892

Eigenvalues --- 0.52575 0.57120 0.58572

Eigenvalue 1 is -2.10D-03 should be greater than 0.000000 Eigenvector:

D27 D20 D112 D12 D98

1 -0.23565 -0.23388 -0.23223 0.23151 0.22992

D113 D13 D85 D28 D19

1 -0.22644 0.22400 0.21521 -0.17257 -0.17187

Eigenvalue 2 is -3.04D-04 should be greater than 0.000000 Eigenvector:

D85 D13 D27 D81 D57

1 0.21109 0.20338 0.19992 -0.19652 -0.19553

D30 D51 D113 D87 D14

1 -0.19527 -0.19488 0.18854 0.18270 0.18071

Cosine: 0.354 < 0.500

Cut down GDIIS temporarily because of the cosine check. E 7

DIIS coeff's: 0.43964 0.22022 -0.05911 -0.12660 0.14557

DIIS coeff's: 0.20726 0.14726 0.01290 -0.01783 0.03070

Cosine: 0.506 > 0.500

Length: 1.178

GDIIS step was calculated using 10 of the last 11 vectors.

Iteration 1 RMS(Cart)= 0.01210040 RMS(Int)= 0.00002976

Iteration 2 RMS(Cart)= 0.00003914 RMS(Int)= 0.00002486

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002486

ITry= 1 IFail=0 DXMaxC= 5.59D-02 DCOld= 1.00D+10 DXMaxT= 2.01D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.65649 0.00010 0.00200 0.00007 0.00207 2.65856

R2 2.64158 -0.00004 -0.00178 0.00009 -0.00172 2.63986

R3 2.03714 0.00001 -0.00006 0.00006 0.00001 2.03715

R4 2.59907 -0.00015 0.00010 -0.00009 0.00003 2.59910

R5 2.71704 -0.00016 -0.00247 -0.00013 -0.00260 2.71444

R6 2.59889 -0.00019 0.00020 -0.00015 0.00007 2.59896

R7 1.90990 -0.00030 0.00002 -0.00016 -0.00014 1.90977

R8 2.65605 0.00017 0.00148 -0.00006 0.00142 2.65747

R9 2.71791 -0.00017 -0.00206 0.00017 -0.00189 2.71602

R10 2.03711 0.00003 0.00002 0.00004 0.00006 2.03717

R11 2.64096 0.00033 0.00033 0.00028 0.00061 2.64157

R12 2.80357 0.00004 0.00032 -0.00022 0.00010 2.80367

R13 2.59617 0.00003 0.00110 0.00031 0.00143 2.59760

R14 2.76249 -0.00008 -0.00201 0.00011 -0.00191 2.76058

R15 2.59419 0.00022 -0.00185 0.00010 -0.00173 2.59246

R16 2.76258 -0.00007 -0.00140 0.00018 -0.00123 2.76135

R17 2.64223 0.00026 0.00362 0.00025 0.00388 2.64610

R18 2.55420 0.00008 0.00153 -0.00010 0.00139 2.55559

R19 2.03909 0.00002 -0.00003 0.00006 0.00004 2.03913

R20 2.03914 -0.00001 -0.00001 0.00005 0.00004 2.03918

R21 2.64241 0.00027 0.00345 0.00035 0.00380 2.64620

R22 2.80355 0.00002 -0.00020 -0.00011 -0.00031 2.80325

R23 2.76260 -0.00007 -0.00141 0.00012 -0.00130 2.76130

R24 2.59415 0.00021 -0.00178 0.00001 -0.00175 2.59240

R25 2.55419 0.00009 0.00154 -0.00010 0.00140 2.55559

R26 2.03908 0.00002 -0.00002 0.00009 0.00007 2.03915

R27 2.76247 -0.00007 -0.00199 0.00017 -0.00183 2.76064

R28 2.03914 -0.00001 -0.00001 0.00003 0.00002 2.03916

R29 2.59626 0.00003 0.00102 0.00037 0.00141 2.59767

R30 2.64079 0.00034 0.00047 0.00018 0.00066 2.64145

R31 2.71771 -0.00015 -0.00192 0.00013 -0.00179 2.71593

R32 2.80400 0.00004 -0.00003 0.00020 0.00017 2.80417

R33 2.65619 0.00018 0.00138 0.00013 0.00150 2.65769

R34 2.59900 -0.00019 0.00009 -0.00004 0.00008 2.59908

R35 2.64145 -0.00004 -0.00167 -0.00005 -0.00175 2.63970

R36 2.03707 0.00003 0.00005 0.00001 0.00006 2.03713

R37 2.65671 0.00009 0.00185 0.00022 0.00206 2.65877

R38 2.03711 0.00001 -0.00003 0.00003 -0.00000 2.03711

R39 2.59922 -0.00017 -0.00002 -0.00002 -0.00001 2.59922

R40 2.71680 -0.00015 -0.00228 -0.00018 -0.00245 2.71435

R41 1.91016 -0.00032 -0.00021 0.00004 -0.00016 1.91000

R42 2.80406 0.00003 -0.00062 0.00030 -0.00032 2.80374

R43 2.65164 -0.00010 -0.00018 0.00009 -0.00009 2.65155

R44 2.65010 0.00004 -0.00009 0.00007 -0.00002 2.65007

R45 2.62865 -0.00002 -0.00001 -0.00001 -0.00002 2.62863

R46 2.04845 -0.00000 -0.00003 0.00002 -0.00000 2.04845

R47 2.63635 0.00000 -0.00006 0.00003 -0.00003 2.63632

R48 2.05016 0.00001 -0.00004 0.00005 0.00001 2.05017

R49 2.63415 0.00002 0.00004 0.00002 0.00006 2.63421

R50 2.05004 0.00002 0.00000 0.00002 0.00003 2.05006

R51 2.63077 0.00004 0.00006 -0.00006 0.00000 2.63077

R52 2.05011 0.00001 -0.00003 0.00004 0.00001 2.05013

R53 2.04843 0.00003 0.00001 -0.00001 0.00000 2.04843

R54 2.63634 0.00000 -0.00009 0.00002 -0.00007 2.63627

R55 2.63417 0.00004 0.00014 0.00001 0.00015 2.63431

R56 2.05004 0.00002 0.00000 0.00003 0.00003 2.05007

R57 2.62870 -0.00001 0.00004 0.00002 0.00005 2.62875

R58 2.05014 0.00002 0.00000 0.00001 0.00001 2.05016

R59 2.65154 -0.00010 0.00010 -0.00004 0.00006 2.65161

R60 2.04843 0.00001 -0.00007 0.00006 -0.00001 2.04842

R61 2.65023 -0.00002 0.00020 -0.00001 0.00019 2.65042

R62 2.63076 0.00002 -0.00012 -0.00002 -0.00015 2.63061

R63 2.04852 0.00001 -0.00003 0.00003 -0.00000 2.04851

R64 2.05013 0.00001 -0.00002 0.00004 0.00002 2.05015

R65 2.65002 -0.00002 0.00038 -0.00016 0.00022 2.65024

R66 2.65132 -0.00008 0.00028 -0.00010 0.00018 2.65150

R67 2.63084 0.00002 -0.00019 0.00004 -0.00015 2.63069

R68 2.04857 0.00001 -0.00007 0.00004 -0.00003 2.04854

R69 2.63416 0.00004 0.00015 0.00000 0.00015 2.63431

R70 2.05013 0.00001 -0.00002 0.00004 0.00002 2.05015

R71 2.63630 0.00000 -0.00005 -0.00003 -0.00008 2.63622

R72 2.05004 0.00002 -0.00000 0.00003 0.00003 2.05007

R73 2.62879 -0.00001 -0.00003 0.00005 0.00002 2.62880

R74 2.05015 0.00002 -0.00001 0.00001 0.00001 2.05016

R75 2.04845 0.00001 -0.00008 0.00005 -0.00003 2.04842

R76 2.64992 0.00005 0.00004 -0.00006 -0.00002 2.64990

R77 2.65148 -0.00010 -0.00006 0.00001 -0.00005 2.65143

R78 2.63082 0.00004 0.00001 0.00001 0.00002 2.63084

R79 2.04846 0.00003 -0.00002 0.00002 0.00000 2.04846

R80 2.63414 0.00003 0.00004 0.00002 0.00006 2.63420

R81 2.05012 0.00001 -0.00003 0.00004 0.00001 2.05012

R82 2.63632 0.00000 -0.00003 -0.00001 -0.00005 2.63627

R83 2.05004 0.00002 0.00000 0.00002 0.00003 2.05006

R84 2.62873 -0.00002 -0.00007 0.00003 -0.00004 2.62868

R85 2.05017 0.00001 -0.00005 0.00006 0.00001 2.05018

R86 2.04846 -0.00001 -0.00003 0.00001 -0.00002 2.04844

A1 1.88147 -0.00001 0.00031 -0.00008 0.00024 1.88171

A2 2.18770 -0.00003 -0.00017 -0.00036 -0.00054 2.18717

A3 2.21399 0.00005 -0.00013 0.00043 0.00030 2.21429

A4 1.86798 -0.00005 -0.00054 -0.00002 -0.00055 1.86743

A5 2.22157 0.00014 0.00024 0.00030 0.00046 2.22203

A6 2.19320 -0.00009 0.00023 -0.00025 0.00007 2.19327

A7 1.92524 0.00014 0.00026 0.00010 0.00034 1.92557

A8 2.17869 -0.00007 -0.00015 0.00010 -0.00002 2.17866

A9 2.17855 -0.00007 -0.00034 0.00001 -0.00029 2.17825

A10 1.86816 -0.00005 -0.00027 -0.00001 -0.00027 1.86789

A11 2.19358 -0.00013 -0.00018 0.00012 0.00004 2.19363

A12 2.22110 0.00018 0.00036 -0.00007 0.00022 2.22132

A13 1.88159 -0.00003 0.00021 0.00002 0.00025 1.88183

A14 2.21392 0.00006 -0.00012 0.00047 0.00035 2.21427

A15 2.18765 -0.00003 -0.00009 -0.00051 -0.00061 2.18705

A16 2.18552 0.00006 0.00043 -0.00045 0.00011 2.18563

A17 2.02350 -0.00010 0.00033 -0.00015 0.00013 2.02362

A18 2.07410 0.00004 -0.00076 0.00058 -0.00023 2.07387

A19 2.19161 0.00011 -0.00048 -0.00025 -0.00063 2.19098

A20 2.16562 -0.00007 0.00058 0.00026 0.00075 2.16637

A21 1.92592 -0.00004 -0.00013 -0.00002 -0.00012 1.92580

A22 1.84724 0.00004 0.00004 -0.00009 -0.00008 1.84715

A23 1.92647 -0.00008 0.00048 0.00002 0.00051 1.92699

A24 2.19246 0.00011 -0.00090 0.00014 -0.00067 2.19180

A25 2.16424 -0.00003 0.00040 -0.00016 0.00015 2.16439

A26 1.86207 0.00003 -0.00025 0.00004 -0.00019 1.86188

A27 2.19669 0.00000 0.00056 -0.00015 0.00041 2.19710

A28 2.22403 -0.00003 -0.00031 0.00010 -0.00022 2.22381

A29 1.86205 0.00006 -0.00018 0.00004 -0.00013 1.86192

A30 2.19696 -0.00004 0.00026 -0.00013 0.00013 2.19709

A31 2.22381 -0.00002 -0.00009 0.00009 0.00000 2.22381

A32 2.18563 0.00009 -0.00051 -0.00018 -0.00057 2.18506

A33 2.02439 -0.00018 0.00119 0.00013 0.00126 2.02566

A34 2.07311 0.00009 -0.00068 0.00004 -0.00069 2.07243

A35 2.16442 -0.00001 0.00028 -0.00016 0.00004 2.16446

A36 2.19227 0.00010 -0.00077 0.00009 -0.00059 2.19168

A37 1.92648 -0.00008 0.00047 0.00006 0.00055 1.92703

A38 1.86209 0.00002 -0.00026 0.00004 -0.00021 1.86188

A39 2.19670 0.00000 0.00056 -0.00025 0.00031 2.19701

A40 2.22399 -0.00002 -0.00029 0.00019 -0.00010 2.22390

A41 1.86204 0.00006 -0.00017 0.00003 -0.00012 1.86192

A42 2.22380 -0.00002 -0.00008 0.00001 -0.00007 2.22373

A43 2.19698 -0.00004 0.00023 -0.00003 0.00020 2.19718

A44 1.92594 -0.00005 -0.00013 -0.00007 -0.00018 1.92575

A45 2.16533 -0.00005 0.00076 0.00031 0.00098 2.16630

A46 2.19190 0.00011 -0.00067 -0.00024 -0.00081 2.19110

A47 1.84722 0.00005 0.00005 -0.00008 -0.00006 1.84715

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D3 -3.11931 -0.00002 -0.00027 0.00067 0.00041 -3.11891

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D5 -0.00084 0.00002 -0.00002 -0.00029 -0.00030 -0.00115

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D11 3.08697 -0.00004 -0.00215 0.00118 -0.00099 3.08598

D12 -0.09359 -0.00001 -0.00754 0.00702 -0.00053 -0.09412

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D14 0.18797 -0.00000 -0.00512 0.00287 -0.00224 0.18573

D15 0.23503 -0.00000 -0.00562 0.00329 -0.00230 0.23273

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D175 -0.01390 -0.00002 0.00004 0.00023 0.00027 -0.01363

D176 -3.13561 -0.00001 0.00085 0.00017 0.00102 -3.13459

D177 0.00850 -0.00001 -0.00024 0.00041 0.00016 0.00866

D178 -3.13054 -0.00002 0.00017 -0.00023 -0.00005 -3.13060

D179 3.13184 0.00001 -0.00052 0.00083 0.00031 3.13215

D180 -0.00720 0.00001 -0.00010 0.00020 0.00010 -0.00710

D181 -0.00670 0.00000 0.00015 -0.00017 -0.00002 -0.00672

D182 3.13713 -0.00001 -0.00005 -0.00034 -0.00039 3.13674

D183 3.13233 0.00001 -0.00027 0.00046 0.00019 3.13252

D184 -0.00702 -0.00000 -0.00047 0.00030 -0.00018 -0.00720

D185 -0.00541 0.00000 0.00004 -0.00003 0.00001 -0.00540

D186 3.13552 0.00000 -0.00010 -0.00015 -0.00025 3.13527

D187 3.13395 0.00001 0.00024 0.00014 0.00038 3.13433

D188 -0.00830 0.00001 0.00010 0.00001 0.00011 -0.00819

D189 0.01584 0.00001 -0.00013 -0.00000 -0.00014 0.01570

D190 3.13746 -0.00000 -0.00095 0.00006 -0.00089 3.13656

D191 -3.12510 0.00001 0.00001 0.00012 0.00013 -3.12497

D192 -0.00348 -0.00000 -0.00081 0.00019 -0.00063 -0.00410

D193 3.14070 -0.00001 0.00097 -0.00183 -0.00086 3.13984

D194 -0.01840 -0.00000 0.00021 -0.00092 -0.00071 -0.01911

D195 -0.00349 -0.00001 0.00037 -0.00042 -0.00005 -0.00354

D196 3.12059 0.00000 -0.00039 0.00049 0.00010 3.12069

D197 -3.12868 0.00002 -0.00061 0.00178 0.00117 -3.12752

D198 -0.00788 0.00001 -0.00076 0.00134 0.00057 -0.00731

D199 0.01551 0.00001 -0.00001 0.00037 0.00036 0.01587

D200 3.13631 0.00000 -0.00016 -0.00008 -0.00024 3.13608

D201 -0.00757 0.00000 -0.00057 0.00032 -0.00025 -0.00782

D202 3.13120 0.00001 -0.00023 0.00011 -0.00012 3.13108

D203 -3.13155 -0.00001 0.00019 -0.00059 -0.00040 -3.13195

D204 0.00721 -0.00001 0.00054 -0.00080 -0.00026 0.00695

D205 0.00673 0.00001 0.00042 -0.00017 0.00025 0.00698

D206 -3.13670 0.00000 0.00014 0.00005 0.00019 -3.13651

D207 -3.13202 0.00000 0.00007 0.00004 0.00011 -3.13190

D208 0.00774 -0.00000 -0.00021 0.00026 0.00005 0.00779

D209 0.00524 -0.00000 -0.00007 0.00012 0.00005 0.00530

D210 -3.13573 -0.00001 -0.00012 0.00002 -0.00010 -3.13583

D211 -3.13451 0.00000 0.00021 -0.00010 0.00012 -3.13440

D212 0.00770 -0.00000 0.00016 -0.00020 -0.00003 0.00766

D213 -0.01651 -0.00000 -0.00014 -0.00023 -0.00036 -0.01687

D214 -3.13722 0.00000 0.00002 0.00022 0.00024 -3.13698

D215 3.12447 -0.00000 -0.00008 -0.00013 -0.00021 3.12426

D216 0.00376 0.00001 0.00007 0.00032 0.00039 0.00415

Item Value Threshold Converged?

Maximum Force 0.000341 0.000450 YES

RMS Force 0.000068 0.000300 YES

Maximum Displacement 0.055918 0.001800 NO

RMS Displacement 0.012100 0.001200 NO

Predicted change in Energy=-1.946384D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Aug 27 17:40:44 2019, MaxMem= 4294967296 cpu: 2.5

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

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=1 Diff= 7.32D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.699540 -4.165816 0.562770

2 6 0 1.130953 -2.876300 0.201867

3 7 0 0.002334 -2.116335 0.000976

4 6 0 -1.126736 -2.878949 0.188312

5 6 0 -0.697382 -4.167354 0.553365

6 6 0 -2.480312 -2.432196 0.004048

7 6 0 -2.878702 -1.098564 -0.125281

8 7 0 -2.067626 -0.002206 0.046942

9 6 0 -2.880007 1.092396 -0.107720

10 6 0 -4.239565 0.674636 -0.442848

11 6 0 -4.238248 -0.677673 -0.454719

12 6 0 2.484491 -2.427566 0.029033

13 6 0 2.880110 -1.091726 -0.111993

14 6 0 4.239648 -0.672718 -0.445518

15 6 0 4.238300 0.679624 -0.452454

16 6 0 2.878738 1.099284 -0.121375

17 7 0 2.067694 0.002225 0.046747

18 6 0 2.480114 2.432428 0.011507

19 6 0 1.126860 2.879384 0.197231

20 6 0 0.697344 4.171523 0.549113

21 6 0 -0.699489 4.169969 0.558608

22 6 0 -1.130900 2.876697 0.210946

23 7 0 -0.002189 2.114376 0.019300

24 6 0 -2.484141 2.427733 0.036793

25 6 0 -3.515197 -3.494660 -0.032832

26 6 0 -3.431527 -4.541178 -0.963744

27 6 0 -4.409657 -5.529190 -1.008529

28 6 0 -5.477456 -5.500555 -0.111183

29 6 0 -5.563530 -4.473324 0.827176

30 6 0 -4.593370 -3.475570 0.863711

31 6 0 5.498129 -5.481732 -0.012656

32 6 0 4.441381 -5.527657 -0.922246

33 6 0 3.458194 -4.543755 -0.902904

34 6 0 3.524895 -3.484868 0.015351

35 6 0 4.593049 -3.447885 0.923536

36 6 0 5.568249 -4.441208 0.912375

37 6 0 -3.524871 3.485022 0.019271

38 6 0 -4.593333 3.450970 0.927063

39 6 0 -5.569697 4.443135 0.910812

40 6 0 -5.500292 5.479475 -0.018951

41 6 0 -4.443191 5.522365 -0.928239

42 6 0 -3.458938 4.539606 -0.903890

43 6 0 3.515248 3.494886 -0.029120

44 6 0 4.593651 3.478654 0.867058

45 6 0 5.564770 4.475345 0.825766

46 6 0 5.479278 5.498558 -0.117020

47 6 0 4.411231 5.524204 -1.014121

48 6 0 3.432244 4.537223 -0.964677

49 1 0 1.345621 -4.993423 0.807223

50 1 0 -1.344863 -4.996410 0.789098

51 1 0 -5.066660 1.331420 -0.664032

52 1 0 -5.064081 -1.332099 -0.687448

53 1 0 5.066678 -1.328750 -0.669215

54 1 0 5.064193 1.334833 -0.682701

55 1 0 1.344519 5.003650 0.774532

56 1 0 -1.345401 5.000648 0.792777

57 1 0 -2.605842 -4.565513 -1.665662

58 1 0 -4.338558 -6.322573 -1.745079

59 1 0 -6.236173 -6.275327 -0.142313

60 1 0 -6.385692 -4.448941 1.534578

61 1 0 -4.658415 -2.683589 1.600972

62 1 0 6.260633 -6.253329 -0.023966

63 1 0 4.383071 -6.331174 -1.648853

64 1 0 2.641398 -4.581521 -1.614540

65 1 0 4.645747 -2.645399 1.650414

66 1 0 6.382018 -4.402902 1.628829

67 1 0 -4.645738 2.651407 1.657200

68 1 0 -6.383916 4.407084 1.626870

69 1 0 -6.263755 6.250053 -0.034313

70 1 0 -4.385470 6.322471 -1.658654

71 1 0 -2.642081 4.574781 -1.615586

72 1 0 4.658461 2.689465 1.607351

73 1 0 6.387311 4.453174 1.532798

74 1 0 6.238770 6.272408 -0.151921

75 1 0 4.340636 6.314304 -1.754245

76 1 0 2.606549 4.559029 -1.666660

77 1 0 0.002262 -1.129661 -0.217650

78 1 0 -0.001969 1.123434 -0.179710

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

Rotational constants (GHZ): 0.0587979 0.0582696 0.0300930

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

Standard basis: 6-311G(d) (5D, 7F)

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

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5357.0761283461 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122269372 Hartrees.

Nuclear repulsion after empirical dispersion term = 5356.8639014089 Hartrees.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5765

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.15D-10

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 294

GePol: Fraction of low-weight points (<1% of avg) = 5.10%

GePol: Cavity surface area = 611.340 Ang\*\*2

GePol: Cavity volume = 627.771 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021057771 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5356.8617956318 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.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Aug 27 17:40:46 2019, MaxMem= 4294967296 cpu: 2.5

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

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= -0.000000 0.000000 0.000000

Rot= 0.999997 -0.000004 0.000007 -0.002563 Ang= -0.29 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0183

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30451432297

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 580000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 99705675.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.55D-15 for 5760.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.93D-15 for 2944 992.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.10D-15 for 5760.

Iteration 1 A^-1\*A deviation from orthogonality is 1.21D-13 for 4994 4990.

E= -1914.33283359208

DIIS: error= 5.35D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.33283359208 IErMin= 1 ErrMin= 5.35D-04

ErrMax= 5.35D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-03 BMatP= 1.03D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.35D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.640 Goal= None Shift= 0.000

Gap= 0.706 Goal= None Shift= 0.000

RMSDP=2.24D-05 MaxDP=7.45D-04 OVMax= 3.72D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.24D-05 CP: 1.00D+00

E= -1914.33332265480 Delta-E= -0.000489062724 Rises=F Damp=F

DIIS: error= 7.69D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33332265480 IErMin= 2 ErrMin= 7.69D-05

ErrMax= 7.69D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D-05 BMatP= 1.03D-03

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

Coeff-Com: -0.632D-01 0.106D+01

Coeff: -0.632D-01 0.106D+01

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.35D-06 MaxDP=1.68D-04 DE=-4.89D-04 OVMax= 2.03D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.89D-06 CP: 1.00D+00 1.09D+00

E= -1914.33332977858 Delta-E= -0.000007123776 Rises=F Damp=F

DIIS: error= 4.49D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33332977858 IErMin= 3 ErrMin= 4.49D-05

ErrMax= 4.49D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.37D-06 BMatP= 1.37D-05

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

Coeff-Com: -0.310D-01 0.427D+00 0.604D+00

Coeff: -0.310D-01 0.427D+00 0.604D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.84D-06 MaxDP=1.10D-04 DE=-7.12D-06 OVMax= 7.21D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.73D-06 CP: 1.00D+00 1.10D+00 8.61D-01

E= -1914.33333084741 Delta-E= -0.000001068830 Rises=F Damp=F

DIIS: error= 2.63D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33333084741 IErMin= 4 ErrMin= 2.63D-05

ErrMax= 2.63D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.00D-06 BMatP= 5.37D-06

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

Coeff-Com: -0.866D-02 0.919D-01 0.376D+00 0.541D+00

Coeff: -0.866D-02 0.919D-01 0.376D+00 0.541D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.22D-06 MaxDP=9.45D-05 DE=-1.07D-06 OVMax= 9.29D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 9.53D-07 CP: 1.00D+00 1.11D+00 1.02D+00 7.65D-01

E= -1914.33333149607 Delta-E= -0.000000648663 Rises=F Damp=F

DIIS: error= 1.52D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33333149607 IErMin= 5 ErrMin= 1.52D-05

ErrMax= 1.52D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.62D-07 BMatP= 2.00D-06

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

Coeff-Com: -0.116D-02-0.118D-02 0.138D+00 0.314D+00 0.550D+00

Coeff: -0.116D-02-0.118D-02 0.138D+00 0.314D+00 0.550D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.86D-07 MaxDP=3.31D-05 DE=-6.49D-07 OVMax= 4.82D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.76D-07 CP: 1.00D+00 1.11D+00 1.08D+00 9.64D-01 1.16D+00

E= -1914.33333164741 Delta-E= -0.000000151334 Rises=F Damp=F

DIIS: error= 1.07D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33333164741 IErMin= 6 ErrMin= 1.07D-05

ErrMax= 1.07D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.12D-08 BMatP= 2.62D-07

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

Coeff-Com: 0.191D-02-0.294D-01-0.298D-01 0.439D-01 0.293D+00 0.721D+00

Coeff: 0.191D-02-0.294D-01-0.298D-01 0.439D-01 0.293D+00 0.721D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=6.60D-07 MaxDP=5.17D-05 DE=-1.51D-07 OVMax= 6.91D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.19D-07 CP: 1.00D+00 1.11D+00 1.17D+00 1.10D+00 1.62D+00

CP: 1.50D+00

E= -1914.33333175511 Delta-E= -0.000000107701 Rises=F Damp=F

DIIS: error= 7.85D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33333175511 IErMin= 7 ErrMin= 7.85D-06

ErrMax= 7.85D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.75D-08 BMatP= 6.12D-08

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

Coeff-Com: 0.614D-03-0.342D-02-0.459D-01-0.601D-01-0.172D+00 0.149D+00

Coeff-Com: 0.113D+01

Coeff: 0.614D-03-0.342D-02-0.459D-01-0.601D-01-0.172D+00 0.149D+00

Coeff: 0.113D+01

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.93D-07 MaxDP=6.06D-05 DE=-1.08D-07 OVMax= 8.38D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.16D-07 CP: 1.00D+00 1.11D+00 1.25D+00 1.27D+00 2.15D+00

CP: 2.44D+00 1.72D+00

E= -1914.33333184538 Delta-E= -0.000000090278 Rises=F Damp=F

DIIS: error= 5.90D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33333184538 IErMin= 8 ErrMin= 5.90D-06

ErrMax= 5.90D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.69D-08 BMatP= 2.75D-08

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

Coeff-Com: -0.118D-02 0.242D-01-0.153D-01-0.739D-01-0.445D+00-0.495D+00

Coeff-Com: 0.983D+00 0.102D+01

Coeff: -0.118D-02 0.242D-01-0.153D-01-0.739D-01-0.445D+00-0.495D+00

Coeff: 0.983D+00 0.102D+01

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.09D-06 MaxDP=8.60D-05 DE=-9.03D-08 OVMax= 1.19D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.87D-07 CP: 1.00D+00 1.12D+00 1.37D+00 1.50D+00 2.89D+00

CP: 3.00D+00 3.00D+00 1.64D+00

E= -1914.33333191401 Delta-E= -0.000000068625 Rises=F Damp=F

DIIS: error= 2.16D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33333191401 IErMin= 9 ErrMin= 2.16D-06

ErrMax= 2.16D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.16D-09 BMatP= 1.69D-08

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

Coeff-Com: -0.513D-03 0.821D-02 0.369D-02 0.183D-02-0.102D+00-0.185D+00

Coeff-Com: -0.422D-02 0.389D+00 0.888D+00

Coeff: -0.513D-03 0.821D-02 0.369D-02 0.183D-02-0.102D+00-0.185D+00

Coeff: -0.422D-02 0.389D+00 0.888D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.69D-07 MaxDP=2.92D-05 DE=-6.86D-08 OVMax= 4.06D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.66D-07 CP: 1.00D+00 1.12D+00 1.41D+00 1.57D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.31D+00 1.62D+00

E= -1914.33333192378 Delta-E= -0.000000009770 Rises=F Damp=F

DIIS: error= 1.16D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33333192378 IErMin=10 ErrMin= 1.16D-06

ErrMax= 1.16D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.42D-09 BMatP= 4.16D-09

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

Coeff-Com: 0.178D-03-0.546D-02 0.850D-02 0.413D-01 0.136D+00 0.105D+00

Coeff-Com: -0.480D+00-0.157D+00 0.637D+00 0.715D+00

Coeff: 0.178D-03-0.546D-02 0.850D-02 0.413D-01 0.136D+00 0.105D+00

Coeff: -0.480D+00-0.157D+00 0.637D+00 0.715D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.85D-07 MaxDP=1.56D-05 DE=-9.77D-09 OVMax= 2.03D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.36D-08 CP: 1.00D+00 1.12D+00 1.42D+00 1.60D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.69D+00 1.98D+00 1.61D+00

E= -1914.33333192684 Delta-E= -0.000000003060 Rises=F Damp=F

DIIS: error= 5.16D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33333192684 IErMin=11 ErrMin= 5.16D-07

ErrMax= 5.16D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.55D-10 BMatP= 2.42D-09

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

Coeff-Com: 0.240D-03-0.507D-02 0.172D-02 0.204D-01 0.939D-01 0.108D+00

Coeff-Com: -0.241D+00-0.178D+00 0.236D-01 0.338D+00 0.838D+00

Coeff: 0.240D-03-0.507D-02 0.172D-02 0.204D-01 0.939D-01 0.108D+00

Coeff: -0.241D+00-0.178D+00 0.236D-01 0.338D+00 0.838D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=9.71D-08 MaxDP=7.88D-06 DE=-3.06D-09 OVMax= 1.05D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.21D-08 CP: 1.00D+00 1.12D+00 1.43D+00 1.62D+00 3.00D+00

CP: 3.00D+00 3.00D+00 2.98D+00 2.16D+00 1.96D+00

CP: 1.27D+00

E= -1914.33333192766 Delta-E= -0.000000000816 Rises=F Damp=F

DIIS: error= 2.19D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.33333192766 IErMin=12 ErrMin= 2.19D-07

ErrMax= 2.19D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.65D-10 BMatP= 4.55D-10

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

Coeff-Com: 0.843D-04-0.129D-02-0.174D-02 0.632D-03 0.147D-01 0.329D-01

Coeff-Com: -0.359D-02-0.485D-01-0.171D+00-0.239D-01 0.473D+00 0.729D+00

Coeff: 0.843D-04-0.129D-02-0.174D-02 0.632D-03 0.147D-01 0.329D-01

Coeff: -0.359D-02-0.485D-01-0.171D+00-0.239D-01 0.473D+00 0.729D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.55D-08 MaxDP=3.02D-06 DE=-8.16D-10 OVMax= 3.61D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.40D-08 CP: 1.00D+00 1.12D+00 1.43D+00 1.62D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.23D+00 2.06D+00

CP: 1.45D+00 1.23D+00

E= -1914.33333192779 Delta-E= -0.000000000130 Rises=F Damp=F

DIIS: error= 1.27D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.33333192779 IErMin=13 ErrMin= 1.27D-07

ErrMax= 1.27D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.89D-11 BMatP= 1.65D-10

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

Coeff-Com: -0.235D-04 0.720D-03-0.128D-02-0.442D-02-0.174D-01-0.138D-01

Coeff-Com: 0.547D-01 0.268D-01-0.796D-01-0.924D-01-0.363D-04 0.306D+00

Coeff-Com: 0.820D+00

Coeff: -0.235D-04 0.720D-03-0.128D-02-0.442D-02-0.174D-01-0.138D-01

Coeff: 0.547D-01 0.268D-01-0.796D-01-0.924D-01-0.363D-04 0.306D+00

Coeff: 0.820D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.87D-08 MaxDP=1.62D-06 DE=-1.30D-10 OVMax= 1.98D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 4.93D-09 CP: 1.00D+00 1.12D+00 1.43D+00 1.62D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.27D+00 2.13D+00

CP: 1.52D+00 1.43D+00 1.35D+00

E= -1914.33333192783 Delta-E= -0.000000000040 Rises=F Damp=F

DIIS: error= 7.16D-08 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.33333192783 IErMin=14 ErrMin= 7.16D-08

ErrMax= 7.16D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-11 BMatP= 2.89D-11

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

Coeff-Com: -0.337D-04 0.703D-03-0.224D-03-0.233D-02-0.131D-01-0.159D-01

Coeff-Com: 0.286D-01 0.279D-01 0.305D-02-0.415D-01-0.124D+00-0.278D-01

Coeff-Com: 0.439D+00 0.725D+00

Coeff: -0.337D-04 0.703D-03-0.224D-03-0.233D-02-0.131D-01-0.159D-01

Coeff: 0.286D-01 0.279D-01 0.305D-02-0.415D-01-0.124D+00-0.278D-01

Coeff: 0.439D+00 0.725D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.26D-09 MaxDP=6.38D-07 DE=-4.00D-11 OVMax= 7.24D-06

Error on total polarization charges = 0.08258

SCF Done: E(UB3LYP) = -1914.33333193 A.U. after 14 cycles

NFock= 14 Conv=0.73D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0183

<L.S>= 0.000000000000E+00

KE= 1.906375566043D+03 PE=-1.516333940239D+04 EE= 5.985768708790D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0551, after 2.0017

Leave Link 502 at Tue Aug 27 17:47:11 2019, MaxMem= 4294967296 cpu: 5994.0

(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: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48041167D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64239607D-01

Leave Link 801 at Tue Aug 27 17:47:11 2019, MaxMem= 4294967296 cpu: 1.0

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

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

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

Leave Link 1101 at Tue Aug 27 17:47:18 2019, MaxMem= 4294967296 cpu: 109.8

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

Symmetrizing basis deriv contribution to polar:

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

Leave Link 1102 at Tue Aug 27 17:47:18 2019, MaxMem= 4294967296 cpu: 2.5

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

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 186

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 27 18:07:10 2019, MaxMem= 4294967296 cpu: 19062.8

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

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 580000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.47D+03 4.57D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.60D+02 3.68D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.68D+00 4.73D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.04D-01 3.98D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.67D-04 2.12D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.66D-06 1.34D-04.

191 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 2.02D-08 1.02D-05.

84 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.41D-11 6.32D-07.

46 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.30D-13 4.02D-08.

4 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 9.18D-15 7.27D-09.

3 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 5.33D-15 2.95D-09.

3 vectors produced by pass 11 Test12= 2.55D-13 1.00D-09 XBig12= 3.91D-15 2.27D-09.

3 vectors produced by pass 12 Test12= 2.55D-13 1.00D-09 XBig12= 5.77D-15 2.15D-09.

3 vectors produced by pass 13 Test12= 2.55D-13 1.00D-09 XBig12= 7.97D-15 2.74D-09.

2 vectors produced by pass 14 Test12= 2.55D-13 1.00D-09 XBig12= 4.57D-15 2.26D-09.

InvSVY: IOpt=1 It= 1 EMax= 2.13D-14

Solved reduced A of dimension 1746 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1129.45 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 27 22:00:46 2019, MaxMem= 4294967296 cpu: 224191.8

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 186

Leave Link 701 at Tue Aug 27 22:02:15 2019, MaxMem= 4294967296 cpu: 1426.5

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

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

Leave Link 702 at Tue Aug 27 22:02:15 2019, MaxMem= 4294967296 cpu: 0.0

(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=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

Leave Link 703 at Tue Aug 27 22:20:46 2019, MaxMem= 4294967296 cpu: 17769.5

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

Dipole =-1.15337678D-04-7.70090841D-03-4.87792313D-01

Polarizability= 1.25872055D+03-3.30480677D+00 1.67658937D+03

1.10797878D-02 1.22784892D-01 4.53042066D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000427993 0.000100471 0.000497718

2 6 0.000564700 -0.000182184 -0.000581408

3 7 0.000168535 -0.000040793 -0.000074294

4 6 0.000396637 -0.000146881 0.000646315

5 6 -0.000320088 0.000050544 -0.000445915

6 6 -0.000479734 0.000156816 -0.000561925

7 6 0.000257339 -0.000183493 0.000470402

8 7 0.000287554 0.000142167 0.000147173

9 6 -0.000971106 -0.000171085 0.000331385

10 6 0.000458745 0.000023080 -0.000252663

11 6 -0.000484595 0.000036720 -0.000255481

12 6 -0.000939824 0.000219161 0.000684848

13 6 0.000960748 -0.000210056 -0.000323990

14 6 -0.000457896 0.000020450 0.000250127

15 6 0.000482682 0.000040400 0.000254213

16 6 -0.000260413 -0.000135509 -0.000470867

17 7 -0.000287764 0.000138976 -0.000144020

18 6 0.000471207 0.000164495 0.000562236

19 6 -0.000375477 -0.000232444 -0.000638156

20 6 0.000314998 0.000070389 0.000444787

21 6 0.000421401 0.000117901 -0.000496657

22 6 -0.000543370 -0.000262520 0.000576384

23 7 -0.000191055 0.000080822 0.000070758

24 6 0.000944806 0.000226926 -0.000688065

25 6 0.000005081 0.000049035 0.000017618

26 6 -0.000006935 -0.000038837 -0.000001983

27 6 -0.000012620 0.000024671 0.000042154

28 6 -0.000018676 -0.000010959 -0.000022083

29 6 0.000044365 0.000021916 -0.000010679

30 6 0.000021297 -0.000004584 -0.000042210

31 6 -0.000001667 -0.000040185 0.000014353

32 6 -0.000048886 0.000031696 -0.000012159

33 6 0.000039130 -0.000063464 -0.000030511

34 6 0.000017456 0.000036696 0.000047242

35 6 0.000012000 -0.000016779 -0.000017647

36 6 0.000017659 0.000052343 0.000017432

37 6 -0.000036977 0.000022972 -0.000041896

38 6 -0.000020109 -0.000031515 0.000028516

39 6 -0.000019293 0.000050839 -0.000018278

40 6 0.000003537 -0.000043289 -0.000014962

41 6 0.000048596 0.000031209 0.000010579

42 6 -0.000026095 -0.000052454 0.000019923

43 6 -0.000015951 0.000029390 -0.000025833

44 6 -0.000029228 -0.000015451 0.000031967

45 6 -0.000044108 0.000020078 0.000010889

46 6 0.000019816 -0.000014395 0.000022215

47 6 0.000013060 0.000022362 -0.000041061

48 6 0.000018687 -0.000028432 0.000012131

49 1 -0.000001428 0.000027390 0.000017980

50 1 -0.000001340 0.000006355 -0.000039628

51 1 -0.000000416 0.000021818 -0.000009701

52 1 -0.000019612 0.000017815 0.000012914

53 1 0.000001073 0.000025327 0.000008131

54 1 0.000018800 0.000012638 -0.000011675

55 1 0.000001123 0.000007067 0.000040482

56 1 0.000002250 0.000024824 -0.000018032

57 1 -0.000009858 -0.000017458 0.000006058

58 1 0.000001788 0.000001265 -0.000000361

59 1 0.000008330 -0.000001545 -0.000002281

60 1 0.000000860 0.000001349 -0.000010848

61 1 -0.000024054 -0.000011898 0.000011595

62 1 0.000006298 0.000004543 0.000007603

63 1 0.000006329 0.000010485 -0.000003815

64 1 -0.000020040 -0.000011611 -0.000017110

65 1 -0.000015692 0.000000326 -0.000027612

66 1 -0.000001235 0.000000388 0.000004191

67 1 0.000019537 0.000001023 0.000026667

68 1 0.000002096 -0.000001553 -0.000004396

69 1 -0.000005907 0.000001705 -0.000008003

70 1 -0.000007706 0.000006692 0.000004391

71 1 0.000020531 -0.000015498 0.000016976

72 1 0.000025184 -0.000013034 -0.000008610

73 1 0.000000385 -0.000000770 0.000011152

74 1 -0.000008129 -0.000004373 0.000002988

75 1 -0.000002796 -0.000002280 0.000000210

76 1 0.000008067 -0.000019641 -0.000005617

77 1 0.000199619 -0.000016934 0.000048789

78 1 -0.000174232 -0.000111627 -0.000051060

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

Cartesian Forces: Max 0.000971106 RMS 0.000230683

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

Leave Link 716 at Tue Aug 27 22:20:46 2019, MaxMem= 4294967296 cpu: 2.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000713708 RMS 0.000105917

Search for a local minimum.

Step number 12 out of a maximum of 452

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

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= 1.42D-06 DEPred=-1.95D-06 R=-7.31D-01

Trust test=-7.31D-01 RLast= 3.02D-02 DXMaxT set to 1.00D-01

ITU= -1 1 1 -1 1 -1 -1 1 1 -1 1 0

Eigenvalues --- -0.00076 -0.00015 0.00525 0.00620 0.00737

Eigenvalues --- 0.00871 0.00995 0.01026 0.01028 0.01087

Eigenvalues --- 0.01117 0.01218 0.01239 0.01288 0.01299

Eigenvalues --- 0.01304 0.01341 0.01390 0.01428 0.01441

Eigenvalues --- 0.01466 0.01489 0.01520 0.01637 0.01718

Eigenvalues --- 0.01719 0.01726 0.01740 0.01747 0.01752

Eigenvalues --- 0.01759 0.01784 0.01803 0.01825 0.01884

Eigenvalues --- 0.01923 0.01936 0.01944 0.01966 0.02146

Eigenvalues --- 0.02189 0.02243 0.02266 0.02269 0.02307

Eigenvalues --- 0.02329 0.02428 0.02441 0.02535 0.02540

Eigenvalues --- 0.02550 0.02552 0.02594 0.02596 0.02603

Eigenvalues --- 0.02606 0.02612 0.02733 0.02739 0.02764

Eigenvalues --- 0.02789 0.02866 0.02869 0.02871 0.02873

Eigenvalues --- 0.03055 0.03066 0.03881 0.04090 0.04195

Eigenvalues --- 0.04318 0.04352 0.04432 0.04515 0.04529

Eigenvalues --- 0.08086 0.09706 0.09716 0.09863 0.09915

Eigenvalues --- 0.09942 0.10253 0.10458 0.10578 0.10689

Eigenvalues --- 0.10690 0.10697 0.10699 0.10743 0.10909

Eigenvalues --- 0.11391 0.11393 0.11401 0.11403 0.12002

Eigenvalues --- 0.12004 0.12007 0.12011 0.12267 0.12269

Eigenvalues --- 0.12277 0.12279 0.12768 0.12771 0.12774

Eigenvalues --- 0.12775 0.15643 0.15961 0.16257 0.16985

Eigenvalues --- 0.17194 0.17299 0.17429 0.17663 0.17976

Eigenvalues --- 0.18037 0.18073 0.18582 0.19246 0.19280

Eigenvalues --- 0.19336 0.19343 0.19366 0.19379 0.19399

Eigenvalues --- 0.19453 0.19549 0.19550 0.19553 0.19555

Eigenvalues --- 0.20285 0.21516 0.22040 0.22784 0.22882

Eigenvalues --- 0.23387 0.23746 0.24308 0.24718 0.25602

Eigenvalues --- 0.26178 0.26593 0.26607 0.27162 0.28469

Eigenvalues --- 0.28516 0.28612 0.28824 0.29653 0.30982

Eigenvalues --- 0.31676 0.31909 0.32730 0.33106 0.33313

Eigenvalues --- 0.33460 0.34236 0.35069 0.35591 0.35619

Eigenvalues --- 0.35625 0.35631 0.35643 0.35705 0.35751

Eigenvalues --- 0.35761 0.35817 0.35834 0.35921 0.35924

Eigenvalues --- 0.35927 0.35930 0.36009 0.36019 0.36020

Eigenvalues --- 0.36020 0.36208 0.36254 0.36272 0.36275

Eigenvalues --- 0.37073 0.37078 0.37258 0.37396 0.37405

Eigenvalues --- 0.37556 0.38173 0.38510 0.38575 0.38752

Eigenvalues --- 0.39542 0.40570 0.40629 0.41000 0.41009

Eigenvalues --- 0.41052 0.41065 0.41096 0.41162 0.41369

Eigenvalues --- 0.41524 0.41817 0.42378 0.43000 0.44775

Eigenvalues --- 0.45526 0.45895 0.45905 0.45938 0.45967

Eigenvalues --- 0.46222 0.46228 0.46250 0.46260 0.46270

Eigenvalues --- 0.48230 0.48615 0.48736 0.49258 0.50491

Eigenvalues --- 0.50755 0.50755 0.50781 0.50809 0.51840

Eigenvalues --- 0.52539 0.56970 0.58482

Eigenvalue 1 is -7.56D-04 should be greater than 0.000000 Eigenvector:

D13 D12 D98 D20 D112

1 0.23935 0.23825 0.23387 -0.23304 -0.22965

D85 D27 D113 D14 D10

1 0.22687 -0.22306 -0.20580 0.17886 0.17494

Eigenvalue 2 is -1.49D-04 should be greater than 0.000000 Eigenvector:

D27 D113 D30 D81 D51

1 0.21602 0.20599 -0.19654 -0.19636 -0.19573

D57 D85 D13 D28 D114

1 -0.19394 0.19388 0.18632 0.18536 0.18337

Cosine: 0.802 < 0.840

Cut down GDIIS temporarily because of the cosine check. E 6

DIIS coeff's: 0.40366 0.59634

Cosine: 0.988 > 0.970

Length: 0.972

GDIIS step was calculated using 2 of the last 12 vectors.

Iteration 1 RMS(Cart)= 0.01600516 RMS(Int)= 0.00004807

Iteration 2 RMS(Cart)= 0.00009845 RMS(Int)= 0.00000462

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000462

ITry= 1 IFail=0 DXMaxC= 9.35D-02 DCOld= 1.00D+10 DXMaxT= 1.00D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.65856 -0.00045 -0.00123 -0.00074 -0.00198 2.65658

R2 2.63986 0.00044 0.00103 0.00056 0.00158 2.64144

R3 2.03715 0.00000 -0.00000 0.00009 0.00009 2.03724

R4 2.59910 -0.00020 -0.00002 -0.00034 -0.00037 2.59873

R5 2.71444 0.00045 0.00155 0.00089 0.00244 2.71688

R6 2.59896 -0.00025 -0.00004 -0.00050 -0.00054 2.59842

R7 1.90977 -0.00020 0.00008 -0.00052 -0.00044 1.90933

R8 2.65747 -0.00033 -0.00085 -0.00026 -0.00111 2.65636

R9 2.71602 0.00052 0.00112 0.00035 0.00147 2.71750

R10 2.03717 0.00002 -0.00003 0.00013 0.00010 2.03727

R11 2.64157 -0.00021 -0.00036 0.00092 0.00056 2.64213

R12 2.80367 0.00002 -0.00006 -0.00073 -0.00079 2.80288

R13 2.59760 -0.00005 -0.00085 -0.00126 -0.00211 2.59550

R14 2.76058 0.00031 0.00114 0.00040 0.00154 2.76212

R15 2.59246 0.00032 0.00103 0.00139 0.00242 2.59488

R16 2.76135 0.00022 0.00073 0.00017 0.00090 2.76226

R17 2.64610 -0.00071 -0.00231 -0.00141 -0.00372 2.64238

R18 2.55559 -0.00041 -0.00083 -0.00026 -0.00110 2.55450

R19 2.03913 0.00001 -0.00002 0.00003 0.00001 2.03914

R20 2.03918 -0.00002 -0.00003 -0.00001 -0.00004 2.03915

R21 2.64620 -0.00071 -0.00227 -0.00105 -0.00331 2.64289

R22 2.80325 -0.00000 0.00018 -0.00060 -0.00041 2.80283

R23 2.76130 0.00022 0.00078 0.00010 0.00087 2.76216

R24 2.59240 0.00032 0.00104 0.00118 0.00222 2.59463

R25 2.55559 -0.00041 -0.00084 -0.00024 -0.00108 2.55451

R26 2.03915 0.00001 -0.00004 0.00007 0.00003 2.03918

R27 2.76064 0.00031 0.00109 0.00045 0.00154 2.76218

R28 2.03916 -0.00002 -0.00001 -0.00004 -0.00005 2.03911

R29 2.59767 -0.00005 -0.00084 -0.00109 -0.00193 2.59574

R30 2.64145 -0.00021 -0.00039 0.00058 0.00019 2.64164

R31 2.71593 0.00051 0.00107 0.00001 0.00108 2.71701

R32 2.80417 0.00002 -0.00010 0.00047 0.00037 2.80454

R33 2.65769 -0.00033 -0.00090 0.00024 -0.00066 2.65703

R34 2.59908 -0.00025 -0.00005 -0.00013 -0.00016 2.59892

R35 2.63970 0.00044 0.00104 0.00015 0.00119 2.64088

R36 2.03713 0.00002 -0.00003 0.00004 0.00000 2.03713

R37 2.65877 -0.00045 -0.00123 -0.00031 -0.00154 2.65723

R38 2.03711 0.00000 0.00000 -0.00000 -0.00000 2.03711

R39 2.59922 -0.00020 0.00001 -0.00005 -0.00003 2.59918

R40 2.71435 0.00044 0.00146 0.00063 0.00210 2.71644

R41 1.91000 -0.00019 0.00010 0.00011 0.00020 1.91020

R42 2.80374 0.00000 0.00019 0.00057 0.00077 2.80450

R43 2.65155 -0.00005 0.00005 0.00020 0.00025 2.65180

R44 2.65007 0.00005 0.00001 0.00038 0.00039 2.65046

R45 2.62863 -0.00003 0.00001 -0.00019 -0.00018 2.62845

R46 2.04845 -0.00001 0.00000 -0.00005 -0.00005 2.04839

R47 2.63632 0.00002 0.00002 0.00008 0.00010 2.63641

R48 2.05017 0.00000 -0.00001 0.00001 -0.00000 2.05017

R49 2.63421 -0.00001 -0.00004 0.00003 -0.00000 2.63420

R50 2.05006 0.00001 -0.00002 0.00003 0.00002 2.05008

R51 2.63077 0.00005 -0.00000 -0.00002 -0.00002 2.63075

R52 2.05013 0.00001 -0.00001 0.00003 0.00003 2.05015

R53 2.04843 0.00003 -0.00000 0.00004 0.00004 2.04847

R54 2.63627 0.00003 0.00004 0.00010 0.00014 2.63641

R55 2.63431 -0.00001 -0.00009 0.00002 -0.00007 2.63424

R56 2.05007 0.00001 -0.00002 0.00003 0.00001 2.05009

R57 2.62875 -0.00002 -0.00003 -0.00021 -0.00024 2.62852

R58 2.05016 0.00001 -0.00001 0.00003 0.00002 2.05018

R59 2.65161 -0.00005 -0.00004 0.00016 0.00012 2.65173

R60 2.04842 0.00000 0.00000 -0.00003 -0.00002 2.04840

R61 2.65042 -0.00003 -0.00011 0.00018 0.00007 2.65049

R62 2.63061 0.00003 0.00009 -0.00001 0.00007 2.63069

R63 2.04851 0.00001 0.00000 -0.00002 -0.00002 2.04850

R64 2.05015 0.00000 -0.00001 0.00002 0.00000 2.05016

R65 2.65024 -0.00003 -0.00013 -0.00023 -0.00037 2.64987

R66 2.65150 -0.00005 -0.00011 -0.00014 -0.00024 2.65125

R67 2.63069 0.00003 0.00009 0.00016 0.00025 2.63093

R68 2.04854 0.00001 0.00002 0.00005 0.00007 2.04861

R69 2.63431 -0.00001 -0.00009 -0.00001 -0.00010 2.63421

R70 2.05015 0.00000 -0.00001 0.00001 0.00000 2.05015

R71 2.63622 0.00003 0.00005 0.00001 0.00005 2.63628

R72 2.05007 0.00001 -0.00002 0.00003 0.00002 2.05009

R73 2.62880 -0.00002 -0.00001 -0.00007 -0.00008 2.62872

R74 2.05016 0.00001 -0.00001 0.00004 0.00003 2.05020

R75 2.04842 0.00000 0.00002 -0.00004 -0.00002 2.04840

R76 2.64990 0.00005 0.00001 -0.00005 -0.00003 2.64986

R77 2.65143 -0.00005 0.00003 -0.00014 -0.00011 2.65132

R78 2.63084 0.00005 -0.00001 0.00015 0.00014 2.63098

R79 2.04846 0.00003 -0.00000 0.00013 0.00012 2.04859

R80 2.63420 -0.00001 -0.00003 0.00001 -0.00003 2.63417

R81 2.05012 0.00001 -0.00000 0.00003 0.00003 2.05015

R82 2.63627 0.00002 0.00003 -0.00003 0.00000 2.63627

R83 2.05006 0.00001 -0.00002 0.00004 0.00002 2.05008

R84 2.62868 -0.00002 0.00003 -0.00004 -0.00001 2.62867

R85 2.05018 0.00000 -0.00001 0.00002 0.00001 2.05019

R86 2.04844 -0.00001 0.00001 -0.00006 -0.00004 2.04839

A1 1.88171 -0.00006 -0.00014 -0.00006 -0.00021 1.88150

A2 2.18717 0.00001 0.00032 -0.00048 -0.00016 2.18700

A3 2.21429 0.00005 -0.00018 0.00054 0.00036 2.21465

A4 1.86743 -0.00001 0.00033 0.00003 0.00037 1.86780

A5 2.22203 0.00022 -0.00028 0.00066 0.00038 2.22241

A6 2.19327 -0.00021 -0.00004 -0.00062 -0.00067 2.19260

A7 1.92557 0.00019 -0.00020 0.00028 0.00007 1.92564

A8 2.17866 -0.00014 0.00001 -0.00018 -0.00019 2.17847

A9 2.17825 -0.00005 0.00018 0.00034 0.00049 2.17874

A10 1.86789 -0.00006 0.00016 -0.00009 0.00008 1.86796

A11 2.19363 -0.00008 -0.00003 -0.00042 -0.00045 2.19317

A12 2.22132 0.00013 -0.00013 0.00054 0.00042 2.22174

A13 1.88183 -0.00006 -0.00015 -0.00015 -0.00030 1.88154

A14 2.21427 0.00006 -0.00021 0.00073 0.00052 2.21479

A15 2.18705 -0.00001 0.00036 -0.00060 -0.00023 2.18682

A16 2.18563 0.00010 -0.00007 -0.00127 -0.00134 2.18429

A17 2.02362 -0.00011 -0.00008 -0.00023 -0.00030 2.02332

A18 2.07387 0.00001 0.00014 0.00148 0.00162 2.07549

A19 2.19098 0.00016 0.00038 -0.00015 0.00023 2.19121

A20 2.16637 -0.00014 -0.00045 -0.00004 -0.00048 2.16588

A21 1.92580 -0.00001 0.00007 0.00018 0.00026 1.92605

A22 1.84715 -0.00008 0.00005 0.00011 0.00016 1.84731

A23 1.92699 -0.00003 -0.00031 -0.00047 -0.00077 1.92621

A24 2.19180 0.00013 0.00040 -0.00016 0.00025 2.19204

A25 2.16439 -0.00010 -0.00009 0.00063 0.00053 2.16492

A26 1.86188 0.00003 0.00011 0.00006 0.00017 1.86205

A27 2.19710 -0.00000 -0.00024 0.00019 -0.00006 2.19704

A28 2.22381 -0.00002 0.00013 -0.00026 -0.00013 2.22368

A29 1.86192 0.00010 0.00008 0.00009 0.00016 1.86209

A30 2.19709 -0.00004 -0.00007 -0.00011 -0.00018 2.19691

A31 2.22381 -0.00006 -0.00000 -0.00001 -0.00001 2.22381

A32 2.18506 -0.00001 0.00034 -0.00104 -0.00070 2.18435

A33 2.02566 -0.00003 -0.00075 -0.00071 -0.00147 2.02419

A34 2.07243 0.00004 0.00041 0.00173 0.00214 2.07457

A35 2.16446 -0.00010 -0.00002 0.00082 0.00079 2.16525

A36 2.19168 0.00013 0.00035 -0.00041 -0.00006 2.19162

A37 1.92703 -0.00003 -0.00033 -0.00041 -0.00074 1.92629

A38 1.86188 0.00003 0.00012 0.00008 0.00021 1.86209

A39 2.19701 -0.00001 -0.00018 -0.00002 -0.00020 2.19681

A40 2.22390 -0.00002 0.00006 -0.00008 -0.00002 2.22387

A41 1.86192 0.00010 0.00007 0.00005 0.00013 1.86205

A42 2.22373 -0.00006 0.00004 -0.00013 -0.00008 2.22364

A43 2.19718 -0.00004 -0.00012 0.00006 -0.00006 2.19713

A44 1.92575 -0.00001 0.00011 0.00011 0.00022 1.92597

A45 2.16630 -0.00014 -0.00058 -0.00011 -0.00071 2.16560

A46 2.19110 0.00015 0.00048 0.00001 0.00050 2.19160

A47 1.84715 -0.00008 0.00004 0.00012 0.00016 1.84731

A48 2.18635 0.00010 -0.00011 0.00034 0.00024 2.18659

A49 2.07297 0.00001 0.00016 -0.00065 -0.00051 2.07246

A50 2.02384 -0.00011 -0.00005 0.00036 0.00029 2.02413

A51 2.22134 0.00013 -0.00012 0.00042 0.00027 2.22161

A52 2.19353 -0.00007 -0.00007 -0.00054 -0.00060 2.19293

A53 1.86784 -0.00006 0.00021 -0.00014 0.00008 1.86792

A54 1.88186 -0.00006 -0.00016 -0.00006 -0.00022 1.88165

A55 2.18729 -0.00001 0.00030 -0.00007 0.00023 2.18752

A56 2.21401 0.00006 -0.00014 0.00015 0.00001 2.21402

A57 1.88174 -0.00006 -0.00014 -0.00000 -0.00014 1.88161

A58 2.21403 0.00005 -0.00020 0.00006 -0.00014 2.21389

A59 2.18740 0.00001 0.00034 -0.00004 0.00029 2.18769

A60 1.86738 -0.00001 0.00033 0.00006 0.00039 1.86778

A61 2.22201 0.00022 -0.00028 0.00046 0.00015 2.22216

A62 2.19320 -0.00021 -0.00001 -0.00077 -0.00077 2.19243

A63 1.92553 0.00018 -0.00022 0.00007 -0.00015 1.92538

A64 2.17806 -0.00004 0.00014 -0.00000 0.00011 2.17817

A65 2.17852 -0.00014 0.00007 -0.00059 -0.00055 2.17797

A66 2.18577 -0.00001 0.00039 0.00046 0.00086 2.18663

A67 2.07151 0.00004 0.00040 -0.00028 0.00010 2.07161

A68 2.02589 -0.00003 -0.00080 -0.00014 -0.00095 2.02494

A69 2.10483 -0.00012 0.00038 -0.00107 -0.00069 2.10414

A70 2.10673 0.00013 -0.00024 0.00135 0.00111 2.10784

A71 2.07162 -0.00001 -0.00013 -0.00029 -0.00042 2.07120

A72 2.10504 0.00003 0.00002 0.00029 0.00031 2.10535

A73 2.08492 -0.00003 0.00009 -0.00036 -0.00027 2.08465

A74 2.09304 0.00000 -0.00010 0.00005 -0.00005 2.09299

A75 2.09778 -0.00000 0.00007 -0.00010 -0.00003 2.09775

A76 2.08886 0.00000 -0.00005 0.00011 0.00006 2.08892

A77 2.09654 0.00000 -0.00002 -0.00001 -0.00003 2.09652

A78 2.08907 -0.00000 -0.00006 -0.00001 -0.00007 2.08900

A79 2.09693 0.00000 0.00002 0.00004 0.00006 2.09699

A80 2.09719 0.00000 0.00004 -0.00003 0.00001 2.09720

A81 2.09761 0.00000 -0.00002 0.00012 0.00010 2.09771

A82 2.09705 -0.00000 0.00003 -0.00009 -0.00006 2.09699

A83 2.08852 0.00000 -0.00001 -0.00003 -0.00004 2.08848

A84 2.10511 -0.00002 0.00013 -0.00003 0.00010 2.10521

A85 2.08392 -0.00001 0.00008 -0.00009 -0.00001 2.08391

A86 2.09402 0.00002 -0.00021 0.00011 -0.00010 2.09392

A87 2.08901 -0.00001 -0.00001 -0.00000 -0.00001 2.08900

A88 2.09694 0.00000 -0.00002 0.00004 0.00002 2.09696

A89 2.09723 0.00001 0.00003 -0.00004 -0.00001 2.09722

A90 2.09790 -0.00000 0.00002 -0.00010 -0.00009 2.09782

A91 2.09645 0.00001 -0.00000 0.00003 0.00002 2.09647

A92 2.08883 -0.00000 -0.00002 0.00008 0.00006 2.08889

A93 2.10511 0.00001 -0.00004 0.00017 0.00013 2.10524

A94 2.09301 0.00002 -0.00003 0.00009 0.00006 2.09308

A95 2.08488 -0.00003 0.00007 -0.00028 -0.00021 2.08467

A96 2.10664 -0.00007 -0.00014 -0.00119 -0.00133 2.10531

A97 2.10526 0.00005 0.00008 0.00127 0.00135 2.10661

A98 2.07128 0.00002 0.00006 -0.00009 -0.00003 2.07125

A99 2.10542 -0.00002 -0.00001 -0.00013 -0.00014 2.10528

A100 2.08373 -0.00002 0.00015 -0.00016 -0.00001 2.08371

A101 2.09389 0.00004 -0.00013 0.00028 0.00015 2.09404

A102 2.09752 0.00000 -0.00001 0.00013 0.00012 2.09763

A103 2.09706 -0.00000 0.00002 -0.00006 -0.00004 2.09702

A104 2.08861 -0.00000 -0.00000 -0.00008 -0.00008 2.08853

A105 2.10535 0.00004 -0.00016 0.00122 0.00105 2.10640

A106 2.10646 -0.00007 0.00004 -0.00141 -0.00137 2.10509

A107 2.07137 0.00003 0.00012 0.00020 0.00032 2.07169

A108 2.10537 -0.00002 -0.00002 -0.00027 -0.00030 2.10507

A109 2.08370 -0.00002 0.00013 -0.00027 -0.00013 2.08357

A110 2.09397 0.00004 -0.00011 0.00056 0.00046 2.09443

A111 2.09753 0.00000 -0.00004 0.00013 0.00008 2.09761

A112 2.08862 -0.00000 0.00001 -0.00004 -0.00003 2.08859

A113 2.09704 -0.00000 0.00003 -0.00009 -0.00006 2.09698

A114 2.08900 -0.00001 0.00001 0.00002 0.00002 2.08902

A115 2.09724 0.00001 0.00002 -0.00003 -0.00001 2.09723

A116 2.09694 0.00000 -0.00003 0.00002 -0.00001 2.09693

A117 2.09788 -0.00000 0.00003 -0.00017 -0.00014 2.09774

A118 2.09650 0.00001 -0.00002 0.00013 0.00011 2.09661

A119 2.08880 -0.00000 -0.00000 0.00003 0.00003 2.08883

A120 2.10511 0.00001 -0.00009 0.00009 -0.00000 2.10511

A121 2.08493 -0.00003 0.00007 -0.00022 -0.00015 2.08478

A122 2.09297 0.00003 0.00002 0.00010 0.00013 2.09310

A123 2.10677 0.00013 -0.00045 0.00113 0.00067 2.10744

A124 2.10469 -0.00012 0.00055 -0.00114 -0.00059 2.10411

A125 2.07172 -0.00001 -0.00010 0.00001 -0.00008 2.07163

A126 2.10506 -0.00002 0.00013 -0.00015 -0.00002 2.10503

A127 2.08387 -0.00000 0.00006 -0.00018 -0.00013 2.08375

A128 2.09412 0.00002 -0.00019 0.00035 0.00016 2.09429

A129 2.09762 0.00000 -0.00004 0.00009 0.00005 2.09767

A130 2.08853 0.00000 -0.00000 0.00002 0.00001 2.08855

A131 2.09703 -0.00000 0.00004 -0.00010 -0.00006 2.09697

A132 2.08906 -0.00000 -0.00005 -0.00000 -0.00005 2.08901

A133 2.09720 0.00000 0.00003 -0.00002 0.00002 2.09722

A134 2.09692 0.00000 0.00001 0.00002 0.00003 2.09695

A135 2.09776 -0.00000 0.00007 -0.00013 -0.00006 2.09770

A136 2.09659 0.00000 -0.00003 0.00008 0.00005 2.09664

A137 2.08883 0.00000 -0.00004 0.00005 0.00001 2.08885

A138 2.10502 0.00003 -0.00001 0.00018 0.00017 2.10518

A139 2.08497 -0.00003 0.00008 -0.00023 -0.00015 2.08482

A140 2.09300 0.00000 -0.00006 0.00003 -0.00003 2.09297

D1 0.01576 0.00000 -0.00021 -0.00064 -0.00085 0.01492

D2 -3.09464 0.00002 -0.00066 -0.00326 -0.00392 -3.09856

D3 -3.11891 -0.00002 -0.00024 0.00055 0.00030 -3.11860

D4 0.05388 0.00000 -0.00069 -0.00207 -0.00277 0.05111

D5 -0.00115 0.00000 0.00018 0.00043 0.00061 -0.00054

D6 -3.13455 -0.00001 -0.00018 0.00156 0.00138 -3.13317

D7 3.13338 0.00002 0.00022 -0.00079 -0.00057 3.13282

D8 -0.00002 0.00000 -0.00014 0.00035 0.00020 0.00018

D9 -0.02508 -0.00001 0.00016 0.00061 0.00077 -0.02431

D10 3.07801 0.00002 -0.00012 0.01289 0.01277 3.09077

D11 3.08598 -0.00002 0.00059 0.00321 0.00380 3.08978

D12 -0.09412 0.00001 0.00032 0.01548 0.01580 -0.07832

D13 -2.94558 -0.00001 0.00191 0.01878 0.02069 -2.92489

D14 0.18573 -0.00000 0.00134 0.01634 0.01768 0.20341

D15 0.23273 0.00000 0.00137 0.01568 0.01705 0.24978

D16 -2.91915 0.00002 0.00080 0.01324 0.01404 -2.90510

D17 0.02438 0.00001 -0.00005 -0.00035 -0.00040 0.02398

D18 -3.09026 0.00003 -0.00040 -0.00170 -0.00210 -3.09236

D19 -3.07872 -0.00002 0.00023 -0.01261 -0.01238 -3.09110

D20 0.08983 0.00000 -0.00012 -0.01396 -0.01408 0.07575

D21 -0.01391 -0.00001 -0.00009 -0.00006 -0.00014 -0.01405

D22 3.11966 0.00001 0.00027 -0.00116 -0.00089 3.11876

D23 3.10017 -0.00003 0.00028 0.00130 0.00158 3.10175

D24 -0.04945 -0.00001 0.00063 0.00020 0.00083 -0.04862

D25 -0.24211 -0.00004 0.00187 -0.01573 -0.01386 -0.25597

D26 2.91159 -0.00007 0.00240 -0.01421 -0.01181 2.89978

D27 2.93187 -0.00002 0.00144 -0.01734 -0.01590 2.91597

D28 -0.19761 -0.00004 0.00197 -0.01582 -0.01385 -0.21146

D29 -0.13069 0.00001 0.00204 -0.00292 -0.00088 -0.13157

D30 3.02152 0.00001 0.00110 -0.00239 -0.00129 3.02023

D31 2.99848 0.00004 0.00149 -0.00450 -0.00300 2.99548

D32 -0.13250 0.00003 0.00056 -0.00397 -0.00341 -0.13591

D33 -0.98854 0.00004 -0.00054 0.00888 0.00834 -0.98021

D34 2.14960 0.00004 -0.00089 0.00830 0.00741 2.15701

D35 2.16434 0.00002 -0.00005 0.01032 0.01027 2.17461

D36 -0.98071 0.00002 -0.00040 0.00974 0.00935 -0.97136

D37 -3.08989 0.00003 -0.00094 0.00098 0.00004 -3.08986

D38 0.04233 0.00003 -0.00012 0.00051 0.00039 0.04272

D39 3.10490 -0.00002 0.00074 -0.00059 0.00015 3.10505

D40 -0.06381 -0.00002 0.00086 -0.00170 -0.00084 -0.06466

D41 -0.02748 -0.00003 -0.00008 -0.00013 -0.00020 -0.02768

D42 3.08699 -0.00002 0.00004 -0.00124 -0.00120 3.08579

D43 -0.04152 -0.00003 0.00025 -0.00070 -0.00044 -0.04197

D44 3.09514 -0.00001 0.00049 0.00070 0.00119 3.09633

D45 0.02529 0.00002 -0.00031 0.00063 0.00032 0.02561

D46 -3.08794 0.00002 -0.00033 0.00109 0.00076 -3.08718

D47 -3.11146 -0.00000 -0.00055 -0.00074 -0.00128 -3.11275

D48 0.05849 0.00000 -0.00057 -0.00027 -0.00084 0.05765

D49 0.13923 -0.00004 -0.00420 0.00005 -0.00415 0.13508

D50 -2.99671 -0.00006 -0.00230 -0.00776 -0.01006 -3.00677

D51 -3.00794 -0.00001 -0.00393 0.00162 -0.00230 -3.01024

D52 0.13930 -0.00004 -0.00203 -0.00618 -0.00821 0.13109

D53 0.00130 0.00000 0.00021 -0.00031 -0.00010 0.00120

D54 -3.11263 -0.00000 0.00009 0.00083 0.00092 -3.11171

D55 3.11396 -0.00000 0.00022 -0.00077 -0.00055 3.11341

D56 0.00003 -0.00001 0.00010 0.00037 0.00047 0.00050

D57 -3.00826 -0.00002 -0.00388 0.00030 -0.00358 -3.01185

D58 0.14042 -0.00004 -0.00475 0.00182 -0.00293 0.13749

D59 0.14387 -0.00003 -0.00329 0.00281 -0.00048 0.14339

D60 -2.99063 -0.00005 -0.00416 0.00434 0.00018 -2.99046

D61 0.98644 -0.00004 0.00237 -0.00862 -0.00625 0.98019

D62 -2.15162 -0.00004 0.00286 -0.00810 -0.00524 -2.15686

D63 -2.16474 -0.00002 0.00184 -0.01091 -0.00907 -2.17381

D64 0.98039 -0.00002 0.00233 -0.01039 -0.00806 0.97233

D65 -3.11024 0.00000 -0.00089 0.00216 0.00127 -3.10897

D66 0.05992 0.00000 -0.00083 0.00280 0.00197 0.06189

D67 0.02520 0.00002 -0.00014 0.00084 0.00070 0.02590

D68 -3.08783 0.00002 -0.00008 0.00148 0.00140 -3.08643

D69 3.09382 -0.00001 0.00108 -0.00230 -0.00122 3.09260

D70 -0.04150 -0.00003 0.00031 -0.00096 -0.00065 -0.04215

D71 0.00142 -0.00000 -0.00010 -0.00037 -0.00048 0.00095

D72 -3.11270 -0.00000 0.00000 0.00014 0.00014 -3.11256

D73 3.11388 -0.00000 -0.00017 -0.00103 -0.00120 3.11268

D74 -0.00025 -0.00001 -0.00006 -0.00051 -0.00058 -0.00083

D75 -0.02760 -0.00002 0.00029 -0.00022 0.00007 -0.02753

D76 3.10607 -0.00002 0.00116 0.00111 0.00226 3.10833

D77 3.08707 -0.00002 0.00019 -0.00072 -0.00053 3.08653

D78 -0.06245 -0.00001 0.00105 0.00060 0.00165 -0.06080

D79 0.04239 0.00003 -0.00037 0.00073 0.00036 0.04274

D80 -3.09115 0.00003 -0.00124 -0.00062 -0.00186 -3.09301

D81 3.02130 0.00000 0.00008 -0.00260 -0.00252 3.01879

D82 -0.12796 0.00004 -0.00127 0.00519 0.00392 -0.12404

D83 -0.12942 0.00001 0.00108 -0.00107 0.00000 -0.12941

D84 3.00450 0.00004 -0.00028 0.00672 0.00644 3.01094

D85 2.94719 0.00002 0.00004 0.01735 0.01739 2.96458

D86 -0.23174 -0.00002 0.00087 0.00744 0.00831 -0.22343

D87 -0.18692 -0.00001 0.00136 0.00976 0.01112 -0.17581

D88 2.91733 -0.00005 0.00219 -0.00015 0.00204 2.91936

D89 -0.98698 -0.00000 -0.00025 -0.00527 -0.00552 -0.99250

D90 2.15644 -0.00000 0.00024 -0.00819 -0.00795 2.14849

D91 2.14765 0.00003 -0.00148 0.00180 0.00032 2.14797

D92 -0.99212 0.00003 -0.00099 -0.00112 -0.00211 -0.99422

D93 3.09476 -0.00004 0.00115 -0.01020 -0.00905 3.08571

D94 -0.05272 -0.00002 0.00116 -0.00670 -0.00554 -0.05826

D95 -0.01511 -0.00001 0.00045 -0.00177 -0.00132 -0.01643

D96 3.12059 0.00002 0.00045 0.00173 0.00219 3.12278

D97 -3.08415 0.00004 -0.00166 0.01078 0.00912 -3.07503

D98 0.10521 0.00005 -0.00149 0.02238 0.02089 0.12610

D99 0.02637 0.00001 -0.00098 0.00255 0.00157 0.02794

D100 -3.06746 0.00002 -0.00080 0.01415 0.01334 -3.05411

D101 -0.00114 0.00000 0.00022 0.00039 0.00061 -0.00054

D102 3.13563 0.00003 -0.00009 0.00381 0.00373 3.13935

D103 -3.13673 -0.00002 0.00021 -0.00318 -0.00297 -3.13970

D104 0.00004 0.00000 -0.00010 0.00024 0.00015 0.00019

D105 0.01695 0.00000 -0.00080 0.00114 0.00034 0.01729

D106 -3.08919 0.00004 -0.00194 0.00869 0.00675 -3.08243

D107 -3.11991 -0.00002 -0.00050 -0.00222 -0.00271 -3.12263

D108 0.05713 0.00001 -0.00163 0.00533 0.00370 0.06083

D109 -0.02707 -0.00001 0.00111 -0.00231 -0.00120 -0.02827

D110 3.06675 -0.00001 0.00094 -0.01389 -0.01295 3.05379

D111 3.07982 -0.00003 0.00221 -0.00966 -0.00745 3.07237

D112 -0.10955 -0.00003 0.00204 -0.02125 -0.01920 -0.12875

D113 -2.96091 -0.00006 0.00296 -0.01516 -0.01219 -2.97310

D114 0.17517 -0.00003 0.00111 -0.00754 -0.00642 0.16875

D115 0.22242 -0.00002 0.00162 -0.00630 -0.00468 0.21774

D116 -2.92469 0.00000 -0.00023 0.00132 0.00109 -2.92360

D117 0.98664 -0.00000 0.00297 0.00398 0.00695 0.99359

D118 -2.15668 0.00000 0.00190 0.00760 0.00949 -2.14719

D119 -2.14981 -0.00002 0.00470 -0.00312 0.00158 -2.14824

D120 0.99005 -0.00002 0.00362 0.00050 0.00412 0.99417

D121 -3.12888 0.00000 -0.00042 0.00015 -0.00027 -3.12915

D122 -0.00845 0.00001 -0.00021 -0.00026 -0.00047 -0.00892

D123 0.01610 0.00001 -0.00008 0.00070 0.00063 0.01673

D124 3.13653 0.00001 0.00013 0.00030 0.00043 3.13696

D125 3.14131 -0.00001 0.00023 0.00009 0.00032 -3.14156

D126 -0.01829 -0.00000 0.00018 -0.00042 -0.00024 -0.01853

D127 -0.00367 -0.00001 -0.00011 -0.00048 -0.00059 -0.00426

D128 3.11991 -0.00000 -0.00017 -0.00098 -0.00115 3.11877

D129 -0.01703 0.00000 0.00015 -0.00037 -0.00022 -0.01724

D130 3.12429 0.00000 0.00009 -0.00017 -0.00008 3.12421

D131 -3.13736 -0.00000 -0.00006 0.00004 -0.00002 -3.13737

D132 0.00396 -0.00000 -0.00012 0.00024 0.00011 0.00408

D133 0.00527 -0.00000 -0.00004 -0.00021 -0.00025 0.00502

D134 -3.13417 0.00000 -0.00010 0.00031 0.00020 -3.13397

D135 -3.13605 -0.00000 0.00002 -0.00040 -0.00038 -3.13643

D136 0.00770 0.00000 -0.00004 0.00011 0.00007 0.00776

D137 0.00712 0.00000 -0.00015 0.00043 0.00028 0.00740

D138 -3.13157 0.00000 -0.00002 0.00054 0.00052 -3.13105

D139 -3.13663 -0.00000 -0.00008 -0.00008 -0.00017 -3.13679

D140 0.00787 -0.00000 0.00005 0.00002 0.00007 0.00794

D141 -0.00788 0.00000 0.00023 -0.00008 0.00014 -0.00773

D142 -3.13136 -0.00000 0.00028 0.00043 0.00071 -3.13065

D143 3.13083 0.00001 0.00010 -0.00019 -0.00009 3.13074

D144 0.00735 0.00000 0.00015 0.00032 0.00047 0.00782

D145 -0.00539 -0.00000 0.00005 0.00006 0.00010 -0.00529

D146 3.13548 0.00000 0.00011 0.00041 0.00052 3.13599

D147 3.13408 -0.00000 -0.00013 -0.00006 -0.00019 3.13389

D148 -0.00824 0.00000 -0.00006 0.00029 0.00023 -0.00801

D149 -0.00682 0.00000 -0.00003 -0.00032 -0.00034 -0.00716

D150 3.13221 -0.00000 -0.00012 -0.00059 -0.00071 3.13150

D151 3.13690 0.00000 0.00015 -0.00020 -0.00005 3.13684

D152 -0.00726 -0.00000 0.00005 -0.00047 -0.00042 -0.00768

D153 0.01582 0.00001 0.00012 0.00089 0.00101 0.01683

D154 3.13700 -0.00000 0.00032 -0.00005 0.00027 3.13727

D155 -3.12505 0.00001 0.00005 0.00055 0.00060 -3.12445

D156 -0.00387 -0.00001 0.00026 -0.00040 -0.00014 -0.00401

D157 3.13128 -0.00002 0.00019 -0.00105 -0.00086 3.13042

D158 -0.01378 -0.00002 -0.00030 -0.00155 -0.00185 -0.01563

D159 0.01000 -0.00001 -0.00001 -0.00011 -0.00012 0.00988

D160 -3.13506 -0.00001 -0.00050 -0.00062 -0.00112 -3.13618

D161 3.13966 0.00002 -0.00017 0.00078 0.00060 3.14027

D162 0.01675 0.00001 -0.00019 0.00103 0.00084 0.01759

D163 0.00154 0.00002 0.00031 0.00129 0.00160 0.00314

D164 -3.12138 0.00001 0.00030 0.00154 0.00184 -3.11954

D165 0.00872 -0.00001 -0.00016 -0.00037 -0.00052 0.00820

D166 -3.13032 -0.00001 -0.00006 -0.00010 -0.00016 -3.13048

D167 3.13153 0.00000 -0.00014 -0.00062 -0.00077 3.13076

D168 -0.00752 0.00000 -0.00004 -0.00036 -0.00040 -0.00792

D169 3.14137 0.00003 -0.00089 0.00456 0.00368 -3.13814

D170 0.01777 0.00001 -0.00079 0.00299 0.00220 0.01997

D171 0.00147 0.00002 0.00017 0.00102 0.00118 0.00266

D172 -3.12212 0.00001 0.00026 -0.00056 -0.00030 -3.12242

D173 3.12966 -0.00003 0.00089 -0.00459 -0.00370 3.12596

D174 0.00870 -0.00001 0.00045 -0.00320 -0.00275 0.00595

D175 -0.01363 -0.00002 -0.00016 -0.00104 -0.00120 -0.01483

D176 -3.13459 -0.00001 -0.00061 0.00035 -0.00025 -3.13485

D177 0.00866 -0.00001 -0.00010 -0.00047 -0.00057 0.00809

D178 -3.13060 -0.00001 0.00003 -0.00077 -0.00074 -3.13133

D179 3.13215 0.00000 -0.00019 0.00110 0.00092 3.13307

D180 -0.00710 0.00001 -0.00006 0.00081 0.00075 -0.00635

D181 -0.00672 0.00000 0.00001 -0.00007 -0.00006 -0.00678

D182 3.13674 -0.00000 0.00023 -0.00055 -0.00032 3.13642

D183 3.13252 0.00000 -0.00011 0.00023 0.00011 3.13264

D184 -0.00720 -0.00000 0.00011 -0.00026 -0.00015 -0.00735

D185 -0.00540 -0.00000 -0.00001 0.00005 0.00004 -0.00535

D186 3.13527 0.00000 0.00015 -0.00002 0.00013 3.13540

D187 3.13433 -0.00000 -0.00023 0.00053 0.00030 3.13463

D188 -0.00819 0.00000 -0.00007 0.00046 0.00039 -0.00780

D189 0.01570 0.00001 0.00008 0.00052 0.00060 0.01630

D190 3.13656 -0.00000 0.00053 -0.00089 -0.00036 3.13621

D191 -3.12497 0.00001 -0.00008 0.00059 0.00051 -3.12446

D192 -0.00410 -0.00001 0.00037 -0.00081 -0.00044 -0.00455

D193 3.13984 -0.00001 0.00051 -0.00297 -0.00246 3.13738

D194 -0.01911 -0.00000 0.00042 -0.00185 -0.00143 -0.02054

D195 -0.00354 -0.00001 0.00003 -0.00011 -0.00008 -0.00362

D196 3.12069 0.00000 -0.00006 0.00101 0.00095 3.12164

D197 -3.12752 0.00001 -0.00070 0.00293 0.00224 -3.12528

D198 -0.00731 0.00001 -0.00034 0.00227 0.00193 -0.00538

D199 0.01587 0.00000 -0.00021 0.00007 -0.00015 0.01572

D200 3.13608 0.00001 0.00014 -0.00060 -0.00045 3.13562

D201 -0.00782 0.00000 0.00015 0.00003 0.00019 -0.00764

D202 3.13108 0.00001 0.00007 0.00040 0.00047 3.13155

D203 -3.13195 -0.00000 0.00024 -0.00109 -0.00085 -3.13280

D204 0.00695 -0.00000 0.00016 -0.00072 -0.00056 0.00639

D205 0.00698 0.00000 -0.00015 0.00008 -0.00007 0.00691

D206 -3.13651 -0.00000 -0.00011 0.00019 0.00008 -3.13643

D207 -3.13190 -0.00000 -0.00007 -0.00029 -0.00036 -3.13226

D208 0.00779 -0.00001 -0.00003 -0.00018 -0.00021 0.00758

D209 0.00530 -0.00000 -0.00003 -0.00012 -0.00015 0.00514

D210 -3.13583 -0.00000 0.00006 0.00003 0.00009 -3.13574

D211 -3.13440 0.00000 -0.00007 -0.00023 -0.00030 -3.13470

D212 0.00766 0.00000 0.00002 -0.00008 -0.00006 0.00760

D213 -0.01687 0.00000 0.00022 0.00004 0.00026 -0.01661

D214 -3.13698 -0.00000 -0.00014 0.00072 0.00057 -3.13641

D215 3.12426 0.00000 0.00013 -0.00010 0.00002 3.12428

D216 0.00415 -0.00000 -0.00023 0.00057 0.00033 0.00448

Item Value Threshold Converged?

Maximum Force 0.000714 0.000450 NO

RMS Force 0.000106 0.000300 YES

Maximum Displacement 0.093485 0.001800 NO

RMS Displacement 0.016009 0.001200 NO

Predicted change in Energy=-1.970969D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Aug 27 22:20:46 2019, MaxMem= 4294967296 cpu: 2.3

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

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=1 Diff= 1.87D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.757206 -4.149004 0.581433

2 6 0 1.169901 -2.859597 0.202765

3 7 0 0.031033 -2.117643 -0.006124

4 6 0 -1.087240 -2.892203 0.194396

5 6 0 -0.640426 -4.169244 0.575802

6 6 0 -2.447598 -2.464395 0.009042

7 6 0 -2.863128 -1.135615 -0.119468

8 7 0 -2.067592 -0.029733 0.055429

9 6 0 -2.894688 1.055361 -0.099587

10 6 0 -4.248008 0.619087 -0.438443

11 6 0 -4.228242 -0.732486 -0.451704

12 6 0 2.517976 -2.392821 0.024363

13 6 0 2.894808 -1.052880 -0.111726

14 6 0 4.247868 -0.612994 -0.446720

15 6 0 4.227978 0.738646 -0.446114

16 6 0 2.862858 1.138173 -0.109448

17 7 0 2.067564 0.030277 0.054454

18 6 0 2.446752 2.465504 0.028985

19 6 0 1.087399 2.894345 0.217304

20 6 0 0.640044 4.183676 0.555607

21 6 0 -0.757291 4.163404 0.561643

22 6 0 -1.169944 2.861664 0.226331

23 7 0 -0.030805 2.112314 0.045668

24 6 0 -2.517113 2.393846 0.045689

25 6 0 -3.466906 -3.541268 -0.026942

26 6 0 -3.361752 -4.592599 -0.950421

27 6 0 -4.324667 -5.595311 -0.995304

28 6 0 -5.398679 -5.577018 -0.105051

29 6 0 -5.505944 -4.545475 0.826367

30 6 0 -4.551052 -3.533112 0.862862

31 6 0 5.564074 -5.413878 -0.041699

32 6 0 4.498999 -5.472143 -0.940927

33 6 0 3.505424 -4.499134 -0.912554

34 6 0 3.570016 -3.438116 0.003489

35 6 0 4.645984 -3.389203 0.901891

36 6 0 5.631701 -4.372007 0.881943

37 6 0 -3.570521 3.438768 0.014686

38 6 0 -4.644023 3.399725 0.916008

39 6 0 -5.633538 4.378533 0.882823

40 6 0 -5.571681 5.406089 -0.057091

41 6 0 -4.508982 5.453996 -0.959621

42 6 0 -3.511894 4.484895 -0.918342

43 6 0 3.467514 3.541857 -0.016348

44 6 0 4.548785 3.542525 0.876485

45 6 0 5.507444 4.550992 0.828131

46 6 0 5.406347 5.569391 -0.118297

47 6 0 4.335213 5.578311 -1.012035

48 6 0 3.368828 4.579363 -0.955657

49 1 0 1.415200 -4.964180 0.835884

50 1 0 -1.276702 -5.003041 0.825167

51 1 0 -5.083439 1.264671 -0.661291

52 1 0 -5.044311 -1.397825 -0.687808

53 1 0 5.083040 -1.256361 -0.676939

54 1 0 5.044163 1.406299 -0.675093

55 1 0 1.275371 5.027347 0.771634

56 1 0 -1.414817 4.988433 0.783117

57 1 0 -2.531227 -4.609010 -1.646794

58 1 0 -4.236894 -6.392201 -1.726248

59 1 0 -6.145498 -6.363284 -0.136006

60 1 0 -6.332744 -4.529203 1.528599

61 1 0 -4.632345 -2.738133 1.595297

62 1 0 6.334797 -6.177145 -0.059810

63 1 0 4.442211 -6.277040 -1.666142

64 1 0 2.681990 -4.546449 -1.615903

65 1 0 4.696473 -2.586047 1.628174

66 1 0 6.451623 -4.324581 1.590800

67 1 0 -4.690812 2.606391 1.653339

68 1 0 -6.452211 4.338794 1.593591

69 1 0 -6.345477 6.165918 -0.085750

70 1 0 -4.456856 6.247319 -1.697839

71 1 0 -2.690761 4.523425 -1.624910

72 1 0 4.626012 2.756546 1.619094

73 1 0 6.332643 4.541597 1.532368

74 1 0 6.156184 6.352351 -0.158715

75 1 0 4.252483 6.364511 -1.755058

76 1 0 2.540987 4.587878 -1.655360

77 1 0 0.017856 -1.136773 -0.248149

78 1 0 -0.017178 1.117403 -0.132532

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

Rotational constants (GHZ): 0.0587828 0.0583030 0.0300966

Leave Link 202 at Tue Aug 27 22:20:46 2019, MaxMem= 4294967296 cpu: 0.0

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

Standard basis: 6-311G(d) (5D, 7F)

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

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5357.2765776070 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122339786 Hartrees.

Nuclear repulsion after empirical dispersion term = 5357.0643436284 Hartrees.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5773

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.12D-10

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 305

GePol: Fraction of low-weight points (<1% of avg) = 5.28%

GePol: Cavity surface area = 611.433 Ang\*\*2

GePol: Cavity volume = 627.994 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021067989 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5357.0622368295 Hartrees.

Leave Link 301 at Tue Aug 27 22:20:47 2019, MaxMem= 4294967296 cpu: 2.3

(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.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Tue Aug 27 22:20:48 2019, MaxMem= 4294967296 cpu: 27.8

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

DipDrv: MaxL=1.

Leave Link 303 at Tue Aug 27 22:20:49 2019, MaxMem= 4294967296 cpu: 2.3

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

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= 0.000000 0.000000 -0.000000

Rot= 0.999978 0.000138 0.000004 -0.006616 Ang= 0.76 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0183

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30453232690

Leave Link 401 at Tue Aug 27 22:20:54 2019, MaxMem= 4294967296 cpu: 81.5

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 590000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 99982587.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.55D-15 for 5758.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.33D-15 for 5747 2023.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.11D-15 for 5758.

Iteration 1 A^-1\*A deviation from orthogonality is 1.73D-08 for 5152 4565.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.22D-15 for 222.

Iteration 2 A\*A^-1 deviation from orthogonality is 1.98D-15 for 4725 2505.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 478.

Iteration 2 A^-1\*A deviation from orthogonality is 4.44D-16 for 5485 3289.

E= -1914.33209626882

DIIS: error= 8.74D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.33209626882 IErMin= 1 ErrMin= 8.74D-04

ErrMax= 8.74D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.70D-03 BMatP= 2.70D-03

IDIUse=3 WtCom= 9.91D-01 WtEn= 8.74D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.641 Goal= None Shift= 0.000

Gap= 0.706 Goal= None Shift= 0.000

RMSDP=6.16D-05 MaxDP=3.10D-03 OVMax= 5.86D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.16D-05 CP: 1.00D+00

E= -1914.33331960986 Delta-E= -0.001223341041 Rises=F Damp=F

DIIS: error= 8.92D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33331960986 IErMin= 2 ErrMin= 8.92D-05

ErrMax= 8.92D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.44D-05 BMatP= 2.70D-03

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

Coeff-Com: -0.572D-01 0.106D+01

Coeff: -0.572D-01 0.106D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.44D-06 MaxDP=3.63D-04 DE=-1.22D-03 OVMax= 2.64D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 6.73D-06 CP: 1.00D+00 1.05D+00

E= -1914.33333498890 Delta-E= -0.000015379037 Rises=F Damp=F

DIIS: error= 7.26D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33333498890 IErMin= 3 ErrMin= 7.26D-05

ErrMax= 7.26D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.84D-05 BMatP= 3.44D-05

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

Coeff-Com: -0.321D-01 0.472D+00 0.560D+00

Coeff: -0.321D-01 0.472D+00 0.560D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.29D-06 MaxDP=2.38D-04 DE=-1.54D-05 OVMax= 9.19D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.91D-06 CP: 1.00D+00 1.05D+00 7.74D-01

E= -1914.33333854579 Delta-E= -0.000003556891 Rises=F Damp=F

DIIS: error= 3.23D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33333854579 IErMin= 4 ErrMin= 3.23D-05

ErrMax= 3.23D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.24D-06 BMatP= 1.84D-05

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

Coeff-Com: -0.990D-02 0.113D+00 0.347D+00 0.550D+00

Coeff: -0.990D-02 0.113D+00 0.347D+00 0.550D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.73D-06 MaxDP=1.37D-04 DE=-3.56D-06 OVMax= 1.11D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.33D-06 CP: 1.00D+00 1.05D+00 9.05D-01 7.78D-01

E= -1914.33334002803 Delta-E= -0.000001482236 Rises=F Damp=F

DIIS: error= 1.68D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33334002803 IErMin= 5 ErrMin= 1.68D-05

ErrMax= 1.68D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.71D-07 BMatP= 5.24D-06

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

Coeff-Com: -0.188D-02 0.961D-02 0.119D+00 0.284D+00 0.590D+00

Coeff: -0.188D-02 0.961D-02 0.119D+00 0.284D+00 0.590D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.98D-07 MaxDP=5.16D-05 DE=-1.48D-06 OVMax= 6.32D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.00D-07 CP: 1.00D+00 1.06D+00 9.37D-01 9.30D-01 1.13D+00

E= -1914.33334027275 Delta-E= -0.000000244725 Rises=F Damp=F

DIIS: error= 1.36D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33334027275 IErMin= 6 ErrMin= 1.36D-05

ErrMax= 1.36D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.41D-07 BMatP= 4.71D-07

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

Coeff-Com: 0.145D-02-0.244D-01-0.206D-01 0.348D-01 0.352D+00 0.656D+00

Coeff: 0.145D-02-0.244D-01-0.206D-01 0.348D-01 0.352D+00 0.656D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.75D-07 MaxDP=6.71D-05 DE=-2.45D-07 OVMax= 8.05D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.43D-07 CP: 1.00D+00 1.06D+00 9.83D-01 1.01D+00 1.53D+00

CP: 1.39D+00

E= -1914.33334044141 Delta-E= -0.000000168663 Rises=F Damp=F

DIIS: error= 9.85D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33334044141 IErMin= 7 ErrMin= 9.85D-06

ErrMax= 9.85D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.52D-08 BMatP= 1.41D-07

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

Coeff-Com: 0.725D-03-0.811D-02-0.268D-01-0.304D-01-0.298D-01 0.215D+00

Coeff-Com: 0.879D+00

Coeff: 0.725D-03-0.811D-02-0.268D-01-0.304D-01-0.298D-01 0.215D+00

Coeff: 0.879D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.19D-07 MaxDP=5.82D-05 DE=-1.69D-07 OVMax= 7.47D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.42D-07 CP: 1.00D+00 1.06D+00 1.02D+00 1.10D+00 1.87D+00

CP: 2.02D+00 1.57D+00

E= -1914.33334055239 Delta-E= -0.000000110979 Rises=F Damp=F

DIIS: error= 8.37D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33334055239 IErMin= 8 ErrMin= 8.37D-06

ErrMax= 8.37D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.80D-08 BMatP= 4.52D-08

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

Coeff-Com: -0.102D-02 0.220D-01-0.456D-02-0.664D-01-0.499D+00-0.565D+00

Coeff-Com: 0.857D+00 0.126D+01

Coeff: -0.102D-02 0.220D-01-0.456D-02-0.664D-01-0.499D+00-0.565D+00

Coeff: 0.857D+00 0.126D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.57D-06 MaxDP=1.32D-04 DE=-1.11D-07 OVMax= 1.70D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.74D-07 CP: 1.00D+00 1.06D+00 1.09D+00 1.28D+00 2.62D+00

CP: 3.00D+00 3.00D+00 1.66D+00

E= -1914.33334068900 Delta-E= -0.000000136607 Rises=F Damp=F

DIIS: error= 2.85D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33334068900 IErMin= 9 ErrMin= 2.85D-06

ErrMax= 2.85D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.25D-09 BMatP= 2.80D-08

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

Coeff-Com: -0.602D-03 0.112D-01 0.344D-02-0.167D-01-0.210D+00-0.286D+00

Coeff-Com: 0.110D+00 0.634D+00 0.754D+00

Coeff: -0.602D-03 0.112D-01 0.344D-02-0.167D-01-0.210D+00-0.286D+00

Coeff: 0.110D+00 0.634D+00 0.754D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.64D-07 MaxDP=3.68D-05 DE=-1.37D-07 OVMax= 5.03D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.79D-07 CP: 1.00D+00 1.06D+00 1.11D+00 1.33D+00 2.83D+00

CP: 3.00D+00 3.00D+00 2.25D+00 1.88D+00

E= -1914.33334070454 Delta-E= -0.000000015541 Rises=F Damp=F

DIIS: error= 1.41D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33334070454 IErMin=10 ErrMin= 1.41D-06

ErrMax= 1.41D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.66D-09 BMatP= 8.25D-09

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

Coeff-Com: 0.587D-04-0.256D-02 0.394D-02 0.224D-01 0.897D-01 0.726D-01

Coeff-Com: -0.355D+00-0.855D-01 0.515D+00 0.740D+00

Coeff: 0.587D-04-0.256D-02 0.394D-02 0.224D-01 0.897D-01 0.726D-01

Coeff: -0.355D+00-0.855D-01 0.515D+00 0.740D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.26D-07 MaxDP=1.93D-05 DE=-1.55D-08 OVMax= 2.50D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.70D-08 CP: 1.00D+00 1.06D+00 1.11D+00 1.35D+00 2.92D+00

CP: 3.00D+00 3.00D+00 2.54D+00 2.43D+00 1.29D+00

E= -1914.33334070918 Delta-E= -0.000000004640 Rises=F Damp=F

DIIS: error= 7.27D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33334070918 IErMin=11 ErrMin= 7.27D-07

ErrMax= 7.27D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.42D-10 BMatP= 3.66D-09

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

Coeff-Com: 0.176D-03-0.394D-02 0.176D-03 0.147D-01 0.920D-01 0.105D+00

Coeff-Com: -0.205D+00-0.173D+00 0.244D-01 0.317D+00 0.829D+00

Coeff: 0.176D-03-0.394D-02 0.176D-03 0.147D-01 0.920D-01 0.105D+00

Coeff: -0.205D+00-0.173D+00 0.244D-01 0.317D+00 0.829D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.05D-07 MaxDP=9.62D-06 DE=-4.64D-09 OVMax= 1.11D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.16D-08 CP: 1.00D+00 1.06D+00 1.12D+00 1.36D+00 2.96D+00

CP: 3.00D+00 3.00D+00 2.75D+00 2.67D+00 1.44D+00

CP: 1.28D+00

E= -1914.33334071040 Delta-E= -0.000000001216 Rises=F Damp=F

DIIS: error= 3.86D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.33334071040 IErMin=12 ErrMin= 3.86D-07

ErrMax= 3.86D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.19D-10 BMatP= 7.42D-10

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

Coeff-Com: 0.793D-04-0.127D-02-0.170D-02 0.427D-03 0.188D-01 0.348D-01

Coeff-Com: 0.121D-01-0.519D-01-0.187D+00-0.110D+00 0.490D+00 0.796D+00

Coeff: 0.793D-04-0.127D-02-0.170D-02 0.427D-03 0.188D-01 0.348D-01

Coeff: 0.121D-01-0.519D-01-0.187D+00-0.110D+00 0.490D+00 0.796D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.68D-08 MaxDP=4.14D-06 DE=-1.22D-09 OVMax= 4.23D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.70D-08 CP: 1.00D+00 1.06D+00 1.12D+00 1.36D+00 2.97D+00

CP: 3.00D+00 3.00D+00 2.84D+00 2.78D+00 1.48D+00

CP: 1.61D+00 1.40D+00

E= -1914.33334071078 Delta-E= -0.000000000384 Rises=F Damp=F

DIIS: error= 1.59D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.33334071078 IErMin=13 ErrMin= 1.59D-07

ErrMax= 1.59D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.27D-11 BMatP= 3.19D-10

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

Coeff-Com: -0.924D-05 0.471D-03-0.106D-02-0.386D-02-0.169D-01-0.127D-01

Coeff-Com: 0.606D-01 0.272D-01-0.109D+00-0.146D+00 0.294D-01 0.418D+00

Coeff-Com: 0.753D+00

Coeff: -0.924D-05 0.471D-03-0.106D-02-0.386D-02-0.169D-01-0.127D-01

Coeff: 0.606D-01 0.272D-01-0.109D+00-0.146D+00 0.294D-01 0.418D+00

Coeff: 0.753D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.67D-08 MaxDP=2.58D-06 DE=-3.84D-10 OVMax= 2.72D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 6.54D-09 CP: 1.00D+00 1.06D+00 1.12D+00 1.36D+00 2.98D+00

CP: 3.00D+00 3.00D+00 2.88D+00 2.85D+00 1.51D+00

CP: 1.73D+00 1.67D+00 1.16D+00

E= -1914.33334071083 Delta-E= -0.000000000052 Rises=F Damp=F

DIIS: error= 9.89D-08 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.33334071083 IErMin=14 ErrMin= 9.89D-08

ErrMax= 9.89D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.25D-11 BMatP= 8.27D-11

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

Coeff-Com: -0.282D-04 0.620D-03-0.106D-04-0.195D-02-0.144D-01-0.171D-01

Coeff-Com: 0.253D-01 0.309D-01 0.108D-02-0.396D-01-0.140D+00-0.262D-01

Coeff-Com: 0.396D+00 0.785D+00

Coeff: -0.282D-04 0.620D-03-0.106D-04-0.195D-02-0.144D-01-0.171D-01

Coeff: 0.253D-01 0.309D-01 0.108D-02-0.396D-01-0.140D+00-0.262D-01

Coeff: 0.396D+00 0.785D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.40D-08 MaxDP=1.33D-06 DE=-5.18D-11 OVMax= 1.45D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 4.04D-09 CP: 1.00D+00 1.06D+00 1.12D+00 1.36D+00 2.98D+00

CP: 3.00D+00 3.00D+00 2.90D+00 2.87D+00 1.53D+00

CP: 1.80D+00 1.78D+00 1.28D+00 1.22D+00

E= -1914.33334071086 Delta-E= -0.000000000032 Rises=F Damp=F

DIIS: error= 4.68D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.33334071086 IErMin=15 ErrMin= 4.68D-08

ErrMax= 4.68D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.19D-12 BMatP= 2.25D-11

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

Coeff-Com: -0.826D-05 0.108D-03 0.301D-03 0.306D-03-0.108D-02-0.320D-02

Coeff-Com: -0.686D-02 0.513D-02 0.289D-01 0.251D-01-0.629D-01-0.120D+00

Coeff-Com: -0.451D-01 0.305D+00 0.875D+00

Coeff: -0.826D-05 0.108D-03 0.301D-03 0.306D-03-0.108D-02-0.320D-02

Coeff: -0.686D-02 0.513D-02 0.289D-01 0.251D-01-0.629D-01-0.120D+00

Coeff: -0.451D-01 0.305D+00 0.875D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.94D-09 MaxDP=5.83D-07 DE=-3.18D-11 OVMax= 5.91D-06

Error on total polarization charges = 0.08258

SCF Done: E(UB3LYP) = -1914.33334071 A.U. after 15 cycles

NFock= 15 Conv=0.59D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0183

<L.S>= 0.000000000000E+00

KE= 1.906377885167D+03 PE=-1.516373795754D+04 EE= 5.985964494830D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0551, after 2.0017

Leave Link 502 at Tue Aug 27 22:27:43 2019, MaxMem= 4294967296 cpu: 6468.3

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

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

Range of M.O.s used for correlation: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.10470005D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48658331D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64386619D-01

Leave Link 801 at Tue Aug 27 22:27:43 2019, MaxMem= 4294967296 cpu: 1.0

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

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

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

Leave Link 1101 at Tue Aug 27 22:27:50 2019, MaxMem= 4294967296 cpu: 110.0

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

Symmetrizing basis deriv contribution to polar:

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

Leave Link 1102 at Tue Aug 27 22:27:50 2019, MaxMem= 4294967296 cpu: 2.0

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

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 188

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 27 22:47:23 2019, MaxMem= 4294967296 cpu: 18770.3

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

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 590000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.44D+03 4.54D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.56D+02 3.73D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.63D+00 4.69D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.03D-01 3.95D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.64D-04 2.11D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.62D-06 1.35D-04.

191 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 2.00D-08 1.01D-05.

84 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.30D-11 6.29D-07.

47 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.27D-13 3.95D-08.

6 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 1.14D-14 5.58D-09.

3 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 4.47D-15 2.04D-09.

3 vectors produced by pass 11 Test12= 2.55D-13 1.00D-09 XBig12= 6.31D-15 2.50D-09.

3 vectors produced by pass 12 Test12= 2.55D-13 1.00D-09 XBig12= 3.14D-15 2.48D-09.

3 vectors produced by pass 13 Test12= 2.55D-13 1.00D-09 XBig12= 3.57D-15 1.83D-09.

3 vectors produced by pass 14 Test12= 2.55D-13 1.00D-09 XBig12= 7.15D-15 1.98D-09.

3 vectors produced by pass 15 Test12= 2.55D-13 1.00D-09 XBig12= 8.97D-15 2.53D-09.

3 vectors produced by pass 16 Test12= 2.55D-13 1.00D-09 XBig12= 8.77D-15 2.66D-09.

2 vectors produced by pass 17 Test12= 2.55D-13 1.00D-09 XBig12= 5.88D-15 2.52D-09.

InvSVY: IOpt=1 It= 1 EMax= 7.11D-14

Solved reduced A of dimension 1758 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1127.66 Bohr\*\*3.

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

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

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

Leave Link 1002 at Wed Aug 28 02:41:02 2019, MaxMem= 4294967296 cpu: 224231.5

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 188

Leave Link 701 at Wed Aug 28 02:42:31 2019, MaxMem= 4294967296 cpu: 1425.8

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

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

Leave Link 702 at Wed Aug 28 02:42:31 2019, MaxMem= 4294967296 cpu: 0.0

(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=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

Leave Link 703 at Wed Aug 28 03:01:59 2019, MaxMem= 4294967296 cpu: 18673.8

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

Dipole = 2.01812143D-04-2.51181116D-02-5.10448684D-01

Polarizability= 1.25652100D+03-5.93322988D+00 1.67393500D+03

-3.77550587D-04 1.24771365D-01 4.52527723D+02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000015545 -0.000019683 0.000001079

2 6 0.000001171 0.000062904 0.000001196

3 7 -0.000027227 -0.000072269 0.000034012

4 6 0.000025477 0.000040740 -0.000000148

5 6 0.000002603 -0.000009869 -0.000008109

6 6 0.000005189 0.000002523 -0.000003560

7 6 -0.000005710 -0.000032196 -0.000006814

8 7 -0.000060503 -0.000043906 -0.000001187

9 6 0.000000142 0.000024402 0.000008959

10 6 0.000008346 -0.000001610 -0.000016408

11 6 0.000007067 0.000003937 0.000011929

12 6 0.000001229 -0.000007418 -0.000006614

13 6 -0.000002608 -0.000034642 -0.000008449

14 6 -0.000007662 -0.000006085 0.000019398

15 6 -0.000009997 0.000009123 -0.000012259

16 6 0.000001947 0.000028567 0.000002982

17 7 0.000031092 -0.000011481 0.000031434

18 6 -0.000014376 -0.000001902 0.000001882

19 6 0.000008237 -0.000059000 0.000009240

20 6 -0.000010495 0.000016730 0.000010657

21 6 0.000010199 0.000005876 0.000001241

22 6 0.000015748 -0.000042829 -0.000012613

23 7 0.000001825 0.000068748 -0.000021361

24 6 -0.000005859 0.000000073 0.000010390

25 6 0.000011391 -0.000004067 0.000028015

26 6 -0.000027728 0.000020672 -0.000034754

27 6 0.000013972 -0.000007894 0.000027007

28 6 -0.000016891 0.000014858 -0.000005719

29 6 0.000032391 -0.000019505 0.000018065

30 6 -0.000031116 0.000031938 -0.000024512

31 6 0.000010046 -0.000008682 -0.000000753

32 6 -0.000011455 0.000010707 0.000031037

33 6 0.000047830 -0.000017293 -0.000035579

34 6 -0.000025006 0.000039002 0.000017538

35 6 0.000020794 -0.000001976 -0.000029858

36 6 -0.000037697 0.000018609 0.000016431

37 6 0.000012825 0.000004068 -0.000011220

38 6 -0.000028556 -0.000019178 0.000036523

39 6 0.000038921 0.000013131 -0.000018854

40 6 -0.000013623 -0.000016513 0.000002101

41 6 0.000004211 -0.000003072 -0.000026337

42 6 -0.000028085 0.000005505 0.000014739

43 6 -0.000022491 -0.000023542 -0.000029098

44 6 0.000019659 0.000013451 0.000009303

45 6 -0.000032035 -0.000022424 -0.000014801

46 6 0.000017915 0.000005775 0.000001306

47 6 -0.000010752 -0.000010254 -0.000021782

48 6 0.000045040 0.000016730 0.000039402

49 1 0.000005969 0.000013632 -0.000006696

50 1 -0.000006626 -0.000013248 0.000001650

51 1 -0.000007890 0.000000833 -0.000001652

52 1 -0.000008447 -0.000001471 -0.000002811

53 1 0.000006499 0.000008167 0.000000025

54 1 0.000007605 -0.000009148 0.000004133

55 1 -0.000001796 -0.000012685 -0.000001390

56 1 0.000002095 0.000005647 0.000009587

57 1 0.000009604 0.000008718 -0.000004347

58 1 -0.000002513 0.000005267 -0.000004393

59 1 0.000003278 0.000002217 0.000005757

60 1 -0.000001426 0.000005156 -0.000000891

61 1 0.000001398 -0.000002216 -0.000006006

62 1 -0.000001661 0.000006003 0.000002878

63 1 0.000000141 0.000002299 -0.000002803

64 1 -0.000009496 0.000000358 -0.000001797

65 1 0.000007896 0.000000411 -0.000000245

66 1 0.000003885 -0.000000542 -0.000001716

67 1 -0.000002871 -0.000000525 -0.000001154

68 1 -0.000000834 -0.000005217 0.000000752

69 1 0.000002319 -0.000002243 -0.000002660

70 1 -0.000001173 -0.000004888 0.000002371

71 1 0.000003984 -0.000006716 0.000002889

72 1 0.000002162 -0.000005495 0.000009792

73 1 0.000004589 -0.000000298 0.000000884

74 1 -0.000002937 -0.000005426 -0.000004549

75 1 -0.000001038 -0.000003735 0.000003493

76 1 -0.000013976 0.000001572 0.000004508

77 1 -0.000007831 -0.000081512 -0.000003327

78 1 0.000059241 0.000134307 -0.000037360

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

Cartesian Forces: Max 0.000134307 RMS 0.000021480

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

Leave Link 716 at Wed Aug 28 03:01:59 2019, MaxMem= 4294967296 cpu: 1.8

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000112790 RMS 0.000026174

Search for a local minimum.

Step number 13 out of a maximum of 452

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

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -8.78D-06 DEPred=-1.97D-05 R= 4.46D-01

Trust test= 4.46D-01 RLast= 7.97D-02 DXMaxT set to 1.00D-01

ITU= 0 -1 1 1 -1 1 -1 -1 1 1 -1 1 0

Eigenvalues --- 0.00030 0.00503 0.00564 0.00622 0.00754

Eigenvalues --- 0.00873 0.01015 0.01034 0.01042 0.01118

Eigenvalues --- 0.01133 0.01217 0.01254 0.01286 0.01301

Eigenvalues --- 0.01310 0.01343 0.01421 0.01450 0.01471

Eigenvalues --- 0.01491 0.01517 0.01538 0.01643 0.01721

Eigenvalues --- 0.01727 0.01737 0.01743 0.01751 0.01756

Eigenvalues --- 0.01770 0.01787 0.01807 0.01828 0.01889

Eigenvalues --- 0.01933 0.01958 0.01981 0.02026 0.02151

Eigenvalues --- 0.02225 0.02252 0.02277 0.02300 0.02327

Eigenvalues --- 0.02333 0.02436 0.02448 0.02541 0.02552

Eigenvalues --- 0.02554 0.02597 0.02602 0.02604 0.02609

Eigenvalues --- 0.02615 0.02668 0.02740 0.02749 0.02774

Eigenvalues --- 0.02825 0.02865 0.02868 0.02871 0.02875

Eigenvalues --- 0.03061 0.03079 0.04059 0.04084 0.04204

Eigenvalues --- 0.04324 0.04382 0.04438 0.04517 0.04534

Eigenvalues --- 0.08558 0.09705 0.09714 0.09881 0.09908

Eigenvalues --- 0.09933 0.10334 0.10456 0.10601 0.10690

Eigenvalues --- 0.10693 0.10708 0.10708 0.10740 0.11079

Eigenvalues --- 0.11389 0.11399 0.11414 0.11422 0.11998

Eigenvalues --- 0.12008 0.12015 0.12024 0.12270 0.12270

Eigenvalues --- 0.12285 0.12288 0.12764 0.12775 0.12784

Eigenvalues --- 0.12793 0.15715 0.15971 0.16282 0.17077

Eigenvalues --- 0.17224 0.17337 0.17510 0.17785 0.17972

Eigenvalues --- 0.18079 0.18110 0.18616 0.19250 0.19287

Eigenvalues --- 0.19341 0.19350 0.19370 0.19391 0.19403

Eigenvalues --- 0.19464 0.19548 0.19550 0.19554 0.19556

Eigenvalues --- 0.20281 0.21511 0.22044 0.22871 0.22888

Eigenvalues --- 0.23406 0.23728 0.24308 0.24716 0.25675

Eigenvalues --- 0.26237 0.26565 0.26609 0.27195 0.28486

Eigenvalues --- 0.28525 0.28648 0.28889 0.29700 0.30979

Eigenvalues --- 0.31681 0.32004 0.32804 0.33112 0.33324

Eigenvalues --- 0.33574 0.34227 0.35122 0.35588 0.35619

Eigenvalues --- 0.35625 0.35634 0.35645 0.35711 0.35750

Eigenvalues --- 0.35765 0.35818 0.35845 0.35919 0.35925

Eigenvalues --- 0.35928 0.35930 0.36005 0.36017 0.36022

Eigenvalues --- 0.36026 0.36210 0.36261 0.36274 0.36287

Eigenvalues --- 0.37073 0.37085 0.37252 0.37389 0.37410

Eigenvalues --- 0.37558 0.38147 0.38551 0.38591 0.38737

Eigenvalues --- 0.39516 0.40509 0.40723 0.41010 0.41019

Eigenvalues --- 0.41084 0.41115 0.41125 0.41168 0.41406

Eigenvalues --- 0.41559 0.41830 0.42297 0.42993 0.44737

Eigenvalues --- 0.45433 0.45892 0.45920 0.45925 0.45978

Eigenvalues --- 0.46226 0.46236 0.46262 0.46264 0.46283

Eigenvalues --- 0.48459 0.48622 0.49070 0.49284 0.50684

Eigenvalues --- 0.50752 0.50754 0.50781 0.50868 0.51880

Eigenvalues --- 0.52597 0.57102 0.58731

DIIS coeff's: 0.30328 0.25179 0.20775 0.06340 -0.02607

DIIS coeff's: -0.07119 0.09043 0.09158 0.10211 -0.01567

DIIS coeff's: 0.00360 0.01411 -0.01511

Cosine: 0.823 > 0.500

Length: 1.830

GDIIS step was calculated using 13 of the last 13 vectors.

Iteration 1 RMS(Cart)= 0.01058421 RMS(Int)= 0.00003369

Iteration 2 RMS(Cart)= 0.00005300 RMS(Int)= 0.00001620

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001620

ITry= 1 IFail=0 DXMaxC= 7.84D-02 DCOld= 1.00D+10 DXMaxT= 1.00D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.65658 -0.00000 0.00030 0.00006 0.00035 2.65693

R2 2.64144 0.00000 -0.00007 0.00003 -0.00006 2.64138

R3 2.03724 -0.00000 -0.00007 0.00002 -0.00005 2.03719

R4 2.59873 -0.00000 0.00021 -0.00012 0.00011 2.59884

R5 2.71688 -0.00001 -0.00026 0.00001 -0.00024 2.71664

R6 2.59842 0.00001 0.00015 0.00002 0.00018 2.59859

R7 1.90933 -0.00001 0.00029 -0.00010 0.00018 1.90951

R8 2.65636 0.00000 -0.00004 -0.00003 -0.00008 2.65628

R9 2.71750 0.00003 0.00022 -0.00002 0.00020 2.71770

R10 2.03727 -0.00000 -0.00008 0.00002 -0.00006 2.03720

R11 2.64213 0.00002 -0.00124 0.00020 -0.00105 2.64108

R12 2.80288 -0.00000 0.00058 -0.00000 0.00058 2.80346

R13 2.59550 0.00001 0.00085 0.00018 0.00105 2.59654

R14 2.76212 0.00001 -0.00016 0.00015 -0.00001 2.76211

R15 2.59488 -0.00003 -0.00127 0.00022 -0.00103 2.59385

R16 2.76226 -0.00000 0.00010 0.00013 0.00022 2.76248

R17 2.64238 -0.00005 0.00090 0.00017 0.00107 2.64345

R18 2.55450 -0.00000 0.00012 -0.00019 -0.00009 2.55441

R19 2.03914 0.00001 -0.00003 0.00003 -0.00001 2.03913

R20 2.03915 -0.00000 0.00000 -0.00000 -0.00000 2.03914

R21 2.64289 -0.00003 0.00058 0.00019 0.00076 2.64366

R22 2.80283 0.00000 0.00035 0.00003 0.00038 2.80321

R23 2.76216 0.00001 0.00015 0.00018 0.00032 2.76248

R24 2.59463 -0.00005 -0.00110 0.00018 -0.00090 2.59373

R25 2.55451 0.00001 0.00011 -0.00018 -0.00009 2.55441

R26 2.03918 0.00001 -0.00006 0.00002 -0.00004 2.03915

R27 2.76218 0.00000 -0.00018 0.00012 -0.00006 2.76212

R28 2.03911 -0.00000 0.00002 0.00000 0.00002 2.03913

R29 2.59574 -0.00002 0.00070 0.00016 0.00088 2.59661

R30 2.64164 -0.00001 -0.00095 0.00017 -0.00079 2.64086

R31 2.71701 0.00001 0.00052 -0.00005 0.00047 2.71747

R32 2.80454 -0.00001 -0.00041 0.00002 -0.00039 2.80414

R33 2.65703 0.00000 -0.00044 -0.00002 -0.00047 2.65656

R34 2.59892 0.00009 -0.00018 0.00008 -0.00009 2.59882

R35 2.64088 -0.00003 0.00027 0.00002 0.00027 2.64115

R36 2.03713 0.00000 0.00000 0.00002 0.00002 2.03715

R37 2.65723 -0.00002 -0.00007 0.00001 -0.00006 2.65717

R38 2.03711 -0.00001 0.00001 0.00002 0.00002 2.03713

R39 2.59918 0.00004 -0.00006 -0.00009 -0.00014 2.59904

R40 2.71644 -0.00004 -0.00000 -0.00001 -0.00001 2.71644

R41 1.91020 0.00008 -0.00026 -0.00005 -0.00031 1.90990

R42 2.80450 0.00001 -0.00065 0.00002 -0.00063 2.80387

R43 2.65180 0.00001 -0.00018 0.00005 -0.00013 2.65166

R44 2.65046 0.00001 -0.00030 0.00002 -0.00028 2.65019

R45 2.62845 -0.00002 0.00006 -0.00000 0.00006 2.62851

R46 2.04839 0.00000 0.00002 0.00000 0.00002 2.04842

R47 2.63641 -0.00001 -0.00003 -0.00001 -0.00004 2.63637

R48 2.05017 0.00000 -0.00002 0.00002 0.00000 2.05017

R49 2.63420 -0.00000 -0.00003 -0.00001 -0.00004 2.63417

R50 2.05008 -0.00000 -0.00002 0.00001 -0.00001 2.05007

R51 2.63075 0.00001 0.00010 -0.00001 0.00009 2.63083

R52 2.05015 -0.00000 -0.00004 0.00002 -0.00002 2.05013

R53 2.04847 0.00000 -0.00001 0.00000 -0.00001 2.04846

R54 2.63641 0.00001 -0.00006 0.00001 -0.00005 2.63636

R55 2.63424 -0.00000 -0.00000 0.00001 0.00001 2.63425

R56 2.05009 0.00000 -0.00002 0.00001 -0.00001 2.05008

R57 2.62852 0.00002 0.00010 0.00003 0.00013 2.62865

R58 2.05018 0.00000 -0.00002 0.00001 -0.00001 2.05017

R59 2.65173 0.00002 -0.00005 -0.00001 -0.00006 2.65166

R60 2.04840 -0.00000 -0.00003 0.00002 -0.00001 2.04839

R61 2.65049 -0.00002 -0.00007 -0.00003 -0.00010 2.65039

R62 2.63069 -0.00001 0.00002 -0.00002 -0.00000 2.63068

R63 2.04850 -0.00000 0.00000 0.00001 0.00001 2.04851

R64 2.05016 0.00000 -0.00002 0.00002 -0.00001 2.05015

R65 2.64987 -0.00001 0.00030 -0.00003 0.00027 2.65014

R66 2.65125 0.00002 0.00023 -0.00001 0.00022 2.65147

R67 2.63093 -0.00002 -0.00013 -0.00002 -0.00015 2.63079

R68 2.04861 -0.00000 -0.00007 0.00001 -0.00006 2.04856

R69 2.63421 -0.00000 0.00002 0.00001 0.00003 2.63424

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R71 2.63628 0.00001 0.00002 0.00001 0.00003 2.63631

R72 2.05009 0.00000 -0.00002 0.00001 -0.00001 2.05008

R73 2.62872 0.00003 -0.00003 0.00004 0.00001 2.62873

R74 2.05020 -0.00000 -0.00003 0.00001 -0.00002 2.05018

R75 2.04840 -0.00000 -0.00002 0.00002 -0.00000 2.04840

R76 2.64986 0.00001 0.00005 0.00002 0.00007 2.64994

R77 2.65132 -0.00001 0.00010 0.00002 0.00012 2.65144

R78 2.63098 0.00000 -0.00004 -0.00001 -0.00005 2.63093

R79 2.04859 0.00000 -0.00008 0.00001 -0.00007 2.04852

R80 2.63417 -0.00001 -0.00001 -0.00001 -0.00002 2.63416

R81 2.05015 -0.00000 -0.00003 0.00002 -0.00001 2.05013

R82 2.63627 -0.00001 0.00005 -0.00001 0.00004 2.63631

R83 2.05008 -0.00000 -0.00002 0.00001 -0.00001 2.05007

R84 2.62867 -0.00001 -0.00007 0.00001 -0.00006 2.62861

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R86 2.04839 -0.00000 0.00002 0.00000 0.00003 2.04842

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A2 2.18700 0.00001 0.00046 -0.00012 0.00033 2.18733

A3 2.21465 -0.00001 -0.00048 0.00015 -0.00033 2.21432

A4 1.86780 -0.00000 -0.00008 -0.00004 -0.00012 1.86768

A5 2.22241 0.00003 -0.00007 0.00016 0.00004 2.22245

A6 2.19260 -0.00003 0.00005 -0.00013 -0.00001 2.19259

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A8 2.17847 -0.00000 0.00001 -0.00002 0.00002 2.17849

A9 2.17874 -0.00001 -0.00027 -0.00005 -0.00029 2.17845

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A12 2.22174 -0.00003 -0.00008 0.00006 -0.00007 2.22167

A13 1.88154 0.00001 0.00002 0.00003 0.00005 1.88159

A14 2.21479 -0.00000 -0.00059 0.00023 -0.00037 2.21442

A15 2.18682 -0.00000 0.00059 -0.00026 0.00033 2.18714

A16 2.18429 0.00008 0.00086 0.00003 0.00098 2.18526

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A18 2.07549 -0.00001 -0.00082 0.00003 -0.00083 2.07467

A19 2.19121 0.00004 0.00009 0.00009 0.00024 2.19145

A20 2.16588 -0.00003 0.00013 -0.00005 0.00003 2.16591

A21 1.92605 -0.00001 -0.00024 -0.00004 -0.00026 1.92579

A22 1.84731 -0.00001 0.00010 -0.00008 0.00001 1.84732

A23 1.92621 0.00003 0.00024 -0.00001 0.00024 1.92645

A24 2.19204 -0.00007 -0.00006 0.00007 0.00008 2.19212

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A26 1.86205 -0.00002 -0.00003 0.00003 0.00001 1.86206

A27 2.19704 0.00000 -0.00005 -0.00006 -0.00012 2.19693

A28 2.22368 0.00001 0.00008 0.00002 0.00010 2.22379

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A31 2.22381 -0.00001 -0.00003 -0.00001 -0.00004 2.22377

A32 2.18435 -0.00005 0.00049 -0.00006 0.00052 2.18487

A33 2.02419 0.00009 0.00052 0.00023 0.00072 2.02491

A34 2.07457 -0.00004 -0.00100 -0.00017 -0.00121 2.07336

A35 2.16525 0.00003 -0.00037 -0.00004 -0.00047 2.16478

A36 2.19162 -0.00003 0.00018 0.00008 0.00032 2.19194

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A38 1.86209 -0.00001 -0.00005 0.00003 -0.00001 1.86208

A39 2.19681 0.00000 0.00009 -0.00005 0.00005 2.19685

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A42 2.22364 -0.00000 0.00006 0.00002 0.00008 2.22372

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A44 1.92597 -0.00000 -0.00019 -0.00003 -0.00021 1.92577

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A46 2.19160 -0.00003 -0.00010 0.00001 -0.00003 2.19157

A47 1.84731 0.00001 0.00010 -0.00005 0.00003 1.84734

A48 2.18659 0.00004 -0.00049 -0.00000 -0.00040 2.18619

A49 2.07246 0.00001 0.00099 -0.00000 0.00095 2.07341

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A56 2.21402 -0.00001 -0.00012 0.00020 0.00007 2.21409

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A62 2.19243 -0.00003 0.00014 -0.00016 0.00004 2.19247

A63 1.92538 -0.00005 0.00009 0.00004 0.00011 1.92549

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A65 2.17797 -0.00001 0.00033 -0.00016 0.00019 2.17816

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A71 2.07120 -0.00001 0.00027 -0.00007 0.00021 2.07141

A72 2.10535 0.00002 -0.00016 0.00004 -0.00012 2.10523

A73 2.08465 0.00001 0.00019 0.00001 0.00019 2.08484

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A75 2.09775 -0.00001 -0.00000 0.00000 0.00000 2.09775

A76 2.08892 0.00000 -0.00002 -0.00000 -0.00002 2.08890

A77 2.09652 0.00000 0.00003 -0.00000 0.00002 2.09654

A78 2.08900 0.00000 0.00005 -0.00003 0.00002 2.08902

A79 2.09699 -0.00001 -0.00006 0.00001 -0.00004 2.09695

A80 2.09720 0.00000 0.00000 0.00002 0.00002 2.09722

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A104 2.08853 0.00000 0.00004 0.00001 0.00005 2.08858

A105 2.10640 -0.00008 -0.00033 -0.00032 -0.00065 2.10575

A106 2.10509 0.00009 0.00062 0.00026 0.00089 2.10598

A107 2.07169 -0.00000 -0.00030 0.00006 -0.00023 2.07146

A108 2.10507 0.00002 0.00019 0.00004 0.00023 2.10529

A109 2.08357 -0.00001 0.00021 -0.00017 0.00004 2.08361

A110 2.09443 -0.00001 -0.00041 0.00013 -0.00028 2.09415

A111 2.09761 -0.00001 -0.00000 -0.00007 -0.00007 2.09755

A112 2.08859 0.00000 -0.00000 0.00001 0.00001 2.08860

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A114 2.08902 -0.00000 -0.00004 0.00002 -0.00002 2.08900

A115 2.09723 -0.00000 -0.00001 0.00002 0.00002 2.09725

A116 2.09693 0.00000 0.00005 -0.00004 0.00000 2.09693

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D2 -3.09856 0.00003 0.00400 0.00037 0.00437 -3.09419

D3 -3.11860 0.00001 -0.00088 -0.00006 -0.00094 -3.11955

D4 0.05111 0.00000 0.00248 -0.00001 0.00247 0.05358

D5 -0.00054 -0.00000 -0.00033 -0.00004 -0.00037 -0.00091

D6 -3.13317 -0.00002 -0.00188 0.00011 -0.00177 -3.13494

D7 3.13282 0.00002 0.00122 0.00035 0.00157 3.13439

D8 0.00018 0.00001 -0.00033 0.00050 0.00017 0.00036

D9 -0.02431 -0.00006 -0.00072 -0.00049 -0.00121 -0.02552

D10 3.09077 -0.00004 -0.01147 0.00057 -0.01089 3.07988

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D14 0.20341 -0.00003 -0.01221 -0.00039 -0.01261 0.19080

D15 0.24978 -0.00006 -0.01098 -0.00084 -0.01181 0.23796

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D18 -3.09236 0.00006 0.00319 0.00050 0.00371 -3.08865

D19 -3.09110 0.00003 0.01127 -0.00060 0.01066 -3.08044

D20 0.07575 0.00003 0.01394 -0.00057 0.01338 0.08913

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D23 3.10175 -0.00003 -0.00285 -0.00029 -0.00314 3.09861

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D43 -0.04197 0.00002 0.00013 -0.00004 0.00010 -0.04187

D44 3.09633 -0.00000 -0.00074 -0.00028 -0.00103 3.09530

D45 0.02561 -0.00002 -0.00015 0.00000 -0.00015 0.02547

D46 -3.08718 -0.00001 -0.00031 0.00029 -0.00002 -3.08720

D47 -3.11275 -0.00000 0.00071 0.00025 0.00096 -3.11179

D48 0.05765 0.00001 0.00055 0.00053 0.00108 0.05873

D49 0.13508 0.00003 0.00163 0.00076 0.00239 0.13747

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D51 -3.01024 0.00001 0.00063 0.00048 0.00112 -3.00912

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D53 0.00120 0.00001 0.00011 0.00003 0.00014 0.00134

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D57 -3.01185 -0.00002 0.00166 0.00004 0.00170 -3.01015

D58 0.13749 -0.00004 0.00034 0.00010 0.00045 0.13794

D59 0.14339 -0.00004 -0.00113 -0.00048 -0.00162 0.14177

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D62 -2.15686 -0.00002 0.00285 -0.00016 0.00269 -2.15417

D63 -2.17381 -0.00000 0.00617 0.00069 0.00686 -2.16696

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D69 3.09260 0.00002 0.00148 -0.00029 0.00118 3.09378

D70 -0.04215 -0.00000 0.00031 -0.00023 0.00008 -0.04207

D71 0.00095 -0.00002 0.00026 -0.00009 0.00017 0.00112

D72 -3.11256 -0.00001 0.00020 -0.00017 0.00003 -3.11253

D73 3.11268 -0.00001 0.00065 -0.00030 0.00036 3.11304

D74 -0.00083 -0.00001 0.00059 -0.00038 0.00022 -0.00061

D75 -0.02753 0.00002 -0.00007 -0.00005 -0.00012 -0.02764

D76 3.10833 -0.00001 -0.00128 -0.00040 -0.00168 3.10665

D77 3.08653 0.00001 -0.00001 0.00003 0.00003 3.08656

D78 -0.06080 -0.00001 -0.00122 -0.00032 -0.00154 -0.06233

D79 0.04274 -0.00001 -0.00015 0.00017 0.00002 0.04277

D80 -3.09301 0.00001 0.00107 0.00053 0.00161 -3.09140

D81 3.01879 -0.00002 0.00242 0.00003 0.00244 3.02123

D82 -0.12404 -0.00005 -0.00319 0.00007 -0.00312 -0.12716

D83 -0.12941 -0.00004 0.00102 -0.00037 0.00064 -0.12877

D84 3.01094 -0.00008 -0.00459 -0.00033 -0.00492 3.00602

D85 2.96458 -0.00007 -0.01694 0.00032 -0.01663 2.94795

D86 -0.22343 -0.00007 -0.01041 0.00013 -0.01029 -0.23373

D87 -0.17581 -0.00003 -0.01149 0.00028 -0.01121 -0.18702

D88 2.91936 -0.00004 -0.00497 0.00009 -0.00488 2.91449

D89 -0.99250 -0.00001 0.00525 0.00016 0.00541 -0.98709

D90 2.14849 0.00000 0.00769 -0.00023 0.00745 2.15594

D91 2.14797 -0.00004 0.00016 0.00020 0.00036 2.14833

D92 -0.99422 -0.00003 0.00260 -0.00020 0.00240 -0.99182

D93 3.08571 0.00004 0.00668 0.00011 0.00680 3.09251

D94 -0.05826 0.00001 0.00445 -0.00027 0.00418 -0.05408

D95 -0.01643 0.00004 0.00114 0.00027 0.00141 -0.01502

D96 3.12278 0.00001 -0.00109 -0.00011 -0.00120 3.12158

D97 -3.07503 -0.00006 -0.00700 -0.00025 -0.00723 -3.08226

D98 0.12610 -0.00004 -0.01652 0.00011 -0.01640 0.10970

D99 0.02794 -0.00007 -0.00156 -0.00040 -0.00196 0.02598

D100 -3.05411 -0.00005 -0.01108 -0.00005 -0.01113 -3.06525

D101 -0.00054 -0.00000 -0.00032 -0.00005 -0.00037 -0.00091

D102 3.13935 -0.00003 -0.00256 0.00003 -0.00252 3.13683

D103 -3.13970 0.00003 0.00195 0.00035 0.00230 -3.13741

D104 0.00019 0.00001 -0.00029 0.00043 0.00014 0.00033

D105 0.01729 -0.00004 -0.00062 -0.00020 -0.00081 0.01648

D106 -3.08243 -0.00004 -0.00560 0.00010 -0.00549 -3.08793

D107 -3.12263 -0.00002 0.00157 -0.00028 0.00130 -3.12133

D108 0.06083 -0.00002 -0.00341 0.00002 -0.00338 0.05745

D109 -0.02827 0.00007 0.00137 0.00037 0.00174 -0.02653

D110 3.05379 0.00005 0.01087 0.00003 0.01090 3.06470

D111 3.07237 0.00007 0.00624 0.00009 0.00632 3.07869

D112 -0.12875 0.00005 0.01575 -0.00025 0.01549 -0.11327

D113 -2.97310 0.00005 0.01354 -0.00040 0.01315 -2.95995

D114 0.16875 0.00001 0.00819 -0.00011 0.00807 0.17682

D115 0.21774 0.00005 0.00769 -0.00005 0.00764 0.22539

D116 -2.92360 0.00001 0.00234 0.00023 0.00257 -2.92103

D117 0.99359 -0.00002 -0.00718 0.00013 -0.00705 0.98654

D118 -2.14719 -0.00002 -0.00970 0.00064 -0.00905 -2.15624

D119 -2.14824 0.00002 -0.00219 -0.00013 -0.00233 -2.15056

D120 0.99417 0.00002 -0.00471 0.00038 -0.00432 0.98985

D121 -3.12915 -0.00001 0.00018 0.00038 0.00056 -3.12859

D122 -0.00892 -0.00000 0.00047 0.00028 0.00074 -0.00817

D123 0.01673 -0.00002 -0.00035 -0.00009 -0.00044 0.01629

D124 3.13696 -0.00001 -0.00007 -0.00019 -0.00026 3.13670

D125 -3.14156 0.00002 -0.00028 -0.00033 -0.00060 3.14102

D126 -0.01853 0.00000 0.00001 -0.00024 -0.00022 -0.01876

D127 -0.00426 0.00002 0.00026 0.00014 0.00040 -0.00386

D128 3.11877 0.00001 0.00055 0.00024 0.00078 3.11955

D129 -0.01724 0.00001 0.00020 -0.00000 0.00019 -0.01705

D130 3.12421 0.00000 0.00005 -0.00004 0.00002 3.12422

D131 -3.13737 -0.00000 -0.00009 0.00010 0.00001 -3.13736

D132 0.00408 -0.00001 -0.00024 0.00007 -0.00017 0.00391

D133 0.00502 -0.00000 0.00006 0.00004 0.00010 0.00512

D134 -3.13397 0.00000 -0.00016 0.00006 -0.00010 -3.13407

D135 -3.13643 0.00000 0.00020 0.00007 0.00028 -3.13615

D136 0.00776 0.00000 -0.00001 0.00009 0.00008 0.00784

D137 0.00740 0.00000 -0.00015 0.00001 -0.00013 0.00727

D138 -3.13105 -0.00000 -0.00043 0.00003 -0.00040 -3.13146

D139 -3.13679 0.00000 0.00007 -0.00000 0.00007 -3.13672

D140 0.00794 -0.00000 -0.00022 0.00001 -0.00020 0.00773

D141 -0.00773 -0.00001 -0.00001 -0.00011 -0.00012 -0.00786

D142 -3.13065 -0.00000 -0.00030 -0.00020 -0.00050 -3.13116

D143 3.13074 -0.00001 0.00027 -0.00012 0.00015 3.13089

D144 0.00782 0.00001 -0.00002 -0.00022 -0.00023 0.00759

D145 -0.00529 -0.00000 -0.00002 0.00002 -0.00000 -0.00529

D146 3.13599 0.00000 -0.00027 0.00005 -0.00022 3.13577

D147 3.13389 0.00000 0.00015 0.00008 0.00023 3.13413

D148 -0.00801 0.00000 -0.00010 0.00011 0.00001 -0.00800

D149 -0.00716 0.00000 0.00032 -0.00009 0.00023 -0.00693

D150 3.13150 -0.00000 0.00034 -0.00000 0.00034 3.13184

D151 3.13684 0.00000 0.00015 -0.00016 -0.00000 3.13684

D152 -0.00768 -0.00000 0.00017 -0.00007 0.00010 -0.00757

D153 0.01683 0.00001 -0.00056 0.00019 -0.00037 0.01646

D154 3.13727 -0.00001 -0.00030 -0.00008 -0.00038 3.13689

D155 -3.12445 0.00001 -0.00031 0.00016 -0.00015 -3.12460

D156 -0.00401 -0.00001 -0.00005 -0.00011 -0.00016 -0.00417

D157 3.13042 -0.00002 0.00007 -0.00069 -0.00063 3.12979

D158 -0.01563 -0.00002 0.00082 -0.00032 0.00050 -0.01513

D159 0.00988 -0.00001 -0.00020 -0.00042 -0.00062 0.00926

D160 -3.13618 -0.00000 0.00056 -0.00005 0.00051 -3.13567

D161 3.14027 0.00003 0.00025 0.00062 0.00086 3.14113

D162 0.01759 0.00001 -0.00012 0.00046 0.00033 0.01793

D163 0.00314 0.00002 -0.00052 0.00025 -0.00027 0.00287

D164 -3.11954 0.00001 -0.00089 0.00009 -0.00080 -3.12034

D165 0.00820 -0.00001 -0.00005 -0.00004 -0.00009 0.00811

D166 -3.13048 -0.00001 -0.00007 -0.00013 -0.00020 -3.13068

D167 3.13076 0.00000 0.00033 0.00012 0.00044 3.13120

D168 -0.00792 0.00001 0.00031 0.00003 0.00033 -0.00758

D169 -3.13814 0.00002 -0.00269 0.00071 -0.00199 -3.14012

D170 0.01997 0.00000 -0.00157 0.00043 -0.00115 0.01882

D171 0.00266 0.00002 -0.00023 0.00021 -0.00003 0.00263

D172 -3.12242 0.00000 0.00089 -0.00007 0.00081 -3.12161

D173 3.12596 -0.00001 0.00282 -0.00072 0.00209 3.12805

D174 0.00595 -0.00001 0.00225 -0.00058 0.00167 0.00761

D175 -0.01483 -0.00001 0.00035 -0.00022 0.00013 -0.01470

D176 -3.13485 -0.00000 -0.00022 -0.00007 -0.00029 -3.13514

D177 0.00809 -0.00001 0.00001 -0.00008 -0.00007 0.00802

D178 -3.13133 -0.00001 0.00046 -0.00018 0.00028 -3.13106

D179 3.13307 -0.00000 -0.00111 0.00020 -0.00091 3.13216

D180 -0.00635 0.00001 -0.00066 0.00009 -0.00057 -0.00692

D181 -0.00678 0.00001 0.00010 -0.00004 0.00006 -0.00671

D182 3.13642 0.00000 0.00042 -0.00014 0.00028 3.13671

D183 3.13264 -0.00000 -0.00035 0.00007 -0.00028 3.13235

D184 -0.00735 -0.00000 -0.00003 -0.00004 -0.00006 -0.00741

D185 -0.00535 -0.00000 0.00001 0.00003 0.00004 -0.00531

D186 3.13540 0.00000 0.00008 0.00001 0.00009 3.13549

D187 3.13463 0.00000 -0.00031 0.00013 -0.00018 3.13445

D188 -0.00780 0.00000 -0.00024 0.00012 -0.00012 -0.00793

D189 0.01630 0.00000 -0.00024 0.00010 -0.00014 0.01616

D190 3.13621 -0.00000 0.00033 -0.00004 0.00029 3.13650

D191 -3.12446 0.00000 -0.00031 0.00012 -0.00019 -3.12465

D192 -0.00455 -0.00000 0.00027 -0.00003 0.00024 -0.00431

D193 3.13738 0.00002 0.00231 -0.00027 0.00203 3.13942

D194 -0.02054 0.00001 0.00121 -0.00006 0.00115 -0.01939

D195 -0.00362 0.00002 -0.00009 0.00012 0.00003 -0.00359

D196 3.12164 0.00000 -0.00118 0.00033 -0.00086 3.12079

D197 -3.12528 -0.00002 -0.00215 0.00028 -0.00187 -3.12715

D198 -0.00538 -0.00001 -0.00168 0.00029 -0.00139 -0.00677

D199 0.01572 -0.00002 0.00024 -0.00011 0.00013 0.01585

D200 3.13562 -0.00000 0.00071 -0.00009 0.00061 3.13624

D201 -0.00764 -0.00001 -0.00011 -0.00004 -0.00015 -0.00778

D202 3.13155 -0.00001 -0.00024 -0.00008 -0.00032 3.13123

D203 -3.13280 0.00000 0.00099 -0.00025 0.00074 -3.13206

D204 0.00639 0.00001 0.00086 -0.00030 0.00057 0.00696

D205 0.00691 0.00000 0.00016 -0.00005 0.00011 0.00702

D206 -3.13643 -0.00000 -0.00015 -0.00003 -0.00018 -3.13661

D207 -3.13226 -0.00000 0.00029 -0.00000 0.00028 -3.13198

D208 0.00758 -0.00000 -0.00002 0.00002 -0.00001 0.00757

D209 0.00514 -0.00000 -0.00001 0.00006 0.00005 0.00519

D210 -3.13574 -0.00000 -0.00019 0.00004 -0.00014 -3.13589

D211 -3.13470 0.00000 0.00030 0.00003 0.00034 -3.13436

D212 0.00760 0.00000 0.00013 0.00002 0.00015 0.00775

D213 -0.01661 0.00001 -0.00019 0.00002 -0.00017 -0.01678

D214 -3.13641 -0.00001 -0.00066 0.00001 -0.00066 -3.13706

D215 3.12428 0.00001 -0.00002 0.00004 0.00002 3.12430

D216 0.00448 -0.00001 -0.00049 0.00002 -0.00047 0.00402

Item Value Threshold Converged?

Maximum Force 0.000113 0.000450 YES

RMS Force 0.000026 0.000300 YES

Maximum Displacement 0.078432 0.001800 NO

RMS Displacement 0.010585 0.001200 NO

Predicted change in Energy=-1.761982D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

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

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=1 Diff= 4.68D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.768915 -4.151417 0.573121

2 6 0 1.178370 -2.856992 0.207589

3 7 0 0.037466 -2.116201 0.005410

4 6 0 -1.078761 -2.896374 0.195979

5 6 0 -0.628610 -4.175793 0.565147

6 6 0 -2.440100 -2.471863 0.009436

7 6 0 -2.859802 -1.145095 -0.120275

8 7 0 -2.067381 -0.035850 0.051794

9 6 0 -2.897830 1.045825 -0.104365

10 6 0 -4.250309 0.604802 -0.440929

11 6 0 -4.226453 -0.746677 -0.451840

12 6 0 2.525003 -2.385785 0.030995

13 6 0 2.897882 -1.044754 -0.109333

14 6 0 4.250281 -0.602380 -0.444450

15 6 0 4.226373 0.749134 -0.450211

16 6 0 2.859674 1.146199 -0.117197

17 7 0 2.067352 0.036204 0.050738

18 6 0 2.439767 2.472392 0.016379

19 6 0 1.078823 2.897366 0.203847

20 6 0 0.628497 4.181804 0.555520

21 6 0 -0.768904 4.157456 0.563893

22 6 0 -1.178386 2.858025 0.216111

23 7 0 -0.037411 2.114271 0.024775

24 6 0 -2.524690 2.386331 0.039173

25 6 0 -3.456503 -3.551773 -0.030196

26 6 0 -3.350664 -4.597564 -0.959761

27 6 0 -4.311270 -5.602369 -1.008167

28 6 0 -5.383505 -5.591520 -0.115687

29 6 0 -5.491464 -4.565284 0.821466

30 6 0 -4.538880 -3.550822 0.861565

31 6 0 5.585872 -5.392316 -0.027738

32 6 0 4.524654 -5.454661 -0.931199

33 6 0 3.526031 -4.486659 -0.905479

34 6 0 3.581531 -3.426873 0.012531

35 6 0 4.653767 -3.373746 0.915062

36 6 0 5.644658 -4.351380 0.897568

37 6 0 -3.581890 3.427165 0.016947

38 6 0 -4.652684 3.378021 0.921210

39 6 0 -5.645251 4.353926 0.898726

40 6 0 -5.589359 5.388991 -0.033312

41 6 0 -4.529560 5.447138 -0.938674

42 6 0 -3.529412 4.480789 -0.908152

43 6 0 3.456911 3.551987 -0.026269

44 6 0 4.537339 3.554421 0.867641

45 6 0 5.491589 4.567222 0.823652

46 6 0 5.387016 5.588245 -0.119552

47 6 0 4.316735 5.595465 -1.014363

48 6 0 3.354591 4.592245 -0.962235

49 1 0 1.428697 -4.967713 0.819094

50 1 0 -1.262386 -5.014508 0.804017

51 1 0 -5.087854 1.247544 -0.664040

52 1 0 -5.040859 -1.414876 -0.685590

53 1 0 5.087745 -1.244291 -0.670277

54 1 0 5.040856 1.418211 -0.681139

55 1 0 1.261901 5.024498 0.780861

56 1 0 -1.428473 4.977732 0.796716

57 1 0 -2.521533 -4.608231 -1.657923

58 1 0 -4.223121 -6.394958 -1.743730

59 1 0 -6.128511 -6.379376 -0.149518

60 1 0 -6.317076 -4.554623 1.525187

61 1 0 -4.620852 -2.759701 1.598086

62 1 0 6.360569 -6.151584 -0.044013

63 1 0 4.474842 -6.258717 -1.657851

64 1 0 2.705829 -4.536994 -1.612382

65 1 0 4.697586 -2.571099 1.642348

66 1 0 6.461697 -4.300623 1.609512

67 1 0 -4.694569 2.579396 1.653062

68 1 0 -6.461449 4.306259 1.611847

69 1 0 -6.365391 6.146800 -0.053548

70 1 0 -4.482096 6.246430 -1.670726

71 1 0 -2.710480 4.527578 -1.616773

72 1 0 4.616958 2.766823 1.608226

73 1 0 6.315950 4.559203 1.528873

74 1 0 6.133338 6.374718 -0.156488

75 1 0 4.231333 6.383824 -1.754786

76 1 0 2.527110 4.599873 -1.662394

77 1 0 0.021367 -1.130874 -0.218024

78 1 0 -0.021270 1.123201 -0.172662

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

Rotational constants (GHZ): 0.0587921 0.0582828 0.0300939

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

Standard basis: 6-311G(d) (5D, 7F)

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

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5357.1312726687 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122295624 Hartrees.

Nuclear repulsion after empirical dispersion term = 5356.9190431063 Hartrees.

Force inversion solution in PCM.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5781

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.12D-10

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 313

GePol: Fraction of low-weight points (<1% of avg) = 5.41%

GePol: Cavity surface area = 611.272 Ang\*\*2

GePol: Cavity volume = 627.909 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0021059013 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5356.9169372050 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.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

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

DipDrv: MaxL=1.

Leave Link 303 at Wed Aug 28 03:02:01 2019, MaxMem= 4294967296 cpu: 2.3

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

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= -0.000000 0.000000 0.000000

Rot= 0.999999 -0.000117 -0.000002 -0.001608 Ang= -0.18 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0183

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30455921922

Leave Link 401 at Wed Aug 28 03:02:06 2019, MaxMem= 4294967296 cpu: 80.8

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 590000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

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

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

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 100259883.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.77D-15 for 5764.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.66D-15 for 3593 355.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.77D-15 for 5764.

Iteration 1 A^-1\*A deviation from orthogonality is 4.55D-07 for 4574 4548.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.44D-15 for 2504.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.63D-15 for 3049 2817.

Iteration 2 A^-1\*A deviation from unit magnitude is 8.88D-16 for 109.

Iteration 2 A^-1\*A deviation from orthogonality is 5.00D-16 for 5331 393.

E= -1914.33267476345

DIIS: error= 7.66D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.33267476345 IErMin= 1 ErrMin= 7.66D-04

ErrMax= 7.66D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.42D-03 BMatP= 1.42D-03

IDIUse=3 WtCom= 9.92D-01 WtEn= 7.66D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.641 Goal= None Shift= 0.000

Gap= 0.706 Goal= None Shift= 0.000

RMSDP=5.22D-05 MaxDP=2.79D-03 OVMax= 4.97D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.22D-05 CP: 1.00D+00

E= -1914.33333211154 Delta-E= -0.000657348087 Rises=F Damp=F

DIIS: error= 8.54D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33333211154 IErMin= 2 ErrMin= 8.54D-05

ErrMax= 8.54D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.86D-05 BMatP= 1.42D-03

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

Coeff-Com: -0.566D-01 0.106D+01

Coeff: -0.566D-01 0.106D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.41D-06 MaxDP=2.85D-04 DE=-6.57D-04 OVMax= 1.34D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.78D-06 CP: 1.00D+00 1.05D+00

E= -1914.33334092227 Delta-E= -0.000008810728 Rises=F Damp=F

DIIS: error= 6.18D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33334092227 IErMin= 3 ErrMin= 6.18D-05

ErrMax= 6.18D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.24D-06 BMatP= 1.86D-05

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

Coeff-Com: -0.306D-01 0.438D+00 0.593D+00

Coeff: -0.306D-01 0.438D+00 0.593D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.12D-06 MaxDP=2.19D-04 DE=-8.81D-06 OVMax= 6.80D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.92D-06 CP: 1.00D+00 1.05D+00 8.09D-01

E= -1914.33334231885 Delta-E= -0.000001396584 Rises=F Damp=F

DIIS: error= 3.36D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33334231885 IErMin= 4 ErrMin= 3.36D-05

ErrMax= 3.36D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.74D-06 BMatP= 8.24D-06

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

Coeff-Com: -0.102D-01 0.113D+00 0.367D+00 0.530D+00

Coeff: -0.102D-01 0.113D+00 0.367D+00 0.530D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.03D-06 MaxDP=8.41D-05 DE=-1.40D-06 OVMax= 5.43D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 7.93D-07 CP: 1.00D+00 1.05D+00 8.91D-01 7.36D-01

E= -1914.33334301503 Delta-E= -0.000000696181 Rises=F Damp=F

DIIS: error= 8.78D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33334301503 IErMin= 5 ErrMin= 8.78D-06

ErrMax= 8.78D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.73D-07 BMatP= 2.74D-06

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

Coeff-Com: -0.161D-02 0.625D-02 0.105D+00 0.245D+00 0.646D+00

Coeff: -0.161D-02 0.625D-02 0.105D+00 0.245D+00 0.646D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.51D-07 MaxDP=3.01D-05 DE=-6.96D-07 OVMax= 3.10D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.73D-07 CP: 1.00D+00 1.05D+00 9.14D-01 8.53D-01 1.05D+00

E= -1914.33334308322 Delta-E= -0.000000068189 Rises=F Damp=F

DIIS: error= 6.46D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33334308322 IErMin= 6 ErrMin= 6.46D-06

ErrMax= 6.46D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.83D-08 BMatP= 1.73D-07

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

Coeff-Com: 0.111D-02-0.204D-01-0.126D-01 0.461D-01 0.415D+00 0.570D+00

Coeff: 0.111D-02-0.204D-01-0.126D-01 0.461D-01 0.415D+00 0.570D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.39D-07 MaxDP=2.96D-05 DE=-6.82D-08 OVMax= 3.32D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.19D-07 CP: 1.00D+00 1.05D+00 9.36D-01 8.83D-01 1.32D+00

CP: 1.21D+00

E= -1914.33334312705 Delta-E= -0.000000043835 Rises=F Damp=F

DIIS: error= 4.52D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33334312705 IErMin= 7 ErrMin= 4.52D-06

ErrMax= 4.52D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.20D-08 BMatP= 6.83D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.560D-03-0.767D-02-0.154D-01-0.559D-02 0.667D-01 0.232D+00

Coeff-Com: 0.729D+00

Coeff: 0.560D-03-0.767D-02-0.154D-01-0.559D-02 0.667D-01 0.232D+00

Coeff: 0.729D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.64D-07 MaxDP=2.21D-05 DE=-4.38D-08 OVMax= 2.67D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 7.20D-08 CP: 1.00D+00 1.05D+00 9.47D-01 9.23D-01 1.50D+00

CP: 1.64D+00 1.46D+00

E= -1914.33334314801 Delta-E= -0.000000020959 Rises=F Damp=F

DIIS: error= 4.14D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33334314801 IErMin= 8 ErrMin= 4.14D-06

ErrMax= 4.14D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.91D-09 BMatP= 1.20D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.774D-03 0.170D-01-0.969D-03-0.564D-01-0.455D+00-0.430D+00

Coeff-Com: 0.614D+00 0.131D+01

Coeff: -0.774D-03 0.170D-01-0.969D-03-0.564D-01-0.455D+00-0.430D+00

Coeff: 0.614D+00 0.131D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=6.57D-07 MaxDP=5.74D-05 DE=-2.10D-08 OVMax= 7.05D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 8.35D-08 CP: 1.00D+00 1.05D+00 9.76D-01 1.00D+00 1.98D+00

CP: 2.67D+00 2.85D+00 1.77D+00

E= -1914.33334317995 Delta-E= -0.000000031939 Rises=F Damp=F

DIIS: error= 1.73D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33334317995 IErMin= 9 ErrMin= 1.73D-06

ErrMax= 1.73D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.33D-09 BMatP= 6.91D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.458D-03 0.861D-02 0.424D-02-0.162D-01-0.194D+00-0.223D+00

Coeff-Com: -0.546D-01 0.621D+00 0.854D+00

Coeff: -0.458D-03 0.861D-02 0.424D-02-0.162D-01-0.194D+00-0.223D+00

Coeff: -0.546D-01 0.621D+00 0.854D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.75D-07 MaxDP=2.28D-05 DE=-3.19D-08 OVMax= 2.96D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.07D-07 CP: 1.00D+00 1.05D+00 9.87D-01 1.03D+00 2.16D+00

CP: 3.00D+00 3.00D+00 2.48D+00 1.47D+00

E= -1914.33334318585 Delta-E= -0.000000005899 Rises=F Damp=F

DIIS: error= 9.72D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33334318585 IErMin=10 ErrMin= 9.72D-07

ErrMax= 9.72D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.01D-09 BMatP= 2.33D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.299D-04-0.167D-02 0.304D-02 0.153D-01 0.684D-01 0.415D-01

Coeff-Com: -0.338D+00-0.851D-01 0.550D+00 0.747D+00

Coeff: 0.299D-04-0.167D-02 0.304D-02 0.153D-01 0.684D-01 0.415D-01

Coeff: -0.338D+00-0.851D-01 0.550D+00 0.747D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.45D-07 MaxDP=1.22D-05 DE=-5.90D-09 OVMax= 1.61D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.38D-08 CP: 1.00D+00 1.05D+00 9.92D-01 1.05D+00 2.25D+00

CP: 3.00D+00 3.00D+00 2.85D+00 1.98D+00 1.82D+00

E= -1914.33334318756 Delta-E= -0.000000001709 Rises=F Damp=F

DIIS: error= 4.50D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33334318756 IErMin=11 ErrMin= 4.50D-07

ErrMax= 4.50D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.05D-10 BMatP= 1.01D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.140D-03-0.322D-02 0.956D-04 0.131D-01 0.887D-01 0.826D-01

Coeff-Com: -0.188D+00-0.185D+00 0.421D-01 0.406D+00 0.743D+00

Coeff: 0.140D-03-0.322D-02 0.956D-04 0.131D-01 0.887D-01 0.826D-01

Coeff: -0.188D+00-0.185D+00 0.421D-01 0.406D+00 0.743D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=6.65D-08 MaxDP=6.16D-06 DE=-1.71D-09 OVMax= 7.23D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.84D-08 CP: 1.00D+00 1.05D+00 9.94D-01 1.05D+00 2.29D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.26D+00 2.21D+00

CP: 1.30D+00

E= -1914.33334318799 Delta-E= -0.000000000427 Rises=F Damp=F

DIIS: error= 2.55D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.33334318799 IErMin=12 ErrMin= 2.55D-07

ErrMax= 2.55D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-10 BMatP= 3.05D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.604D-04-0.972D-03-0.145D-02 0.987D-03 0.181D-01 0.274D-01

Coeff-Com: 0.304D-01-0.361D-01-0.215D+00-0.911D-01 0.403D+00 0.865D+00

Coeff: 0.604D-04-0.972D-03-0.145D-02 0.987D-03 0.181D-01 0.274D-01

Coeff: 0.304D-01-0.361D-01-0.215D+00-0.911D-01 0.403D+00 0.865D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.38D-08 MaxDP=3.22D-06 DE=-4.27D-10 OVMax= 3.48D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.38D-08 CP: 1.00D+00 1.05D+00 9.95D-01 1.05D+00 2.30D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.46D+00 2.39D+00

CP: 1.47D+00 1.35D+00

E= -1914.33334318815 Delta-E= -0.000000000166 Rises=F Damp=F

DIIS: error= 1.29D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.33334318815 IErMin=13 ErrMin= 1.29D-07

ErrMax= 1.29D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.90D-11 BMatP= 1.05D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.168D-04 0.638D-03-0.998D-03-0.415D-02-0.231D-01-0.153D-01

Coeff-Com: 0.816D-01 0.556D-01-0.150D+00-0.201D+00-0.328D-01 0.511D+00

Coeff-Com: 0.779D+00

Coeff: -0.168D-04 0.638D-03-0.998D-03-0.415D-02-0.231D-01-0.153D-01

Coeff: 0.816D-01 0.556D-01-0.150D+00-0.201D+00-0.328D-01 0.511D+00

Coeff: 0.779D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.30D-08 MaxDP=2.36D-06 DE=-1.66D-10 OVMax= 2.43D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 4.50D-09 CP: 1.00D+00 1.05D+00 9.96D-01 1.06D+00 2.32D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.57D+00 2.52D+00

CP: 1.57D+00 1.76D+00 1.37D+00

E= -1914.33334318820 Delta-E= -0.000000000042 Rises=F Damp=F

DIIS: error= 7.65D-08 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.33334318820 IErMin=14 ErrMin= 7.65D-08

ErrMax= 7.65D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.01D-12 BMatP= 3.90D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.267D-04 0.614D-03-0.312D-04-0.224D-02-0.172D-01-0.160D-01

Coeff-Com: 0.288D-01 0.416D-01-0.961D-02-0.712D-01-0.145D+00-0.106D-01

Coeff-Com: 0.390D+00 0.811D+00

Coeff: -0.267D-04 0.614D-03-0.312D-04-0.224D-02-0.172D-01-0.160D-01

Coeff: 0.288D-01 0.416D-01-0.961D-02-0.712D-01-0.145D+00-0.106D-01

Coeff: 0.390D+00 0.811D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.07D-08 MaxDP=1.05D-06 DE=-4.18D-11 OVMax= 1.14D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 2.40D-09 CP: 1.00D+00 1.05D+00 9.96D-01 1.06D+00 2.32D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.62D+00 2.58D+00

CP: 1.63D+00 1.92D+00 1.58D+00 1.17D+00

E= -1914.33334318821 Delta-E= -0.000000000019 Rises=F Damp=F

DIIS: error= 3.40D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.33334318821 IErMin=15 ErrMin= 3.40D-08

ErrMax= 3.40D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.79D-12 BMatP= 9.01D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.604D-05 0.717D-04 0.266D-03 0.240D-03-0.868D-03-0.218D-02

Coeff-Com: -0.107D-01 0.258D-02 0.352D-01 0.245D-01-0.493D-01-0.138D+00

Coeff-Com: -0.449D-01 0.329D+00 0.854D+00

Coeff: -0.604D-05 0.717D-04 0.266D-03 0.240D-03-0.868D-03-0.218D-02

Coeff: -0.107D-01 0.258D-02 0.352D-01 0.245D-01-0.493D-01-0.138D+00

Coeff: -0.449D-01 0.329D+00 0.854D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.37D-09 MaxDP=4.02D-07 DE=-1.91D-11 OVMax= 4.49D-06

Error on total polarization charges = 0.08258

SCF Done: E(UB3LYP) = -1914.33334319 A.U. after 15 cycles

NFock= 15 Conv=0.44D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0183

<L.S>= 0.000000000000E+00

KE= 1.906377219962D+03 PE=-1.516345116117D+04 EE= 5.985823660814D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0551, after 2.0017

Leave Link 502 at Wed Aug 28 03:08:47 2019, MaxMem= 4294967296 cpu: 6332.0

(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: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48668731D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64381337D-01

Leave Link 801 at Wed Aug 28 03:08:47 2019, MaxMem= 4294967296 cpu: 1.0

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Wed Aug 28 03:08:54 2019, MaxMem= 4294967296 cpu: 112.8

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Wed Aug 28 03:08:54 2019, MaxMem= 4294967296 cpu: 2.3

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 187

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Wed Aug 28 03:28:41 2019, MaxMem= 4294967296 cpu: 18982.0

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 590000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.44D+03 4.54D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.56D+02 3.70D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.62D+00 4.69D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.03D-01 3.95D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.64D-04 2.11D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.62D-06 1.35D-04.

190 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 2.00D-08 1.01D-05.

81 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.31D-11 6.29D-07.

38 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.25D-13 3.97D-08.

5 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 1.03D-14 7.16D-09.

4 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 8.36D-15 3.18D-09.

4 vectors produced by pass 11 Test12= 2.55D-13 1.00D-09 XBig12= 8.27D-15 3.34D-09.

4 vectors produced by pass 12 Test12= 2.55D-13 1.00D-09 XBig12= 7.42D-15 2.38D-09.

4 vectors produced by pass 13 Test12= 2.55D-13 1.00D-09 XBig12= 8.71D-15 3.05D-09.

4 vectors produced by pass 14 Test12= 2.55D-13 1.00D-09 XBig12= 8.38D-15 2.69D-09.

3 vectors produced by pass 15 Test12= 2.55D-13 1.00D-09 XBig12= 5.94D-15 2.20D-09.

3 vectors produced by pass 16 Test12= 2.55D-13 1.00D-09 XBig12= 7.60D-15 3.05D-09.

3 vectors produced by pass 17 Test12= 2.55D-13 1.00D-09 XBig12= 7.66D-15 2.95D-09.

3 vectors produced by pass 18 Test12= 2.55D-13 1.00D-09 XBig12= 3.46D-15 1.84D-09.

3 vectors produced by pass 19 Test12= 2.55D-13 1.00D-09 XBig12= 7.96D-15 2.42D-09.

3 vectors produced by pass 20 Test12= 2.55D-13 1.00D-09 XBig12= 6.44D-15 2.38D-09.

3 vectors produced by pass 21 Test12= 2.55D-13 1.00D-09 XBig12= 6.47D-15 2.50D-09.

3 vectors produced by pass 22 Test12= 2.55D-13 1.00D-09 XBig12= 6.82D-15 2.44D-09.

3 vectors produced by pass 23 Test12= 2.55D-13 1.00D-09 XBig12= 7.08D-15 2.45D-09.

3 vectors produced by pass 24 Test12= 2.55D-13 1.00D-09 XBig12= 6.05D-15 2.12D-09.

3 vectors produced by pass 25 Test12= 2.55D-13 1.00D-09 XBig12= 7.76D-15 2.91D-09.

2 vectors produced by pass 26 Test12= 2.55D-13 1.00D-09 XBig12= 5.92D-15 2.42D-09.

InvSVY: IOpt=1 It= 1 EMax= 1.28D-13

Solved reduced A of dimension 1776 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1127.50 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Wed Aug 28 07:24:41 2019, MaxMem= 4294967296 cpu: 226493.8

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 187

Leave Link 701 at Wed Aug 28 07:26:10 2019, MaxMem= 4294967296 cpu: 1418.8

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Wed Aug 28 07:26:10 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

Compute integral second derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

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= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Wed Aug 28 07:44:24 2019, MaxMem= 4294967296 cpu: 17502.0

(Enter /home/kira/g09/l716.exe)

Dipole =-2.10329538D-04-1.02749051D-02-5.01478783D-01

Polarizability= 1.25627096D+03-8.67755003D+00 1.67358312D+03

-8.78047033D-03-2.02013578D-02 4.52659189D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000019152 0.000008918 -0.000036323

2 6 0.000013220 -0.000002291 0.000076843

3 7 -0.000004798 -0.000010589 -0.000010808

4 6 -0.000060516 0.000012535 -0.000022366

5 6 0.000048761 -0.000018002 0.000054520

6 6 0.000116312 -0.000008177 0.000067663

7 6 -0.000157051 0.000014573 -0.000014286

8 7 0.000045612 0.000041754 0.000026046

9 6 -0.000154022 -0.000008253 -0.000052225

10 6 -0.000035045 -0.000028247 0.000017985

11 6 0.000040331 0.000003840 0.000042097

12 6 -0.000102735 0.000021735 -0.000041957

13 6 0.000150385 -0.000005403 0.000054392

14 6 0.000035591 -0.000028848 -0.000018982

15 6 -0.000041034 0.000005589 -0.000043701

16 6 0.000157546 0.000017903 0.000017788

17 7 -0.000056927 0.000045254 -0.000019303

18 6 -0.000119009 -0.000010729 -0.000070134

19 6 0.000062117 0.000010526 0.000025768

20 6 -0.000048004 -0.000019493 -0.000054337

21 6 0.000019596 0.000005094 0.000036004

22 6 -0.000014664 -0.000002800 -0.000077235

23 7 0.000002945 -0.000006045 0.000010058

24 6 0.000109635 0.000021901 0.000041573

25 6 0.000029831 0.000001439 0.000034872

26 6 -0.000048354 -0.000003129 -0.000021698

27 6 0.000010454 -0.000001359 0.000023953

28 6 -0.000019788 0.000013943 -0.000006062

29 6 0.000034072 -0.000010808 0.000015875

30 6 -0.000000300 0.000012316 -0.000037336

31 6 0.000010162 -0.000013484 -0.000003301

32 6 -0.000025403 0.000012016 0.000028326

33 6 0.000027236 -0.000034816 -0.000030279

34 6 0.000005296 0.000020894 0.000027464

35 6 0.000029319 -0.000014591 -0.000032053

36 6 -0.000028758 0.000027928 0.000009163

37 6 -0.000009398 0.000019520 -0.000027313

38 6 -0.000027734 -0.000016826 0.000031985

39 6 0.000027470 0.000024781 -0.000008178

40 6 -0.000008997 -0.000016349 0.000002944

41 6 0.000023851 0.000009263 -0.000028524

42 6 -0.000027014 -0.000035784 0.000029779

43 6 -0.000028595 -0.000000651 -0.000035790

44 6 0.000001810 0.000012232 0.000037352

45 6 -0.000034597 -0.000013615 -0.000017353

46 6 0.000020495 0.000011546 0.000006126

47 6 -0.000010523 -0.000003570 -0.000023806

48 6 0.000047855 -0.000007892 0.000020042

49 1 0.000001477 0.000014307 -0.000004659

50 1 -0.000000241 -0.000010609 -0.000016917

51 1 -0.000013560 0.000007843 -0.000007959

52 1 -0.000012707 0.000000270 0.000002180

53 1 0.000013486 0.000007987 0.000007703

54 1 0.000011900 -0.000000340 -0.000002113

55 1 -0.000001324 -0.000009552 0.000018178

56 1 -0.000000010 0.000011604 0.000004676

57 1 0.000000430 -0.000002144 -0.000001313

58 1 0.000001133 0.000000342 -0.000002098

59 1 0.000005578 -0.000000384 0.000001895

60 1 -0.000000666 0.000000813 -0.000005299

61 1 -0.000012867 -0.000008425 -0.000006309

62 1 0.000000351 0.000005679 0.000006607

63 1 0.000004762 0.000004171 -0.000004192

64 1 -0.000016358 -0.000002576 -0.000009474

65 1 -0.000004362 0.000000074 -0.000006303

66 1 0.000003063 -0.000002677 0.000000427

67 1 0.000005434 -0.000000733 0.000006690

68 1 -0.000002363 -0.000004930 -0.000000288

69 1 -0.000000346 0.000002730 -0.000006711

70 1 -0.000005535 0.000001005 0.000004178

71 1 0.000016537 -0.000005077 0.000009176

72 1 0.000012729 -0.000010446 0.000007220

73 1 0.000001474 -0.000001044 0.000005265

74 1 -0.000005648 -0.000002771 -0.000001480

75 1 -0.000001981 -0.000002513 0.000001962

76 1 -0.000001204 -0.000003581 0.000001597

77 1 0.000118007 0.000018578 0.000070333

78 1 -0.000104676 -0.000061349 -0.000078245

-------------------------------------------------------------------

Cartesian Forces: Max 0.000157546 RMS 0.000036250

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Wed Aug 28 07:44:24 2019, MaxMem= 4294967296 cpu: 2.3

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000204307 RMS 0.000038077

Search for a local minimum.

Step number 14 out of a maximum of 452

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -2.48D-06 DEPred=-1.76D-06 R= 1.41D+00

TightC=F SS= 1.41D+00 RLast= 6.55D-02 DXNew= 1.6886D-01 1.9658D-01

Trust test= 1.41D+00 RLast= 6.55D-02 DXMaxT set to 1.69D-01

ITU= 1 0 -1 1 1 -1 1 -1 -1 1 1 -1 1 0

Eigenvalues --- 0.00014 0.00054 0.00520 0.00618 0.00734

Eigenvalues --- 0.00871 0.01012 0.01034 0.01045 0.01108

Eigenvalues --- 0.01122 0.01215 0.01250 0.01287 0.01301

Eigenvalues --- 0.01308 0.01340 0.01422 0.01448 0.01457

Eigenvalues --- 0.01467 0.01502 0.01526 0.01645 0.01720

Eigenvalues --- 0.01724 0.01728 0.01742 0.01749 0.01755

Eigenvalues --- 0.01762 0.01786 0.01806 0.01827 0.01888

Eigenvalues --- 0.01926 0.01955 0.01960 0.01981 0.02149

Eigenvalues --- 0.02191 0.02251 0.02274 0.02279 0.02306

Eigenvalues --- 0.02331 0.02434 0.02449 0.02537 0.02547

Eigenvalues --- 0.02551 0.02553 0.02602 0.02603 0.02609

Eigenvalues --- 0.02612 0.02615 0.02742 0.02748 0.02773

Eigenvalues --- 0.02797 0.02866 0.02869 0.02871 0.02873

Eigenvalues --- 0.03060 0.03072 0.03899 0.04085 0.04188

Eigenvalues --- 0.04322 0.04367 0.04436 0.04522 0.04537

Eigenvalues --- 0.08263 0.09701 0.09713 0.09847 0.09910

Eigenvalues --- 0.09936 0.10332 0.10455 0.10599 0.10689

Eigenvalues --- 0.10689 0.10709 0.10710 0.10738 0.11079

Eigenvalues --- 0.11397 0.11403 0.11416 0.11423 0.12009

Eigenvalues --- 0.12012 0.12017 0.12023 0.12264 0.12265

Eigenvalues --- 0.12288 0.12289 0.12772 0.12779 0.12787

Eigenvalues --- 0.12792 0.15689 0.15960 0.16285 0.17055

Eigenvalues --- 0.17224 0.17301 0.17519 0.17796 0.17966

Eigenvalues --- 0.18082 0.18116 0.18572 0.19251 0.19287

Eigenvalues --- 0.19343 0.19349 0.19370 0.19393 0.19404

Eigenvalues --- 0.19458 0.19549 0.19550 0.19554 0.19556

Eigenvalues --- 0.20282 0.21511 0.22042 0.22816 0.22881

Eigenvalues --- 0.23402 0.23733 0.24279 0.24712 0.25540

Eigenvalues --- 0.26244 0.26535 0.26609 0.27196 0.28488

Eigenvalues --- 0.28526 0.28657 0.28901 0.29708 0.30984

Eigenvalues --- 0.31683 0.32003 0.32809 0.33113 0.33322

Eigenvalues --- 0.33440 0.34201 0.35111 0.35586 0.35619

Eigenvalues --- 0.35627 0.35634 0.35645 0.35698 0.35751

Eigenvalues --- 0.35762 0.35810 0.35823 0.35921 0.35924

Eigenvalues --- 0.35928 0.35930 0.36009 0.36018 0.36023

Eigenvalues --- 0.36023 0.36212 0.36254 0.36273 0.36278

Eigenvalues --- 0.37077 0.37087 0.37250 0.37397 0.37407

Eigenvalues --- 0.37548 0.38149 0.38543 0.38591 0.38750

Eigenvalues --- 0.39505 0.40501 0.40689 0.40997 0.41007

Eigenvalues --- 0.41082 0.41125 0.41128 0.41180 0.41387

Eigenvalues --- 0.41556 0.41829 0.42319 0.42959 0.44736

Eigenvalues --- 0.45442 0.45899 0.45911 0.45943 0.45971

Eigenvalues --- 0.46213 0.46229 0.46236 0.46269 0.46282

Eigenvalues --- 0.48338 0.48608 0.49043 0.49305 0.50478

Eigenvalues --- 0.50753 0.50755 0.50780 0.50809 0.51884

Eigenvalues --- 0.52543 0.57114 0.58505

Cosine: 0.484 < 0.500

Cut down GDIIS temporarily because of the cosine check. E 6

DIIS coeff's: 0.18480 0.26447 0.24972 0.13720 0.05066

DIIS coeff's: -0.01368 -0.08199 0.08552 0.06079 0.07171

DIIS coeff's: -0.00919

Cosine: 0.554 > 0.500

Length: 0.178

GDIIS step was calculated using 11 of the last 14 vectors.

Iteration 1 RMS(Cart)= 0.00076250 RMS(Int)= 0.00001089

Iteration 2 RMS(Cart)= 0.00000024 RMS(Int)= 0.00001089

ITry= 1 IFail=0 DXMaxC= 5.12D-03 DCOld= 1.00D+10 DXMaxT= 1.69D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.65693 -0.00002 -0.00005 0.00005 -0.00001 2.65692

R2 2.64138 -0.00001 -0.00007 0.00001 -0.00007 2.64131

R3 2.03719 -0.00000 -0.00001 0.00002 0.00001 2.03719

R4 2.59884 -0.00008 0.00012 -0.00013 -0.00001 2.59884

R5 2.71664 -0.00011 -0.00007 0.00002 -0.00005 2.71659

R6 2.59859 -0.00006 -0.00010 0.00001 -0.00008 2.59851

R7 1.90951 -0.00011 0.00005 -0.00011 -0.00005 1.90946

R8 2.65628 0.00007 0.00016 0.00000 0.00016 2.65644

R9 2.71770 0.00002 -0.00007 -0.00010 -0.00017 2.71753

R10 2.03720 0.00001 -0.00001 0.00001 0.00000 2.03721

R11 2.64108 0.00020 0.00029 0.00018 0.00046 2.64154

R12 2.80346 0.00000 -0.00002 -0.00000 -0.00003 2.80343

R13 2.59654 0.00000 -0.00047 0.00008 -0.00037 2.59617

R14 2.76211 -0.00000 -0.00014 0.00010 -0.00005 2.76206

R15 2.59385 0.00010 0.00017 0.00021 0.00039 2.59424

R16 2.76248 -0.00005 -0.00023 0.00008 -0.00016 2.76231

R17 2.64345 -0.00010 -0.00041 0.00010 -0.00031 2.64314

R18 2.55441 0.00003 0.00025 -0.00014 0.00009 2.55450

R19 2.03913 0.00002 -0.00002 0.00003 0.00001 2.03914

R20 2.03914 -0.00001 0.00001 -0.00001 -0.00000 2.03914

R21 2.64366 -0.00010 -0.00041 0.00012 -0.00029 2.64337

R22 2.80321 -0.00001 -0.00003 0.00004 0.00000 2.80321

R23 2.76248 -0.00006 -0.00028 0.00012 -0.00016 2.76232

R24 2.59373 0.00010 0.00019 0.00018 0.00038 2.59411

R25 2.55441 0.00004 0.00024 -0.00013 0.00010 2.55451

R26 2.03915 0.00002 -0.00002 0.00003 0.00001 2.03916

R27 2.76212 -0.00000 -0.00011 0.00007 -0.00005 2.76207

R28 2.03913 -0.00001 -0.00000 -0.00000 -0.00000 2.03913

R29 2.59661 -0.00001 -0.00044 0.00006 -0.00037 2.59624

R30 2.64086 0.00020 0.00030 0.00014 0.00045 2.64130

R31 2.71747 0.00002 -0.00006 -0.00013 -0.00019 2.71728

R32 2.80414 -0.00000 0.00001 0.00002 0.00003 2.80417

R33 2.65656 0.00007 0.00018 0.00001 0.00019 2.65675

R34 2.59882 -0.00006 -0.00014 0.00007 -0.00006 2.59877

R35 2.64115 -0.00000 -0.00007 -0.00001 -0.00009 2.64106

R36 2.03715 0.00001 -0.00001 0.00001 0.00000 2.03715

R37 2.65717 -0.00002 0.00000 0.00001 0.00001 2.65717

R38 2.03713 -0.00001 -0.00001 0.00001 0.00000 2.03713

R39 2.59904 -0.00009 0.00010 -0.00010 0.00001 2.59906

R40 2.71644 -0.00011 -0.00006 -0.00001 -0.00007 2.71637

R41 1.90990 -0.00011 0.00003 -0.00005 -0.00002 1.90988

R42 2.80387 -0.00000 0.00002 0.00004 0.00006 2.80394

R43 2.65166 -0.00003 -0.00004 0.00005 0.00000 2.65167

R44 2.65019 0.00003 0.00001 0.00001 0.00002 2.65021

R45 2.62851 -0.00001 0.00001 -0.00002 -0.00001 2.62850

R46 2.04842 -0.00000 0.00000 0.00000 0.00000 2.04842

R47 2.63637 -0.00001 0.00001 -0.00001 -0.00001 2.63637

R48 2.05017 0.00000 -0.00001 0.00002 0.00000 2.05018

R49 2.63417 -0.00000 0.00002 -0.00001 0.00001 2.63418

R50 2.05007 0.00000 -0.00000 0.00001 0.00000 2.05007

R51 2.63083 0.00002 -0.00000 0.00000 0.00000 2.63083

R52 2.05013 0.00000 -0.00001 0.00001 0.00001 2.05014

R53 2.04846 0.00002 0.00000 0.00001 0.00001 2.04848

R54 2.63636 0.00001 -0.00000 0.00000 0.00000 2.63637

R55 2.63425 -0.00000 -0.00001 0.00001 0.00000 2.63425

R56 2.05008 0.00000 -0.00001 0.00001 0.00000 2.05008

R57 2.62865 0.00001 -0.00005 0.00004 -0.00000 2.62864

R58 2.05017 0.00001 -0.00001 0.00001 0.00000 2.05017

R59 2.65166 -0.00002 -0.00000 -0.00000 -0.00001 2.65166

R60 2.04839 0.00000 -0.00001 0.00002 0.00000 2.04840

R61 2.65039 -0.00002 0.00001 -0.00003 -0.00002 2.65037

R62 2.63068 -0.00001 0.00002 -0.00003 -0.00000 2.63068

R63 2.04851 0.00000 -0.00001 0.00000 -0.00000 2.04850

R64 2.05015 0.00000 -0.00001 0.00002 0.00000 2.05015

R65 2.65014 -0.00002 -0.00000 -0.00003 -0.00004 2.65010

R66 2.65147 -0.00002 -0.00001 -0.00001 -0.00003 2.65145

R67 2.63079 -0.00001 0.00003 -0.00003 0.00000 2.63079

R68 2.04856 0.00000 -0.00000 0.00000 0.00000 2.04856

R69 2.63424 0.00000 -0.00001 0.00001 0.00000 2.63424

R70 2.05015 0.00000 -0.00002 0.00002 0.00000 2.05015

R71 2.63631 0.00001 -0.00001 0.00001 -0.00000 2.63631

R72 2.05008 0.00001 -0.00001 0.00001 0.00001 2.05008

R73 2.62873 0.00001 -0.00005 0.00005 0.00000 2.62873

R74 2.05018 0.00001 -0.00001 0.00001 0.00000 2.05018

R75 2.04840 0.00000 -0.00002 0.00002 0.00000 2.04840

R76 2.64994 0.00003 -0.00000 0.00000 0.00000 2.64994

R77 2.65144 -0.00004 -0.00002 0.00001 -0.00002 2.65142

R78 2.63093 0.00002 0.00001 0.00000 0.00001 2.63094

R79 2.04852 0.00002 0.00000 0.00002 0.00002 2.04853

R80 2.63416 -0.00000 0.00002 -0.00001 0.00001 2.63417

R81 2.05013 0.00000 -0.00001 0.00002 0.00001 2.05014

R82 2.63631 -0.00001 0.00000 -0.00001 -0.00001 2.63630

R83 2.05007 0.00000 -0.00000 0.00001 0.00000 2.05008

R84 2.62861 -0.00001 0.00001 -0.00001 -0.00000 2.62861

R85 2.05018 0.00000 -0.00001 0.00001 0.00000 2.05019

R86 2.04842 -0.00000 -0.00000 0.00000 0.00000 2.04842

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A2 2.18733 0.00001 0.00009 -0.00013 -0.00005 2.18728

A3 2.21432 0.00001 -0.00012 0.00016 0.00004 2.21436

A4 1.86768 0.00001 0.00003 -0.00003 0.00000 1.86768

A5 2.22245 0.00016 -0.00004 0.00021 0.00013 2.22258

A6 2.19259 -0.00017 0.00001 -0.00018 -0.00013 2.19246

A7 1.92562 0.00005 -0.00004 0.00009 0.00004 1.92567

A8 2.17849 -0.00009 -0.00007 -0.00009 -0.00015 2.17835

A9 2.17845 0.00004 0.00008 0.00004 0.00013 2.17859

A10 1.86800 -0.00005 0.00003 -0.00008 -0.00005 1.86795

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A12 2.22167 -0.00003 0.00002 0.00001 -0.00001 2.22167

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A15 2.18714 -0.00001 0.00019 -0.00026 -0.00008 2.18707

A16 2.18526 0.00016 -0.00012 0.00006 0.00000 2.18526

A17 2.02320 -0.00015 0.00008 -0.00008 -0.00003 2.02317

A18 2.07467 -0.00002 0.00003 0.00003 0.00003 2.07469

A19 2.19145 0.00010 -0.00011 0.00009 0.00003 2.19148

A20 2.16591 -0.00007 0.00002 -0.00010 -0.00012 2.16579

A21 1.92579 -0.00003 0.00008 0.00001 0.00009 1.92588

A22 1.84732 0.00001 0.00007 -0.00006 -0.00001 1.84732

A23 1.92645 -0.00000 -0.00005 -0.00003 -0.00008 1.92637

A24 2.19212 -0.00001 -0.00012 0.00002 -0.00006 2.19207

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A27 2.19693 0.00000 0.00010 -0.00009 0.00001 2.19694

A28 2.22379 0.00001 -0.00004 0.00004 -0.00001 2.22378

A29 1.86210 0.00004 -0.00005 0.00004 -0.00001 1.86209

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A31 2.22377 -0.00003 -0.00002 0.00000 -0.00002 2.22375

A32 2.18487 -0.00011 0.00003 -0.00009 -0.00001 2.18486

A33 2.02491 0.00008 -0.00025 0.00022 -0.00006 2.02485

A34 2.07336 0.00003 0.00021 -0.00012 0.00007 2.07343

A35 2.16478 0.00002 0.00015 0.00004 0.00015 2.16493

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D3 -3.11955 -0.00001 0.00008 -0.00005 0.00003 -3.11951

D4 0.05358 -0.00001 0.00001 -0.00008 -0.00007 0.05351

D5 -0.00091 -0.00000 0.00010 -0.00006 0.00005 -0.00086

D6 -3.13494 0.00000 -0.00002 0.00021 0.00020 -3.13475

D7 3.13439 0.00000 -0.00033 0.00034 0.00002 3.13441

D8 0.00036 0.00001 -0.00045 0.00061 0.00016 0.00052

D9 -0.02552 0.00001 0.00046 -0.00051 -0.00005 -0.02557

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D11 3.08523 0.00001 0.00053 -0.00048 0.00005 3.08528

D12 -0.09255 0.00003 0.00018 0.00076 0.00093 -0.09162

D13 -2.94072 -0.00001 0.00127 -0.00060 0.00068 -2.94004

D14 0.19080 -0.00002 0.00079 -0.00017 0.00062 0.19142

D15 0.23796 -0.00002 0.00118 -0.00063 0.00056 0.23852

D16 -2.91370 -0.00002 0.00070 -0.00020 0.00050 -2.91320

D17 0.02496 -0.00001 -0.00039 0.00048 0.00008 0.02505

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D21 -0.01441 0.00001 0.00017 -0.00025 -0.00008 -0.01449

D22 3.11977 0.00000 0.00029 -0.00051 -0.00022 3.11955

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D24 -0.05039 -0.00001 0.00041 -0.00056 -0.00015 -0.05054

D25 -0.24685 -0.00005 -0.00067 0.00022 -0.00046 -0.24731

D26 2.90612 -0.00006 0.00003 -0.00053 -0.00050 2.90562

D27 2.92837 -0.00004 -0.00082 0.00029 -0.00054 2.92783

D28 -0.20185 -0.00004 -0.00012 -0.00046 -0.00058 -0.20243

D29 -0.12928 -0.00003 -0.00019 0.00005 -0.00014 -0.12942

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D31 3.00063 -0.00003 -0.00091 0.00082 -0.00009 3.00053

D32 -0.13152 -0.00001 -0.00052 0.00058 0.00007 -0.13146

D33 -0.98559 0.00000 -0.00029 0.00033 0.00004 -0.98555

D34 2.15265 -0.00000 -0.00075 0.00081 0.00006 2.15272

D35 2.16662 -0.00000 0.00037 -0.00037 -0.00000 2.16662

D36 -0.97833 -0.00000 -0.00009 0.00011 0.00002 -0.97830

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D39 3.10564 -0.00002 -0.00036 0.00011 -0.00026 3.10538

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D43 -0.04187 -0.00001 -0.00002 0.00002 0.00001 -0.04186

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D47 -3.11179 -0.00000 -0.00031 0.00016 -0.00015 -3.11193

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D57 -3.01015 -0.00001 -0.00017 -0.00004 -0.00021 -3.01036

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D62 -2.15417 -0.00000 -0.00012 -0.00007 -0.00018 -2.15435

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D74 -0.00061 -0.00001 0.00032 -0.00049 -0.00017 -0.00078

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D87 -0.18702 -0.00002 0.00029 0.00040 0.00070 -0.18632

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D92 -0.99182 0.00001 -0.00002 -0.00044 -0.00046 -0.99228

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D101 -0.00091 -0.00000 0.00011 -0.00006 0.00004 -0.00086

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D103 -3.13741 -0.00001 -0.00040 0.00038 -0.00003 -3.13743

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D109 -0.02653 -0.00002 -0.00043 0.00031 -0.00012 -0.02665

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D134 -3.13407 0.00000 -0.00005 0.00010 0.00005 -3.13402

D135 -3.13615 -0.00000 -0.00009 0.00009 0.00000 -3.13615

D136 0.00784 0.00000 -0.00009 0.00014 0.00005 0.00789

D137 0.00727 0.00000 0.00000 0.00004 0.00004 0.00731

D138 -3.13146 -0.00000 0.00000 -0.00001 -0.00001 -3.13147

D139 -3.13672 -0.00000 0.00000 -0.00001 -0.00001 -3.13673

D140 0.00773 -0.00001 0.00000 -0.00006 -0.00006 0.00767

D141 -0.00786 -0.00001 0.00009 -0.00020 -0.00011 -0.00797

D142 -3.13116 -0.00000 0.00018 -0.00025 -0.00007 -3.13123

D143 3.13089 -0.00000 0.00009 -0.00015 -0.00006 3.13083

D144 0.00759 0.00000 0.00018 -0.00020 -0.00002 0.00757

D145 -0.00529 -0.00000 -0.00000 -0.00000 -0.00000 -0.00529

D146 3.13577 0.00000 -0.00002 0.00007 0.00005 3.13582

D147 3.13413 0.00000 -0.00007 0.00009 0.00002 3.13415

D148 -0.00800 0.00000 -0.00009 0.00017 0.00007 -0.00793

D149 -0.00693 0.00000 0.00006 -0.00009 -0.00004 -0.00697

D150 3.13184 -0.00000 -0.00001 -0.00006 -0.00006 3.13178

D151 3.13684 -0.00000 0.00013 -0.00019 -0.00006 3.13678

D152 -0.00757 -0.00000 0.00006 -0.00015 -0.00009 -0.00766

D153 0.01646 0.00001 -0.00012 0.00026 0.00014 0.01660

D154 3.13689 -0.00001 0.00003 -0.00005 -0.00003 3.13687

D155 -3.12460 0.00001 -0.00010 0.00019 0.00009 -3.12451

D156 -0.00417 -0.00001 0.00005 -0.00013 -0.00008 -0.00425

D157 3.12979 -0.00002 0.00044 -0.00068 -0.00025 3.12954

D158 -0.01513 -0.00002 0.00019 -0.00042 -0.00023 -0.01536

D159 0.00926 -0.00001 0.00029 -0.00037 -0.00008 0.00918

D160 -3.13567 -0.00000 0.00004 -0.00010 -0.00006 -3.13573

D161 3.14113 0.00002 -0.00038 0.00059 0.00021 3.14134

D162 0.01793 0.00001 -0.00029 0.00045 0.00015 0.01808

D163 0.00287 0.00002 -0.00014 0.00033 0.00019 0.00306

D164 -3.12034 0.00000 -0.00005 0.00018 0.00013 -3.12020

D165 0.00811 -0.00001 0.00002 -0.00007 -0.00006 0.00805

D166 -3.13068 -0.00001 0.00008 -0.00011 -0.00003 -3.13071

D167 3.13120 0.00000 -0.00007 0.00007 -0.00000 3.13120

D168 -0.00758 0.00001 -0.00001 0.00003 0.00002 -0.00756

D169 -3.14012 0.00003 -0.00029 0.00064 0.00034 -3.13978

D170 0.01882 0.00001 -0.00017 0.00038 0.00021 0.01903

D171 0.00263 0.00002 -0.00010 0.00027 0.00016 0.00279

D172 -3.12161 0.00000 0.00002 0.00001 0.00003 -3.12158

D173 3.12805 -0.00003 0.00031 -0.00068 -0.00037 3.12768

D174 0.00761 -0.00001 0.00029 -0.00049 -0.00020 0.00741

D175 -0.01470 -0.00002 0.00011 -0.00030 -0.00019 -0.01489

D176 -3.13514 -0.00000 0.00009 -0.00012 -0.00002 -3.13516

D177 0.00802 -0.00001 0.00004 -0.00010 -0.00006 0.00797

D178 -3.13106 -0.00001 0.00009 -0.00015 -0.00006 -3.13111

D179 3.13216 0.00001 -0.00008 0.00016 0.00008 3.13224

D180 -0.00692 0.00001 -0.00002 0.00010 0.00008 -0.00685

D181 -0.00671 0.00000 0.00001 -0.00004 -0.00002 -0.00674

D182 3.13671 -0.00000 0.00009 -0.00017 -0.00007 3.13663

D183 3.13235 -0.00000 -0.00004 0.00002 -0.00002 3.13233

D184 -0.00741 -0.00000 0.00004 -0.00011 -0.00007 -0.00748

D185 -0.00531 -0.00000 -0.00001 -0.00000 -0.00001 -0.00532

D186 3.13549 0.00000 -0.00001 0.00004 0.00003 3.13552

D187 3.13445 0.00000 -0.00009 0.00013 0.00004 3.13450

D188 -0.00793 0.00000 -0.00009 0.00017 0.00008 -0.00785

D189 0.01616 0.00001 -0.00006 0.00018 0.00012 0.01628

D190 3.13650 -0.00001 -0.00004 -0.00001 -0.00006 3.13644

D191 -3.12465 0.00001 -0.00005 0.00013 0.00008 -3.12457

D192 -0.00431 -0.00001 -0.00004 -0.00005 -0.00009 -0.00440

D193 3.13942 0.00001 0.00014 -0.00012 0.00002 3.13943

D194 -0.01939 0.00001 0.00001 0.00003 0.00004 -0.01935

D195 -0.00359 0.00001 -0.00011 0.00028 0.00017 -0.00342

D196 3.12079 0.00000 -0.00024 0.00043 0.00019 3.12098

D197 -3.12715 -0.00001 -0.00015 0.00017 0.00002 -3.12714

D198 -0.00677 -0.00000 -0.00018 0.00026 0.00008 -0.00669

D199 0.01585 -0.00001 0.00009 -0.00023 -0.00013 0.01572

D200 3.13624 -0.00000 0.00007 -0.00014 -0.00007 3.13616

D201 -0.00778 -0.00001 0.00004 -0.00016 -0.00012 -0.00790

D202 3.13123 -0.00000 0.00008 -0.00012 -0.00004 3.13120

D203 -3.13206 -0.00000 0.00017 -0.00031 -0.00014 -3.13220

D204 0.00696 0.00000 0.00021 -0.00027 -0.00006 0.00690

D205 0.00702 0.00001 0.00004 -0.00002 0.00002 0.00705

D206 -3.13661 0.00000 0.00003 -0.00003 0.00000 -3.13660

D207 -3.13198 -0.00000 0.00000 -0.00006 -0.00005 -3.13203

D208 0.00757 -0.00001 -0.00001 -0.00007 -0.00007 0.00750

D209 0.00519 -0.00000 -0.00006 0.00007 0.00001 0.00520

D210 -3.13589 -0.00000 -0.00005 0.00007 0.00002 -3.13586

D211 -3.13436 0.00000 -0.00005 0.00008 0.00003 -3.13433

D212 0.00775 0.00000 -0.00004 0.00008 0.00005 0.00779

D213 -0.01678 0.00001 -0.00001 0.00006 0.00005 -0.01673

D214 -3.13706 -0.00000 0.00001 -0.00003 -0.00001 -3.13708

D215 3.12430 0.00000 -0.00002 0.00005 0.00003 3.12433

D216 0.00402 -0.00000 0.00000 -0.00003 -0.00003 0.00399

Item Value Threshold Converged?

Maximum Force 0.000204 0.000450 YES

RMS Force 0.000038 0.000300 YES

Maximum Displacement 0.005121 0.001800 NO

RMS Displacement 0.000763 0.001200 YES

Predicted change in Energy=-9.324257D-07

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Wed Aug 28 07:44:24 2019, MaxMem= 4294967296 cpu: 2.5

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=1 Diff= 1.39D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 0.809595 -4.143593 0.574058

2 6 0 1.206465 -2.845447 0.207863

3 7 0 0.058428 -2.115837 0.005431

4 6 0 -1.050174 -2.906635 0.196394

5 6 0 -0.587590 -4.181514 0.566226

6 6 0 -2.415495 -2.495468 0.009751

7 6 0 -2.848201 -1.172634 -0.120043

8 7 0 -2.066844 -0.055832 0.052178

9 6 0 -2.908016 1.017802 -0.103894

10 6 0 -4.255965 0.563458 -0.440538

11 6 0 -4.218681 -0.787765 -0.451697

12 6 0 2.548370 -2.361119 0.030987

13 6 0 2.908066 -1.016640 -0.109253

14 6 0 4.255903 -0.560847 -0.444388

15 6 0 4.218566 0.790415 -0.450012

16 6 0 2.848058 1.173828 -0.116769

17 7 0 2.066821 0.056225 0.051043

18 6 0 2.415134 2.496041 0.017173

19 6 0 1.050232 2.907725 0.204759

20 6 0 0.587408 4.188055 0.555582

21 6 0 -0.809642 4.150172 0.563848

22 6 0 -1.206493 2.846592 0.216930

23 7 0 -0.058353 2.113764 0.026261

24 6 0 -2.548036 2.361722 0.039753

25 6 0 -3.421253 -3.585275 -0.029989

26 6 0 -3.304911 -4.629913 -0.959597

27 6 0 -4.255457 -5.644224 -1.008225

28 6 0 -5.327887 -5.644077 -0.115919

29 6 0 -5.446191 -4.619006 0.821267

30 6 0 -4.503785 -3.595089 0.861548

31 6 0 5.638385 -5.337603 -0.029038

32 6 0 4.577416 -5.410322 -0.932018

33 6 0 3.569332 -4.452197 -0.905764

34 6 0 3.614946 -3.391908 0.012204

35 6 0 4.686948 -3.328344 0.914325

36 6 0 5.687369 -4.296210 0.896326

37 6 0 -3.615351 3.392216 0.016949

38 6 0 -4.685751 3.332979 0.921043

39 6 0 -5.687976 4.298947 0.897724

40 6 0 -5.642154 5.333937 -0.034947

41 6 0 -4.582762 5.402093 -0.940085

42 6 0 -3.573032 4.445785 -0.908712

43 6 0 3.421710 3.585503 -0.025768

44 6 0 4.502044 3.598931 0.868160

45 6 0 5.446267 4.621075 0.823764

46 6 0 5.331739 5.640570 -0.119942

47 6 0 4.261520 5.636833 -1.014840

48 6 0 3.309293 4.624218 -0.962276

49 1 0 1.477311 -4.953309 0.820384

50 1 0 -1.213258 -5.026124 0.805708

51 1 0 -5.099833 1.197884 -0.663652

52 1 0 -5.026414 -1.463964 -0.685593

53 1 0 5.099667 -1.194381 -0.670444

54 1 0 5.026366 1.467559 -0.680895

55 1 0 1.212635 5.036983 0.780363

56 1 0 -1.477165 4.964207 0.795903

57 1 0 -2.475579 -4.632315 -1.657599

58 1 0 -4.159316 -6.435862 -1.743814

59 1 0 -6.064996 -6.439326 -0.149872

60 1 0 -6.271994 -4.616593 1.524846

61 1 0 -4.593775 -2.804817 1.598057

62 1 0 6.420519 -6.089203 -0.045741

63 1 0 4.535159 -6.214806 -1.658678

64 1 0 2.749336 -4.510500 -1.612296

65 1 0 4.723164 -2.525343 1.641636

66 1 0 6.504171 -4.237513 1.607933

67 1 0 -4.719843 2.534363 1.653308

68 1 0 -6.503835 4.243607 1.610679

69 1 0 -6.425723 6.083935 -0.055875

70 1 0 -4.543067 6.201385 -1.672602

71 1 0 -2.754435 4.500232 -1.617175

72 1 0 4.589403 2.812428 1.609050

73 1 0 6.270642 4.621488 1.529020

74 1 0 6.070286 6.434338 -0.157182

75 1 0 4.168441 6.423945 -1.755667

76 1 0 2.481823 4.623367 -1.662492

77 1 0 0.032941 -1.130994 -0.219137

78 1 0 -0.032780 1.122683 -0.170077

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0587909 0.0582855 0.0300946

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(Enter /home/kira/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5357.1553607236 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122295531 Hartrees.

Nuclear repulsion after empirical dispersion term = 5356.9431311704 Hartrees.

Force inversion solution in PCM.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5794

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.17D-10

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 321

GePol: Fraction of low-weight points (<1% of avg) = 5.54%

GePol: Cavity surface area = 611.130 Ang\*\*2

GePol: Cavity volume = 627.924 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0021062206 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5356.9410249499 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.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

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(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Wed Aug 28 07:44:27 2019, MaxMem= 4294967296 cpu: 2.3

(Enter /home/kira/g09/l401.exe)

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 0.999988 0.000007 0.000000 -0.004898 Ang= 0.56 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0183

Leave Link 401 at Wed Aug 28 07:44:30 2019, MaxMem= 4294967296 cpu: 47.0

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 590000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 100711308.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.77D-15 for 5778.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.52D-15 for 3603 355.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.22D-15 for 5778.

Iteration 1 A^-1\*A deviation from orthogonality is 5.76D-07 for 4884 4846.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.89D-15 for 175.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.33D-15 for 5316 404.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 1673.

Iteration 2 A^-1\*A deviation from orthogonality is 3.96D-16 for 4478 2548.

E= -1914.33333831172

DIIS: error= 4.22D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.33333831172 IErMin= 1 ErrMin= 4.22D-05

ErrMax= 4.22D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.38D-06 BMatP= 7.38D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.641 Goal= None Shift= 0.000

Gap= 0.706 Goal= None Shift= 0.000

RMSDP=3.35D-06 MaxDP=1.56D-04 OVMax= 5.89D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.35D-06 CP: 1.00D+00

E= -1914.33334164537 Delta-E= -0.000003333650 Rises=F Damp=F

DIIS: error= 5.45D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33334164537 IErMin= 2 ErrMin= 5.45D-06

ErrMax= 5.45D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D-07 BMatP= 7.38D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.444D-01 0.104D+01

Coeff: -0.444D-01 0.104D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.89D-07 MaxDP=3.84D-05 DE=-3.33D-06 OVMax= 4.23D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 5.60D-07 CP: 1.00D+00 1.05D+00

E= -1914.33334168406 Delta-E= -0.000000038684 Rises=F Damp=F

DIIS: error= 1.14D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33334168406 IErMin= 2 ErrMin= 5.45D-06

ErrMax= 1.14D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.80D-07 BMatP= 1.37D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.365D-01 0.588D+00 0.448D+00

Coeff: -0.365D-01 0.588D+00 0.448D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.93D-07 MaxDP=1.82D-05 DE=-3.87D-08 OVMax= 1.03D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.63D-07 CP: 1.00D+00 1.07D+00 7.78D-01

E= -1914.33334173205 Delta-E= -0.000000047996 Rises=F Damp=F

DIIS: error= 3.86D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33334173205 IErMin= 4 ErrMin= 3.86D-06

ErrMax= 3.86D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.16D-08 BMatP= 1.37D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.118D-01 0.141D+00 0.255D+00 0.615D+00

Coeff: -0.118D-01 0.141D+00 0.255D+00 0.615D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.89D-07 MaxDP=1.48D-05 DE=-4.80D-08 OVMax= 1.76D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.23D-07 CP: 1.00D+00 1.07D+00 1.03D+00 1.04D+00

E= -1914.33334174410 Delta-E= -0.000000012046 Rises=F Damp=F

DIIS: error= 2.35D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33334174410 IErMin= 5 ErrMin= 2.35D-06

ErrMax= 2.35D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.61D-09 BMatP= 2.16D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.154D-02-0.147D-02 0.736D-01 0.371D+00 0.559D+00

Coeff: -0.154D-02-0.147D-02 0.736D-01 0.371D+00 0.559D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.18D-07 MaxDP=8.13D-06 DE=-1.20D-08 OVMax= 1.17D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.83D-08 CP: 1.00D+00 1.08D+00 1.15D+00 1.31D+00 1.32D+00

E= -1914.33334174958 Delta-E= -0.000000005476 Rises=F Damp=F

DIIS: error= 2.14D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33334174958 IErMin= 6 ErrMin= 2.14D-06

ErrMax= 2.14D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.64D-09 BMatP= 5.61D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.523D-02-0.716D-01-0.107D+00-0.822D-01 0.152D+00 0.110D+01

Coeff: 0.523D-02-0.716D-01-0.107D+00-0.822D-01 0.152D+00 0.110D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.08D-07 MaxDP=1.68D-05 DE=-5.48D-09 OVMax= 2.20D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.57D-08 CP: 1.00D+00 1.08D+00 1.39D+00 1.72D+00 2.15D+00

CP: 2.02D+00

E= -1914.33334175571 Delta-E= -0.000000006133 Rises=F Damp=F

DIIS: error= 1.40D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33334175571 IErMin= 7 ErrMin= 1.40D-06

ErrMax= 1.40D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.48D-10 BMatP= 1.64D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.250D-02-0.211D-01-0.808D-01-0.149D+00-0.253D+00 0.347D+00

Coeff-Com: 0.115D+01

Coeff: 0.250D-02-0.211D-01-0.808D-01-0.149D+00-0.253D+00 0.347D+00

Coeff: 0.115D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.01D-07 MaxDP=1.58D-05 DE=-6.13D-09 OVMax= 2.15D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.74D-08 CP: 1.00D+00 1.09D+00 1.60D+00 2.11D+00 2.94D+00

CP: 3.00D+00 1.79D+00

E= -1914.33334175934 Delta-E= -0.000000003629 Rises=F Damp=F

DIIS: error= 8.53D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33334175934 IErMin= 8 ErrMin= 8.53D-07

ErrMax= 8.53D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.12D-10 BMatP= 9.48D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.172D-02 0.354D-01 0.337D-02-0.413D-01-0.317D+00-0.530D+00

Coeff-Com: 0.949D+00 0.902D+00

Coeff: -0.172D-02 0.354D-01 0.337D-02-0.413D-01-0.317D+00-0.530D+00

Coeff: 0.949D+00 0.902D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.91D-07 MaxDP=1.53D-05 DE=-3.63D-09 OVMax= 2.09D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.01D-07 CP: 1.00D+00 1.10D+00 1.80D+00 2.47D+00 3.00D+00

CP: 3.00D+00 2.86D+00 2.64D+00

E= -1914.33334176087 Delta-E= -0.000000001529 Rises=F Damp=F

DIIS: error= 3.20D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33334176087 IErMin= 9 ErrMin= 3.20D-07

ErrMax= 3.20D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.76D-11 BMatP= 5.12D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.797D-03 0.118D-01 0.829D-02 0.204D-01-0.125D-01-0.177D+00

Coeff-Com: 0.856D-02 0.289D+00 0.853D+00

Coeff: -0.797D-03 0.118D-01 0.829D-02 0.204D-01-0.125D-01-0.177D+00

Coeff: 0.856D-02 0.289D+00 0.853D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.74D-08 MaxDP=2.17D-06 DE=-1.53D-09 OVMax= 2.88D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.05D-08 CP: 1.00D+00 1.10D+00 1.82D+00 2.51D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.13D+00

E= -1914.33334176100 Delta-E= -0.000000000138 Rises=F Damp=F

DIIS: error= 1.98D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33334176100 IErMin=10 ErrMin= 1.98D-07

ErrMax= 1.98D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.03D-11 BMatP= 7.76D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.210D-03-0.761D-02 0.982D-03 0.322D-01 0.139D+00 0.113D+00

Coeff-Com: -0.435D+00-0.172D+00 0.552D+00 0.778D+00

Coeff: 0.210D-03-0.761D-02 0.982D-03 0.322D-01 0.139D+00 0.113D+00

Coeff: -0.435D+00-0.172D+00 0.552D+00 0.778D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.95D-08 MaxDP=1.44D-06 DE=-1.38D-10 OVMax= 1.92D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.04D-08 CP: 1.00D+00 1.10D+00 1.83D+00 2.53D+00 3.00D+00

CP: 3.00D+00 3.00D+00 3.00D+00 1.21D+00 2.04D+00

E= -1914.33334176099 Delta-E= 0.000000000015 Rises=F Damp=F

DIIS: error= 7.34D-08 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=10 EnMin= -1914.33334176100 IErMin=11 ErrMin= 7.34D-08

ErrMax= 7.34D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.99D-12 BMatP= 4.03D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.309D-03-0.671D-02-0.298D-02 0.104D-01 0.729D-01 0.102D+00

Coeff-Com: -0.221D+00-0.147D+00 0.420D-01 0.375D+00 0.775D+00

Coeff: 0.309D-03-0.671D-02-0.298D-02 0.104D-01 0.729D-01 0.102D+00

Coeff: -0.221D+00-0.147D+00 0.420D-01 0.375D+00 0.775D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=8.14D-09 MaxDP=6.55D-07 DE= 1.46D-11 OVMax= 7.40D-06

Error on total polarization charges = 0.08257

SCF Done: E(UB3LYP) = -1914.33334176 A.U. after 11 cycles

NFock= 11 Conv=0.81D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0183

<L.S>= 0.000000000000E+00

KE= 1.906377411476D+03 PE=-1.516350013609D+04 EE= 5.985848357904D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0551, after 2.0017

Leave Link 502 at Wed Aug 28 07:49:31 2019, MaxMem= 4294967296 cpu: 4752.3

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48637977D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64374222D-01

Leave Link 801 at Wed Aug 28 07:49:31 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Wed Aug 28 07:49:38 2019, MaxMem= 4294967296 cpu: 111.5

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Wed Aug 28 07:49:38 2019, MaxMem= 4294967296 cpu: 2.0

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 188

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Wed Aug 28 08:09:15 2019, MaxMem= 4294967296 cpu: 18815.0

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 590000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.44D+03 4.54D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.56D+02 3.71D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.62D+00 4.69D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.03D-01 3.95D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.64D-04 2.11D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.62D-06 1.35D-04.

188 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 2.00D-08 1.01D-05.

80 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.31D-11 6.28D-07.

39 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.28D-13 3.99D-08.

6 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 1.08D-14 7.54D-09.

6 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 7.69D-15 2.79D-09.

3 vectors produced by pass 11 Test12= 2.55D-13 1.00D-09 XBig12= 4.81D-15 2.20D-09.

2 vectors produced by pass 12 Test12= 2.55D-13 1.00D-09 XBig12= 3.39D-15 2.21D-09.

InvSVY: IOpt=1 It= 1 EMax= 8.53D-14

Solved reduced A of dimension 1731 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1127.63 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Wed Aug 28 12:00:26 2019, MaxMem= 4294967296 cpu: 221887.5

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 188

Leave Link 701 at Wed Aug 28 12:01:56 2019, MaxMem= 4294967296 cpu: 1428.3

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Wed Aug 28 12:01:56 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

Compute integral second derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

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= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Wed Aug 28 12:21:29 2019, MaxMem= 4294967296 cpu: 18765.8

(Enter /home/kira/g09/l716.exe)

Dipole =-1.44383910D-04-1.11272051D-02-5.02728136D-01

Polarizability= 1.25661424D+03-1.23757096D+01 1.67352651D+03

-9.76196670D-03-3.46258331D-02 4.52744644D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000036656 0.000010628 -0.000003588

2 6 0.000017329 -0.000001997 0.000033587

3 7 -0.000015206 -0.000015675 0.000014401

4 6 -0.000008268 -0.000012172 -0.000009432

5 6 0.000012857 -0.000008960 0.000009022

6 6 0.000029860 0.000004716 0.000018187

7 6 -0.000035507 0.000000639 0.000002486

8 7 -0.000019295 0.000010632 0.000023509

9 6 -0.000102949 -0.000017015 -0.000005912

10 6 0.000013575 -0.000008002 -0.000008348

11 6 0.000001484 0.000001457 0.000019885

12 6 -0.000069159 0.000014753 -0.000014629

13 6 0.000100530 -0.000014755 0.000008215

14 6 -0.000013194 -0.000010021 0.000008379

15 6 -0.000002184 0.000004547 -0.000021334

16 6 0.000035857 0.000003018 0.000000390

17 7 -0.000000392 0.000023372 -0.000016431

18 6 -0.000032434 0.000001520 -0.000020837

19 6 0.000010703 -0.000013324 0.000013535

20 6 -0.000011047 -0.000010691 -0.000007771

21 6 0.000038153 0.000006209 0.000002455

22 6 -0.000020837 -0.000004153 -0.000034074

23 7 0.000009649 -0.000008397 -0.000009733

24 6 0.000074850 0.000015615 0.000013855

25 6 0.000028949 0.000006098 0.000047689

26 6 -0.000056132 0.000013887 -0.000038755

27 6 0.000017537 -0.000009610 0.000032054

28 6 -0.000028107 0.000013860 -0.000010834

29 6 0.000041857 -0.000020426 0.000016289

30 6 -0.000015989 0.000026181 -0.000027595

31 6 0.000017404 -0.000019593 0.000000198

32 6 -0.000020341 0.000010664 0.000035200

33 6 0.000039330 -0.000028554 -0.000029461

34 6 -0.000013827 0.000034838 0.000021149

35 6 0.000037961 -0.000014054 -0.000049610

36 6 -0.000044728 0.000030598 0.000017730

37 6 0.000009779 0.000031126 -0.000019515

38 6 -0.000034875 -0.000015046 0.000047438

39 6 0.000042794 0.000026489 -0.000015172

40 6 -0.000016838 -0.000022563 -0.000001193

41 6 0.000016945 0.000004964 -0.000032994

42 6 -0.000037572 -0.000026802 0.000025393

43 6 -0.000027590 0.000005586 -0.000048140

44 6 0.000017852 0.000026795 0.000026674

45 6 -0.000042948 -0.000023336 -0.000018088

46 6 0.000029175 0.000010959 0.000010632

47 6 -0.000017260 -0.000011834 -0.000031513

48 6 0.000056664 0.000006325 0.000036087

49 1 0.000005863 0.000015611 -0.000013476

50 1 -0.000000085 -0.000016209 -0.000007236

51 1 -0.000012061 0.000004575 -0.000008513

52 1 -0.000016897 -0.000004363 0.000001224

53 1 0.000011774 0.000004745 0.000008142

54 1 0.000015988 -0.000005145 -0.000000966

55 1 -0.000003932 -0.000013461 0.000009522

56 1 -0.000002668 0.000012738 0.000014434

57 1 0.000009176 0.000001816 -0.000005776

58 1 -0.000001180 -0.000000014 -0.000004450

59 1 0.000005361 -0.000001215 0.000006110

60 1 -0.000002993 0.000002427 -0.000003491

61 1 -0.000007574 -0.000011125 -0.000014219

62 1 -0.000003588 0.000005413 0.000005405

63 1 0.000003835 0.000002915 -0.000004964

64 1 -0.000016432 -0.000003676 -0.000007890

65 1 0.000002138 -0.000003732 0.000001266

66 1 0.000005536 -0.000002866 -0.000001050

67 1 -0.000000791 -0.000004618 -0.000000381

68 1 -0.000004647 -0.000005260 0.000001075

69 1 0.000003448 0.000002270 -0.000005590

70 1 -0.000004446 0.000000012 0.000004499

71 1 0.000016388 -0.000005757 0.000007564

72 1 0.000007066 -0.000013761 0.000015284

73 1 0.000003758 0.000000347 0.000003436

74 1 -0.000005587 -0.000003791 -0.000005722

75 1 0.000000005 -0.000002951 0.000004005

76 1 -0.000009812 0.000000482 0.000005952

77 1 0.000093539 0.000033634 0.000067601

78 1 -0.000068941 -0.000017530 -0.000081277

-------------------------------------------------------------------

Cartesian Forces: Max 0.000102949 RMS 0.000024258

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Wed Aug 28 12:21:29 2019, MaxMem= 4294967296 cpu: 2.3

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000161094 RMS 0.000032775

Search for a local minimum.

Step number 15 out of a maximum of 452

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= 1.43D-06 DEPred=-9.32D-07 R=-1.53D+00

Trust test=-1.53D+00 RLast= 4.35D-03 DXMaxT set to 8.44D-02

ITU= -1 1 0 -1 1 1 -1 1 -1 -1 1 1 -1 1 0

Eigenvalues --- 0.00069 0.00106 0.00513 0.00617 0.00735

Eigenvalues --- 0.00877 0.01008 0.01046 0.01061 0.01119

Eigenvalues --- 0.01127 0.01211 0.01261 0.01288 0.01302

Eigenvalues --- 0.01311 0.01338 0.01432 0.01460 0.01474

Eigenvalues --- 0.01478 0.01522 0.01544 0.01653 0.01721

Eigenvalues --- 0.01725 0.01731 0.01743 0.01750 0.01756

Eigenvalues --- 0.01763 0.01787 0.01808 0.01825 0.01892

Eigenvalues --- 0.01930 0.01963 0.01974 0.01991 0.02153

Eigenvalues --- 0.02191 0.02256 0.02280 0.02289 0.02306

Eigenvalues --- 0.02334 0.02431 0.02455 0.02535 0.02548

Eigenvalues --- 0.02551 0.02553 0.02605 0.02606 0.02615

Eigenvalues --- 0.02622 0.02626 0.02751 0.02756 0.02783

Eigenvalues --- 0.02805 0.02867 0.02871 0.02872 0.02874

Eigenvalues --- 0.03058 0.03073 0.03910 0.04088 0.04194

Eigenvalues --- 0.04327 0.04376 0.04444 0.04527 0.04545

Eigenvalues --- 0.08329 0.09697 0.09712 0.09825 0.09908

Eigenvalues --- 0.09933 0.10329 0.10454 0.10598 0.10686

Eigenvalues --- 0.10687 0.10715 0.10717 0.10737 0.11070

Eigenvalues --- 0.11400 0.11405 0.11420 0.11428 0.12010

Eigenvalues --- 0.12014 0.12018 0.12024 0.12261 0.12262

Eigenvalues --- 0.12295 0.12296 0.12776 0.12781 0.12788

Eigenvalues --- 0.12795 0.15716 0.15956 0.16303 0.17082

Eigenvalues --- 0.17241 0.17306 0.17554 0.17861 0.17962

Eigenvalues --- 0.18094 0.18163 0.18528 0.19251 0.19289

Eigenvalues --- 0.19348 0.19353 0.19371 0.19400 0.19407

Eigenvalues --- 0.19456 0.19549 0.19550 0.19555 0.19557

Eigenvalues --- 0.20288 0.21511 0.22046 0.22817 0.22880

Eigenvalues --- 0.23407 0.23753 0.24278 0.24724 0.25453

Eigenvalues --- 0.26278 0.26506 0.26639 0.27217 0.28499

Eigenvalues --- 0.28538 0.28691 0.28948 0.29733 0.30997

Eigenvalues --- 0.31692 0.32014 0.32829 0.33118 0.33337

Eigenvalues --- 0.33412 0.34191 0.35105 0.35582 0.35613

Eigenvalues --- 0.35628 0.35635 0.35645 0.35673 0.35751

Eigenvalues --- 0.35762 0.35790 0.35818 0.35921 0.35923

Eigenvalues --- 0.35928 0.35931 0.36008 0.36015 0.36022

Eigenvalues --- 0.36024 0.36212 0.36248 0.36270 0.36277

Eigenvalues --- 0.37079 0.37086 0.37252 0.37394 0.37404

Eigenvalues --- 0.37542 0.38165 0.38531 0.38585 0.38771

Eigenvalues --- 0.39494 0.40493 0.40722 0.40997 0.41007

Eigenvalues --- 0.41104 0.41133 0.41164 0.41218 0.41395

Eigenvalues --- 0.41565 0.41826 0.42321 0.42946 0.44709

Eigenvalues --- 0.45395 0.45901 0.45912 0.45951 0.45974

Eigenvalues --- 0.46169 0.46229 0.46236 0.46277 0.46290

Eigenvalues --- 0.48183 0.48541 0.49044 0.49320 0.50282

Eigenvalues --- 0.50753 0.50755 0.50781 0.50798 0.51882

Eigenvalues --- 0.52473 0.57123 0.58353

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: -0.67152 1.23731 0.32477 0.10945

Cosine: 0.817 > 0.500

Length: 0.588

GDIIS step was calculated using 4 of the last 15 vectors.

Iteration 1 RMS(Cart)= 0.02706790 RMS(Int)= 0.00003391

Iteration 2 RMS(Cart)= 0.00012824 RMS(Int)= 0.00000298

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000298

ITry= 1 IFail=0 DXMaxC= 1.25D-01 DCOld= 1.00D+10 DXMaxT= 8.44D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.65692 -0.00003 0.00008 -0.00004 0.00004 2.65696

R2 2.64131 0.00001 -0.00003 0.00007 0.00005 2.64136

R3 2.03719 -0.00001 0.00000 -0.00002 -0.00001 2.03718

R4 2.59884 -0.00007 0.00000 0.00008 0.00008 2.59892

R5 2.71659 -0.00007 -0.00008 -0.00047 -0.00055 2.71604

R6 2.59851 -0.00001 0.00012 -0.00044 -0.00032 2.59819

R7 1.90946 -0.00008 0.00005 -0.00013 -0.00007 1.90939

R8 2.65644 0.00003 -0.00012 0.00010 -0.00001 2.65643

R9 2.71753 0.00004 0.00004 0.00053 0.00056 2.71809

R10 2.03721 0.00001 0.00001 0.00004 0.00005 2.03726

R11 2.64154 0.00010 -0.00038 -0.00008 -0.00046 2.64108

R12 2.80343 -0.00000 -0.00012 0.00024 0.00012 2.80355

R13 2.59617 0.00003 0.00040 0.00022 0.00061 2.59678

R14 2.76206 0.00001 -0.00008 0.00013 0.00004 2.76211

R15 2.59424 0.00005 -0.00047 -0.00002 -0.00050 2.59375

R16 2.76231 -0.00002 0.00008 -0.00012 -0.00004 2.76227

R17 2.64314 -0.00009 0.00046 0.00004 0.00050 2.64364

R18 2.55450 -0.00001 0.00000 -0.00002 -0.00001 2.55449

R19 2.03914 0.00001 -0.00002 0.00007 0.00005 2.03920

R20 2.03914 -0.00001 0.00001 -0.00005 -0.00004 2.03910

R21 2.64337 -0.00008 0.00051 0.00002 0.00053 2.64390

R22 2.80321 -0.00000 -0.00013 -0.00008 -0.00020 2.80301

R23 2.76232 -0.00002 0.00004 -0.00009 -0.00005 2.76226

R24 2.59411 0.00005 -0.00049 -0.00003 -0.00052 2.59359

R25 2.55451 -0.00000 -0.00000 -0.00001 -0.00000 2.55451

R26 2.03916 0.00001 -0.00001 0.00006 0.00006 2.03921

R27 2.76207 0.00001 -0.00006 0.00009 0.00004 2.76211

R28 2.03913 -0.00001 -0.00000 -0.00004 -0.00004 2.03909

R29 2.59624 0.00001 0.00045 0.00018 0.00063 2.59687

R30 2.64130 0.00009 -0.00043 -0.00005 -0.00048 2.64083

R31 2.71728 0.00003 -0.00000 0.00052 0.00052 2.71780

R32 2.80417 -0.00001 0.00009 0.00010 0.00019 2.80436

R33 2.65675 0.00003 -0.00004 0.00006 0.00002 2.65677

R34 2.59877 -0.00001 0.00015 -0.00044 -0.00029 2.59848

R35 2.64106 0.00001 -0.00009 0.00012 0.00003 2.64109

R36 2.03715 0.00001 -0.00001 0.00005 0.00004 2.03720

R37 2.65717 -0.00004 0.00018 -0.00012 0.00007 2.65724

R38 2.03713 -0.00001 -0.00001 -0.00000 -0.00001 2.03712

R39 2.59906 -0.00007 0.00004 0.00004 0.00008 2.59914

R40 2.71637 -0.00008 -0.00011 -0.00045 -0.00056 2.71580

R41 1.90988 -0.00007 0.00014 -0.00019 -0.00006 1.90982

R42 2.80394 -0.00000 0.00009 -0.00021 -0.00012 2.80381

R43 2.65167 -0.00002 0.00003 -0.00002 0.00001 2.65168

R44 2.65021 0.00003 0.00004 -0.00003 0.00002 2.65022

R45 2.62850 -0.00002 0.00001 -0.00007 -0.00006 2.62845

R46 2.04842 -0.00000 -0.00001 -0.00001 -0.00002 2.04840

R47 2.63637 -0.00001 0.00002 -0.00002 -0.00000 2.63636

R48 2.05018 -0.00000 -0.00001 -0.00000 -0.00001 2.05017

R49 2.63418 -0.00001 0.00000 -0.00004 -0.00004 2.63413

R50 2.05007 -0.00000 -0.00000 0.00001 0.00000 2.05008

R51 2.63083 0.00001 -0.00004 0.00009 0.00005 2.63089

R52 2.05014 0.00000 -0.00000 0.00001 0.00000 2.05014

R53 2.04848 0.00001 -0.00003 0.00003 -0.00000 2.04848

R54 2.63637 0.00001 0.00000 0.00000 0.00000 2.63637

R55 2.63425 -0.00001 0.00000 0.00002 0.00002 2.63427

R56 2.05008 0.00000 -0.00001 0.00002 0.00001 2.05010

R57 2.62864 0.00002 -0.00002 0.00007 0.00004 2.62868

R58 2.05017 0.00000 -0.00000 0.00002 0.00001 2.05018

R59 2.65166 -0.00001 0.00003 -0.00006 -0.00003 2.65163

R60 2.04840 0.00000 0.00000 0.00000 0.00000 2.04840

R61 2.65037 -0.00002 0.00007 -0.00003 0.00004 2.65041

R62 2.63068 -0.00002 0.00000 -0.00008 -0.00008 2.63060

R63 2.04850 0.00000 0.00000 0.00001 0.00002 2.04852

R64 2.05015 0.00000 -0.00000 0.00001 0.00001 2.05016

R65 2.65010 -0.00002 -0.00001 0.00002 0.00000 2.65011

R66 2.65145 -0.00001 -0.00002 -0.00004 -0.00006 2.65138

R67 2.63079 -0.00001 0.00003 -0.00010 -0.00006 2.63072

R68 2.04856 0.00000 0.00002 0.00001 0.00002 2.04858

R69 2.63424 -0.00000 -0.00000 0.00002 0.00002 2.63426

R70 2.05015 0.00000 -0.00000 0.00001 0.00001 2.05016

R71 2.63631 0.00001 -0.00002 0.00002 -0.00000 2.63631

R72 2.05008 0.00000 -0.00001 0.00002 0.00001 2.05010

R73 2.62873 0.00002 -0.00000 0.00006 0.00006 2.62879

R74 2.05018 0.00000 0.00000 0.00001 0.00002 2.05019

R75 2.04840 0.00000 -0.00000 0.00001 0.00000 2.04841

R76 2.64994 0.00003 -0.00003 0.00002 -0.00001 2.64993

R77 2.65142 -0.00002 -0.00001 0.00000 -0.00001 2.65141

R78 2.63094 0.00001 -0.00001 0.00007 0.00006 2.63100

R79 2.04853 0.00001 -0.00001 0.00002 0.00001 2.04854

R80 2.63417 -0.00001 -0.00000 -0.00004 -0.00004 2.63412

R81 2.05014 0.00000 -0.00001 0.00001 0.00000 2.05014

R82 2.63630 -0.00001 -0.00000 -0.00001 -0.00001 2.63630

R83 2.05008 -0.00000 -0.00000 0.00001 0.00000 2.05008

R84 2.62861 -0.00002 0.00003 -0.00007 -0.00004 2.62857

R85 2.05019 -0.00000 -0.00001 -0.00000 -0.00001 2.05018

R86 2.04842 -0.00000 -0.00001 -0.00001 -0.00002 2.04840

A1 1.88153 -0.00001 0.00000 -0.00017 -0.00017 1.88135

A2 2.18728 0.00002 -0.00005 0.00022 0.00017 2.18745

A3 2.21436 -0.00000 0.00004 -0.00004 0.00001 2.21436

A4 1.86768 0.00001 0.00001 -0.00001 -0.00000 1.86768

A5 2.22258 0.00014 -0.00028 0.00161 0.00135 2.22393

A6 2.19246 -0.00015 0.00029 -0.00169 -0.00140 2.19106

A7 1.92567 0.00004 -0.00007 0.00016 0.00009 1.92576

A8 2.17835 -0.00008 0.00025 -0.00187 -0.00161 2.17674

A9 2.17859 0.00005 -0.00015 0.00168 0.00153 2.18012

A10 1.86795 -0.00004 0.00006 -0.00011 -0.00005 1.86790

A11 2.19319 0.00008 -0.00003 0.00096 0.00093 2.19412

A12 2.22167 -0.00004 -0.00001 -0.00085 -0.00084 2.22082

A13 1.88159 0.00001 0.00001 0.00011 0.00013 1.88171

A14 2.21450 -0.00000 -0.00003 0.00021 0.00019 2.21469

A15 2.18707 -0.00001 0.00001 -0.00033 -0.00032 2.18675

A16 2.18526 0.00016 -0.00028 0.00085 0.00055 2.18582

A17 2.02317 -0.00012 0.00013 -0.00127 -0.00113 2.02205

A18 2.07469 -0.00003 0.00014 0.00042 0.00056 2.07526

A19 2.19148 0.00010 -0.00018 0.00016 -0.00002 2.19146

A20 2.16579 -0.00007 0.00024 -0.00000 0.00025 2.16604

A21 1.92588 -0.00003 -0.00007 -0.00018 -0.00025 1.92564

A22 1.84732 -0.00000 -0.00001 0.00001 -0.00000 1.84731

A23 1.92637 0.00001 0.00011 0.00009 0.00020 1.92657

A24 2.19207 -0.00003 0.00003 0.00013 0.00015 2.19221

A25 2.16474 0.00002 -0.00014 -0.00020 -0.00034 2.16440

A26 1.86206 -0.00001 -0.00002 -0.00001 -0.00003 1.86203

A27 2.19694 0.00000 0.00004 -0.00014 -0.00010 2.19684

A28 2.22378 0.00001 -0.00001 0.00010 0.00009 2.22387

A29 1.86209 0.00004 -0.00001 0.00007 0.00006 1.86215

A30 2.19697 -0.00001 -0.00004 0.00016 0.00013 2.19709

A31 2.22375 -0.00003 0.00005 -0.00021 -0.00016 2.22359

A32 2.18486 -0.00012 -0.00013 -0.00057 -0.00071 2.18415

A33 2.02485 0.00012 -0.00006 0.00114 0.00109 2.02594

A34 2.07343 0.00000 0.00018 -0.00055 -0.00037 2.07306

A35 2.16493 0.00002 -0.00014 -0.00017 -0.00030 2.16463

A36 2.19186 -0.00003 -0.00000 0.00012 0.00010 2.19196

A37 1.92638 0.00000 0.00014 0.00007 0.00021 1.92659

A38 1.86207 -0.00001 -0.00001 -0.00001 -0.00003 1.86205

A39 2.19686 0.00000 -0.00000 -0.00011 -0.00011 2.19674

A40 2.22384 0.00001 0.00002 0.00008 0.00010 2.22394

A41 1.86206 0.00003 -0.00001 0.00007 0.00006 1.86212

A42 2.22371 -0.00003 0.00000 -0.00016 -0.00016 2.22355

A43 2.19705 -0.00001 0.00000 0.00013 0.00013 2.19718

A44 1.92586 -0.00003 -0.00009 -0.00016 -0.00025 1.92561

A45 2.16570 -0.00006 0.00019 0.00003 0.00023 2.16593

A46 2.19160 0.00008 -0.00010 0.00011 0.00000 2.19160

A47 1.84734 0.00000 -0.00003 0.00002 -0.00000 1.84733

A48 2.18627 0.00016 0.00001 0.00067 0.00067 2.18694

A49 2.07333 -0.00003 -0.00022 0.00060 0.00039 2.07373

A50 2.02356 -0.00013 0.00021 -0.00128 -0.00106 2.02250

A51 2.22153 -0.00005 0.00003 -0.00086 -0.00081 2.22073

A52 2.19316 0.00010 -0.00011 0.00101 0.00089 2.19405

A53 1.86794 -0.00004 0.00005 -0.00010 -0.00006 1.86788

A54 1.88165 0.00001 0.00002 0.00012 0.00013 1.88178

A55 2.18739 -0.00001 0.00009 -0.00039 -0.00029 2.18710

A56 2.21413 -0.00000 -0.00011 0.00027 0.00016 2.21429

A57 1.88157 -0.00001 0.00002 -0.00019 -0.00017 1.88140

A58 2.21403 -0.00000 -0.00006 0.00004 -0.00002 2.21401

A59 2.18758 0.00002 0.00005 0.00015 0.00020 2.18778

A60 1.86771 0.00002 -0.00002 0.00003 0.00000 1.86771

A61 2.22249 0.00014 -0.00031 0.00161 0.00131 2.22380

A62 2.19233 -0.00016 0.00030 -0.00170 -0.00141 2.19092

A63 1.92552 0.00003 -0.00008 0.00016 0.00009 1.92561

A64 2.17848 0.00006 -0.00032 0.00183 0.00151 2.18000

A65 2.17798 -0.00009 0.00029 -0.00195 -0.00165 2.17632

A66 2.18580 -0.00013 0.00019 -0.00077 -0.00060 2.18520

A67 2.07214 0.00001 -0.00020 -0.00031 -0.00050 2.07164

A68 2.02524 0.00012 0.00001 0.00108 0.00110 2.02634

A69 2.10416 -0.00004 0.00023 -0.00131 -0.00108 2.10308

A70 2.10764 0.00005 -0.00022 0.00137 0.00114 2.10878

A71 2.07138 -0.00001 -0.00001 -0.00006 -0.00006 2.07132

A72 2.10527 0.00002 -0.00004 0.00018 0.00013 2.10540

A73 2.08481 0.00000 -0.00001 -0.00005 -0.00006 2.08476

A74 2.09291 -0.00002 0.00005 -0.00013 -0.00008 2.09283

A75 2.09773 -0.00000 0.00004 -0.00012 -0.00009 2.09764

A76 2.08892 0.00001 -0.00003 0.00007 0.00005 2.08896

A77 2.09654 -0.00000 -0.00001 0.00005 0.00004 2.09658

A78 2.08902 0.00000 0.00000 -0.00000 -0.00000 2.08901

A79 2.09695 -0.00001 0.00001 0.00001 0.00002 2.09697

A80 2.09722 0.00000 -0.00001 -0.00001 -0.00002 2.09720

A81 2.09769 0.00000 -0.00002 0.00010 0.00008 2.09777

A82 2.09701 0.00000 0.00002 -0.00003 -0.00001 2.09699

A83 2.08848 -0.00000 0.00001 -0.00007 -0.00006 2.08842

A84 2.10514 -0.00001 0.00003 -0.00010 -0.00007 2.10507

A85 2.08392 0.00002 -0.00000 0.00020 0.00020 2.08412

A86 2.09399 -0.00001 -0.00003 -0.00010 -0.00013 2.09386

A87 2.08900 -0.00001 -0.00002 0.00001 -0.00001 2.08899

A88 2.09694 0.00001 0.00001 -0.00003 -0.00002 2.09692

A89 2.09724 0.00000 0.00001 0.00003 0.00003 2.09727

A90 2.09788 0.00001 -0.00002 0.00008 0.00007 2.09795

A91 2.09647 -0.00000 -0.00000 -0.00003 -0.00003 2.09644

A92 2.08883 -0.00001 0.00002 -0.00005 -0.00004 2.08879

A93 2.10512 -0.00001 0.00008 -0.00016 -0.00008 2.10504

A94 2.09310 0.00003 -0.00006 0.00019 0.00012 2.09322

A95 2.08477 -0.00001 -0.00001 -0.00004 -0.00005 2.08472

A96 2.10596 0.00006 -0.00006 0.00088 0.00082 2.10678

A97 2.10590 -0.00006 0.00013 -0.00096 -0.00083 2.10508

A98 2.07132 0.00000 -0.00008 0.00008 0.00000 2.07132

A99 2.10536 0.00002 0.00001 0.00007 0.00008 2.10543

A100 2.08365 -0.00001 0.00006 -0.00018 -0.00012 2.08353

A101 2.09403 -0.00001 -0.00007 0.00012 0.00005 2.09408

A102 2.09755 -0.00000 0.00003 -0.00009 -0.00006 2.09750

A103 2.09705 -0.00000 -0.00001 0.00002 0.00001 2.09706

A104 2.08859 0.00000 -0.00002 0.00007 0.00005 2.08863

A105 2.10575 -0.00005 0.00018 -0.00100 -0.00083 2.10492

A106 2.10592 0.00005 -0.00014 0.00093 0.00079 2.10671

A107 2.07152 0.00000 -0.00004 0.00008 0.00004 2.07156

A108 2.10526 0.00002 -0.00001 0.00007 0.00006 2.10532

A109 2.08358 -0.00001 0.00005 -0.00018 -0.00013 2.08345

A110 2.09421 -0.00001 -0.00003 0.00011 0.00008 2.09429

A111 2.09754 -0.00000 0.00003 -0.00009 -0.00006 2.09748

A112 2.08861 0.00000 -0.00002 0.00007 0.00005 2.08866

A113 2.09703 -0.00000 -0.00002 0.00002 0.00001 2.09704

A114 2.08902 -0.00001 -0.00002 0.00002 -0.00000 2.08901

A115 2.09724 0.00000 0.00001 0.00002 0.00003 2.09727

A116 2.09693 0.00001 0.00001 -0.00004 -0.00003 2.09690

A117 2.09785 0.00001 -0.00003 0.00008 0.00006 2.09791

A118 2.09653 0.00000 0.00002 -0.00004 -0.00003 2.09650

A119 2.08880 -0.00001 0.00001 -0.00004 -0.00003 2.08877

A120 2.10505 -0.00001 0.00007 -0.00016 -0.00009 2.10496

A121 2.08482 -0.00001 0.00001 -0.00007 -0.00007 2.08475

A122 2.09312 0.00003 -0.00007 0.00022 0.00015 2.09327

A123 2.10735 0.00005 -0.00018 0.00126 0.00108 2.10843

A124 2.10423 -0.00004 0.00015 -0.00119 -0.00104 2.10320

A125 2.07161 -0.00001 0.00003 -0.00007 -0.00004 2.07156

A126 2.10505 -0.00001 0.00002 -0.00009 -0.00007 2.10498

A127 2.08383 0.00002 -0.00001 0.00021 0.00020 2.08403

A128 2.09417 -0.00001 0.00000 -0.00012 -0.00012 2.09405

A129 2.09766 0.00000 -0.00002 0.00009 0.00007 2.09773

A130 2.08852 -0.00000 0.00001 -0.00007 -0.00006 2.08846

A131 2.09700 0.00000 0.00001 -0.00002 -0.00001 2.09699

A132 2.08903 0.00000 -0.00000 0.00000 -0.00000 2.08903

A133 2.09722 0.00000 0.00000 -0.00002 -0.00002 2.09720

A134 2.09693 -0.00001 0.00000 0.00001 0.00002 2.09695

A135 2.09771 -0.00000 0.00003 -0.00011 -0.00008 2.09763

A136 2.09659 -0.00000 0.00001 0.00003 0.00005 2.09663

A137 2.08889 0.00001 -0.00004 0.00008 0.00004 2.08892

A138 2.10517 0.00002 -0.00005 0.00017 0.00012 2.10529

A139 2.08489 0.00000 0.00001 -0.00005 -0.00003 2.08486

A140 2.09293 -0.00002 0.00003 -0.00012 -0.00009 2.09284

D1 0.01588 -0.00001 -0.00033 0.00100 0.00067 0.01655

D2 -3.09429 -0.00001 -0.00130 0.00395 0.00265 -3.09164

D3 -3.11951 -0.00001 0.00032 -0.00036 -0.00004 -3.11955

D4 0.05351 -0.00001 -0.00065 0.00260 0.00194 0.05545

D5 -0.00086 -0.00000 0.00001 -0.00077 -0.00076 -0.00162

D6 -3.13475 0.00001 0.00029 -0.00055 -0.00026 -3.13501

D7 3.13441 -0.00000 -0.00065 0.00061 -0.00004 3.13437

D8 0.00052 0.00001 -0.00037 0.00083 0.00046 0.00098

D9 -0.02557 0.00001 0.00053 -0.00086 -0.00033 -0.02590

D10 3.08071 0.00002 0.00195 -0.00191 0.00004 3.08075

D11 3.08528 0.00002 0.00148 -0.00368 -0.00220 3.08308

D12 -0.09162 0.00003 0.00289 -0.00472 -0.00183 -0.09345

D13 -2.94004 -0.00000 0.00348 -0.01043 -0.00696 -2.94700

D14 0.19142 -0.00002 0.00250 -0.00804 -0.00554 0.18588

D15 0.23852 -0.00001 0.00233 -0.00700 -0.00467 0.23385

D16 -2.91320 -0.00003 0.00136 -0.00461 -0.00326 -2.91645

D17 0.02505 -0.00001 -0.00052 0.00038 -0.00014 0.02491

D18 -3.08864 -0.00001 -0.00141 -0.00007 -0.00148 -3.09011

D19 -3.08123 -0.00002 -0.00195 0.00152 -0.00043 -3.08166

D20 0.08827 -0.00001 -0.00284 0.00107 -0.00177 0.08650

D21 -0.01449 0.00001 0.00031 0.00025 0.00056 -0.01393

D22 3.11955 -0.00000 0.00003 0.00004 0.00007 3.11962

D23 3.09860 0.00000 0.00121 0.00075 0.00196 3.10056

D24 -0.05054 -0.00001 0.00093 0.00053 0.00147 -0.04908

D25 -0.24731 -0.00006 -0.00168 -0.00469 -0.00637 -0.25367

D26 2.90562 -0.00005 -0.00062 -0.00488 -0.00550 2.90012

D27 2.92783 -0.00005 -0.00274 -0.00525 -0.00799 2.91984

D28 -0.20243 -0.00005 -0.00168 -0.00544 -0.00713 -0.20956

D29 -0.12942 -0.00002 -0.00066 0.00533 0.00466 -0.12476

D30 3.02178 -0.00000 -0.00056 0.00779 0.00724 3.02901

D31 3.00053 -0.00003 -0.00175 0.00552 0.00377 3.00430

D32 -0.13146 -0.00001 -0.00164 0.00798 0.00634 -0.12512

D33 -0.98555 -0.00001 0.00136 -0.00129 0.00007 -0.98548

D34 2.15272 -0.00001 0.00097 -0.00089 0.00009 2.15280

D35 2.16662 -0.00001 0.00235 -0.00147 0.00087 2.16749

D36 -0.97830 -0.00001 0.00197 -0.00107 0.00089 -0.97741

D37 -3.09034 0.00002 -0.00005 0.00316 0.00311 -3.08723

D38 0.04277 0.00000 -0.00015 0.00098 0.00084 0.04361

D39 3.10538 -0.00001 0.00016 -0.00417 -0.00401 3.10138

D40 -0.06379 -0.00001 -0.00009 -0.00296 -0.00304 -0.06683

D41 -0.02788 0.00000 0.00025 -0.00203 -0.00178 -0.02965

D42 3.08614 0.00000 0.00001 -0.00082 -0.00081 3.08533

D43 -0.04186 -0.00001 -0.00000 0.00035 0.00034 -0.04152

D44 3.09537 -0.00000 0.00019 0.00254 0.00274 3.09811

D45 0.02539 0.00001 0.00016 -0.00163 -0.00147 0.02392

D46 -3.08715 0.00000 -0.00015 -0.00009 -0.00025 -3.08740

D47 -3.11193 0.00000 -0.00003 -0.00378 -0.00382 -3.11575

D48 0.05871 -0.00000 -0.00035 -0.00225 -0.00259 0.05612

D49 0.13728 -0.00002 -0.00027 0.00511 0.00484 0.14212

D50 -2.99972 -0.00002 -0.00129 0.00414 0.00285 -2.99687

D51 -3.00924 -0.00002 -0.00004 0.00759 0.00755 -3.00169

D52 0.13695 -0.00001 -0.00107 0.00663 0.00556 0.14250

D53 0.00145 -0.00000 -0.00023 0.00212 0.00189 0.00334

D54 -3.11201 -0.00001 0.00001 0.00088 0.00089 -3.11112

D55 3.11340 -0.00000 0.00009 0.00055 0.00063 3.11404

D56 -0.00006 -0.00000 0.00034 -0.00070 -0.00036 -0.00042

D57 -3.01036 -0.00002 0.00000 0.00753 0.00753 -3.00283

D58 0.13778 -0.00002 0.00039 0.00453 0.00492 0.14270

D59 0.14162 -0.00001 0.00101 0.00507 0.00608 0.14769

D60 -2.99343 -0.00001 0.00140 0.00207 0.00346 -2.98997

D61 0.98386 0.00001 -0.00070 -0.00101 -0.00171 0.98215

D62 -2.15435 0.00000 -0.00028 -0.00184 -0.00213 -2.15648

D63 -2.16718 -0.00001 -0.00162 0.00122 -0.00040 -2.16758

D64 0.97780 -0.00001 -0.00120 0.00038 -0.00082 0.97698

D65 -3.11022 0.00001 0.00041 -0.00415 -0.00374 -3.11396

D66 0.06059 0.00000 0.00019 -0.00266 -0.00247 0.05812

D67 0.02569 0.00001 0.00008 -0.00155 -0.00147 0.02422

D68 -3.08668 0.00000 -0.00014 -0.00006 -0.00020 -3.08689

D69 3.09372 -0.00001 -0.00029 0.00294 0.00265 3.09638

D70 -0.04208 -0.00001 0.00005 0.00029 0.00034 -0.04174

D71 0.00120 -0.00000 -0.00016 0.00205 0.00189 0.00309

D72 -3.11257 -0.00001 0.00003 0.00079 0.00083 -3.11174

D73 3.11298 0.00000 0.00007 0.00052 0.00059 3.11357

D74 -0.00078 -0.00000 0.00026 -0.00073 -0.00047 -0.00125

D75 -0.02774 -0.00001 0.00021 -0.00199 -0.00178 -0.02952

D76 3.10649 -0.00001 0.00076 -0.00478 -0.00402 3.10247

D77 3.08657 0.00000 0.00002 -0.00077 -0.00075 3.08583

D78 -0.06239 -0.00001 0.00057 -0.00355 -0.00298 -0.06537

D79 0.04283 0.00001 -0.00016 0.00099 0.00084 0.04367

D80 -3.09126 0.00002 -0.00072 0.00383 0.00311 -3.08815

D81 3.02114 -0.00000 -0.00063 0.00775 0.00711 3.02825

D82 -0.12683 -0.00000 0.00038 0.00630 0.00668 -0.12016

D83 -0.12894 -0.00001 0.00000 0.00453 0.00454 -0.12441

D84 3.00627 -0.00001 0.00101 0.00308 0.00410 3.01037

D85 2.94906 -0.00002 0.00347 -0.00939 -0.00593 2.94313

D86 -0.23306 -0.00003 0.00244 -0.00747 -0.00503 -0.23809

D87 -0.18632 -0.00002 0.00248 -0.00799 -0.00551 -0.19182

D88 2.91475 -0.00003 0.00145 -0.00607 -0.00461 2.91014

D89 -0.98777 -0.00001 -0.00060 0.00059 -0.00001 -0.98778

D90 2.15511 -0.00001 -0.00097 0.00073 -0.00024 2.15487

D91 2.14803 -0.00001 0.00031 -0.00072 -0.00040 2.14763

D92 -0.99228 -0.00001 -0.00005 -0.00058 -0.00063 -0.99291

D93 3.09203 -0.00001 -0.00115 0.00246 0.00131 3.09334

D94 -0.05449 -0.00001 -0.00052 0.00157 0.00104 -0.05345

D95 -0.01513 -0.00000 -0.00028 0.00080 0.00053 -0.01461

D96 3.12153 -0.00000 0.00036 -0.00009 0.00026 3.12180

D97 -3.08176 0.00001 0.00129 -0.00211 -0.00082 -3.08258

D98 0.11058 0.00001 0.00337 -0.00302 0.00035 0.11093

D99 0.02612 0.00001 0.00044 -0.00053 -0.00010 0.02602

D100 -3.06473 0.00000 0.00251 -0.00144 0.00107 -3.06366

D101 -0.00086 -0.00000 0.00002 -0.00078 -0.00076 -0.00162

D102 3.13704 0.00001 0.00034 -0.00013 0.00021 3.13725

D103 -3.13743 -0.00000 -0.00062 0.00014 -0.00048 -3.13792

D104 0.00047 0.00001 -0.00031 0.00079 0.00048 0.00095

D105 0.01653 0.00000 0.00024 0.00045 0.00069 0.01722

D106 -3.08755 0.00000 0.00102 0.00225 0.00327 -3.08428

D107 -3.12145 -0.00000 -0.00007 -0.00019 -0.00026 -3.12170

D108 0.05766 -0.00000 0.00071 0.00162 0.00233 0.05999

D109 -0.02665 -0.00001 -0.00042 0.00005 -0.00037 -0.02702

D110 3.06422 0.00000 -0.00252 0.00109 -0.00142 3.06280

D111 3.07825 0.00000 -0.00120 -0.00162 -0.00282 3.07544

D112 -0.11406 0.00001 -0.00329 -0.00058 -0.00387 -0.11793

D113 -2.96086 -0.00003 -0.00286 -0.00606 -0.00891 -2.96977

D114 0.17625 -0.00003 -0.00186 -0.00512 -0.00697 0.16928

D115 0.22487 -0.00003 -0.00193 -0.00399 -0.00592 0.21894

D116 -2.92121 -0.00004 -0.00093 -0.00305 -0.00398 -2.92519

D117 0.98701 -0.00001 0.00151 -0.00129 0.00022 0.98723

D118 -2.15558 -0.00000 0.00179 -0.00085 0.00095 -2.15463

D119 -2.15041 -0.00000 0.00058 -0.00217 -0.00159 -2.15200

D120 0.99018 0.00000 0.00086 -0.00172 -0.00086 0.98932

D121 -3.12866 -0.00002 -0.00010 0.00088 0.00078 -3.12787

D122 -0.00818 -0.00000 -0.00026 0.00091 0.00064 -0.00753

D123 0.01620 -0.00002 0.00027 0.00049 0.00077 0.01696

D124 3.13667 -0.00000 0.00011 0.00051 0.00063 3.13730

D125 3.14114 0.00002 0.00004 -0.00074 -0.00070 3.14044

D126 -0.01868 0.00001 0.00000 -0.00057 -0.00057 -0.01926

D127 -0.00372 0.00002 -0.00034 -0.00035 -0.00069 -0.00441

D128 3.11964 0.00001 -0.00037 -0.00019 -0.00056 3.11909

D129 -0.01703 0.00001 -0.00010 -0.00024 -0.00034 -0.01736

D130 3.12425 0.00001 -0.00004 -0.00012 -0.00016 3.12409

D131 -3.13740 -0.00000 0.00006 -0.00026 -0.00020 -3.13760

D132 0.00387 -0.00001 0.00013 -0.00015 -0.00002 0.00385

D133 0.00512 -0.00000 -0.00002 -0.00016 -0.00018 0.00494

D134 -3.13402 0.00000 -0.00007 0.00006 -0.00000 -3.13403

D135 -3.13615 -0.00000 -0.00008 -0.00028 -0.00036 -3.13651

D136 0.00789 0.00000 -0.00013 -0.00006 -0.00019 0.00771

D137 0.00731 0.00000 -0.00004 0.00031 0.00026 0.00757

D138 -3.13147 -0.00000 0.00014 0.00018 0.00031 -3.13116

D139 -3.13673 -0.00000 0.00000 0.00008 0.00008 -3.13665

D140 0.00767 -0.00001 0.00018 -0.00005 0.00013 0.00780

D141 -0.00797 -0.00001 0.00023 -0.00005 0.00018 -0.00779

D142 -3.13123 0.00000 0.00026 -0.00021 0.00005 -3.13118

D143 3.13083 -0.00001 0.00005 0.00008 0.00013 3.13095

D144 0.00757 0.00001 0.00008 -0.00008 -0.00001 0.00756

D145 -0.00529 -0.00000 -0.00000 -0.00014 -0.00015 -0.00544

D146 3.13582 0.00000 -0.00004 -0.00012 -0.00016 3.13566

D147 3.13415 0.00000 -0.00011 0.00014 0.00003 3.13417

D148 -0.00793 0.00000 -0.00015 0.00017 0.00001 -0.00791

D149 -0.00697 0.00000 0.00000 0.00007 0.00007 -0.00690

D150 3.13178 -0.00000 0.00004 0.00014 0.00018 3.13196

D151 3.13678 0.00000 0.00011 -0.00021 -0.00010 3.13668

D152 -0.00766 -0.00001 0.00015 -0.00014 0.00000 -0.00766

D153 0.01660 0.00001 -0.00018 0.00019 0.00001 0.01661

D154 3.13687 -0.00001 0.00018 -0.00047 -0.00029 3.13658

D155 -3.12451 0.00001 -0.00015 0.00016 0.00002 -3.12449

D156 -0.00425 -0.00001 0.00022 -0.00050 -0.00028 -0.00453

D157 3.12954 -0.00002 0.00078 -0.00098 -0.00020 3.12934

D158 -0.01536 -0.00002 0.00037 -0.00016 0.00021 -0.01516

D159 0.00918 -0.00001 0.00042 -0.00032 0.00009 0.00927

D160 -3.13573 -0.00000 0.00001 0.00049 0.00050 -3.13523

D161 3.14134 0.00003 -0.00078 0.00091 0.00013 3.14147

D162 0.01808 0.00001 -0.00049 0.00052 0.00003 0.01811

D163 0.00306 0.00002 -0.00037 0.00009 -0.00028 0.00278

D164 -3.12020 0.00001 -0.00008 -0.00030 -0.00038 -3.12058

D165 0.00805 -0.00002 0.00019 -0.00005 0.00015 0.00819

D166 -3.13071 -0.00001 0.00015 -0.00012 0.00004 -3.13067

D167 3.13120 0.00000 -0.00010 0.00034 0.00024 3.13144

D168 -0.00756 0.00001 -0.00014 0.00027 0.00013 -0.00743

D169 -3.13978 0.00003 -0.00011 0.00059 0.00047 -3.13931

D170 0.01903 0.00001 -0.00009 0.00027 0.00018 0.01921

D171 0.00279 0.00002 -0.00039 0.00015 -0.00024 0.00255

D172 -3.12158 0.00001 -0.00037 -0.00016 -0.00053 -3.12211

D173 3.12768 -0.00002 0.00012 -0.00067 -0.00055 3.12713

D174 0.00741 -0.00001 -0.00009 -0.00011 -0.00019 0.00722

D175 -0.01489 -0.00002 0.00040 -0.00023 0.00017 -0.01473

D176 -3.13516 -0.00000 0.00019 0.00033 0.00052 -3.13464

D177 0.00797 -0.00001 0.00019 -0.00006 0.00013 0.00810

D178 -3.13111 -0.00001 0.00006 -0.00008 -0.00002 -3.13114

D179 3.13224 0.00000 0.00017 0.00025 0.00042 3.13266

D180 -0.00685 0.00001 0.00004 0.00023 0.00027 -0.00658

D181 -0.00674 0.00000 0.00002 0.00005 0.00007 -0.00667

D182 3.13663 -0.00000 0.00004 -0.00018 -0.00014 3.13649

D183 3.13233 -0.00000 0.00015 0.00007 0.00022 3.13255

D184 -0.00748 -0.00001 0.00016 -0.00016 0.00001 -0.00747

D185 -0.00532 -0.00000 -0.00001 -0.00013 -0.00014 -0.00546

D186 3.13552 0.00000 -0.00011 -0.00004 -0.00015 3.13538

D187 3.13450 0.00000 -0.00003 0.00009 0.00007 3.13456

D188 -0.00785 0.00000 -0.00012 0.00019 0.00006 -0.00778

D189 0.01628 0.00001 -0.00020 0.00022 0.00002 0.01630

D190 3.13644 -0.00001 0.00001 -0.00034 -0.00034 3.13611

D191 -3.12457 0.00001 -0.00010 0.00013 0.00003 -3.12454

D192 -0.00440 -0.00001 0.00010 -0.00044 -0.00033 -0.00474

D193 3.13943 0.00002 -0.00064 -0.00023 -0.00088 3.13856

D194 -0.01935 0.00001 -0.00041 -0.00022 -0.00063 -0.01998

D195 -0.00342 0.00002 -0.00029 -0.00037 -0.00065 -0.00408

D196 3.12098 0.00000 -0.00005 -0.00036 -0.00041 3.12057

D197 -3.12714 -0.00002 0.00054 0.00038 0.00092 -3.12622

D198 -0.00669 -0.00001 0.00026 0.00054 0.00080 -0.00589

D199 0.01572 -0.00002 0.00018 0.00051 0.00070 0.01641

D200 3.13616 -0.00000 -0.00009 0.00067 0.00058 3.13674

D201 -0.00790 -0.00001 0.00024 -0.00003 0.00021 -0.00769

D202 3.13120 -0.00001 0.00015 0.00004 0.00019 3.13138

D203 -3.13220 0.00000 0.00000 -0.00005 -0.00004 -3.13224

D204 0.00690 0.00001 -0.00009 0.00002 -0.00006 0.00684

D205 0.00705 0.00001 -0.00008 0.00030 0.00021 0.00726

D206 -3.13660 -0.00000 0.00006 0.00004 0.00010 -3.13651

D207 -3.13203 -0.00000 0.00001 0.00022 0.00023 -3.13180

D208 0.00750 -0.00001 0.00015 -0.00004 0.00012 0.00761

D209 0.00520 -0.00000 -0.00002 -0.00015 -0.00017 0.00503

D210 -3.13586 -0.00000 0.00001 -0.00032 -0.00031 -3.13617

D211 -3.13433 0.00000 -0.00016 0.00011 -0.00006 -3.13439

D212 0.00779 0.00000 -0.00013 -0.00006 -0.00020 0.00760

D213 -0.01673 0.00001 -0.00003 -0.00026 -0.00029 -0.01702

D214 -3.13708 -0.00001 0.00025 -0.00042 -0.00017 -3.13725

D215 3.12433 0.00001 -0.00006 -0.00009 -0.00015 3.12418

D216 0.00399 -0.00001 0.00022 -0.00025 -0.00003 0.00395

Item Value Threshold Converged?

Maximum Force 0.000161 0.000450 YES

RMS Force 0.000033 0.000300 YES

Maximum Displacement 0.124685 0.001800 NO

RMS Displacement 0.027071 0.001200 NO

Predicted change in Energy=-2.960508D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Wed Aug 28 12:21:29 2019, MaxMem= 4294967296 cpu: 2.3

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=1 Diff= 1.28D-01

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 1.176006 -4.054903 0.581406

2 6 0 1.458232 -2.726607 0.216953

3 7 0 0.251152 -2.101926 0.006831

4 6 0 -0.783893 -2.988038 0.190791

5 6 0 -0.212214 -4.216889 0.563844

6 6 0 -2.179824 -2.700460 -0.002921

7 6 0 -2.730086 -1.421730 -0.126805

8 7 0 -2.053223 -0.239522 0.053616

9 6 0 -2.988364 0.754120 -0.094986

10 6 0 -4.289780 0.181811 -0.434751

11 6 0 -4.129695 -1.160269 -0.457158

12 6 0 2.751756 -2.123951 0.045672

13 6 0 2.988362 -0.752826 -0.100915

14 6 0 4.289461 -0.178931 -0.439193

15 6 0 4.129269 1.163230 -0.455628

16 6 0 2.729809 1.423095 -0.123390

17 7 0 2.053208 0.239979 0.052359

18 6 0 2.179384 2.701151 0.005123

19 6 0 0.783884 2.989336 0.199923

20 6 0 0.211254 4.224071 0.552173

21 6 0 -1.176819 4.062127 0.570208

22 6 0 -1.458333 2.727915 0.226858

23 7 0 -0.250746 2.099787 0.029567

24 6 0 -2.751393 2.124645 0.055291

25 6 0 -3.081540 -3.877353 -0.056049

26 6 0 -2.863071 -4.900215 -0.991471

27 6 0 -3.716219 -5.996938 -1.054547

28 6 0 -4.790575 -6.101659 -0.170743

29 6 0 -5.008945 -5.098874 0.772526

30 6 0 -4.164734 -3.993180 0.827188

31 6 0 6.102365 -4.804087 0.020508

32 6 0 5.057694 -4.979871 -0.887282

33 6 0 3.965467 -4.118583 -0.872607

34 6 0 3.908099 -3.052910 0.038418

35 6 0 4.964746 -2.885086 0.945300

36 6 0 6.050100 -3.756742 0.938966

37 6 0 -3.908565 3.053207 0.043661

38 6 0 -4.963762 2.890372 0.952892

39 6 0 -6.051016 3.759696 0.940619

40 6 0 -6.106332 4.799540 0.013866

41 6 0 -5.063034 4.970101 -0.896446

42 6 0 -3.969063 4.111057 -0.876039

43 6 0 3.082046 3.877701 -0.051441

44 6 0 4.162491 3.997127 0.834433

45 6 0 5.008916 5.100973 0.775362

46 6 0 4.795253 6.098095 -0.174954

47 6 0 3.723691 5.989479 -1.061616

48 6 0 2.868494 4.894520 -0.994347

49 1 0 1.911340 -4.802177 0.832423

50 1 0 -0.762167 -5.113728 0.799364

51 1 0 -5.187851 0.738764 -0.653205

52 1 0 -4.872723 -1.905051 -0.697038

53 1 0 5.187321 -0.734944 -0.660933

54 1 0 4.872233 1.909086 -0.692328

55 1 0 0.760189 5.125556 0.771625

56 1 0 -1.912482 4.814103 0.805599

57 1 0 -2.031880 -4.821539 -1.682784

58 1 0 -3.542497 -6.770992 -1.794598

59 1 0 -5.451466 -6.960783 -0.215877

60 1 0 -5.836392 -5.177499 1.469759

61 1 0 -4.332128 -3.220206 1.568513

62 1 0 6.950481 -5.480524 0.012753

63 1 0 5.093826 -5.789349 -1.608718

64 1 0 3.158405 -4.256375 -1.582994

65 1 0 4.922831 -2.077383 1.667090

66 1 0 6.854085 -3.618488 1.654158

67 1 0 -4.919804 2.087774 1.680280

68 1 0 -6.854220 3.625288 1.657418

69 1 0 -6.955961 5.474005 0.001383

70 1 0 -5.101620 5.773530 -1.624495

71 1 0 -3.163217 4.244402 -1.588655

72 1 0 4.326613 3.227967 1.580490

73 1 0 5.834541 5.182428 1.474428

74 1 0 5.457902 6.955673 -0.223616

75 1 0 3.553796 6.758923 -1.807349

76 1 0 2.039655 4.812591 -1.688106

77 1 0 0.141270 -1.123105 -0.218449

78 1 0 -0.139957 1.114241 -0.164880

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0588014 0.0582761 0.0300992

Leave Link 202 at Wed Aug 28 12:21:29 2019, MaxMem= 4294967296 cpu: 0.0

(Enter /home/kira/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5357.2504926482 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122340100 Hartrees.

Nuclear repulsion after empirical dispersion term = 5357.0382586382 Hartrees.

Force inversion solution in PCM.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5820

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.92D-11

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 409

GePol: Fraction of low-weight points (<1% of avg) = 7.03%

GePol: Cavity surface area = 611.218 Ang\*\*2

GePol: Cavity volume = 628.957 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0021075676 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5357.0361510706 Hartrees.

Leave Link 301 at Wed Aug 28 12:21:30 2019, MaxMem= 4294967296 cpu: 1.8

(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.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Wed Aug 28 12:21:31 2019, MaxMem= 4294967296 cpu: 28.0

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Wed Aug 28 12:21:32 2019, MaxMem= 4294967296 cpu: 2.0

(Enter /home/kira/g09/l401.exe)

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 0.998972 0.000009 -0.000000 -0.045338 Ang= 5.20 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0183

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30525592444

Leave Link 401 at Wed Aug 28 12:21:37 2019, MaxMem= 4294967296 cpu: 83.0

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 580000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 101617200.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.33D-15 for 5818.

Iteration 1 A\*A^-1 deviation from orthogonality is 6.66D-15 for 5815 4752.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.77D-15 for 5818.

Iteration 1 A^-1\*A deviation from orthogonality is 6.39D-11 for 5408 5388.

E= -1914.33217037357

DIIS: error= 1.35D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.33217037357 IErMin= 1 ErrMin= 1.35D-03

ErrMax= 1.35D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.60D-03 BMatP= 2.60D-03

IDIUse=3 WtCom= 9.87D-01 WtEn= 1.35D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.641 Goal= None Shift= 0.000

Gap= 0.706 Goal= None Shift= 0.000

GapD= 0.641 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=3.05D-05 MaxDP=9.08D-04 OVMax= 3.86D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.05D-05 CP: 1.00D+00

E= -1914.33322149268 Delta-E= -0.001051119102 Rises=F Damp=F

DIIS: error= 1.05D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33322149268 IErMin= 2 ErrMin= 1.05D-04

ErrMax= 1.05D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.30D-05 BMatP= 2.60D-03

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.05D-03

Coeff-Com: -0.610D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.610D-01 0.106D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.65D-06 MaxDP=2.57D-04 DE=-1.05D-03 OVMax= 1.05D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 5.18D-06 CP: 1.00D+00 1.07D+00

E= -1914.33322995807 Delta-E= -0.000008465394 Rises=F Damp=F

DIIS: error= 6.36D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33322995807 IErMin= 3 ErrMin= 6.36D-05

ErrMax= 6.36D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.55D-05 BMatP= 2.30D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.351D-01 0.545D+00 0.490D+00

Coeff: -0.351D-01 0.545D+00 0.490D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.31D-06 MaxDP=1.75D-04 DE=-8.47D-06 OVMax= 4.83D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.79D-06 CP: 1.00D+00 1.08D+00 7.26D-01

E= -1914.33323364823 Delta-E= -0.000003690162 Rises=F Damp=F

DIIS: error= 2.01D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33323364823 IErMin= 4 ErrMin= 2.01D-05

ErrMax= 2.01D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.59D-06 BMatP= 1.55D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.481D-02 0.526D-01 0.242D+00 0.710D+00

Coeff: -0.481D-02 0.526D-01 0.242D+00 0.710D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=8.12D-07 MaxDP=3.85D-05 DE=-3.69D-06 OVMax= 4.03D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 6.30D-07 CP: 1.00D+00 1.09D+00 8.14D-01 8.76D-01

E= -1914.33323407220 Delta-E= -0.000000423966 Rises=F Damp=F

DIIS: error= 7.54D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33323407220 IErMin= 5 ErrMin= 7.54D-06

ErrMax= 7.54D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.18D-07 BMatP= 1.59D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.207D-03-0.947D-02 0.982D-01 0.382D+00 0.529D+00

Coeff: -0.207D-03-0.947D-02 0.982D-01 0.382D+00 0.529D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.08D-07 MaxDP=3.02D-05 DE=-4.24D-07 OVMax= 2.84D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.59D-07 CP: 1.00D+00 1.09D+00 8.22D-01 9.74D-01 9.00D-01

E= -1914.33323413898 Delta-E= -0.000000066783 Rises=F Damp=F

DIIS: error= 5.51D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33323413898 IErMin= 6 ErrMin= 5.51D-06

ErrMax= 5.51D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.47D-08 BMatP= 2.18D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.778D-03-0.157D-01 0.116D-01 0.872D-01 0.319D+00 0.597D+00

Coeff: 0.778D-03-0.157D-01 0.116D-01 0.872D-01 0.319D+00 0.597D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.54D-07 MaxDP=1.33D-05 DE=-6.68D-08 OVMax= 1.88D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.62D-07 CP: 1.00D+00 1.09D+00 8.37D-01 9.98D-01 1.16D+00

CP: 1.15D+00

E= -1914.33323416560 Delta-E= -0.000000026622 Rises=F Damp=F

DIIS: error= 3.88D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33323416560 IErMin= 7 ErrMin= 3.88D-06

ErrMax= 3.88D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.22D-09 BMatP= 4.47D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.392D-03-0.615D-02-0.742D-02-0.821D-02 0.927D-01 0.270D+00

Coeff-Com: 0.659D+00

Coeff: 0.392D-03-0.615D-02-0.742D-02-0.821D-02 0.927D-01 0.270D+00

Coeff: 0.659D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.05D-07 MaxDP=1.52D-05 DE=-2.66D-08 OVMax= 2.02D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.62D-08 CP: 1.00D+00 1.09D+00 8.44D-01 1.03D+00 1.31D+00

CP: 1.56D+00 1.35D+00

E= -1914.33323417868 Delta-E= -0.000000013073 Rises=F Damp=F

DIIS: error= 2.86D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33323417868 IErMin= 8 ErrMin= 2.86D-06

ErrMax= 2.86D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.42D-09 BMatP= 8.22D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.351D-03 0.823D-02-0.129D-01-0.674D-01-0.171D+00-0.340D+00

Coeff-Com: 0.441D+00 0.114D+01

Coeff: -0.351D-03 0.823D-02-0.129D-01-0.674D-01-0.171D+00-0.340D+00

Coeff: 0.441D+00 0.114D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.84D-07 MaxDP=2.65D-05 DE=-1.31D-08 OVMax= 3.88D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 5.87D-08 CP: 1.00D+00 1.09D+00 8.54D-01 1.08D+00 1.64D+00

CP: 2.23D+00 2.38D+00 1.70D+00

E= -1914.33323419616 Delta-E= -0.000000017481 Rises=F Damp=F

DIIS: error= 1.97D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33323419616 IErMin= 9 ErrMin= 1.97D-06

ErrMax= 1.97D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.47D-09 BMatP= 5.42D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.263D-03 0.486D-02-0.462D-03-0.136D-01-0.736D-01-0.244D+00

Coeff-Com: -0.106D+00 0.322D+00 0.111D+01

Coeff: -0.263D-03 0.486D-02-0.462D-03-0.136D-01-0.736D-01-0.244D+00

Coeff: -0.106D+00 0.322D+00 0.111D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.92D-07 MaxDP=2.26D-05 DE=-1.75D-08 OVMax= 3.12D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 5.21D-08 CP: 1.00D+00 1.09D+00 8.62D-01 1.11D+00 1.87D+00

CP: 2.75D+00 3.00D+00 2.65D+00 1.78D+00

E= -1914.33323420275 Delta-E= -0.000000006596 Rises=F Damp=F

DIIS: error= 1.05D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33323420275 IErMin=10 ErrMin= 1.05D-06

ErrMax= 1.05D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.48D-09 BMatP= 1.47D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.712D-04 0.605D-03 0.467D-02 0.159D-01 0.131D-01-0.742D-01

Coeff-Com: -0.256D+00-0.196D+00 0.901D+00 0.591D+00

Coeff: -0.712D-04 0.605D-03 0.467D-02 0.159D-01 0.131D-01-0.742D-01

Coeff: -0.256D+00-0.196D+00 0.901D+00 0.591D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.53D-07 MaxDP=1.16D-05 DE=-6.60D-09 OVMax= 1.63D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.01D-08 CP: 1.00D+00 1.09D+00 8.66D-01 1.13D+00 1.98D+00

CP: 3.00D+00 3.00D+00 3.00D+00 2.51D+00 1.71D+00

E= -1914.33323420460 Delta-E= -0.000000001851 Rises=F Damp=F

DIIS: error= 5.60D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33323420460 IErMin=11 ErrMin= 5.60D-07

ErrMax= 5.60D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.73D-10 BMatP= 1.47D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.546D-04-0.130D-02 0.188D-02 0.106D-01 0.337D-01 0.383D-01

Coeff-Com: -0.593D-01-0.160D+00-0.189D-01 0.163D+00 0.992D+00

Coeff: 0.546D-04-0.130D-02 0.188D-02 0.106D-01 0.337D-01 0.383D-01

Coeff: -0.593D-01-0.160D+00-0.189D-01 0.163D+00 0.992D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=8.03D-08 MaxDP=6.97D-06 DE=-1.85D-09 OVMax= 9.03D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 4.78D-08 CP: 1.00D+00 1.09D+00 8.68D-01 1.14D+00 2.03D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 2.39D+00

CP: 1.42D+00

E= -1914.33323420509 Delta-E= -0.000000000487 Rises=F Damp=F

DIIS: error= 2.82D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.33323420509 IErMin=12 ErrMin= 2.82D-07

ErrMax= 2.82D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.06D-10 BMatP= 1.73D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.514D-04-0.889D-03-0.483D-03 0.871D-03 0.169D-01 0.381D-01

Coeff-Com: 0.516D-01-0.142D-01-0.297D+00-0.126D+00 0.602D+00 0.729D+00

Coeff: 0.514D-04-0.889D-03-0.483D-03 0.871D-03 0.169D-01 0.381D-01

Coeff: 0.516D-01-0.142D-01-0.297D+00-0.126D+00 0.602D+00 0.729D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.42D-08 MaxDP=2.87D-06 DE=-4.87D-10 OVMax= 3.61D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.93D-08 CP: 1.00D+00 1.09D+00 8.69D-01 1.14D+00 2.05D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 2.68D+00

CP: 1.61D+00 1.39D+00

E= -1914.33323420527 Delta-E= -0.000000000183 Rises=F Damp=F

DIIS: error= 1.36D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.33323420527 IErMin=13 ErrMin= 1.36D-07

ErrMax= 1.36D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.56D-11 BMatP= 1.06D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.231D-05 0.117D-03-0.111D-02-0.407D-02-0.481D-02-0.178D-02

Coeff-Com: 0.521D-01 0.669D-01-0.139D+00-0.150D+00-0.926D-01 0.339D+00

Coeff-Com: 0.935D+00

Coeff: 0.231D-05 0.117D-03-0.111D-02-0.407D-02-0.481D-02-0.178D-02

Coeff: 0.521D-01 0.669D-01-0.139D+00-0.150D+00-0.926D-01 0.339D+00

Coeff: 0.935D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.30D-08 MaxDP=1.96D-06 DE=-1.83D-10 OVMax= 2.35D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 5.55D-09 CP: 1.00D+00 1.09D+00 8.69D-01 1.14D+00 2.05D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 2.90D+00

CP: 1.71D+00 1.65D+00 1.64D+00

E= -1914.33323420533 Delta-E= -0.000000000056 Rises=F Damp=F

DIIS: error= 6.58D-08 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.33323420533 IErMin=14 ErrMin= 6.58D-08

ErrMax= 6.58D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.34D-12 BMatP= 2.56D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.130D-04 0.309D-03-0.465D-03-0.237D-02-0.710D-02-0.125D-01

Coeff-Com: 0.128D-01 0.385D-01 0.140D-01-0.490D-01-0.221D+00-0.305D-01

Coeff-Com: 0.496D+00 0.761D+00

Coeff: -0.130D-04 0.309D-03-0.465D-03-0.237D-02-0.710D-02-0.125D-01

Coeff: 0.128D-01 0.385D-01 0.140D-01-0.490D-01-0.221D+00-0.305D-01

Coeff: 0.496D+00 0.761D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.04D-08 MaxDP=9.27D-07 DE=-5.64D-11 OVMax= 1.09D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 2.02D-09 CP: 1.00D+00 1.09D+00 8.69D-01 1.14D+00 2.06D+00

CP: 3.00D+00 3.00D+00 3.00D+00 3.00D+00 2.98D+00

CP: 1.76D+00 1.77D+00 1.90D+00 1.24D+00

E= -1914.33323420539 Delta-E= -0.000000000058 Rises=F Damp=F

DIIS: error= 2.35D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.33323420539 IErMin=15 ErrMin= 2.35D-08

ErrMax= 2.35D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.77D-13 BMatP= 7.34D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.452D-05 0.669D-04 0.134D-03 0.262D-03-0.104D-02-0.371D-02

Coeff-Com: -0.871D-02-0.649D-02 0.411D-01 0.190D-01-0.472D-01-0.842D-01

Coeff-Com: -0.541D-01 0.252D+00 0.893D+00

Coeff: -0.452D-05 0.669D-04 0.134D-03 0.262D-03-0.104D-02-0.371D-02

Coeff: -0.871D-02-0.649D-02 0.411D-01 0.190D-01-0.472D-01-0.842D-01

Coeff: -0.541D-01 0.252D+00 0.893D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.76D-09 MaxDP=3.30D-07 DE=-5.82D-11 OVMax= 4.01D-06

Error on total polarization charges = 0.08273

SCF Done: E(UB3LYP) = -1914.33323421 A.U. after 15 cycles

NFock= 15 Conv=0.38D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0183

<L.S>= 0.000000000000E+00

KE= 1.906378004056D+03 PE=-1.516369434217D+04 EE= 5.985946952838D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0551, after 2.0017

Leave Link 502 at Wed Aug 28 12:28:14 2019, MaxMem= 4294967296 cpu: 6284.5

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48659477D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64384192D-01

Leave Link 801 at Wed Aug 28 12:28:14 2019, MaxMem= 4294967296 cpu: 1.0

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Wed Aug 28 12:28:21 2019, MaxMem= 4294967296 cpu: 110.5

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Wed Aug 28 12:28:22 2019, MaxMem= 4294967296 cpu: 1.8

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 192

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Wed Aug 28 12:48:10 2019, MaxMem= 4294967296 cpu: 19004.5

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 580000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.38D+03 4.46D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.49D+02 3.49D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.48D+00 4.58D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.03D-01 3.93D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.64D-04 2.09D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.56D-06 1.33D-04.

192 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 1.98D-08 9.95D-06.

74 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.28D-11 6.17D-07.

32 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.15D-13 3.93D-08.

5 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 8.88D-15 3.82D-09.

4 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 3.93D-15 1.86D-09.

4 vectors produced by pass 11 Test12= 2.55D-13 1.00D-09 XBig12= 9.51D-15 3.69D-09.

4 vectors produced by pass 12 Test12= 2.55D-13 1.00D-09 XBig12= 1.08D-14 3.01D-09.

4 vectors produced by pass 13 Test12= 2.55D-13 1.00D-09 XBig12= 1.18D-14 3.35D-09.

4 vectors produced by pass 14 Test12= 2.55D-13 1.00D-09 XBig12= 7.97D-15 2.55D-09.

4 vectors produced by pass 15 Test12= 2.55D-13 1.00D-09 XBig12= 9.14D-15 3.05D-09.

4 vectors produced by pass 16 Test12= 2.55D-13 1.00D-09 XBig12= 8.00D-15 2.31D-09.

4 vectors produced by pass 17 Test12= 2.55D-13 1.00D-09 XBig12= 7.04D-15 2.66D-09.

3 vectors produced by pass 18 Test12= 2.55D-13 1.00D-09 XBig12= 4.84D-15 1.86D-09.

3 vectors produced by pass 19 Test12= 2.55D-13 1.00D-09 XBig12= 8.31D-15 2.81D-09.

3 vectors produced by pass 20 Test12= 2.55D-13 1.00D-09 XBig12= 5.98D-15 2.09D-09.

3 vectors produced by pass 21 Test12= 2.55D-13 1.00D-09 XBig12= 1.04D-14 2.77D-09.

2 vectors produced by pass 22 Test12= 2.55D-13 1.00D-09 XBig12= 4.64D-15 1.80D-09.

InvSVY: IOpt=1 It= 1 EMax= 5.68D-14

Solved reduced A of dimension 1756 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1127.86 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Wed Aug 28 16:43:52 2019, MaxMem= 4294967296 cpu: 226214.0

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 192

Leave Link 701 at Wed Aug 28 16:45:22 2019, MaxMem= 4294967296 cpu: 1440.0

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Wed Aug 28 16:45:22 2019, MaxMem= 4294967296 cpu: 0.5

(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=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

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= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Wed Aug 28 17:03:53 2019, MaxMem= 4294967296 cpu: 17760.0

(Enter /home/kira/g09/l716.exe)

Dipole = 5.52902009D-04-1.22655760D-02-5.05353224D-01

Polarizability= 1.26275471D+03-5.00056682D+01 1.66789750D+03

2.78177918D-02-6.44006641D-02 4.52918989D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000037096 0.000043498 0.000004808

2 6 -0.000026254 0.000003271 0.000097318

3 7 -0.000095017 -0.000016285 -0.000024753

4 6 0.000005749 -0.000040905 -0.000102584

5 6 -0.000010424 -0.000021784 0.000012620

6 6 0.000015153 -0.000084301 0.000014444

7 6 0.000078637 0.000018282 0.000003995

8 7 -0.000028972 -0.000082381 0.000033523

9 6 -0.000040259 -0.000001992 0.000049691

10 6 0.000024660 0.000053697 0.000046781

11 6 0.000006282 -0.000030028 -0.000053614

12 6 0.000061736 -0.000058277 0.000012858

13 6 0.000039844 0.000001142 -0.000044003

14 6 -0.000025662 0.000043795 -0.000046403

15 6 -0.000005196 -0.000015410 0.000058001

16 6 -0.000075473 0.000015734 -0.000009692

17 7 0.000034838 -0.000063496 -0.000025017

18 6 -0.000010937 -0.000093936 -0.000012321

19 6 -0.000007496 -0.000034711 0.000111648

20 6 0.000030132 -0.000020273 -0.000002365

21 6 0.000033395 0.000023688 -0.000018342

22 6 0.000020708 0.000001345 -0.000108759

23 7 0.000072463 -0.000019953 0.000010029

24 6 -0.000057666 -0.000067910 -0.000013924

25 6 -0.000039049 0.000091945 0.000080281

26 6 -0.000006037 0.000176126 -0.000127228

27 6 0.000040715 -0.000077033 0.000018281

28 6 -0.000034468 0.000018842 -0.000047250

29 6 -0.000012816 -0.000102041 0.000055567

30 6 -0.000062203 0.000118351 0.000103375

31 6 0.000039491 -0.000046321 -0.000020603

32 6 -0.000000065 -0.000008814 0.000022184

33 6 0.000012080 0.000015474 -0.000010317

34 6 -0.000069641 0.000057967 -0.000050903

35 6 0.000085548 0.000019435 -0.000062514

36 6 -0.000098579 0.000011210 0.000009813

37 6 0.000065783 0.000052363 0.000075095

38 6 -0.000077342 0.000032399 0.000061313

39 6 0.000092846 -0.000004784 0.000009837

40 6 -0.000037546 -0.000044966 0.000009092

41 6 -0.000006414 -0.000026258 -0.000015081

42 6 -0.000003270 0.000025421 -0.000005513

43 6 0.000042279 0.000091652 -0.000085378

44 6 0.000063141 0.000127532 -0.000106357

45 6 0.000006977 -0.000115062 -0.000067115

46 6 0.000038171 0.000016560 0.000055780

47 6 -0.000038944 -0.000081983 -0.000019940

48 6 0.000005481 0.000176140 0.000138635

49 1 0.000002387 0.000041286 -0.000054588

50 1 -0.000015228 -0.000062586 0.000088377

51 1 0.000065379 -0.000003302 0.000008949

52 1 -0.000006581 -0.000056337 0.000048432

53 1 -0.000068508 -0.000003299 -0.000010328

54 1 0.000005696 -0.000059394 -0.000044938

55 1 0.000008850 -0.000058140 -0.000100973

56 1 0.000008031 0.000053048 0.000051851

57 1 0.000036114 0.000015516 -0.000032847

58 1 -0.000021527 -0.000009986 -0.000029852

59 1 -0.000013037 -0.000018956 0.000013738

60 1 0.000005131 -0.000001146 0.000012974

61 1 0.000053925 -0.000040503 -0.000080884

62 1 -0.000018017 0.000002941 -0.000009622

63 1 -0.000004705 0.000000573 0.000006022

64 1 0.000040713 0.000046676 0.000026751

65 1 0.000059594 -0.000043741 0.000068490

66 1 0.000023592 0.000000285 -0.000020557

67 1 -0.000064738 -0.000051406 -0.000067013

68 1 -0.000021117 -0.000002806 0.000019705

69 1 0.000015331 -0.000003286 0.000010634

70 1 0.000005252 -0.000000059 -0.000010236

71 1 -0.000040555 0.000054513 -0.000028664

72 1 -0.000062794 -0.000049124 0.000078594

73 1 -0.000005647 -0.000004564 -0.000014524

74 1 0.000012172 -0.000022729 -0.000014999

75 1 0.000019749 -0.000011693 0.000031205

76 1 -0.000032065 0.000019825 0.000036002

77 1 -0.000409843 0.000048070 -0.000036004

78 1 0.000413159 0.000143357 0.000039313

-------------------------------------------------------------------

Cartesian Forces: Max 0.000413159 RMS 0.000064323

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Wed Aug 28 17:03:53 2019, MaxMem= 4294967296 cpu: 2.0

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000509376 RMS 0.000102622

Search for a local minimum.

Step number 16 out of a maximum of 452

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= 1.08D-04 DEPred=-2.96D-06 R=-3.63D+01

Trust test=-3.63D+01 RLast= 3.73D-02 DXMaxT set to 5.00D-02

ITU= -1 -1 1 0 -1 1 1 -1 1 -1 -1 1 1 -1 1 0

Eigenvalues --- 0.00134 0.00171 0.00433 0.00571 0.00675

Eigenvalues --- 0.00700 0.00815 0.01048 0.01067 0.01110

Eigenvalues --- 0.01123 0.01144 0.01256 0.01277 0.01281

Eigenvalues --- 0.01293 0.01311 0.01399 0.01419 0.01570

Eigenvalues --- 0.01585 0.01599 0.01633 0.01680 0.01706

Eigenvalues --- 0.01711 0.01722 0.01732 0.01758 0.01762

Eigenvalues --- 0.01770 0.01775 0.01782 0.01783 0.01875

Eigenvalues --- 0.01941 0.02001 0.02028 0.02037 0.02132

Eigenvalues --- 0.02203 0.02232 0.02279 0.02298 0.02303

Eigenvalues --- 0.02324 0.02377 0.02439 0.02491 0.02506

Eigenvalues --- 0.02541 0.02549 0.02583 0.02626 0.02628

Eigenvalues --- 0.02653 0.02657 0.02750 0.02771 0.02783

Eigenvalues --- 0.02788 0.02832 0.02851 0.02865 0.02865

Eigenvalues --- 0.02866 0.02881 0.03961 0.04089 0.04189

Eigenvalues --- 0.04296 0.04352 0.04468 0.04545 0.04579

Eigenvalues --- 0.08390 0.09657 0.09664 0.09772 0.09841

Eigenvalues --- 0.09872 0.10302 0.10414 0.10561 0.10698

Eigenvalues --- 0.10733 0.10737 0.10738 0.10740 0.11053

Eigenvalues --- 0.11402 0.11405 0.11409 0.11413 0.11972

Eigenvalues --- 0.11978 0.11989 0.11998 0.12321 0.12324

Eigenvalues --- 0.12331 0.12331 0.12765 0.12769 0.12771

Eigenvalues --- 0.12776 0.15763 0.15942 0.16009 0.16348

Eigenvalues --- 0.17211 0.17439 0.17639 0.17993 0.18185

Eigenvalues --- 0.18218 0.18379 0.18535 0.19243 0.19289

Eigenvalues --- 0.19363 0.19391 0.19408 0.19421 0.19429

Eigenvalues --- 0.19434 0.19547 0.19547 0.19549 0.19550

Eigenvalues --- 0.20289 0.21494 0.22043 0.22775 0.22898

Eigenvalues --- 0.23105 0.23793 0.24216 0.24733 0.25378

Eigenvalues --- 0.26275 0.26460 0.26693 0.27013 0.28573

Eigenvalues --- 0.28622 0.28806 0.29058 0.29784 0.30988

Eigenvalues --- 0.31680 0.32028 0.32909 0.33121 0.33316

Eigenvalues --- 0.33335 0.33607 0.34200 0.35110 0.35571

Eigenvalues --- 0.35630 0.35631 0.35641 0.35645 0.35757

Eigenvalues --- 0.35758 0.35769 0.35818 0.35927 0.35927

Eigenvalues --- 0.35934 0.35938 0.35988 0.35994 0.36010

Eigenvalues --- 0.36015 0.36196 0.36199 0.36257 0.36265

Eigenvalues --- 0.36915 0.37044 0.37231 0.37382 0.37392

Eigenvalues --- 0.37468 0.38186 0.38438 0.38543 0.38576

Eigenvalues --- 0.39469 0.40269 0.40799 0.41109 0.41177

Eigenvalues --- 0.41198 0.41258 0.41287 0.41376 0.41421

Eigenvalues --- 0.41618 0.41896 0.42385 0.42656 0.44646

Eigenvalues --- 0.45134 0.45311 0.45934 0.45950 0.45994

Eigenvalues --- 0.46022 0.46182 0.46282 0.46288 0.46317

Eigenvalues --- 0.46332 0.48597 0.49086 0.49495 0.49610

Eigenvalues --- 0.50747 0.50749 0.50777 0.50779 0.51847

Eigenvalues --- 0.52167 0.57116 0.57560

Cosine: 0.539 < 0.970

Cut down GDIIS temporarily because of the cosine check. E 7

Eigenvalues --- 0.00134 0.00171 0.00433 0.00571 0.00675

Eigenvalues --- 0.00700 0.00815 0.01048 0.01067 0.01110

Eigenvalues --- 0.01123 0.01144 0.01256 0.01277 0.01281

Eigenvalues --- 0.01293 0.01311 0.01399 0.01419 0.01570

Eigenvalues --- 0.01585 0.01599 0.01633 0.01680 0.01706

Eigenvalues --- 0.01711 0.01722 0.01732 0.01758 0.01762

Eigenvalues --- 0.01770 0.01775 0.01782 0.01783 0.01875

Eigenvalues --- 0.01941 0.02001 0.02028 0.02037 0.02132

Eigenvalues --- 0.02203 0.02232 0.02279 0.02298 0.02303

Eigenvalues --- 0.02324 0.02377 0.02439 0.02491 0.02506

Eigenvalues --- 0.02541 0.02549 0.02583 0.02626 0.02628

Eigenvalues --- 0.02653 0.02657 0.02750 0.02771 0.02783

Eigenvalues --- 0.02788 0.02832 0.02851 0.02865 0.02865

Eigenvalues --- 0.02866 0.02881 0.03961 0.04089 0.04189

Eigenvalues --- 0.04296 0.04352 0.04468 0.04545 0.04579

Eigenvalues --- 0.08390 0.09657 0.09664 0.09772 0.09841

Eigenvalues --- 0.09872 0.10302 0.10414 0.10561 0.10698

Eigenvalues --- 0.10733 0.10737 0.10738 0.10740 0.11053

Eigenvalues --- 0.11402 0.11405 0.11409 0.11413 0.11972

Eigenvalues --- 0.11978 0.11989 0.11998 0.12321 0.12324

Eigenvalues --- 0.12331 0.12331 0.12765 0.12769 0.12771

Eigenvalues --- 0.12776 0.15763 0.15942 0.16009 0.16348

Eigenvalues --- 0.17211 0.17439 0.17639 0.17993 0.18185

Eigenvalues --- 0.18218 0.18379 0.18535 0.19243 0.19289

Eigenvalues --- 0.19363 0.19391 0.19408 0.19421 0.19429

Eigenvalues --- 0.19434 0.19547 0.19547 0.19549 0.19550

Eigenvalues --- 0.20289 0.21494 0.22043 0.22775 0.22898

Eigenvalues --- 0.23105 0.23793 0.24216 0.24733 0.25378

Eigenvalues --- 0.26275 0.26460 0.26693 0.27013 0.28573

Eigenvalues --- 0.28622 0.28806 0.29058 0.29784 0.30988

Eigenvalues --- 0.31680 0.32028 0.32909 0.33121 0.33316

Eigenvalues --- 0.33335 0.33607 0.34200 0.35110 0.35571

Eigenvalues --- 0.35630 0.35631 0.35641 0.35645 0.35757

Eigenvalues --- 0.35758 0.35769 0.35818 0.35927 0.35927

Eigenvalues --- 0.35934 0.35938 0.35988 0.35994 0.36010

Eigenvalues --- 0.36015 0.36196 0.36199 0.36257 0.36265

Eigenvalues --- 0.36915 0.37044 0.37231 0.37382 0.37392

Eigenvalues --- 0.37468 0.38186 0.38438 0.38543 0.38576

Eigenvalues --- 0.39469 0.40269 0.40799 0.41109 0.41177

Eigenvalues --- 0.41198 0.41258 0.41287 0.41376 0.41421

Eigenvalues --- 0.41618 0.41896 0.42385 0.42656 0.44646

Eigenvalues --- 0.45134 0.45311 0.45934 0.45950 0.45994

Eigenvalues --- 0.46022 0.46182 0.46282 0.46288 0.46317

Eigenvalues --- 0.46332 0.48597 0.49086 0.49495 0.49610

Eigenvalues --- 0.50747 0.50749 0.50777 0.50779 0.51847

Eigenvalues --- 0.52167 0.57116 0.57560

Quadratic step=4.055D-01 exceeds max=5.000D-02 adjusted using Lamda=-1.198D-02.

Angle between NR and scaled steps= 24.66 degrees.

Angle between quadratic step and forces= 59.85 degrees.

Linear search not attempted -- option 19 set.

Iteration 1 RMS(Cart)= 0.02340367 RMS(Int)= 0.00007376

Iteration 2 RMS(Cart)= 0.00018127 RMS(Int)= 0.00000379

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000379

ITry= 1 IFail=0 DXMaxC= 1.25D-01 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.65696 -0.00009 0.00000 -0.00032 -0.00032 2.65664

R2 2.64136 -0.00020 0.00000 -0.00052 -0.00052 2.64084

R3 2.03718 -0.00004 0.00000 -0.00015 -0.00015 2.03703

R4 2.59892 0.00029 0.00000 0.00074 0.00073 2.59965

R5 2.71604 -0.00016 0.00000 -0.00015 -0.00015 2.71589

R6 2.59819 0.00026 0.00000 0.00100 0.00099 2.59918

R7 1.90939 0.00041 0.00000 0.00110 0.00110 1.91049

R8 2.65643 -0.00004 0.00000 -0.00020 -0.00020 2.65623

R9 2.71809 -0.00015 0.00000 -0.00099 -0.00099 2.71710

R10 2.03726 -0.00005 0.00000 -0.00015 -0.00015 2.03711

R11 2.64108 -0.00031 0.00000 -0.00050 -0.00050 2.64058

R12 2.80355 -0.00001 0.00000 0.00025 0.00025 2.80380

R13 2.59678 -0.00010 0.00000 -0.00046 -0.00046 2.59632

R14 2.76211 -0.00008 0.00000 -0.00013 -0.00013 2.76197

R15 2.59375 -0.00011 0.00000 0.00031 0.00031 2.59405

R16 2.76227 0.00001 0.00000 -0.00004 -0.00003 2.76224

R17 2.64364 -0.00021 0.00000 -0.00111 -0.00111 2.64253

R18 2.55449 -0.00008 0.00000 -0.00019 -0.00018 2.55431

R19 2.03920 -0.00005 0.00000 -0.00009 -0.00009 2.03911

R20 2.03910 -0.00005 0.00000 -0.00014 -0.00014 2.03896

R21 2.64390 -0.00020 0.00000 -0.00105 -0.00105 2.64285

R22 2.80301 0.00002 0.00000 0.00033 0.00033 2.80334

R23 2.76226 0.00001 0.00000 0.00004 0.00004 2.76231

R24 2.59359 -0.00012 0.00000 0.00028 0.00028 2.59387

R25 2.55451 -0.00008 0.00000 -0.00018 -0.00018 2.55433

R26 2.03921 -0.00005 0.00000 -0.00011 -0.00011 2.03910

R27 2.76211 -0.00008 0.00000 -0.00017 -0.00017 2.76194

R28 2.03909 -0.00005 0.00000 -0.00011 -0.00011 2.03898

R29 2.59687 -0.00010 0.00000 -0.00045 -0.00046 2.59642

R30 2.64083 -0.00030 0.00000 -0.00054 -0.00054 2.64029

R31 2.71780 -0.00015 0.00000 -0.00104 -0.00104 2.71677

R32 2.80436 -0.00001 0.00000 0.00020 0.00020 2.80456

R33 2.65677 -0.00004 0.00000 -0.00024 -0.00024 2.65653

R34 2.59848 0.00027 0.00000 0.00097 0.00096 2.59944

R35 2.64109 -0.00021 0.00000 -0.00048 -0.00047 2.64062

R36 2.03720 -0.00006 0.00000 -0.00015 -0.00015 2.03705

R37 2.65724 -0.00012 0.00000 -0.00040 -0.00040 2.65684

R38 2.03712 -0.00005 0.00000 -0.00016 -0.00016 2.03696

R39 2.59914 0.00029 0.00000 0.00070 0.00070 2.59984

R40 2.71580 -0.00020 0.00000 -0.00029 -0.00029 2.71551

R41 1.90982 0.00043 0.00000 0.00111 0.00111 1.91093

R42 2.80381 0.00001 0.00000 0.00024 0.00024 2.80406

R43 2.65168 0.00013 0.00000 -0.00016 -0.00016 2.65152

R44 2.65022 -0.00003 0.00000 -0.00016 -0.00016 2.65006

R45 2.62845 0.00005 0.00000 0.00020 0.00020 2.62864

R46 2.04840 -0.00001 0.00000 0.00007 0.00007 2.04846

R47 2.63636 -0.00000 0.00000 -0.00005 -0.00005 2.63631

R48 2.05017 -0.00002 0.00000 -0.00004 -0.00004 2.05013

R49 2.63413 -0.00007 0.00000 -0.00011 -0.00011 2.63403

R50 2.05008 -0.00002 0.00000 -0.00004 -0.00004 2.05004

R51 2.63089 -0.00010 0.00000 -0.00011 -0.00011 2.63078

R52 2.05014 -0.00001 0.00000 -0.00001 -0.00001 2.05013

R53 2.04848 -0.00001 0.00000 0.00007 0.00007 2.04854

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R57 2.62868 0.00002 0.00000 0.00013 0.00013 2.62882

R58 2.05018 -0.00001 0.00000 -0.00001 -0.00001 2.05018

R59 2.65163 0.00009 0.00000 -0.00001 -0.00001 2.65162

R60 2.04840 0.00001 0.00000 0.00009 0.00009 2.04849

R61 2.65041 0.00004 0.00000 -0.00014 -0.00014 2.65026

R62 2.63060 -0.00007 0.00000 -0.00008 -0.00008 2.63052

R63 2.04852 -0.00001 0.00000 0.00002 0.00002 2.04854

R64 2.05016 -0.00001 0.00000 -0.00003 -0.00003 2.05013

R65 2.65011 0.00004 0.00000 -0.00014 -0.00014 2.64997

R66 2.65138 0.00010 0.00000 -0.00004 -0.00004 2.65134

R67 2.63072 -0.00009 0.00000 -0.00011 -0.00011 2.63061

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R69 2.63426 -0.00005 0.00000 -0.00009 -0.00009 2.63416

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R75 2.04841 0.00001 0.00000 0.00012 0.00012 2.04852

R76 2.64993 -0.00003 0.00000 -0.00018 -0.00018 2.64975

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A2 2.18745 -0.00000 0.00000 0.00010 0.00010 2.18756

A3 2.21436 -0.00008 0.00000 -0.00038 -0.00038 2.21399

A4 1.86768 0.00006 0.00000 0.00041 0.00041 1.86809

A5 2.22393 -0.00036 0.00000 -0.00289 -0.00287 2.22105

A6 2.19106 0.00030 0.00000 0.00260 0.00258 2.19364

A7 1.92576 -0.00026 0.00000 -0.00108 -0.00107 1.92469

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A12 2.22082 -0.00014 0.00000 -0.00123 -0.00121 2.21961

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A14 2.21469 -0.00009 0.00000 -0.00056 -0.00055 2.21413

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A19 2.19146 -0.00006 0.00000 0.00022 0.00020 2.19166

A20 2.16604 -0.00004 0.00000 -0.00061 -0.00060 2.16544

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A23 1.92657 0.00005 0.00000 0.00010 0.00009 1.92666

A24 2.19221 -0.00021 0.00000 -0.00051 -0.00052 2.19169

A25 2.16440 0.00016 0.00000 0.00041 0.00043 2.16483

A26 1.86203 -0.00002 0.00000 -0.00003 -0.00003 1.86200

A27 2.19684 0.00006 0.00000 0.00033 0.00033 2.19717

A28 2.22387 -0.00004 0.00000 -0.00026 -0.00026 2.22361

A29 1.86215 -0.00005 0.00000 -0.00010 -0.00010 1.86205

A30 2.19709 -0.00001 0.00000 -0.00039 -0.00039 2.19670

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A32 2.18415 -0.00018 0.00000 0.00014 0.00012 2.18427

A33 2.02594 0.00000 0.00000 -0.00055 -0.00054 2.02540

A34 2.07306 0.00017 0.00000 0.00039 0.00040 2.07346

A35 2.16463 0.00016 0.00000 0.00055 0.00056 2.16519

A36 2.19196 -0.00020 0.00000 -0.00059 -0.00060 2.19136

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A38 1.86205 -0.00002 0.00000 -0.00001 -0.00001 1.86203

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A48 2.18694 -0.00019 0.00000 0.00002 0.00000 2.18694

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A51 2.22073 -0.00015 0.00000 -0.00122 -0.00121 2.21952

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A53 1.86788 0.00007 0.00000 0.00049 0.00049 1.86837

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A59 2.18778 -0.00001 0.00000 0.00000 0.00000 2.18778

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A62 2.19092 0.00031 0.00000 0.00254 0.00252 2.19344

A63 1.92561 -0.00027 0.00000 -0.00108 -0.00107 1.92453

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A65 2.17632 0.00017 0.00000 0.00134 0.00134 2.17766

A66 2.18520 -0.00019 0.00000 0.00005 0.00003 2.18524

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A68 2.02634 -0.00001 0.00000 -0.00056 -0.00055 2.02579

A69 2.10308 0.00047 0.00000 0.00216 0.00216 2.10524

A70 2.10878 -0.00041 0.00000 -0.00220 -0.00220 2.10658

A71 2.07132 -0.00006 0.00000 0.00004 0.00004 2.07136

A72 2.10540 -0.00007 0.00000 -0.00033 -0.00033 2.10507

A73 2.08476 0.00008 0.00000 0.00049 0.00049 2.08525

A74 2.09283 -0.00001 0.00000 -0.00014 -0.00014 2.09269

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A77 2.09658 -0.00004 0.00000 -0.00024 -0.00024 2.09634

A78 2.08901 -0.00000 0.00000 -0.00008 -0.00008 2.08893

A79 2.09697 0.00001 0.00000 0.00005 0.00005 2.09702

A80 2.09720 -0.00001 0.00000 0.00003 0.00003 2.09723

A81 2.09777 -0.00001 0.00000 -0.00019 -0.00019 2.09758

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A103 2.09706 -0.00002 0.00000 -0.00003 -0.00003 2.09702

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A114 2.08901 -0.00001 0.00000 -0.00013 -0.00013 2.08889

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A117 2.09791 0.00003 0.00000 0.00017 0.00017 2.09808

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D7 3.13437 -0.00000 0.00000 -0.00006 -0.00006 3.13430

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D64 0.97698 0.00006 0.00000 0.00532 0.00532 0.98230

D65 -3.11396 0.00003 0.00000 0.00051 0.00051 -3.11345

D66 0.05812 0.00000 0.00000 -0.00076 -0.00076 0.05736

D67 0.02422 0.00002 0.00000 0.00046 0.00046 0.02469

D68 -3.08689 -0.00000 0.00000 -0.00081 -0.00081 -3.08770

D69 3.09638 0.00002 0.00000 0.00106 0.00106 3.09744

D70 -0.04174 0.00002 0.00000 0.00111 0.00111 -0.04063

D71 0.00309 -0.00005 0.00000 -0.00174 -0.00174 0.00135

D72 -3.11174 -0.00001 0.00000 -0.00085 -0.00085 -3.11259

D73 3.11357 -0.00002 0.00000 -0.00042 -0.00042 3.11315

D74 -0.00125 0.00002 0.00000 0.00047 0.00047 -0.00078

D75 -0.02952 0.00007 0.00000 0.00253 0.00253 -0.02699

D76 3.10247 0.00009 0.00000 0.00532 0.00532 3.10779

D77 3.08583 0.00003 0.00000 0.00168 0.00168 3.08750

D78 -0.06537 0.00005 0.00000 0.00447 0.00447 -0.06090

D79 0.04367 -0.00005 0.00000 -0.00219 -0.00219 0.04147

D80 -3.08815 -0.00008 0.00000 -0.00503 -0.00503 -3.09318

D81 3.02825 -0.00001 0.00000 -0.00176 -0.00176 3.02650

D82 -0.12016 -0.00010 0.00000 -0.00349 -0.00349 -0.12365

D83 -0.12441 0.00002 0.00000 0.00146 0.00146 -0.12295

D84 3.01037 -0.00007 0.00000 -0.00027 -0.00027 3.01010

D85 2.94313 -0.00001 0.00000 0.00523 0.00523 2.94836

D86 -0.23809 0.00007 0.00000 0.00795 0.00795 -0.23014

D87 -0.19182 0.00008 0.00000 0.00692 0.00692 -0.18490

D88 2.91014 0.00015 0.00000 0.00965 0.00965 2.91979

D89 -0.98778 -0.00013 0.00000 -0.00880 -0.00880 -0.99659

D90 2.15487 -0.00011 0.00000 -0.00742 -0.00742 2.14745

D91 2.14763 -0.00021 0.00000 -0.01038 -0.01038 2.13725

D92 -0.99291 -0.00019 0.00000 -0.00900 -0.00900 -1.00191

D93 3.09334 0.00006 0.00000 0.00253 0.00253 3.09586

D94 -0.05345 0.00003 0.00000 0.00174 0.00174 -0.05170

D95 -0.01461 -0.00001 0.00000 0.00020 0.00020 -0.01440

D96 3.12180 -0.00004 0.00000 -0.00058 -0.00058 3.12121

D97 -3.08258 -0.00012 0.00000 -0.00377 -0.00377 -3.08634

D98 0.11093 -0.00004 0.00000 -0.00139 -0.00139 0.10954

D99 0.02602 -0.00005 0.00000 -0.00153 -0.00153 0.02449

D100 -3.06366 0.00003 0.00000 0.00084 0.00085 -3.06281

D101 -0.00162 0.00006 0.00000 0.00113 0.00113 -0.00048

D102 3.13725 -0.00002 0.00000 -0.00055 -0.00055 3.13670

D103 -3.13792 0.00009 0.00000 0.00193 0.00193 -3.13599

D104 0.00095 0.00000 0.00000 0.00025 0.00025 0.00120

D105 0.01722 -0.00009 0.00000 -0.00203 -0.00203 0.01518

D106 -3.08428 -0.00017 0.00000 -0.00691 -0.00690 -3.09118

D107 -3.12170 -0.00001 0.00000 -0.00038 -0.00038 -3.12209

D108 0.05999 -0.00009 0.00000 -0.00526 -0.00525 0.05473

D109 -0.02702 0.00009 0.00000 0.00223 0.00223 -0.02479

D110 3.06280 0.00001 0.00000 -0.00020 -0.00021 3.06259

D111 3.07544 0.00015 0.00000 0.00684 0.00685 3.08229

D112 -0.11793 0.00007 0.00000 0.00441 0.00441 -0.11352

D113 -2.96977 0.00012 0.00000 0.00413 0.00413 -2.96564

D114 0.16928 0.00002 0.00000 0.00049 0.00049 0.16977

D115 0.21894 0.00003 0.00000 -0.00152 -0.00152 0.21742

D116 -2.92519 -0.00007 0.00000 -0.00517 -0.00517 -2.93036

D117 0.98723 0.00008 0.00000 0.00536 0.00536 0.99259

D118 -2.15463 0.00004 0.00000 0.00414 0.00414 -2.15050

D119 -2.15200 0.00017 0.00000 0.00875 0.00875 -2.14325

D120 0.98932 0.00013 0.00000 0.00753 0.00753 0.99685

D121 -3.12787 -0.00005 0.00000 -0.00170 -0.00170 -3.12957

D122 -0.00753 -0.00003 0.00000 -0.00089 -0.00090 -0.00843

D123 0.01696 -0.00004 0.00000 -0.00097 -0.00097 0.01599

D124 3.13730 -0.00001 0.00000 -0.00017 -0.00017 3.13713

D125 3.14044 0.00006 0.00000 0.00197 0.00197 -3.14078

D126 -0.01926 0.00001 0.00000 0.00094 0.00094 -0.01832

D127 -0.00441 0.00005 0.00000 0.00125 0.00125 -0.00316

D128 3.11909 -0.00000 0.00000 0.00022 0.00022 3.11930

D129 -0.01736 0.00001 0.00000 0.00038 0.00038 -0.01699

D130 3.12409 0.00001 0.00000 0.00012 0.00012 3.12421

D131 -3.13760 -0.00001 0.00000 -0.00044 -0.00044 -3.13804

D132 0.00385 -0.00002 0.00000 -0.00069 -0.00069 0.00316

D133 0.00494 -0.00000 0.00000 -0.00004 -0.00004 0.00489

D134 -3.13403 0.00001 0.00000 0.00029 0.00029 -3.13374

D135 -3.13651 0.00000 0.00000 0.00021 0.00021 -3.13630

D136 0.00771 0.00002 0.00000 0.00054 0.00054 0.00825

D137 0.00757 0.00002 0.00000 0.00032 0.00032 0.00789

D138 -3.13116 0.00001 0.00000 0.00009 0.00009 -3.13107

D139 -3.13665 0.00000 0.00000 -0.00001 -0.00001 -3.13666

D140 0.00780 -0.00000 0.00000 -0.00024 -0.00024 0.00757

D141 -0.00779 -0.00004 0.00000 -0.00094 -0.00094 -0.00873

D142 -3.13118 0.00001 0.00000 0.00009 0.00008 -3.13110

D143 3.13095 -0.00003 0.00000 -0.00071 -0.00071 3.13025

D144 0.00756 0.00002 0.00000 0.00031 0.00031 0.00788

D145 -0.00544 -0.00001 0.00000 -0.00033 -0.00033 -0.00577

D146 3.13566 -0.00001 0.00000 -0.00028 -0.00028 3.13538

D147 3.13417 -0.00000 0.00000 -0.00000 -0.00000 3.13417

D148 -0.00791 0.00000 0.00000 0.00004 0.00004 -0.00787

D149 -0.00690 0.00001 0.00000 0.00043 0.00043 -0.00647

D150 3.13196 -0.00001 0.00000 -0.00012 -0.00012 3.13184

D151 3.13668 0.00000 0.00000 0.00010 0.00010 3.13678

D152 -0.00766 -0.00002 0.00000 -0.00045 -0.00045 -0.00810

D153 0.01661 0.00001 0.00000 0.00010 0.00010 0.01671

D154 3.13658 -0.00000 0.00000 0.00013 0.00013 3.13670

D155 -3.12449 0.00001 0.00000 0.00006 0.00006 -3.12443

D156 -0.00453 -0.00000 0.00000 0.00008 0.00008 -0.00444

D157 3.12934 0.00002 0.00000 0.00082 0.00082 3.13016

D158 -0.01516 -0.00000 0.00000 0.00003 0.00003 -0.01513

D159 0.00927 0.00003 0.00000 0.00080 0.00080 0.01007

D160 -3.13523 0.00001 0.00000 0.00001 0.00001 -3.13522

D161 3.14147 -0.00002 0.00000 -0.00072 -0.00072 3.14075

D162 0.01811 -0.00001 0.00000 -0.00045 -0.00045 0.01766

D163 0.00278 0.00000 0.00000 0.00007 0.00007 0.00285

D164 -3.12058 0.00002 0.00000 0.00034 0.00034 -3.12024

D165 0.00819 -0.00001 0.00000 -0.00030 -0.00030 0.00790

D166 -3.13067 0.00001 0.00000 0.00025 0.00025 -3.13043

D167 3.13144 -0.00002 0.00000 -0.00055 -0.00055 3.13089

D168 -0.00743 -0.00000 0.00000 -0.00000 -0.00000 -0.00743

D169 -3.13931 -0.00004 0.00000 -0.00138 -0.00138 -3.14068

D170 0.01921 -0.00001 0.00000 -0.00078 -0.00078 0.01843

D171 0.00255 -0.00000 0.00000 -0.00018 -0.00018 0.00237

D172 -3.12211 0.00002 0.00000 0.00041 0.00041 -3.12170

D173 3.12713 0.00004 0.00000 0.00139 0.00140 3.12853

D174 0.00722 0.00005 0.00000 0.00122 0.00122 0.00844

D175 -0.01473 0.00000 0.00000 0.00020 0.00020 -0.01453

D176 -3.13464 0.00001 0.00000 0.00002 0.00002 -3.13462

D177 0.00810 -0.00000 0.00000 -0.00008 -0.00008 0.00801

D178 -3.13114 0.00002 0.00000 0.00038 0.00038 -3.13076

D179 3.13266 -0.00003 0.00000 -0.00067 -0.00067 3.13199

D180 -0.00658 -0.00001 0.00000 -0.00021 -0.00021 -0.00679

D181 -0.00667 0.00001 0.00000 0.00034 0.00034 -0.00633

D182 3.13649 0.00000 0.00000 0.00011 0.00011 3.13660

D183 3.13255 -0.00001 0.00000 -0.00013 -0.00013 3.13242

D184 -0.00747 -0.00002 0.00000 -0.00036 -0.00036 -0.00783

D185 -0.00546 -0.00001 0.00000 -0.00032 -0.00032 -0.00578

D186 3.13538 -0.00001 0.00000 -0.00032 -0.00032 3.13505

D187 3.13456 -0.00001 0.00000 -0.00009 -0.00009 3.13447

D188 -0.00778 -0.00000 0.00000 -0.00009 -0.00009 -0.00788

D189 0.01630 0.00001 0.00000 0.00006 0.00006 0.01635

D190 3.13611 0.00000 0.00000 0.00024 0.00024 3.13635

D191 -3.12454 0.00000 0.00000 0.00005 0.00005 -3.12449

D192 -0.00474 -0.00000 0.00000 0.00024 0.00024 -0.00449

D193 3.13856 0.00008 0.00000 0.00273 0.00273 3.14129

D194 -0.01998 0.00001 0.00000 0.00134 0.00134 -0.01864

D195 -0.00408 0.00006 0.00000 0.00138 0.00138 -0.00270

D196 3.12057 -0.00001 0.00000 -0.00001 -0.00001 3.12056

D197 -3.12622 -0.00006 0.00000 -0.00233 -0.00234 -3.12855

D198 -0.00589 -0.00004 0.00000 -0.00145 -0.00145 -0.00734

D199 0.01641 -0.00004 0.00000 -0.00098 -0.00098 0.01543

D200 3.13674 -0.00002 0.00000 -0.00010 -0.00010 3.13664

D201 -0.00769 -0.00005 0.00000 -0.00110 -0.00110 -0.00879

D202 3.13138 -0.00004 0.00000 -0.00091 -0.00091 3.13047

D203 -3.13224 0.00002 0.00000 0.00029 0.00029 -3.13195

D204 0.00684 0.00003 0.00000 0.00048 0.00048 0.00731

D205 0.00726 0.00002 0.00000 0.00038 0.00038 0.00764

D206 -3.13651 0.00000 0.00000 -0.00004 -0.00004 -3.13655

D207 -3.13180 0.00001 0.00000 0.00020 0.00019 -3.13161

D208 0.00761 -0.00000 0.00000 -0.00023 -0.00023 0.00739

D209 0.00503 0.00000 0.00000 0.00002 0.00002 0.00505

D210 -3.13617 0.00000 0.00000 0.00017 0.00017 -3.13601

D211 -3.13439 0.00002 0.00000 0.00044 0.00044 -3.13395

D212 0.00760 0.00002 0.00000 0.00059 0.00059 0.00818

D213 -0.01702 0.00001 0.00000 0.00029 0.00029 -0.01673

D214 -3.13725 -0.00001 0.00000 -0.00060 -0.00060 -3.13785

D215 3.12418 0.00001 0.00000 0.00014 0.00014 3.12433

D216 0.00395 -0.00002 0.00000 -0.00075 -0.00075 0.00321

Item Value Threshold Converged?

Maximum Force 0.000509 0.000450 NO

RMS Force 0.000103 0.000300 YES

Maximum Displacement 0.124630 0.001800 NO

RMS Displacement 0.023453 0.001200 NO

Predicted change in Energy=-4.215300D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

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(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=1 Diff= 5.73D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 1.015606 -4.099136 0.557887

2 6 0 1.348259 -2.780847 0.200356

3 7 0 0.165750 -2.107210 -0.000586

4 6 0 -0.902433 -2.953692 0.184485

5 6 0 -0.377731 -4.206107 0.547667

6 6 0 -2.286996 -2.611620 0.001962

7 6 0 -2.787203 -1.312647 -0.120532

8 7 0 -2.062419 -0.157806 0.048783

9 6 0 -2.958189 0.871621 -0.100276

10 6 0 -4.283872 0.349812 -0.427213

11 6 0 -4.177909 -0.997637 -0.441315

12 6 0 2.665405 -2.230973 0.032207

13 6 0 2.958402 -0.870376 -0.105034

14 6 0 4.283887 -0.347254 -0.430841

15 6 0 4.177812 1.000239 -0.440153

16 6 0 2.787065 1.313925 -0.118333

17 7 0 2.062523 0.158341 0.047329

18 6 0 2.286679 2.612361 0.007342

19 6 0 0.902476 2.955272 0.189654

20 6 0 0.377224 4.213179 0.533142

21 6 0 -1.015991 4.106241 0.543947

22 6 0 -1.348283 2.782483 0.206431

23 7 0 -0.165543 2.105769 0.016856

24 6 0 -2.664983 2.231768 0.039247

25 6 0 -3.236391 -3.751032 -0.040089

26 6 0 -3.075867 -4.780771 -0.979569

27 6 0 -3.974255 -5.841651 -1.028172

28 6 0 -5.036895 -5.903278 -0.126375

29 6 0 -5.198089 -4.893303 0.820636

30 6 0 -4.308709 -3.823037 0.860767

31 6 0 5.901383 -5.048769 -0.002721

32 6 0 4.855479 -5.171694 -0.917710

33 6 0 3.800121 -4.265546 -0.900360

34 6 0 3.782289 -3.207243 0.020823

35 6 0 4.839910 -3.092745 0.934728

36 6 0 5.887889 -4.008905 0.925500

37 6 0 -3.782885 3.207409 0.024904

38 6 0 -4.836910 3.097882 0.943320

39 6 0 -5.886919 4.011746 0.930436

40 6 0 -5.905891 5.044026 -0.006103

41 6 0 -4.863590 5.161644 -0.925847

42 6 0 -3.806268 4.257752 -0.905003

43 6 0 3.237170 3.751310 -0.036684

44 6 0 4.304712 3.827335 0.869245

45 6 0 5.196022 4.895978 0.826906

46 6 0 5.041368 5.900007 -0.127478

47 6 0 3.983587 5.833985 -1.034619

48 6 0 3.083326 4.774699 -0.983942

49 1 0 1.721918 -4.876391 0.800724

50 1 0 -0.960780 -5.081999 0.782052

51 1 0 -5.160751 0.940606 -0.642606

52 1 0 -4.951632 -1.713927 -0.670346

53 1 0 5.160703 -0.937207 -0.648765

54 1 0 4.951544 1.717431 -0.666366

55 1 0 0.959531 5.093403 0.752503

56 1 0 -1.722420 4.887725 0.772278

57 1 0 -2.253827 -4.736032 -1.684769

58 1 0 -3.845127 -6.621450 -1.771281

59 1 0 -5.732811 -6.734789 -0.160315

60 1 0 -6.016060 -4.938651 1.531857

61 1 0 -4.432304 -3.044883 1.605313

62 1 0 6.720435 -5.760052 -0.012680

63 1 0 4.861795 -5.974951 -1.646931

64 1 0 2.992189 -4.362895 -1.616497

65 1 0 4.828272 -2.291413 1.664709

66 1 0 6.692762 -3.911486 1.646374

67 1 0 -4.821312 2.301800 1.678995

68 1 0 -6.689254 3.918225 1.654655

69 1 0 -6.726565 5.753392 -0.019028

70 1 0 -4.874312 5.958774 -1.661717

71 1 0 -3.001265 4.350677 -1.625042

72 1 0 4.423460 3.053294 1.618902

73 1 0 6.010473 4.944567 1.541945

74 1 0 5.738799 6.730173 -0.163225

75 1 0 3.859721 6.608983 -1.783634

76 1 0 2.265149 4.726368 -1.693406

77 1 0 0.092437 -1.122522 -0.217631

78 1 0 -0.091831 1.115096 -0.172084

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0587919 0.0582516 0.0300945

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(Enter /home/kira/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5356.9485797161 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122058555 Hartrees.

Nuclear repulsion after empirical dispersion term = 5356.7363738605 Hartrees.

Force inversion solution in PCM.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5786

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.27D-10

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 309

GePol: Fraction of low-weight points (<1% of avg) = 5.34%

GePol: Cavity surface area = 610.644 Ang\*\*2

GePol: Cavity volume = 628.190 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0021019020 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5356.7342719586 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.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

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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: "TPP3C1.chk"

B after Tr= -0.000000 0.000000 0.000000

Rot= 0.999796 0.000003 0.000001 0.020219 Ang= 2.32 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0183

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30524590098

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(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 590000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 100433388.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.77D-15 for 5748.

Iteration 1 A\*A^-1 deviation from orthogonality is 7.44D-15 for 5774 4723.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.77D-15 for 5770.

Iteration 1 A^-1\*A deviation from orthogonality is 4.44D-11 for 5573 5555.

E= -1914.33117283867

DIIS: error= 1.28D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.33117283867 IErMin= 1 ErrMin= 1.28D-03

ErrMax= 1.28D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.34D-03 BMatP= 4.34D-03

IDIUse=3 WtCom= 9.87D-01 WtEn= 1.28D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.640 Goal= None Shift= 0.000

Gap= 0.706 Goal= None Shift= 0.000

GapD= 0.640 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=4.36D-05 MaxDP=1.77D-03 OVMax= 6.99D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.36D-05 CP: 1.00D+00

E= -1914.33327532593 Delta-E= -0.002102487259 Rises=F Damp=F

DIIS: error= 1.88D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33327532593 IErMin= 2 ErrMin= 1.88D-04

ErrMax= 1.88D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.40D-05 BMatP= 4.34D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.88D-03

Coeff-Com: -0.669D-01 0.107D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.668D-01 0.107D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=8.13D-06 MaxDP=2.54D-04 DE=-2.10D-03 OVMax= 1.05D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 7.37D-06 CP: 1.00D+00 1.08D+00

E= -1914.33330419521 Delta-E= -0.000028869280 Rises=F Damp=F

DIIS: error= 6.59D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33330419521 IErMin= 3 ErrMin= 6.59D-05

ErrMax= 6.59D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.89D-05 BMatP= 5.40D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.317D-01 0.421D+00 0.610D+00

Coeff: -0.317D-01 0.421D+00 0.610D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.14D-06 MaxDP=2.38D-04 DE=-2.89D-05 OVMax= 5.15D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.61D-06 CP: 1.00D+00 1.09D+00 7.83D-01

E= -1914.33330739171 Delta-E= -0.000003196498 Rises=F Damp=F

DIIS: error= 4.54D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33330739171 IErMin= 4 ErrMin= 4.54D-05

ErrMax= 4.54D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.72D-06 BMatP= 1.89D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.807D-02 0.816D-01 0.372D+00 0.554D+00

Coeff: -0.807D-02 0.816D-01 0.372D+00 0.554D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.35D-06 MaxDP=1.05D-04 DE=-3.20D-06 OVMax= 4.20D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 9.05D-07 CP: 1.00D+00 1.10D+00 8.56D-01 6.83D-01

E= -1914.33330901616 Delta-E= -0.000001624454 Rises=F Damp=F

DIIS: error= 1.08D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33330901616 IErMin= 5 ErrMin= 1.08D-05

ErrMax= 1.08D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.35D-07 BMatP= 6.72D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.415D-03-0.801D-02 0.987D-01 0.240D+00 0.670D+00

Coeff: -0.415D-03-0.801D-02 0.987D-01 0.240D+00 0.670D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.02D-07 MaxDP=3.39D-05 DE=-1.62D-06 OVMax= 2.01D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.02D-07 CP: 1.00D+00 1.10D+00 8.67D-01 7.62D-01 7.86D-01

E= -1914.33330908822 Delta-E= -0.000000072060 Rises=F Damp=F

DIIS: error= 5.99D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33330908822 IErMin= 6 ErrMin= 5.99D-06

ErrMax= 5.99D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.23D-07 BMatP= 3.35D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.897D-03-0.172D-01 0.776D-02 0.715D-01 0.425D+00 0.512D+00

Coeff: 0.897D-03-0.172D-01 0.776D-02 0.715D-01 0.425D+00 0.512D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.47D-07 MaxDP=1.75D-05 DE=-7.21D-08 OVMax= 9.56D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.84D-07 CP: 1.00D+00 1.10D+00 8.78D-01 7.61D-01 8.97D-01

CP: 7.60D-01

E= -1914.33330912358 Delta-E= -0.000000035360 Rises=F Damp=F

DIIS: error= 2.07D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33330912358 IErMin= 7 ErrMin= 2.07D-06

ErrMax= 2.07D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.86D-09 BMatP= 1.23D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.426D-03-0.703D-02-0.354D-02 0.157D-01 0.140D+00 0.234D+00

Coeff-Com: 0.620D+00

Coeff: 0.426D-03-0.703D-02-0.354D-02 0.157D-01 0.140D+00 0.234D+00

Coeff: 0.620D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.19D-07 MaxDP=7.83D-06 DE=-3.54D-08 OVMax= 9.62D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 7.46D-08 CP: 1.00D+00 1.10D+00 8.79D-01 7.70D-01 9.20D-01

CP: 9.45D-01 1.24D+00

E= -1914.33330912951 Delta-E= -0.000000005934 Rises=F Damp=F

DIIS: error= 1.56D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33330912951 IErMin= 8 ErrMin= 1.56D-06

ErrMax= 1.56D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.46D-09 BMatP= 7.86D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.243D-03 0.546D-02-0.663D-02-0.298D-01-0.156D+00-0.143D+00

Coeff-Com: 0.378D+00 0.952D+00

Coeff: -0.243D-03 0.546D-02-0.663D-02-0.298D-01-0.156D+00-0.143D+00

Coeff: 0.378D+00 0.952D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.72D-07 MaxDP=1.06D-05 DE=-5.93D-09 OVMax= 1.59D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 5.05D-08 CP: 1.00D+00 1.10D+00 8.81D-01 7.78D-01 9.78D-01

CP: 1.15D+00 1.92D+00 1.46D+00

E= -1914.33330913566 Delta-E= -0.000000006143 Rises=F Damp=F

DIIS: error= 1.24D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33330913566 IErMin= 9 ErrMin= 1.24D-06

ErrMax= 1.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.55D-10 BMatP= 3.46D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.205D-03 0.396D-02-0.157D-02-0.152D-01-0.985D-01-0.119D+00

Coeff-Com: 0.889D-03 0.384D+00 0.845D+00

Coeff: -0.205D-03 0.396D-02-0.157D-02-0.152D-01-0.985D-01-0.119D+00

Coeff: 0.889D-03 0.384D+00 0.845D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.13D-07 MaxDP=8.46D-06 DE=-6.14D-09 OVMax= 1.15D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 3.04D-08 CP: 1.00D+00 1.10D+00 8.82D-01 7.82D-01 1.00D+00

CP: 1.30D+00 2.30D+00 1.98D+00 1.59D+00

E= -1914.33330913795 Delta-E= -0.000000002292 Rises=F Damp=F

DIIS: error= 8.21D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33330913795 IErMin=10 ErrMin= 8.21D-07

ErrMax= 8.21D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.19D-10 BMatP= 9.55D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.364D-05-0.355D-03 0.251D-02 0.604D-02 0.192D-01-0.467D-02

Coeff-Com: -0.191D+00-0.261D+00 0.584D+00 0.846D+00

Coeff: -0.364D-05-0.355D-03 0.251D-02 0.604D-02 0.192D-01-0.467D-02

Coeff: -0.191D+00-0.261D+00 0.584D+00 0.846D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.03D-07 MaxDP=7.43D-06 DE=-2.29D-09 OVMax= 1.07D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.73D-08 CP: 1.00D+00 1.10D+00 8.82D-01 7.85D-01 1.03D+00

CP: 1.42D+00 2.65D+00 2.48D+00 2.45D+00 1.32D+00

E= -1914.33330913921 Delta-E= -0.000000001260 Rises=F Damp=F

DIIS: error= 5.95D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33330913921 IErMin=11 ErrMin= 5.95D-07

ErrMax= 5.95D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.63D-10 BMatP= 6.19D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.578D-04-0.134D-02 0.171D-02 0.743D-02 0.396D-01 0.302D-01

Coeff-Com: -0.889D-01-0.248D+00 0.659D-01 0.395D+00 0.798D+00

Coeff: 0.578D-04-0.134D-02 0.171D-02 0.743D-02 0.396D-01 0.302D-01

Coeff: -0.889D-01-0.248D+00 0.659D-01 0.395D+00 0.798D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.74D-08 MaxDP=4.74D-06 DE=-1.26D-09 OVMax= 6.36D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.23D-08 CP: 1.00D+00 1.10D+00 8.83D-01 7.87D-01 1.04D+00

CP: 1.48D+00 2.83D+00 2.78D+00 2.97D+00 1.83D+00

CP: 1.32D+00

E= -1914.33330913965 Delta-E= -0.000000000443 Rises=F Damp=F

DIIS: error= 3.50D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.33330913965 IErMin=12 ErrMin= 3.50D-07

ErrMax= 3.50D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.18D-10 BMatP= 1.63D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.398D-04-0.689D-03-0.240D-03 0.158D-02 0.169D-01 0.201D-01

Coeff-Com: 0.471D-01-0.355D-01-0.260D+00-0.221D+00 0.611D+00 0.821D+00

Coeff: 0.398D-04-0.689D-03-0.240D-03 0.158D-02 0.169D-01 0.201D-01

Coeff: 0.471D-01-0.355D-01-0.260D+00-0.221D+00 0.611D+00 0.821D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.07D-08 MaxDP=3.97D-06 DE=-4.43D-10 OVMax= 5.53D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 2.46D-08 CP: 1.00D+00 1.10D+00 8.83D-01 7.88D-01 1.05D+00

CP: 1.53D+00 2.97D+00 3.00D+00 3.00D+00 2.26D+00

CP: 2.07D+00 1.20D+00

E= -1914.33330913984 Delta-E= -0.000000000190 Rises=F Damp=F

DIIS: error= 2.06D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.33330913984 IErMin=13 ErrMin= 2.06D-07

ErrMax= 2.06D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.67D-11 BMatP= 1.18D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.228D-05 0.836D-04-0.770D-03-0.171D-02-0.384D-02-0.468D-03

Coeff-Com: 0.616D-01 0.649D-01-0.157D+00-0.273D+00 0.101D+00 0.398D+00

Coeff-Com: 0.811D+00

Coeff: 0.228D-05 0.836D-04-0.770D-03-0.171D-02-0.384D-02-0.468D-03

Coeff: 0.616D-01 0.649D-01-0.157D+00-0.273D+00 0.101D+00 0.398D+00

Coeff: 0.811D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.54D-08 MaxDP=2.21D-06 DE=-1.90D-10 OVMax= 2.85D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 1.15D-08 CP: 1.00D+00 1.10D+00 8.83D-01 7.88D-01 1.05D+00

CP: 1.55D+00 3.00D+00 3.00D+00 3.00D+00 2.51D+00

CP: 2.45D+00 1.65D+00 1.54D+00

E= -1914.33330913992 Delta-E= -0.000000000075 Rises=F Damp=F

DIIS: error= 1.01D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.33330913992 IErMin=14 ErrMin= 1.01D-07

ErrMax= 1.01D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.46D-11 BMatP= 2.67D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.134D-04 0.314D-03-0.403D-03-0.167D-02-0.878D-02-0.866D-02

Coeff-Com: 0.220D-01 0.529D-01 0.245D-02-0.983D-01-0.153D+00-0.951D-01

Coeff-Com: 0.547D+00 0.742D+00

Coeff: -0.134D-04 0.314D-03-0.403D-03-0.167D-02-0.878D-02-0.866D-02

Coeff: 0.220D-01 0.529D-01 0.245D-02-0.983D-01-0.153D+00-0.951D-01

Coeff: 0.547D+00 0.742D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.60D-08 MaxDP=1.33D-06 DE=-7.55D-11 OVMax= 1.77D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 4.60D-09 CP: 1.00D+00 1.10D+00 8.83D-01 7.88D-01 1.06D+00

CP: 1.56D+00 3.00D+00 3.00D+00 3.00D+00 2.66D+00

CP: 2.72D+00 1.88D+00 1.89D+00 1.74D+00

E= -1914.33330913990 Delta-E= 0.000000000017 Rises=F Damp=F

DIIS: error= 5.51D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=14 EnMin= -1914.33330913992 IErMin=15 ErrMin= 5.51D-08

ErrMax= 5.51D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.63D-12 BMatP= 1.46D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.424D-05 0.360D-04 0.245D-03 0.376D-03-0.451D-03-0.245D-02

Coeff-Com: -0.219D-01-0.167D-01 0.740D-01 0.904D-01-0.662D-01-0.223D+00

Coeff-Com: -0.175D+00 0.162D+00 0.118D+01

Coeff: -0.424D-05 0.360D-04 0.245D-03 0.376D-03-0.451D-03-0.245D-02

Coeff: -0.219D-01-0.167D-01 0.740D-01 0.904D-01-0.662D-01-0.223D+00

Coeff: -0.175D+00 0.162D+00 0.118D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.07D-08 MaxDP=9.12D-07 DE= 1.73D-11 OVMax= 1.18D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 1.93D-09 CP: 1.00D+00 1.10D+00 8.83D-01 7.88D-01 1.06D+00

CP: 1.57D+00 3.00D+00 3.00D+00 3.00D+00 2.75D+00

CP: 2.88D+00 2.07D+00 2.10D+00 2.26D+00 1.57D+00

E= -1914.33330913997 Delta-E= -0.000000000073 Rises=F Damp=F

DIIS: error= 1.97D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1914.33330913997 IErMin=16 ErrMin= 1.97D-08

ErrMax= 1.97D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.15D-12 BMatP= 2.63D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.769D-06-0.552D-04 0.249D-03 0.638D-03 0.186D-02 0.703D-03

Coeff-Com: -0.182D-01-0.223D-01 0.429D-01 0.739D-01-0.496D-03-0.113D+00

Coeff-Com: -0.229D+00-0.909D-01 0.678D+00 0.675D+00

Coeff: 0.769D-06-0.552D-04 0.249D-03 0.638D-03 0.186D-02 0.703D-03

Coeff: -0.182D-01-0.223D-01 0.429D-01 0.739D-01-0.496D-03-0.113D+00

Coeff: -0.229D+00-0.909D-01 0.678D+00 0.675D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.00D-09 MaxDP=3.24D-07 DE=-7.28D-11 OVMax= 4.32D-06

Error on total polarization charges = 0.08260

SCF Done: E(UB3LYP) = -1914.33330914 A.U. after 16 cycles

NFock= 16 Conv=0.40D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0550 S= 1.0182

<L.S>= 0.000000000000E+00

KE= 1.906383071289D+03 PE=-1.516309887873D+04 EE= 5.985648226340D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0550, after 2.0017

Leave Link 502 at Wed Aug 28 17:10:59 2019, MaxMem= 4294967296 cpu: 6624.0

(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: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48629807D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64260133D-01

Leave Link 801 at Wed Aug 28 17:10:59 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Wed Aug 28 17:11:06 2019, MaxMem= 4294967296 cpu: 111.0

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Wed Aug 28 17:11:06 2019, MaxMem= 4294967296 cpu: 2.0

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 188

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Wed Aug 28 17:32:47 2019, MaxMem= 4294967296 cpu: 20792.0

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 590000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.38D+03 4.49D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.51D+02 3.63D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.51D+00 4.64D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.02D-01 3.97D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.58D-04 2.10D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.57D-06 1.35D-04.

188 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 1.99D-08 1.01D-05.

80 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.31D-11 6.20D-07.

42 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.17D-13 3.86D-08.

3 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 8.70D-15 4.58D-09.

3 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 5.62D-15 2.13D-09.

3 vectors produced by pass 11 Test12= 2.55D-13 1.00D-09 XBig12= 5.42D-15 2.47D-09.

3 vectors produced by pass 12 Test12= 2.55D-13 1.00D-09 XBig12= 1.08D-14 3.64D-09.

3 vectors produced by pass 13 Test12= 2.55D-13 1.00D-09 XBig12= 7.85D-15 2.48D-09.

3 vectors produced by pass 14 Test12= 2.55D-13 1.00D-09 XBig12= 8.40D-15 2.84D-09.

3 vectors produced by pass 15 Test12= 2.55D-13 1.00D-09 XBig12= 8.06D-15 2.73D-09.

3 vectors produced by pass 16 Test12= 2.55D-13 1.00D-09 XBig12= 5.35D-15 2.54D-09.

3 vectors produced by pass 17 Test12= 2.55D-13 1.00D-09 XBig12= 4.04D-15 2.28D-09.

3 vectors produced by pass 18 Test12= 2.55D-13 1.00D-09 XBig12= 9.10D-15 2.85D-09.

2 vectors produced by pass 19 Test12= 2.55D-13 1.00D-09 XBig12= 5.32D-15 1.93D-09.

InvSVY: IOpt=1 It= 1 EMax= 8.53D-14

Solved reduced A of dimension 1749 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1125.64 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Wed Aug 28 21:27:48 2019, MaxMem= 4294967296 cpu: 225563.0

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 188

Leave Link 701 at Wed Aug 28 21:29:18 2019, MaxMem= 4294967296 cpu: 1428.5

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Wed Aug 28 21:29:18 2019, MaxMem= 4294967296 cpu: 0.5

(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=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

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= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Wed Aug 28 21:48:40 2019, MaxMem= 4294967296 cpu: 18587.0

(Enter /home/kira/g09/l716.exe)

Dipole =-2.56023809D-04-1.14512620D-02-4.79990113D-01

Polarizability= 1.25674959D+03-3.38351866D+01 1.66479668D+03

1.93639580D-02-2.04706589D-01 4.55360117D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000029719 -0.000042876 -0.000000817

2 6 0.000033662 0.000025290 -0.000022592

3 7 -0.000003317 -0.000075138 0.000034277

4 6 0.000020871 -0.000051574 -0.000004006

5 6 0.000017169 0.000054850 -0.000033122

6 6 0.000014067 0.000068732 0.000059218

7 6 -0.000015824 0.000034361 -0.000036373

8 7 0.000120618 -0.000022007 0.000003572

9 6 -0.000017801 0.000018126 -0.000004764

10 6 -0.000000267 0.000000284 -0.000019893

11 6 -0.000001056 0.000035470 0.000039402

12 6 -0.000039376 0.000016112 -0.000039547

13 6 0.000019629 0.000038549 0.000005714

14 6 0.000000179 -0.000004270 0.000022137

15 6 -0.000000167 0.000039696 -0.000041436

16 6 0.000018071 0.000017243 0.000038968

17 7 -0.000128197 -0.000006548 -0.000012985

18 6 -0.000016505 0.000066222 -0.000072914

19 6 -0.000028748 -0.000002569 0.000003177

20 6 -0.000019581 0.000036058 0.000030007

21 6 0.000034910 -0.000059762 0.000005286

22 6 -0.000052876 0.000070079 0.000026743

23 7 0.000021401 -0.000141997 -0.000017608

24 6 0.000042148 0.000021840 0.000043501

25 6 0.000018737 -0.000097186 -0.000002004

26 6 -0.000099736 0.000022990 -0.000055665

27 6 0.000016249 -0.000013354 0.000027410

28 6 -0.000012835 0.000020220 0.000003603

29 6 0.000044605 -0.000002962 -0.000008606

30 6 0.000012215 -0.000048794 -0.000014046

31 6 0.000016064 -0.000007334 -0.000012743

32 6 0.000012338 0.000008170 0.000018319

33 6 0.000012751 0.000022561 0.000009751

34 6 -0.000024195 0.000062695 0.000054573

35 6 0.000009577 -0.000062513 -0.000057999

36 6 -0.000001774 0.000026791 0.000027026

37 6 0.000029966 0.000054993 -0.000069126

38 6 -0.000005559 -0.000063146 0.000050747

39 6 -0.000000157 0.000024186 -0.000026938

40 6 -0.000013907 -0.000009733 0.000013526

41 6 -0.000017306 0.000001026 -0.000012615

42 6 -0.000012723 0.000021190 -0.000006478

43 6 -0.000002390 -0.000095581 0.000019136

44 6 -0.000011294 -0.000051407 0.000013874

45 6 -0.000044417 -0.000001810 0.000012011

46 6 0.000009196 0.000019454 -0.000008821

47 6 -0.000018200 -0.000016045 -0.000027139

48 6 0.000098004 0.000014769 0.000048415

49 1 0.000028464 0.000008993 -0.000004957

50 1 -0.000000236 -0.000010778 -0.000010267

51 1 -0.000045999 -0.000009644 -0.000015437

52 1 -0.000002717 -0.000020262 -0.000038740

53 1 0.000045523 -0.000007907 0.000016252

54 1 0.000001300 -0.000022461 0.000036933

55 1 -0.000004852 -0.000004801 0.000018970

56 1 -0.000026734 0.000009188 0.000003920

57 1 -0.000000056 0.000001295 0.000009476

58 1 0.000003051 0.000012797 0.000001484

59 1 0.000015085 0.000002313 0.000007994

60 1 -0.000008445 0.000002022 -0.000006051

61 1 -0.000030841 0.000017865 0.000014904

62 1 -0.000006783 0.000004462 0.000012551

63 1 0.000001851 -0.000000852 -0.000010677

64 1 -0.000025322 -0.000026180 -0.000017136

65 1 -0.000015238 0.000013615 -0.000020463

66 1 -0.000003619 -0.000006592 0.000004115

67 1 0.000019094 0.000015493 0.000022354

68 1 0.000004086 -0.000007317 -0.000003779

69 1 0.000006256 0.000001884 -0.000012063

70 1 -0.000001681 -0.000001272 0.000009416

71 1 0.000025590 -0.000030114 0.000016544

72 1 0.000032655 0.000018644 -0.000014225

73 1 0.000008678 0.000000814 0.000005623

74 1 -0.000015959 0.000001313 -0.000008301

75 1 -0.000003342 0.000010807 -0.000002991

76 1 0.000000816 -0.000001478 -0.000010214

77 1 0.000177103 -0.000007072 0.000040363

78 1 -0.000182229 0.000069877 -0.000047755

-------------------------------------------------------------------

Cartesian Forces: Max 0.000182229 RMS 0.000036920

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Wed Aug 28 21:48:40 2019, MaxMem= 4294967296 cpu: 3.5

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000174328 RMS 0.000040801

Search for a local minimum.

Step number 17 out of a maximum of 452

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -7.49D-05 DEPred=-4.22D-05 R= 1.78D+00

TightC=F SS= 1.41D+00 RLast= 5.01D-02 DXNew= 8.4090D-02 1.5024D-01

Trust test= 1.78D+00 RLast= 5.01D-02 DXMaxT set to 8.41D-02

ITU= 1 -1 -1 1 0 -1 1 1 -1 1 -1 -1 1 1 -1 1 0

Eigenvalues --- 0.00183 0.00269 0.00374 0.00593 0.00720

Eigenvalues --- 0.00785 0.00904 0.01048 0.01065 0.01121

Eigenvalues --- 0.01137 0.01152 0.01261 0.01280 0.01300

Eigenvalues --- 0.01301 0.01320 0.01421 0.01427 0.01552

Eigenvalues --- 0.01563 0.01566 0.01600 0.01674 0.01710

Eigenvalues --- 0.01716 0.01727 0.01736 0.01756 0.01761

Eigenvalues --- 0.01763 0.01779 0.01796 0.01801 0.01883

Eigenvalues --- 0.01940 0.01992 0.02017 0.02022 0.02170

Eigenvalues --- 0.02173 0.02250 0.02286 0.02299 0.02304

Eigenvalues --- 0.02328 0.02388 0.02470 0.02472 0.02520

Eigenvalues --- 0.02540 0.02547 0.02584 0.02628 0.02629

Eigenvalues --- 0.02645 0.02648 0.02764 0.02776 0.02794

Eigenvalues --- 0.02800 0.02863 0.02869 0.02872 0.02873

Eigenvalues --- 0.02915 0.02944 0.03946 0.04087 0.04189

Eigenvalues --- 0.04321 0.04366 0.04470 0.04547 0.04578

Eigenvalues --- 0.08232 0.09654 0.09677 0.09742 0.09849

Eigenvalues --- 0.09872 0.10299 0.10430 0.10566 0.10696

Eigenvalues --- 0.10707 0.10712 0.10739 0.10742 0.11006

Eigenvalues --- 0.11397 0.11405 0.11409 0.11415 0.11976

Eigenvalues --- 0.11986 0.11995 0.12007 0.12289 0.12292

Eigenvalues --- 0.12330 0.12331 0.12769 0.12769 0.12775

Eigenvalues --- 0.12778 0.15717 0.15942 0.16313 0.16650

Eigenvalues --- 0.17213 0.17382 0.17610 0.17874 0.18033

Eigenvalues --- 0.18038 0.18324 0.18426 0.19240 0.19283

Eigenvalues --- 0.19360 0.19363 0.19374 0.19413 0.19418

Eigenvalues --- 0.19428 0.19552 0.19553 0.19554 0.19555

Eigenvalues --- 0.20312 0.21484 0.22034 0.22796 0.22916

Eigenvalues --- 0.23223 0.23780 0.24265 0.24757 0.25424

Eigenvalues --- 0.26270 0.26403 0.26679 0.27112 0.28530

Eigenvalues --- 0.28567 0.28765 0.29035 0.29800 0.31032

Eigenvalues --- 0.31702 0.32012 0.32861 0.33089 0.33284

Eigenvalues --- 0.33335 0.34191 0.34426 0.35068 0.35574

Eigenvalues --- 0.35625 0.35629 0.35638 0.35645 0.35760

Eigenvalues --- 0.35764 0.35771 0.35818 0.35928 0.35929

Eigenvalues --- 0.35935 0.35939 0.35985 0.35991 0.36004

Eigenvalues --- 0.36010 0.36191 0.36200 0.36247 0.36258

Eigenvalues --- 0.36975 0.37066 0.37250 0.37395 0.37399

Eigenvalues --- 0.37487 0.38159 0.38434 0.38503 0.38532

Eigenvalues --- 0.39493 0.40369 0.40720 0.41070 0.41094

Eigenvalues --- 0.41104 0.41216 0.41273 0.41386 0.41402

Eigenvalues --- 0.41561 0.41837 0.42291 0.42632 0.44524

Eigenvalues --- 0.45223 0.45753 0.45917 0.45934 0.45980

Eigenvalues --- 0.46016 0.46050 0.46265 0.46273 0.46320

Eigenvalues --- 0.46334 0.48545 0.49027 0.49479 0.49664

Eigenvalues --- 0.50751 0.50754 0.50779 0.50783 0.51871

Eigenvalues --- 0.52188 0.57183 0.57738

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 1.05444 -0.05444

Cosine: 0.995 > 0.500

Length: 0.973

GDIIS step was calculated using 2 of the last 17 vectors.

Iteration 1 RMS(Cart)= 0.01191057 RMS(Int)= 0.00001609

Iteration 2 RMS(Cart)= 0.00003659 RMS(Int)= 0.00000167

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000167

ITry= 1 IFail=0 DXMaxC= 6.39D-02 DCOld= 1.00D+10 DXMaxT= 8.41D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.65664 0.00005 -0.00002 0.00016 0.00014 2.65678

R2 2.64084 0.00007 -0.00003 0.00012 0.00009 2.64094

R3 2.03703 0.00002 -0.00001 0.00005 0.00004 2.03707

R4 2.59965 -0.00015 0.00004 -0.00047 -0.00043 2.59923

R5 2.71589 0.00006 -0.00001 0.00009 0.00008 2.71598

R6 2.59918 -0.00006 0.00005 -0.00007 -0.00001 2.59917

R7 1.91049 -0.00017 0.00006 -0.00030 -0.00024 1.91025

R8 2.65623 -0.00000 -0.00001 0.00027 0.00026 2.65649

R9 2.71710 0.00003 -0.00005 -0.00035 -0.00040 2.71670

R10 2.03711 0.00001 -0.00001 0.00001 -0.00000 2.03711

R11 2.64058 0.00007 -0.00003 0.00020 0.00017 2.64075

R12 2.80380 -0.00002 0.00001 0.00045 0.00046 2.80426

R13 2.59632 0.00001 -0.00003 -0.00023 -0.00025 2.59607

R14 2.76197 0.00003 -0.00001 0.00003 0.00002 2.76199

R15 2.59405 0.00010 0.00002 0.00047 0.00049 2.59454

R16 2.76224 0.00001 -0.00000 0.00016 0.00016 2.76240

R17 2.64253 0.00010 -0.00006 0.00005 -0.00001 2.64253

R18 2.55431 0.00003 -0.00001 0.00002 0.00001 2.55432

R19 2.03911 0.00004 -0.00000 0.00007 0.00007 2.03918

R20 2.03896 0.00002 -0.00001 0.00011 0.00010 2.03906

R21 2.64285 0.00010 -0.00006 -0.00019 -0.00025 2.64260

R22 2.80334 -0.00001 0.00002 0.00046 0.00048 2.80382

R23 2.76231 0.00001 0.00000 0.00010 0.00011 2.76242

R24 2.59387 0.00010 0.00002 0.00062 0.00063 2.59450

R25 2.55433 0.00003 -0.00001 0.00001 -0.00000 2.55433

R26 2.03910 0.00004 -0.00001 0.00008 0.00007 2.03918

R27 2.76194 0.00003 -0.00001 0.00006 0.00005 2.76199

R28 2.03898 0.00002 -0.00001 0.00010 0.00009 2.03906

R29 2.59642 0.00001 -0.00002 -0.00031 -0.00034 2.59608

R30 2.64029 0.00006 -0.00003 0.00041 0.00038 2.64067

R31 2.71677 0.00002 -0.00006 -0.00010 -0.00015 2.71661

R32 2.80456 -0.00002 0.00001 -0.00009 -0.00008 2.80448

R33 2.65653 -0.00000 -0.00001 0.00008 0.00007 2.65660

R34 2.59944 -0.00006 0.00005 -0.00026 -0.00021 2.59924

R35 2.64062 0.00007 -0.00003 0.00027 0.00024 2.64086

R36 2.03705 0.00002 -0.00001 0.00006 0.00005 2.03709

R37 2.65684 0.00005 -0.00002 0.00002 0.00000 2.65685

R38 2.03696 0.00002 -0.00001 0.00010 0.00009 2.03704

R39 2.59984 -0.00014 0.00004 -0.00059 -0.00055 2.59929

R40 2.71551 0.00006 -0.00002 0.00038 0.00037 2.71588

R41 1.91093 -0.00017 0.00006 -0.00060 -0.00054 1.91039

R42 2.80406 -0.00001 0.00001 -0.00005 -0.00003 2.80402

R43 2.65152 -0.00005 -0.00001 -0.00034 -0.00035 2.65117

R44 2.65006 0.00002 -0.00001 -0.00022 -0.00023 2.64983

R45 2.62864 -0.00003 0.00001 0.00001 0.00002 2.62867

R46 2.04846 0.00001 0.00000 0.00005 0.00006 2.04852

R47 2.63631 -0.00001 -0.00000 -0.00004 -0.00004 2.63627

R48 2.05013 0.00001 -0.00000 0.00004 0.00004 2.05017

R49 2.63403 0.00003 -0.00001 0.00006 0.00006 2.63408

R50 2.05004 0.00001 -0.00000 0.00002 0.00002 2.05006

R51 2.63078 0.00005 -0.00001 0.00021 0.00020 2.63098

R52 2.05013 0.00000 -0.00000 0.00002 0.00002 2.05015

R53 2.04854 0.00001 0.00000 0.00009 0.00010 2.04864

R54 2.63631 0.00002 -0.00000 0.00001 0.00001 2.63631

R55 2.63418 0.00002 -0.00000 0.00004 0.00003 2.63421

R56 2.05004 0.00000 -0.00000 0.00002 0.00001 2.05006

R57 2.62882 0.00002 0.00001 0.00011 0.00012 2.62893

R58 2.05018 0.00000 -0.00000 0.00000 0.00000 2.05018

R59 2.65162 -0.00001 -0.00000 -0.00023 -0.00023 2.65139

R60 2.04849 -0.00001 0.00000 0.00001 0.00001 2.04850

R61 2.65026 -0.00003 -0.00001 -0.00021 -0.00021 2.65005

R62 2.63052 0.00002 -0.00000 0.00010 0.00010 2.63062

R63 2.04854 0.00000 0.00000 0.00002 0.00002 2.04856

R64 2.05013 0.00001 -0.00000 0.00003 0.00003 2.05016

R65 2.64997 -0.00003 -0.00001 0.00002 0.00001 2.64997

R66 2.65134 -0.00002 -0.00000 -0.00002 -0.00003 2.65132

R67 2.63061 0.00002 -0.00001 0.00003 0.00003 2.63064

R68 2.04860 0.00000 0.00000 -0.00002 -0.00002 2.04857

R69 2.63416 0.00002 -0.00001 0.00005 0.00005 2.63421

R70 2.05014 0.00001 -0.00000 0.00002 0.00002 2.05016

R71 2.63626 0.00002 -0.00000 0.00005 0.00004 2.63630

R72 2.05005 0.00000 -0.00000 0.00001 0.00001 2.05006

R73 2.62895 0.00002 0.00001 0.00001 0.00001 2.62897

R74 2.05019 0.00000 -0.00000 -0.00000 -0.00000 2.05019

R75 2.04852 -0.00001 0.00001 -0.00002 -0.00002 2.04850

R76 2.64975 0.00002 -0.00001 -0.00000 -0.00001 2.64974

R77 2.65121 -0.00006 -0.00001 -0.00011 -0.00012 2.65108

R78 2.63088 0.00005 -0.00001 0.00014 0.00014 2.63102

R79 2.04861 0.00001 0.00000 0.00004 0.00005 2.04866

R80 2.63401 0.00003 -0.00001 0.00008 0.00007 2.63408

R81 2.05013 0.00000 -0.00000 0.00001 0.00001 2.05015

R82 2.63626 -0.00001 -0.00000 -0.00001 -0.00001 2.63625

R83 2.05004 0.00001 -0.00000 0.00002 0.00002 2.05006

R84 2.62877 -0.00003 0.00001 -0.00008 -0.00007 2.62870

R85 2.05015 0.00001 -0.00000 0.00003 0.00003 2.05018

R86 2.04849 0.00001 0.00000 0.00003 0.00003 2.04853

A1 1.88162 -0.00001 0.00001 -0.00007 -0.00005 1.88157

A2 2.18756 0.00002 0.00001 0.00027 0.00028 2.18783

A3 2.21399 -0.00001 -0.00002 -0.00020 -0.00022 2.21377

A4 1.86809 -0.00004 0.00002 -0.00005 -0.00002 1.86807

A5 2.22105 0.00016 -0.00016 0.00082 0.00066 2.22172

A6 2.19364 -0.00013 0.00014 -0.00077 -0.00063 2.19300

A7 1.92469 0.00011 -0.00006 0.00035 0.00029 1.92498

A8 2.17807 -0.00009 0.00007 -0.00054 -0.00047 2.17760

A9 2.17973 -0.00001 -0.00002 0.00013 0.00011 2.17984

A10 1.86839 -0.00003 0.00003 -0.00024 -0.00022 1.86817

A11 2.19488 -0.00004 0.00004 -0.00040 -0.00036 2.19452

A12 2.21961 0.00007 -0.00007 0.00058 0.00052 2.22013

A13 1.88165 -0.00003 -0.00000 0.00000 -0.00000 1.88165

A14 2.21413 0.00002 -0.00003 -0.00013 -0.00016 2.21397

A15 2.18737 0.00001 0.00003 0.00014 0.00017 2.18754

A16 2.18585 0.00003 0.00000 0.00094 0.00094 2.18679

A17 2.02314 -0.00007 0.00006 -0.00021 -0.00015 2.02299

A18 2.07413 0.00004 -0.00006 -0.00071 -0.00077 2.07336

A19 2.19166 -0.00004 0.00001 0.00022 0.00023 2.19188

A20 2.16544 0.00005 -0.00003 -0.00033 -0.00036 2.16508

A21 1.92606 -0.00001 0.00002 0.00012 0.00014 1.92620

A22 1.84702 0.00002 -0.00002 0.00002 0.00001 1.84702

A23 1.92666 -0.00003 0.00001 -0.00020 -0.00020 1.92647

A24 2.19169 0.00016 -0.00003 0.00051 0.00048 2.19217

A25 2.16483 -0.00013 0.00002 -0.00031 -0.00029 2.16454

A26 1.86200 0.00001 -0.00000 0.00006 0.00006 1.86206

A27 2.19717 -0.00004 0.00002 -0.00024 -0.00022 2.19694

A28 2.22361 0.00002 -0.00001 0.00021 0.00019 2.22380

A29 1.86205 0.00001 -0.00001 -0.00000 -0.00001 1.86204

A30 2.19670 0.00002 -0.00002 0.00011 0.00008 2.19679

A31 2.22406 -0.00003 0.00003 -0.00008 -0.00005 2.22401

A32 2.18427 0.00014 0.00001 0.00113 0.00113 2.18540

A33 2.02540 0.00001 -0.00003 -0.00043 -0.00046 2.02494

A34 2.07346 -0.00015 0.00002 -0.00070 -0.00068 2.07279

A35 2.16519 -0.00013 0.00003 -0.00058 -0.00055 2.16464

A36 2.19136 0.00016 -0.00003 0.00075 0.00071 2.19207

A37 1.92662 -0.00003 0.00000 -0.00017 -0.00016 1.92646

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A44 1.92605 -0.00001 0.00002 0.00013 0.00015 1.92620

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A51 2.21952 0.00006 -0.00007 0.00063 0.00056 2.22008

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A53 1.86837 -0.00002 0.00003 -0.00024 -0.00021 1.86816

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D4 0.05122 -0.00001 -0.00023 -0.00090 -0.00113 0.05009

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D56 0.00006 -0.00000 0.00003 -0.00087 -0.00084 -0.00077

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D125 -3.14078 0.00001 0.00011 0.00059 0.00069 -3.14009

D126 -0.01832 0.00002 0.00005 0.00137 0.00142 -0.01690

D127 -0.00316 0.00002 0.00007 0.00116 0.00123 -0.00193

D128 3.11930 0.00002 0.00001 0.00194 0.00196 3.12126

D129 -0.01699 0.00001 0.00002 0.00079 0.00081 -0.01618

D130 3.12421 0.00001 0.00001 0.00054 0.00055 3.12476

D131 -3.13804 -0.00000 -0.00002 -0.00020 -0.00022 -3.13826

D132 0.00316 -0.00001 -0.00004 -0.00044 -0.00048 0.00268

D133 0.00489 -0.00000 -0.00000 0.00025 0.00025 0.00514

D134 -3.13374 0.00000 0.00002 0.00013 0.00014 -3.13359

D135 -3.13630 0.00000 0.00001 0.00049 0.00051 -3.13579

D136 0.00825 0.00001 0.00003 0.00037 0.00040 0.00865

D137 0.00789 -0.00000 0.00002 -0.00057 -0.00055 0.00734

D138 -3.13107 -0.00001 0.00000 -0.00089 -0.00089 -3.13195

D139 -3.13666 -0.00001 -0.00000 -0.00045 -0.00045 -3.13711

D140 0.00757 -0.00001 -0.00001 -0.00077 -0.00078 0.00678

D141 -0.00873 -0.00000 -0.00005 -0.00015 -0.00020 -0.00893

D142 -3.13110 -0.00000 0.00000 -0.00093 -0.00092 -3.13202

D143 3.13025 -0.00000 -0.00004 0.00017 0.00013 3.13038

D144 0.00788 -0.00000 0.00002 -0.00060 -0.00059 0.00729

D145 -0.00577 0.00001 -0.00002 0.00039 0.00037 -0.00539

D146 3.13538 0.00000 -0.00002 0.00037 0.00036 3.13573

D147 3.13417 0.00001 -0.00000 0.00063 0.00063 3.13480

D148 -0.00787 0.00001 0.00000 0.00061 0.00061 -0.00726

D149 -0.00647 0.00000 0.00002 0.00004 0.00007 -0.00640

D150 3.13184 -0.00000 -0.00001 0.00002 0.00001 3.13184

D151 3.13678 -0.00000 0.00001 -0.00019 -0.00019 3.13659

D152 -0.00810 -0.00000 -0.00002 -0.00022 -0.00024 -0.00835

D153 0.01671 -0.00000 0.00001 -0.00013 -0.00013 0.01658

D154 3.13670 -0.00000 0.00001 0.00018 0.00018 3.13689

D155 -3.12443 -0.00000 0.00000 -0.00011 -0.00011 -3.12454

D156 -0.00444 0.00000 0.00000 0.00020 0.00020 -0.00424

D157 3.13016 -0.00001 0.00004 -0.00034 -0.00029 3.12987

D158 -0.01513 -0.00001 0.00000 -0.00055 -0.00055 -0.01568

D159 0.01007 -0.00001 0.00004 -0.00066 -0.00061 0.00946

D160 -3.13522 -0.00001 0.00000 -0.00087 -0.00087 -3.13609

D161 3.14075 0.00002 -0.00004 0.00078 0.00074 3.14149

D162 0.01766 -0.00000 -0.00002 -0.00038 -0.00040 0.01725

D163 0.00285 0.00002 0.00000 0.00099 0.00100 0.00385

D164 -3.12024 0.00000 0.00002 -0.00016 -0.00014 -3.12038

D165 0.00790 -0.00002 -0.00002 -0.00074 -0.00076 0.00714

D166 -3.13043 -0.00001 0.00001 -0.00072 -0.00070 -3.13113

D167 3.13089 0.00000 -0.00003 0.00041 0.00038 3.13127

D168 -0.00743 0.00001 -0.00000 0.00043 0.00043 -0.00700

D169 -3.14068 0.00001 -0.00007 -0.00040 -0.00048 -3.14116

D170 0.01843 -0.00001 -0.00004 -0.00088 -0.00092 0.01751

D171 0.00237 0.00002 -0.00001 0.00132 0.00131 0.00369

D172 -3.12170 -0.00000 0.00002 0.00085 0.00087 -3.12083

D173 3.12853 -0.00000 0.00008 0.00078 0.00086 3.12938

D174 0.00844 -0.00001 0.00007 0.00048 0.00055 0.00899

D175 -0.01453 -0.00001 0.00001 -0.00095 -0.00094 -0.01547

D176 -3.13462 -0.00001 0.00000 -0.00125 -0.00124 -3.13586

D177 0.00801 -0.00002 -0.00000 -0.00084 -0.00085 0.00717

D178 -3.13076 -0.00001 0.00002 -0.00049 -0.00047 -3.13123

D179 3.13199 0.00000 -0.00004 -0.00037 -0.00040 3.13159

D180 -0.00679 0.00001 -0.00001 -0.00002 -0.00003 -0.00682

D181 -0.00633 0.00000 0.00002 -0.00004 -0.00002 -0.00636

D182 3.13660 0.00000 0.00001 -0.00006 -0.00005 3.13654

D183 3.13242 -0.00000 -0.00001 -0.00039 -0.00040 3.13203

D184 -0.00783 -0.00000 -0.00002 -0.00041 -0.00042 -0.00826

D185 -0.00578 0.00001 -0.00002 0.00042 0.00040 -0.00539

D186 3.13505 0.00000 -0.00002 0.00056 0.00054 3.13560

D187 3.13447 0.00001 -0.00001 0.00043 0.00043 3.13490

D188 -0.00788 0.00001 -0.00000 0.00058 0.00057 -0.00730

D189 0.01635 -0.00000 0.00000 0.00009 0.00009 0.01644

D190 3.13635 0.00000 0.00001 0.00037 0.00039 3.13674

D191 -3.12449 -0.00000 0.00000 -0.00006 -0.00005 -3.12454

D192 -0.00449 0.00000 0.00001 0.00023 0.00024 -0.00425

D193 3.14129 0.00002 0.00015 0.00145 0.00160 -3.14030

D194 -0.01864 0.00002 0.00007 0.00168 0.00175 -0.01689

D195 -0.00270 0.00002 0.00008 0.00082 0.00090 -0.00180

D196 3.12056 0.00002 -0.00000 0.00105 0.00105 3.12161

D197 -3.12855 -0.00003 -0.00013 -0.00172 -0.00185 -3.13040

D198 -0.00734 -0.00001 -0.00008 -0.00078 -0.00086 -0.00820

D199 0.01543 -0.00002 -0.00005 -0.00110 -0.00115 0.01428

D200 3.13664 0.00000 -0.00001 -0.00015 -0.00015 3.13648

D201 -0.00879 -0.00000 -0.00006 -0.00006 -0.00012 -0.00891

D202 3.13047 -0.00000 -0.00005 0.00001 -0.00004 3.13044

D203 -3.13195 -0.00000 0.00002 -0.00028 -0.00026 -3.13222

D204 0.00731 -0.00000 0.00003 -0.00021 -0.00018 0.00713

D205 0.00764 -0.00001 0.00002 -0.00045 -0.00043 0.00722

D206 -3.13655 -0.00001 -0.00000 -0.00056 -0.00056 -3.13711

D207 -3.13161 -0.00001 0.00001 -0.00052 -0.00051 -3.13212

D208 0.00739 -0.00001 -0.00001 -0.00063 -0.00064 0.00674

D209 0.00505 -0.00000 0.00000 0.00017 0.00018 0.00522

D210 -3.13601 0.00000 0.00001 0.00030 0.00031 -3.13570

D211 -3.13395 0.00000 0.00002 0.00028 0.00031 -3.13364

D212 0.00818 0.00000 0.00003 0.00041 0.00044 0.00863

D213 -0.01673 0.00001 0.00002 0.00061 0.00062 -0.01610

D214 -3.13785 -0.00001 -0.00003 -0.00034 -0.00037 -3.13822

D215 3.12433 0.00001 0.00001 0.00048 0.00049 3.12482

D216 0.00321 -0.00001 -0.00004 -0.00047 -0.00051 0.00270

Item Value Threshold Converged?

Maximum Force 0.000174 0.000450 YES

RMS Force 0.000041 0.000300 YES

Maximum Displacement 0.063859 0.001800 NO

RMS Displacement 0.011910 0.001200 NO

Predicted change in Energy=-4.788476D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

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(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=1 Diff= 2.57D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 0.942305 -4.121661 0.545595

2 6 0 1.297740 -2.807223 0.195596

3 7 0 0.127209 -2.110952 0.003418

4 6 0 -0.955816 -2.938816 0.186380

5 6 0 -0.452829 -4.203132 0.539449

6 6 0 -2.333917 -2.570403 0.007929

7 6 0 -2.810287 -1.262725 -0.117924

8 7 0 -2.063959 -0.120893 0.044814

9 6 0 -2.941012 0.924493 -0.106823

10 6 0 -4.276760 0.425640 -0.428967

11 6 0 -4.195797 -0.923601 -0.436643

12 6 0 2.623794 -2.279390 0.026450

13 6 0 2.941125 -0.924159 -0.108399

14 6 0 4.276853 -0.424911 -0.430055

15 6 0 4.195866 0.924340 -0.436217

16 6 0 2.810313 1.263063 -0.117257

17 7 0 2.064027 0.121017 0.044230

18 6 0 2.333883 2.570579 0.009576

19 6 0 0.955891 2.939252 0.187972

20 6 0 0.452803 4.205276 0.534947

21 6 0 -0.942288 4.123816 0.541348

22 6 0 -1.297688 2.807692 0.197571

23 7 0 -0.127119 2.110436 0.008995

24 6 0 -2.623623 2.279600 0.028733

25 6 0 -3.305388 -3.691589 -0.028029

26 6 0 -3.172190 -4.721605 -0.971196

27 6 0 -4.089987 -5.766016 -1.013870

28 6 0 -5.145637 -5.810016 -0.102912

29 6 0 -5.280469 -4.798907 0.847049

30 6 0 -4.371273 -3.745080 0.881520

31 6 0 5.810748 -5.152387 -0.019676

32 6 0 4.764606 -5.251912 -0.937240

33 6 0 3.724921 -4.327808 -0.916279

34 6 0 3.723675 -3.275102 0.011285

35 6 0 4.780810 -3.184544 0.928258

36 6 0 5.813214 -4.118249 0.915042

37 6 0 -3.723824 3.275106 0.012605

38 6 0 -4.780105 3.185842 0.930627

39 6 0 -5.813138 4.118854 0.916208

40 6 0 -5.812120 5.150915 -0.020801

41 6 0 -4.766844 5.249049 -0.939488

42 6 0 -3.726563 4.325614 -0.917385

43 6 0 3.305652 3.691642 -0.027024

44 6 0 4.370206 3.746434 0.883931

45 6 0 5.279828 4.799894 0.848792

46 6 0 5.146681 5.809277 -0.103239

47 6 0 4.092396 5.763857 -1.015692

48 6 0 3.174205 4.719793 -0.972400

49 1 0 1.634957 -4.913670 0.780061

50 1 0 -1.050841 -5.069995 0.769656

51 1 0 -5.143084 1.031698 -0.644842

52 1 0 -4.983558 -1.626567 -0.659275

53 1 0 5.143175 -1.030715 -0.646655

54 1 0 4.983656 1.627578 -0.657893

55 1 0 1.050649 5.073502 0.760365

56 1 0 -1.634934 4.917130 0.771316

57 1 0 -2.355442 -4.690385 -1.683285

58 1 0 -3.981577 -6.546496 -1.759602

59 1 0 -5.856677 -6.628828 -0.132157

60 1 0 -6.093408 -4.830378 1.564773

61 1 0 -4.474425 -2.965325 1.627579

62 1 0 6.617810 -5.877207 -0.032777

63 1 0 4.758431 -6.050779 -1.671272

64 1 0 2.916456 -4.406688 -1.634097

65 1 0 4.781241 -2.387335 1.662846

66 1 0 6.618323 -4.038977 1.637896

67 1 0 -4.779495 2.390058 1.666772

68 1 0 -6.617660 4.040596 1.639827

69 1 0 -6.619682 5.875161 -0.034866

70 1 0 -4.761852 6.046213 -1.675382

71 1 0 -2.918837 4.403306 -1.636166

72 1 0 4.472103 2.967907 1.631454

73 1 0 6.091785 4.832405 1.567581

74 1 0 5.858038 6.627795 -0.133006

75 1 0 3.985343 6.542928 -1.763093

76 1 0 2.358533 4.687431 -1.685675

77 1 0 0.071523 -1.123436 -0.205278

78 1 0 -0.071409 1.121070 -0.191098

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0587862 0.0582466 0.0300930

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(Enter /home/kira/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5356.7582716941 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2121948064 Hartrees.

Nuclear repulsion after empirical dispersion term = 5356.5460768876 Hartrees.

Force inversion solution in PCM.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5782

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.43D-09

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 307

GePol: Fraction of low-weight points (<1% of avg) = 5.31%

GePol: Cavity surface area = 610.762 Ang\*\*2

GePol: Cavity volume = 627.859 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0020975815 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5356.5439793061 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.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

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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: "TPP3C1.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999959 -0.000070 -0.000007 0.009087 Ang= -1.04 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0550 S= 1.0182

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30498212093

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(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 590000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 100294572.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.11D-15 for 5774.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.74D-15 for 4494 1329.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.22D-15 for 5774.

Iteration 1 A^-1\*A deviation from orthogonality is 2.55D-10 for 4658 4650.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.44D-15 for 2529.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.44D-15 for 4918 2627.

Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 3267.

Iteration 2 A^-1\*A deviation from orthogonality is 2.86D-16 for 2719 212.

E= -1914.33285591559

DIIS: error= 4.15D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.33285591559 IErMin= 1 ErrMin= 4.15D-04

ErrMax= 4.15D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.48D-04 BMatP= 9.48D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.15D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.640 Goal= None Shift= 0.000

Gap= 0.705 Goal= None Shift= 0.000

RMSDP=3.05D-05 MaxDP=1.32D-03 OVMax= 2.94D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.05D-05 CP: 1.00D+00

E= -1914.33331135256 Delta-E= -0.000455436972 Rises=F Damp=F

DIIS: error= 5.33D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33331135256 IErMin= 2 ErrMin= 5.33D-05

ErrMax= 5.33D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.19D-05 BMatP= 9.48D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.639D-01 0.106D+01

Coeff: -0.639D-01 0.106D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.08D-06 MaxDP=1.61D-04 DE=-4.55D-04 OVMax= 6.75D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.62D-06 CP: 1.00D+00 1.06D+00

E= -1914.33331757751 Delta-E= -0.000006224952 Rises=F Damp=F

DIIS: error= 3.21D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33331757751 IErMin= 3 ErrMin= 3.21D-05

ErrMax= 3.21D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.75D-06 BMatP= 1.19D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.320D-01 0.437D+00 0.595D+00

Coeff: -0.320D-01 0.437D+00 0.595D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.54D-06 MaxDP=1.32D-04 DE=-6.22D-06 OVMax= 3.81D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.38D-06 CP: 1.00D+00 1.06D+00 8.11D-01

E= -1914.33331842620 Delta-E= -0.000000848690 Rises=F Damp=F

DIIS: error= 1.86D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33331842620 IErMin= 4 ErrMin= 1.86D-05

ErrMax= 1.86D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.52D-06 BMatP= 4.75D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.848D-02 0.867D-01 0.361D+00 0.560D+00

Coeff: -0.848D-02 0.867D-01 0.361D+00 0.560D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=6.62D-07 MaxDP=6.13D-05 DE=-8.49D-07 OVMax= 2.29D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.81D-07 CP: 1.00D+00 1.07D+00 8.84D-01 7.38D-01

E= -1914.33331880974 Delta-E= -0.000000383536 Rises=F Damp=F

DIIS: error= 4.23D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33331880974 IErMin= 5 ErrMin= 4.23D-06

ErrMax= 4.23D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.40D-08 BMatP= 1.52D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.502D-03-0.754D-02 0.910D-01 0.233D+00 0.684D+00

Coeff: -0.502D-03-0.754D-02 0.910D-01 0.233D+00 0.684D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.48D-07 MaxDP=1.51D-05 DE=-3.84D-07 OVMax= 1.16D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.14D-07 CP: 1.00D+00 1.07D+00 9.03D-01 8.11D-01 9.16D-01

E= -1914.33331883041 Delta-E= -0.000000020670 Rises=F Damp=F

DIIS: error= 3.04D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33331883041 IErMin= 6 ErrMin= 3.04D-06

ErrMax= 3.04D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.14D-08 BMatP= 7.40D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.960D-03-0.181D-01 0.228D-02 0.626D-01 0.435D+00 0.517D+00

Coeff: 0.960D-03-0.181D-01 0.228D-02 0.626D-01 0.435D+00 0.517D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.46D-07 MaxDP=1.01D-05 DE=-2.07D-08 OVMax= 1.03D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.22D-07 CP: 1.00D+00 1.07D+00 9.13D-01 8.16D-01 1.06D+00

CP: 9.58D-01

E= -1914.33331884281 Delta-E= -0.000000012396 Rises=F Damp=F

DIIS: error= 1.84D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33331884281 IErMin= 7 ErrMin= 1.84D-06

ErrMax= 1.84D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.57D-09 BMatP= 3.14D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.472D-03-0.726D-02-0.760D-02 0.706D-02 0.124D+00 0.248D+00

Coeff-Com: 0.635D+00

Coeff: 0.472D-03-0.726D-02-0.760D-02 0.706D-02 0.124D+00 0.248D+00

Coeff: 0.635D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=9.08D-08 MaxDP=6.58D-06 DE=-1.24D-08 OVMax= 7.35D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 4.41D-08 CP: 1.00D+00 1.07D+00 9.16D-01 8.30D-01 1.13D+00

CP: 1.24D+00 1.29D+00

E= -1914.33331884650 Delta-E= -0.000000003698 Rises=F Damp=F

DIIS: error= 1.43D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33331884650 IErMin= 8 ErrMin= 1.43D-06

ErrMax= 1.43D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.64D-09 BMatP= 3.57D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.432D-03 0.954D-02-0.753D-02-0.441D-01-0.272D+00-0.222D+00

Coeff-Com: 0.410D+00 0.113D+01

Coeff: -0.432D-03 0.954D-02-0.753D-02-0.441D-01-0.272D+00-0.222D+00

Coeff: 0.410D+00 0.113D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.83D-07 MaxDP=1.46D-05 DE=-3.70D-09 OVMax= 1.78D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.23D-08 CP: 1.00D+00 1.07D+00 9.22D-01 8.47D-01 1.29D+00

CP: 1.72D+00 2.22D+00 1.60D+00

E= -1914.33331885119 Delta-E= -0.000000004684 Rises=F Damp=F

DIIS: error= 8.12D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33331885119 IErMin= 9 ErrMin= 8.12D-07

ErrMax= 8.12D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.15D-10 BMatP= 1.64D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.320D-03 0.617D-02-0.104D-02-0.199D-01-0.156D+00-0.160D+00

Coeff-Com: -0.373D-01 0.573D+00 0.796D+00

Coeff: -0.320D-03 0.617D-02-0.104D-02-0.199D-01-0.156D+00-0.160D+00

Coeff: -0.373D-01 0.573D+00 0.796D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=9.35D-08 MaxDP=7.39D-06 DE=-4.68D-09 OVMax= 9.40D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.02D-08 CP: 1.00D+00 1.07D+00 9.24D-01 8.55D-01 1.36D+00

CP: 1.98D+00 2.66D+00 2.18D+00 1.52D+00

E= -1914.33331885242 Delta-E= -0.000000001230 Rises=F Damp=F

DIIS: error= 6.48D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33331885242 IErMin=10 ErrMin= 6.48D-07

ErrMax= 6.48D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.41D-10 BMatP= 6.15D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.857D-05-0.806D-03 0.296D-02 0.979D-02 0.343D-01 0.110D-01

Coeff-Com: -0.251D+00-0.127D+00 0.465D+00 0.856D+00

Coeff: 0.857D-05-0.806D-03 0.296D-02 0.979D-02 0.343D-01 0.110D-01

Coeff: -0.251D+00-0.127D+00 0.465D+00 0.856D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.48D-08 MaxDP=6.38D-06 DE=-1.23D-09 OVMax= 8.13D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.33D-08 CP: 1.00D+00 1.07D+00 9.26D-01 8.59D-01 1.42D+00

CP: 2.15D+00 3.00D+00 2.67D+00 2.24D+00 1.32D+00

E= -1914.33331885303 Delta-E= -0.000000000615 Rises=F Damp=F

DIIS: error= 3.55D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33331885303 IErMin=11 ErrMin= 3.55D-07

ErrMax= 3.55D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.06D-10 BMatP= 2.41D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.939D-04-0.217D-02 0.180D-02 0.113D-01 0.626D-01 0.523D-01

Coeff-Com: -0.150D+00-0.204D+00 0.244D-02 0.503D+00 0.722D+00

Coeff: 0.939D-04-0.217D-02 0.180D-02 0.113D-01 0.626D-01 0.523D-01

Coeff: -0.150D+00-0.204D+00 0.244D-02 0.503D+00 0.722D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.91D-08 MaxDP=3.21D-06 DE=-6.15D-10 OVMax= 4.29D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.20D-08 CP: 1.00D+00 1.07D+00 9.27D-01 8.61D-01 1.44D+00

CP: 2.23D+00 3.00D+00 2.95D+00 2.66D+00 1.81D+00

CP: 1.37D+00

E= -1914.33331885323 Delta-E= -0.000000000199 Rises=F Damp=F

DIIS: error= 2.50D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.33331885323 IErMin=12 ErrMin= 2.50D-07

ErrMax= 2.50D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.71D-11 BMatP= 1.06D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.442D-04-0.706D-03-0.734D-03 0.117D-02 0.151D-01 0.237D-01

Coeff-Com: 0.336D-01-0.940D-02-0.263D+00-0.138D+00 0.378D+00 0.961D+00

Coeff: 0.442D-04-0.706D-03-0.734D-03 0.117D-02 0.151D-01 0.237D-01

Coeff: 0.336D-01-0.940D-02-0.263D+00-0.138D+00 0.378D+00 0.961D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.22D-08 MaxDP=2.72D-06 DE=-1.99D-10 OVMax= 3.60D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 9.25D-09 CP: 1.00D+00 1.07D+00 9.28D-01 8.62D-01 1.46D+00

CP: 2.30D+00 3.00D+00 3.00D+00 3.00D+00 2.23D+00

CP: 2.12D+00 1.67D+00

E= -1914.33331885334 Delta-E= -0.000000000106 Rises=F Damp=F

DIIS: error= 1.24D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.33331885334 IErMin=13 ErrMin= 1.24D-07

ErrMax= 1.24D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.63D-11 BMatP= 3.71D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.781D-05 0.374D-03-0.118D-02-0.335D-02-0.142D-01-0.473D-02

Coeff-Com: 0.682D-01 0.800D-01-0.174D+00-0.256D+00-0.463D-01 0.576D+00

Coeff-Com: 0.776D+00

Coeff: -0.781D-05 0.374D-03-0.118D-02-0.335D-02-0.142D-01-0.473D-02

Coeff: 0.682D-01 0.800D-01-0.174D+00-0.256D+00-0.463D-01 0.576D+00

Coeff: 0.776D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.93D-08 MaxDP=1.78D-06 DE=-1.06D-10 OVMax= 2.14D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 9.28D-09 CP: 1.00D+00 1.07D+00 9.28D-01 8.62D-01 1.47D+00

CP: 2.33D+00 3.00D+00 3.00D+00 3.00D+00 2.52D+00

CP: 2.53D+00 2.11D+00 1.73D+00

E= -1914.33331885335 Delta-E= -0.000000000017 Rises=F Damp=F

DIIS: error= 6.63D-08 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.33331885335 IErMin=14 ErrMin= 6.63D-08

ErrMax= 6.63D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.53D-12 BMatP= 1.63D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.231D-04 0.524D-03-0.419D-03-0.244D-02-0.152D-01-0.126D-01

Coeff-Com: 0.243D-01 0.589D-01-0.463D-03-0.925D-01-0.195D+00-0.394D-01

Coeff-Com: 0.478D+00 0.796D+00

Coeff: -0.231D-04 0.524D-03-0.419D-03-0.244D-02-0.152D-01-0.126D-01

Coeff: 0.243D-01 0.589D-01-0.463D-03-0.925D-01-0.195D+00-0.394D-01

Coeff: 0.478D+00 0.796D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.10D-08 MaxDP=9.78D-07 DE=-1.73D-11 OVMax= 1.22D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.99D-09 CP: 1.00D+00 1.07D+00 9.28D-01 8.63D-01 1.47D+00

CP: 2.35D+00 3.00D+00 3.00D+00 3.00D+00 2.66D+00

CP: 2.80D+00 2.35D+00 2.22D+00 1.47D+00

E= -1914.33331885336 Delta-E= -0.000000000005 Rises=F Damp=F

DIIS: error= 2.56D-08 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1914.33331885336 IErMin=15 ErrMin= 2.56D-08

ErrMax= 2.56D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.19D-12 BMatP= 5.53D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.613D-05 0.690D-04 0.257D-03 0.280D-03-0.112D-02-0.311D-02

Coeff-Com: -0.159D-01-0.283D-02 0.575D-01 0.552D-01-0.651D-01-0.211D+00

Coeff-Com: -0.815D-01 0.319D+00 0.948D+00

Coeff: -0.613D-05 0.690D-04 0.257D-03 0.280D-03-0.112D-02-0.311D-02

Coeff: -0.159D-01-0.283D-02 0.575D-01 0.552D-01-0.651D-01-0.211D+00

Coeff: -0.815D-01 0.319D+00 0.948D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.82D-09 MaxDP=5.27D-07 DE=-4.55D-12 OVMax= 6.33D-06

Error on total polarization charges = 0.08258

SCF Done: E(UB3LYP) = -1914.33331885 A.U. after 15 cycles

NFock= 15 Conv=0.58D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0550 S= 1.0182

<L.S>= 0.000000000000E+00

KE= 1.906381139441D+03 PE=-1.516271416422D+04 EE= 5.985455726620D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0550, after 2.0017

Leave Link 502 at Wed Aug 28 21:55:25 2019, MaxMem= 4294967296 cpu: 6279.5

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48629407D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64235828D-01

Leave Link 801 at Wed Aug 28 21:55:25 2019, MaxMem= 4294967296 cpu: 1.0

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Wed Aug 28 21:55:32 2019, MaxMem= 4294967296 cpu: 111.5

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Wed Aug 28 21:55:33 2019, MaxMem= 4294967296 cpu: 3.0

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 189

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Wed Aug 28 22:15:48 2019, MaxMem= 4294967296 cpu: 19416.5

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 590000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.38D+03 4.50D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.52D+02 3.62D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.53D+00 4.67D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.02D-01 3.97D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.55D-04 2.10D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.58D-06 1.35D-04.

189 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 1.99D-08 1.02D-05.

81 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.29D-11 6.20D-07.

42 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.18D-13 3.93D-08.

3 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 8.11D-15 4.27D-09.

3 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 4.72D-15 2.53D-09.

3 vectors produced by pass 11 Test12= 2.55D-13 1.00D-09 XBig12= 8.70D-15 3.79D-09.

3 vectors produced by pass 12 Test12= 2.55D-13 1.00D-09 XBig12= 5.18D-15 2.41D-09.

3 vectors produced by pass 13 Test12= 2.55D-13 1.00D-09 XBig12= 8.28D-15 3.47D-09.

3 vectors produced by pass 14 Test12= 2.55D-13 1.00D-09 XBig12= 9.32D-15 2.99D-09.

3 vectors produced by pass 15 Test12= 2.55D-13 1.00D-09 XBig12= 8.79D-15 4.28D-09.

3 vectors produced by pass 16 Test12= 2.55D-13 1.00D-09 XBig12= 5.87D-15 2.30D-09.

2 vectors produced by pass 17 Test12= 2.55D-13 1.00D-09 XBig12= 8.91D-15 2.31D-09.

InvSVY: IOpt=1 It= 1 EMax= 3.55D-14

Solved reduced A of dimension 1745 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1124.66 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 Thu Aug 29 02:11:07 2019, MaxMem= 4294967296 cpu: 225845.0

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 189

Leave Link 701 at Thu Aug 29 02:12:36 2019, MaxMem= 4294967296 cpu: 1416.0

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Thu Aug 29 02:12:36 2019, MaxMem= 4294967296 cpu: 0.5

(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=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

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= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Thu Aug 29 02:31:20 2019, MaxMem= 4294967296 cpu: 17984.0

(Enter /home/kira/g09/l716.exe)

Dipole =-2.56033397D-04-3.31147033D-03-4.73010234D-01

Polarizability= 1.25431592D+03-2.67493657D+01 1.66360276D+03

2.62344170D-03-6.23726273D-02 4.56067261D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000000248 -0.000000845 -0.000003583

2 6 0.000004905 -0.000000287 -0.000015152

3 7 0.000007355 -0.000000738 -0.000002802

4 6 -0.000004020 0.000007331 0.000029723

5 6 0.000005363 0.000002383 0.000000021

6 6 -0.000002646 0.000011526 -0.000018160

7 6 -0.000008693 -0.000003198 -0.000003408

8 7 -0.000042082 0.000027335 0.000000299

9 6 0.000001383 -0.000004057 -0.000010770

10 6 -0.000005311 -0.000009906 -0.000011410

11 6 -0.000000694 -0.000005998 0.000018754

12 6 -0.000009643 0.000015305 -0.000005022

13 6 -0.000001351 -0.000002581 0.000011822

14 6 0.000004761 -0.000009459 0.000011138

15 6 0.000000768 -0.000005991 -0.000019666

16 6 0.000007784 -0.000002777 0.000004861

17 7 0.000039707 0.000027321 0.000001019

18 6 0.000002700 0.000011389 0.000014569

19 6 0.000003690 0.000006828 -0.000026494

20 6 -0.000006287 0.000002121 0.000000931

21 6 0.000000866 -0.000001099 0.000001396

22 6 -0.000004543 0.000000119 0.000015577

23 7 -0.000006676 0.000000628 0.000003443

24 6 0.000010690 0.000014889 0.000004245

25 6 0.000020400 -0.000011320 -0.000015338

26 6 0.000003221 -0.000016624 0.000022938

27 6 0.000003391 0.000005807 0.000000439

28 6 0.000007290 -0.000002206 0.000006104

29 6 0.000004616 0.000009967 -0.000010446

30 6 0.000000564 -0.000017927 -0.000025432

31 6 -0.000004788 0.000006153 0.000002216

32 6 -0.000003194 0.000005071 -0.000002671

33 6 0.000004837 -0.000005886 -0.000005819

34 6 0.000009733 -0.000009983 0.000022127

35 6 -0.000010593 -0.000008937 0.000012413

36 6 0.000008320 0.000003934 0.000010474

37 6 -0.000008916 -0.000010024 -0.000025179

38 6 0.000010365 -0.000009281 -0.000010278

39 6 -0.000008132 0.000003445 -0.000011415

40 6 0.000004222 0.000004218 -0.000000469

41 6 0.000003443 0.000005568 0.000001431

42 6 -0.000005561 -0.000006584 0.000005026

43 6 -0.000023382 -0.000012130 0.000015005

44 6 0.000000740 -0.000018095 0.000026826

45 6 -0.000005609 0.000009156 0.000009456

46 6 -0.000005611 -0.000001972 -0.000005096

47 6 -0.000004502 0.000005090 -0.000001373

48 6 -0.000003296 -0.000015900 -0.000021743

49 1 -0.000003596 -0.000008925 0.000008001

50 1 0.000003734 0.000011839 -0.000026019

51 1 -0.000014985 0.000001894 0.000002402

52 1 -0.000009282 0.000014780 -0.000004209

53 1 0.000014991 0.000001720 -0.000002764

54 1 0.000008956 0.000014362 0.000003934

55 1 -0.000002364 0.000009920 0.000025948

56 1 0.000002613 -0.000010627 -0.000005658

57 1 -0.000007655 -0.000010047 0.000007826

58 1 0.000002076 0.000001155 0.000004668

59 1 0.000002024 0.000003882 -0.000000532

60 1 -0.000003941 0.000001440 -0.000001837

61 1 -0.000012675 0.000014957 0.000015936

62 1 0.000004214 0.000001250 -0.000000703

63 1 0.000001508 0.000000284 -0.000001833

64 1 -0.000006544 -0.000010664 -0.000005610

65 1 -0.000011144 0.000011684 -0.000012915

66 1 -0.000002384 0.000000853 0.000001784

67 1 0.000011001 0.000011588 0.000012263

68 1 0.000002400 0.000000081 -0.000001617

69 1 -0.000003915 0.000000606 0.000000427

70 1 -0.000001945 -0.000001248 0.000002284

71 1 0.000006503 -0.000011235 0.000006148

72 1 0.000014614 0.000014924 -0.000016312

73 1 0.000003919 0.000001308 0.000001945

74 1 -0.000002028 0.000003523 0.000000651

75 1 -0.000002230 0.000000535 -0.000004575

76 1 0.000007799 -0.000010377 -0.000007651

77 1 0.000132489 -0.000027056 0.000009931

78 1 -0.000129986 -0.000024185 -0.000012438

-------------------------------------------------------------------

Cartesian Forces: Max 0.000132489 RMS 0.000016240

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Thu Aug 29 02:31:20 2019, MaxMem= 4294967296 cpu: 2.5

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000135182 RMS 0.000027215

Search for a local minimum.

Step number 18 out of a maximum of 452

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -9.71D-06 DEPred=-4.79D-06 R= 2.03D+00

TightC=F SS= 1.41D+00 RLast= 4.26D-02 DXNew= 1.4142D-01 1.2765D-01

Trust test= 2.03D+00 RLast= 4.26D-02 DXMaxT set to 1.28D-01

ITU= 1 1 -1 -1 1 0 -1 1 1 -1 1 -1 -1 1 1 -1 1 0

Eigenvalues --- 0.00024 0.00226 0.00417 0.00599 0.00723

Eigenvalues --- 0.00817 0.00919 0.01042 0.01055 0.01115

Eigenvalues --- 0.01132 0.01166 0.01262 0.01280 0.01302

Eigenvalues --- 0.01305 0.01321 0.01421 0.01428 0.01525

Eigenvalues --- 0.01540 0.01556 0.01586 0.01670 0.01710

Eigenvalues --- 0.01714 0.01726 0.01736 0.01752 0.01757

Eigenvalues --- 0.01759 0.01782 0.01801 0.01803 0.01881

Eigenvalues --- 0.01931 0.01980 0.01988 0.02007 0.02165

Eigenvalues --- 0.02168 0.02257 0.02288 0.02291 0.02305

Eigenvalues --- 0.02330 0.02389 0.02465 0.02466 0.02519

Eigenvalues --- 0.02534 0.02540 0.02584 0.02624 0.02627

Eigenvalues --- 0.02642 0.02645 0.02769 0.02779 0.02795

Eigenvalues --- 0.02801 0.02869 0.02872 0.02874 0.02875

Eigenvalues --- 0.02950 0.02975 0.03900 0.04090 0.04192

Eigenvalues --- 0.04316 0.04369 0.04458 0.04538 0.04565

Eigenvalues --- 0.08108 0.09631 0.09691 0.09723 0.09872

Eigenvalues --- 0.09897 0.10294 0.10441 0.10570 0.10688

Eigenvalues --- 0.10689 0.10705 0.10727 0.10728 0.10992

Eigenvalues --- 0.11388 0.11390 0.11405 0.11409 0.11983

Eigenvalues --- 0.11987 0.11994 0.12000 0.12269 0.12269

Eigenvalues --- 0.12316 0.12317 0.12765 0.12767 0.12771

Eigenvalues --- 0.12773 0.15709 0.15912 0.16292 0.16837

Eigenvalues --- 0.17209 0.17257 0.17566 0.17804 0.17960

Eigenvalues --- 0.18030 0.18207 0.18277 0.19241 0.19282

Eigenvalues --- 0.19355 0.19355 0.19366 0.19402 0.19406

Eigenvalues --- 0.19426 0.19550 0.19551 0.19555 0.19556

Eigenvalues --- 0.20289 0.21486 0.22038 0.22712 0.22873

Eigenvalues --- 0.23266 0.23767 0.24231 0.24751 0.25023

Eigenvalues --- 0.26285 0.26389 0.26657 0.27169 0.28512

Eigenvalues --- 0.28537 0.28725 0.28993 0.29777 0.31032

Eigenvalues --- 0.31697 0.32011 0.32831 0.33081 0.33166

Eigenvalues --- 0.33324 0.34100 0.34736 0.35068 0.35566

Eigenvalues --- 0.35621 0.35623 0.35630 0.35637 0.35754

Eigenvalues --- 0.35758 0.35762 0.35807 0.35922 0.35923

Eigenvalues --- 0.35928 0.35931 0.35985 0.35987 0.36004

Eigenvalues --- 0.36007 0.36188 0.36199 0.36239 0.36242

Eigenvalues --- 0.36998 0.37063 0.37241 0.37388 0.37400

Eigenvalues --- 0.37496 0.38138 0.38452 0.38529 0.38587

Eigenvalues --- 0.39443 0.40386 0.40715 0.41023 0.41033

Eigenvalues --- 0.41087 0.41177 0.41236 0.41311 0.41343

Eigenvalues --- 0.41555 0.41778 0.42278 0.42684 0.44579

Eigenvalues --- 0.45294 0.45849 0.45922 0.45924 0.45985

Eigenvalues --- 0.45998 0.46131 0.46252 0.46258 0.46312

Eigenvalues --- 0.46321 0.48391 0.49022 0.49452 0.49681

Eigenvalues --- 0.50754 0.50757 0.50782 0.50786 0.51869

Eigenvalues --- 0.52231 0.57190 0.57749

DIIS coeff's: 0.73858 0.00368 0.16459 -0.40687 0.46082

DIIS coeff's: -0.00676 0.11830 -0.07106 0.01885 0.01911

DIIS coeff's: -0.03350 0.02491 -0.03036 -0.01241 -0.00096

DIIS coeff's: 0.00325 -0.00230 0.01211

Cosine: 0.551 > 0.500

Length: 0.857

GDIIS step was calculated using 18 of the last 18 vectors.

Iteration 1 RMS(Cart)= 0.00544669 RMS(Int)= 0.00000926

Iteration 2 RMS(Cart)= 0.00001314 RMS(Int)= 0.00000538

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000538

ITry= 1 IFail=0 DXMaxC= 2.18D-02 DCOld= 1.00D+10 DXMaxT= 1.28D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.65678 0.00001 0.00065 0.00001 0.00065 2.65743

R2 2.64094 0.00005 -0.00051 -0.00002 -0.00054 2.64040

R3 2.03707 0.00000 0.00002 0.00000 0.00002 2.03709

R4 2.59923 -0.00007 -0.00004 -0.00001 -0.00004 2.59919

R5 2.71598 0.00004 -0.00073 0.00003 -0.00071 2.71527

R6 2.59917 -0.00008 -0.00013 -0.00004 -0.00017 2.59899

R7 1.91025 -0.00014 -0.00018 -0.00006 -0.00025 1.91001

R8 2.65649 0.00001 0.00061 0.00001 0.00061 2.65711

R9 2.71670 0.00005 -0.00047 -0.00004 -0.00052 2.71618

R10 2.03711 0.00002 0.00004 -0.00000 0.00003 2.03714

R11 2.64075 0.00011 0.00080 0.00007 0.00087 2.64161

R12 2.80426 0.00001 -0.00019 0.00002 -0.00017 2.80409

R13 2.59607 0.00006 0.00014 0.00004 0.00019 2.59626

R14 2.76199 0.00002 -0.00058 0.00001 -0.00058 2.76141

R15 2.59454 0.00003 -0.00025 0.00002 -0.00023 2.59431

R16 2.76240 -0.00001 -0.00060 -0.00002 -0.00062 2.76178

R17 2.64253 0.00003 0.00101 0.00001 0.00102 2.64355

R18 2.55432 0.00001 0.00056 -0.00003 0.00053 2.55485

R19 2.03918 0.00001 0.00001 -0.00001 -0.00000 2.03917

R20 2.03906 0.00000 0.00002 -0.00002 0.00001 2.03907

R21 2.64260 0.00003 0.00103 0.00004 0.00107 2.64367

R22 2.80382 0.00001 -0.00020 0.00002 -0.00018 2.80364

R23 2.76242 -0.00001 -0.00061 0.00001 -0.00061 2.76181

R24 2.59450 0.00003 -0.00028 0.00002 -0.00026 2.59424

R25 2.55433 0.00001 0.00056 -0.00003 0.00053 2.55486

R26 2.03918 0.00001 0.00001 -0.00002 -0.00000 2.03917

R27 2.76199 0.00001 -0.00057 -0.00001 -0.00059 2.76140

R28 2.03906 0.00000 0.00002 -0.00001 0.00001 2.03907

R29 2.59608 0.00006 0.00016 0.00005 0.00021 2.59630

R30 2.64067 0.00011 0.00078 0.00004 0.00082 2.64148

R31 2.71661 0.00004 -0.00049 -0.00008 -0.00058 2.71604

R32 2.80448 0.00001 -0.00008 0.00005 -0.00003 2.80446

R33 2.65660 0.00001 0.00066 0.00000 0.00066 2.65726

R34 2.59924 -0.00008 -0.00010 -0.00004 -0.00013 2.59911

R35 2.64086 0.00005 -0.00055 -0.00002 -0.00057 2.64029

R36 2.03709 0.00002 0.00003 -0.00001 0.00002 2.03711

R37 2.65685 0.00001 0.00069 0.00001 0.00070 2.65754

R38 2.03704 0.00000 0.00001 -0.00000 0.00001 2.03705

R39 2.59929 -0.00007 -0.00002 -0.00000 -0.00002 2.59927

R40 2.71588 0.00004 -0.00074 -0.00002 -0.00076 2.71512

R41 1.91039 -0.00013 -0.00014 -0.00005 -0.00019 1.91020

R42 2.80402 0.00001 -0.00009 0.00004 -0.00005 2.80397

R43 2.65117 -0.00002 0.00009 0.00004 0.00013 2.65130

R44 2.64983 0.00000 0.00013 -0.00001 0.00012 2.64995

R45 2.62867 -0.00001 -0.00001 -0.00000 -0.00001 2.62865

R46 2.04852 -0.00000 -0.00003 -0.00001 -0.00004 2.04848

R47 2.63627 0.00000 0.00001 -0.00001 0.00000 2.63627

R48 2.05017 0.00000 -0.00000 -0.00000 -0.00000 2.05017

R49 2.63408 0.00002 0.00005 0.00000 0.00005 2.63413

R50 2.05006 0.00000 0.00001 -0.00000 0.00000 2.05006

R51 2.63098 0.00002 -0.00007 -0.00000 -0.00008 2.63091

R52 2.05015 0.00000 0.00000 -0.00001 -0.00000 2.05014

R53 2.04864 -0.00000 -0.00004 -0.00001 -0.00006 2.04859

R54 2.63631 0.00001 -0.00001 -0.00001 -0.00002 2.63630

R55 2.63421 0.00001 0.00004 0.00000 0.00004 2.63426

R56 2.05006 0.00000 0.00001 0.00000 0.00001 2.05007

R57 2.62893 -0.00000 -0.00006 0.00000 -0.00006 2.62887

R58 2.05018 0.00000 0.00000 -0.00000 -0.00000 2.05018

R59 2.65139 -0.00002 0.00004 0.00003 0.00007 2.65146

R60 2.04850 -0.00000 -0.00001 -0.00001 -0.00003 2.04848

R61 2.65005 -0.00000 0.00010 0.00002 0.00012 2.65017

R62 2.63062 0.00001 -0.00001 -0.00001 -0.00002 2.63060

R63 2.04856 0.00000 -0.00001 -0.00001 -0.00002 2.04854

R64 2.05016 0.00000 -0.00000 -0.00000 -0.00000 2.05016

R65 2.64997 -0.00000 0.00006 -0.00000 0.00006 2.65003

R66 2.65132 -0.00002 0.00002 0.00000 0.00002 2.65134

R67 2.63064 0.00001 0.00000 -0.00001 -0.00000 2.63064

R68 2.04857 -0.00000 -0.00000 -0.00001 -0.00001 2.04856

R69 2.63421 0.00001 0.00004 -0.00000 0.00004 2.63425

R70 2.05016 0.00000 -0.00000 -0.00000 -0.00000 2.05016

R71 2.63630 0.00001 -0.00002 -0.00001 -0.00003 2.63627

R72 2.05006 0.00000 0.00001 0.00000 0.00001 2.05007

R73 2.62897 -0.00000 -0.00005 0.00002 -0.00004 2.62893

R74 2.05019 0.00000 0.00000 -0.00000 0.00000 2.05019

R75 2.04850 -0.00000 -0.00002 -0.00000 -0.00002 2.04849

R76 2.64974 0.00000 0.00010 -0.00003 0.00007 2.64981

R77 2.65108 -0.00002 0.00007 0.00001 0.00008 2.65117

R78 2.63102 0.00002 -0.00006 0.00000 -0.00006 2.63096

R79 2.04866 -0.00000 -0.00004 -0.00001 -0.00004 2.04861

R80 2.63408 0.00002 0.00004 0.00000 0.00005 2.63413

R81 2.05015 0.00000 0.00000 -0.00001 -0.00000 2.05014

R82 2.63625 0.00000 -0.00000 -0.00001 -0.00001 2.63625

R83 2.05006 0.00000 0.00001 -0.00000 0.00000 2.05006

R84 2.62870 -0.00001 -0.00000 0.00001 0.00001 2.62871

R85 2.05018 0.00000 -0.00000 -0.00000 -0.00000 2.05017

R86 2.04853 -0.00000 -0.00003 -0.00000 -0.00004 2.04849

A1 1.88157 -0.00002 0.00006 0.00001 0.00007 1.88164

A2 2.18783 0.00000 -0.00022 -0.00004 -0.00027 2.18756

A3 2.21377 0.00002 0.00017 0.00003 0.00020 2.21397

A4 1.86807 -0.00002 -0.00021 -0.00004 -0.00025 1.86782

A5 2.22172 0.00012 0.00039 0.00005 0.00042 2.22213

A6 2.19300 -0.00010 -0.00020 -0.00001 -0.00019 2.19282

A7 1.92498 0.00008 0.00025 0.00004 0.00028 1.92527

A8 2.17760 -0.00005 -0.00009 0.00007 -0.00001 2.17760

A9 2.17984 -0.00003 -0.00015 -0.00011 -0.00025 2.17959

A10 1.86817 -0.00003 -0.00019 -0.00002 -0.00020 1.86796

A11 2.19452 -0.00001 -0.00018 -0.00006 -0.00021 2.19430

A12 2.22013 0.00003 0.00036 0.00007 0.00041 2.22054

A13 1.88165 -0.00001 0.00008 -0.00000 0.00008 1.88173

A14 2.21397 0.00003 0.00015 0.00005 0.00020 2.21417

A15 2.18754 -0.00002 -0.00024 -0.00005 -0.00029 2.18725

A16 2.18679 0.00008 -0.00030 -0.00002 -0.00029 2.18650

A17 2.02299 -0.00012 0.00021 -0.00009 0.00010 2.02309

A18 2.07336 0.00005 0.00009 0.00011 0.00018 2.07354

A19 2.19188 0.00006 -0.00024 0.00007 -0.00014 2.19174

A20 2.16508 -0.00001 0.00027 -0.00005 0.00020 2.16528

A21 1.92620 -0.00004 -0.00004 -0.00003 -0.00007 1.92614

A22 1.84702 0.00002 0.00001 0.00000 0.00000 1.84703

A23 1.92647 -0.00001 0.00013 -0.00001 0.00012 1.92658

A24 2.19217 0.00004 -0.00027 0.00005 -0.00020 2.19197

A25 2.16454 -0.00003 0.00013 -0.00004 0.00008 2.16462

A26 1.86206 0.00001 -0.00009 0.00002 -0.00008 1.86198

A27 2.19694 -0.00002 0.00013 -0.00007 0.00006 2.19700

A28 2.22380 0.00001 -0.00004 0.00005 0.00001 2.22381

A29 1.86204 0.00003 -0.00002 0.00002 -0.00000 1.86204

A30 2.19679 -0.00000 0.00013 -0.00001 0.00012 2.19691

A31 2.22401 -0.00002 -0.00012 -0.00001 -0.00012 2.22389

A32 2.18540 0.00000 -0.00023 -0.00010 -0.00030 2.18511

A33 2.02494 0.00006 0.00032 0.00011 0.00042 2.02536

A34 2.07279 -0.00006 -0.00008 -0.00002 -0.00012 2.07267

A35 2.16464 -0.00003 0.00014 0.00002 0.00014 2.16479

A36 2.19207 0.00004 -0.00029 0.00001 -0.00026 2.19181

A37 1.92646 -0.00001 0.00014 -0.00003 0.00011 1.92657

A38 1.86206 0.00001 -0.00009 0.00002 -0.00007 1.86199

A39 2.19693 -0.00002 0.00010 -0.00005 0.00005 2.19698

A40 2.22380 0.00001 -0.00002 0.00003 0.00001 2.22381

A41 1.86203 0.00003 -0.00002 0.00001 -0.00001 1.86202

A42 2.22402 -0.00002 -0.00014 0.00001 -0.00012 2.22390

A43 2.19680 -0.00000 0.00015 -0.00003 0.00013 2.19692

A44 1.92620 -0.00004 -0.00006 -0.00002 -0.00007 1.92613

A45 2.16502 -0.00001 0.00028 -0.00010 0.00016 2.16518

A46 2.19194 0.00006 -0.00023 0.00011 -0.00010 2.19185

A47 1.84704 0.00002 0.00001 0.00001 0.00001 1.84704

A48 2.18712 0.00007 -0.00015 0.00003 -0.00009 2.18703

A49 2.07297 0.00004 -0.00012 0.00006 -0.00007 2.07290

A50 2.02305 -0.00012 0.00027 -0.00010 0.00017 2.02322

A51 2.22008 0.00003 0.00037 0.00006 0.00041 2.22049

A52 2.19453 -0.00000 -0.00020 -0.00005 -0.00023 2.19430

A53 1.86816 -0.00003 -0.00020 -0.00001 -0.00021 1.86795

A54 1.88167 -0.00001 0.00009 0.00000 0.00010 1.88176

A55 2.18765 -0.00002 -0.00019 -0.00004 -0.00023 2.18742

A56 2.21384 0.00003 0.00010 0.00004 0.00014 2.21398

A57 1.88157 -0.00002 0.00006 0.00001 0.00007 1.88165

A58 2.21371 0.00001 0.00011 0.00003 0.00013 2.21385

A59 2.18789 0.00000 -0.00017 -0.00003 -0.00021 2.18768

A60 1.86809 -0.00002 -0.00022 -0.00003 -0.00024 1.86784

A61 2.22172 0.00012 0.00037 0.00005 0.00041 2.22212

A62 2.19294 -0.00010 -0.00022 -0.00002 -0.00021 2.19272

A63 1.92494 0.00007 0.00025 0.00003 0.00027 1.92520

A64 2.17984 -0.00002 -0.00018 -0.00011 -0.00029 2.17956

A65 2.17747 -0.00005 -0.00014 0.00008 -0.00005 2.17742

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D5 -0.00051 -0.00001 -0.00004 -0.00005 -0.00009 -0.00060

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D11 3.08820 -0.00002 -0.00094 -0.00014 -0.00108 3.08711

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D14 0.18038 -0.00001 0.00147 0.00019 0.00165 0.18204

D15 0.22589 -0.00000 0.00176 0.00002 0.00178 0.22767

D16 -2.92691 0.00001 0.00235 0.00017 0.00251 -2.92439

D17 0.02454 0.00001 0.00020 0.00013 0.00033 0.02487

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D21 -0.01441 0.00000 -0.00009 -0.00005 -0.00014 -0.01455

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D28 -0.19108 -0.00001 -0.00223 0.00007 -0.00216 -0.19324

D29 -0.12375 -0.00002 -0.00277 0.00022 -0.00255 -0.12631

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D31 3.00657 -0.00001 -0.00281 0.00017 -0.00264 3.00393

D32 -0.12703 0.00001 -0.00179 0.00033 -0.00146 -0.12850

D33 -1.00051 0.00005 0.00404 0.00044 0.00448 -0.99603

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D37 -3.09340 0.00003 0.00141 0.00027 0.00168 -3.09171

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D52 0.13687 -0.00000 0.00118 0.00001 0.00118 0.13805

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D94 -0.05145 -0.00001 -0.00081 -0.00004 -0.00084 -0.05229

D95 -0.01451 0.00000 -0.00032 0.00010 -0.00022 -0.01473

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D103 -3.13492 -0.00002 -0.00045 -0.00003 -0.00048 -3.13540

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D137 0.00734 -0.00000 0.00001 -0.00005 -0.00004 0.00730

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D198 -0.00820 -0.00000 0.00022 -0.00027 -0.00005 -0.00825

D199 0.01428 -0.00000 0.00029 -0.00013 0.00016 0.01444

D200 3.13648 0.00001 -0.00023 0.00005 -0.00018 3.13631

D201 -0.00891 0.00001 0.00018 -0.00005 0.00012 -0.00878

D202 3.13044 0.00001 0.00011 -0.00006 0.00005 3.13049

D203 -3.13222 -0.00000 -0.00000 0.00000 0.00000 -3.13221

D204 0.00713 -0.00000 -0.00007 -0.00000 -0.00008 0.00705

D205 0.00722 -0.00000 -0.00001 -0.00004 -0.00006 0.00716

D206 -3.13711 -0.00000 0.00020 -0.00007 0.00013 -3.13698

D207 -3.13212 -0.00000 0.00005 -0.00003 0.00002 -3.13210

D208 0.00674 -0.00000 0.00026 -0.00006 0.00020 0.00695

D209 0.00522 -0.00000 -0.00001 0.00005 0.00004 0.00527

D210 -3.13570 -0.00000 -0.00005 0.00005 -0.00001 -3.13570

D211 -3.13364 -0.00000 -0.00022 0.00008 -0.00014 -3.13378

D212 0.00863 -0.00000 -0.00026 0.00007 -0.00019 0.00844

D213 -0.01610 0.00000 -0.00013 0.00003 -0.00010 -0.01620

D214 -3.13822 -0.00000 0.00039 -0.00015 0.00024 -3.13798

D215 3.12482 0.00000 -0.00008 0.00004 -0.00005 3.12477

D216 0.00270 -0.00000 0.00044 -0.00014 0.00030 0.00300

Item Value Threshold Converged?

Maximum Force 0.000135 0.000450 YES

RMS Force 0.000027 0.000300 YES

Maximum Displacement 0.021800 0.001800 NO

RMS Displacement 0.005447 0.001200 NO

Predicted change in Energy=-8.049563D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

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(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=1 Diff= 4.09D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 0.953545 -4.118023 0.552646

2 6 0 1.305706 -2.803384 0.198731

3 7 0 0.133243 -2.111190 0.003771

4 6 0 -0.947588 -2.941459 0.188121

5 6 0 -0.441060 -4.203491 0.545565

6 6 0 -2.326174 -2.577241 0.007024

7 6 0 -2.805882 -1.270476 -0.120708

8 7 0 -2.063258 -0.126577 0.045282

9 6 0 -2.942840 0.916336 -0.107647

10 6 0 -4.275847 0.414267 -0.434637

11 6 0 -4.190981 -0.935005 -0.443648

12 6 0 2.629829 -2.272281 0.027874

13 6 0 2.942977 -0.915787 -0.109914

14 6 0 4.275927 -0.413078 -0.436201

15 6 0 4.191011 0.936208 -0.442847

16 6 0 2.805863 1.271033 -0.119466

17 7 0 2.063328 0.126781 0.044637

18 6 0 2.326058 2.577540 0.009776

19 6 0 0.947650 2.942170 0.190784

20 6 0 0.440927 4.206821 0.538886

21 6 0 -0.953618 4.121370 0.546247

22 6 0 -1.305681 2.804128 0.201814

23 7 0 -0.133136 2.110428 0.012462

24 6 0 -2.629602 2.272617 0.031338

25 6 0 -3.294410 -3.701082 -0.029618

26 6 0 -3.153618 -4.734336 -0.968231

27 6 0 -4.068398 -5.781345 -1.011731

28 6 0 -5.128531 -5.824842 -0.105968

29 6 0 -5.270896 -4.810596 0.839579

30 6 0 -4.364738 -3.754235 0.874818

31 6 0 5.825669 -5.135299 -0.018130

32 6 0 4.776793 -5.241430 -0.931809

33 6 0 3.734315 -4.320528 -0.910672

34 6 0 3.732768 -3.264468 0.013123

35 6 0 4.792862 -3.167137 0.926073

36 6 0 5.828038 -4.097751 0.912834

37 6 0 -3.733032 3.264502 0.015126

38 6 0 -4.791685 3.169299 0.929862

39 6 0 -5.827803 4.098871 0.914800

40 6 0 -5.827748 5.133111 -0.019835

41 6 0 -4.780327 5.236958 -0.935423

42 6 0 -3.736948 4.317073 -0.912542

43 6 0 3.294787 3.701175 -0.027961

44 6 0 4.363049 3.756360 0.878674

45 6 0 5.269989 4.812045 0.842221

46 6 0 5.130379 5.823456 -0.106764

47 6 0 4.072354 5.777749 -1.014858

48 6 0 3.156834 4.731395 -0.970218

49 1 0 1.648421 -4.907122 0.790370

50 1 0 -1.036979 -5.071260 0.777860

51 1 0 -5.143152 1.018114 -0.652751

52 1 0 -4.975999 -1.639847 -0.670023

53 1 0 5.143219 -1.016517 -0.655493

54 1 0 4.976058 1.641488 -0.667766

55 1 0 1.036561 5.076658 0.763997

56 1 0 -1.648488 4.912502 0.777045

57 1 0 -2.333438 -4.703350 -1.676342

58 1 0 -3.954062 -6.564286 -1.753987

59 1 0 -5.837292 -6.645607 -0.135852

60 1 0 -6.087323 -4.841692 1.553348

61 1 0 -4.473593 -2.972101 1.617525

62 1 0 6.634873 -5.857734 -0.031243

63 1 0 4.770709 -6.042948 -1.662945

64 1 0 2.923818 -4.404518 -1.625592

65 1 0 4.793230 -2.367196 1.657671

66 1 0 6.635327 -4.013337 1.632666

67 1 0 -4.790402 2.371628 1.663954

68 1 0 -6.634096 4.016124 1.635942

69 1 0 -6.637704 5.854675 -0.034415

70 1 0 -4.776118 6.035785 -1.669516

71 1 0 -2.927658 4.399134 -1.629061

72 1 0 4.469868 2.976200 1.623771

73 1 0 6.084900 4.844776 1.557646

74 1 0 5.839745 6.643662 -0.137621

75 1 0 3.960243 6.558388 -1.759878

76 1 0 2.338334 4.698604 -1.680197

77 1 0 0.074775 -1.124677 -0.208251

78 1 0 -0.074563 1.121091 -0.186445

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0587922 0.0582545 0.0300934

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(Enter /home/kira/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5356.8969936457 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122072999 Hartrees.

Nuclear repulsion after empirical dispersion term = 5356.6847863458 Hartrees.

Force inversion solution in PCM.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5793

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.86D-10

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 313

GePol: Fraction of low-weight points (<1% of avg) = 5.40%

GePol: Cavity surface area = 610.609 Ang\*\*2

GePol: Cavity volume = 627.886 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0021014705 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5356.6826848753 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.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

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(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Thu Aug 29 02:31:23 2019, MaxMem= 4294967296 cpu: 2.5

(Enter /home/kira/g09/l401.exe)

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999999 0.000017 0.000002 -0.001444 Ang= 0.17 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0182

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30493935078

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(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 590000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 100676547.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.44D-15 for 5771.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.83D-15 for 3619 321.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.88D-15 for 5787.

Iteration 1 A^-1\*A deviation from orthogonality is 5.09D-11 for 5382 5375.

E= -1914.33309446783

DIIS: error= 4.45D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.33309446783 IErMin= 1 ErrMin= 4.45D-04

ErrMax= 4.45D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.15D-04 BMatP= 4.15D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.45D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.640 Goal= None Shift= 0.000

Gap= 0.705 Goal= None Shift= 0.000

RMSDP=1.52D-05 MaxDP=5.28D-04 OVMax= 2.51D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.52D-05 CP: 1.00D+00

E= -1914.33331419822 Delta-E= -0.000219730390 Rises=F Damp=F

DIIS: error= 6.52D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33331419822 IErMin= 2 ErrMin= 6.52D-05

ErrMax= 6.52D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.93D-06 BMatP= 4.15D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.706D-01 0.107D+01

Coeff: -0.706D-01 0.107D+01

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.64D-06 MaxDP=6.98D-05 DE=-2.20D-04 OVMax= 3.85D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.34D-06 CP: 1.00D+00 1.08D+00

E= -1914.33331787347 Delta-E= -0.000003675259 Rises=F Damp=F

DIIS: error= 1.08D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33331787347 IErMin= 3 ErrMin= 1.08D-05

ErrMax= 1.08D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.99D-07 BMatP= 5.93D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.249D-01 0.291D+00 0.733D+00

Coeff: -0.249D-01 0.291D+00 0.733D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.97D-07 MaxDP=5.58D-05 DE=-3.68D-06 OVMax= 1.59D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 7.15D-07 CP: 1.00D+00 1.09D+00 8.80D-01

E= -1914.33331802326 Delta-E= -0.000000149784 Rises=F Damp=F

DIIS: error= 9.03D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33331802326 IErMin= 4 ErrMin= 9.03D-06

ErrMax= 9.03D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.23D-07 BMatP= 8.99D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.798D-02 0.726D-01 0.412D+00 0.523D+00

Coeff: -0.798D-02 0.726D-01 0.412D+00 0.523D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.98D-07 MaxDP=3.38D-05 DE=-1.50D-07 OVMax= 1.53D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.14D-07 CP: 1.00D+00 1.10D+00 9.24D-01 6.95D-01

E= -1914.33331812573 Delta-E= -0.000000102473 Rises=F Damp=F

DIIS: error= 3.93D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33331812573 IErMin= 5 ErrMin= 3.93D-06

ErrMax= 3.93D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.32D-08 BMatP= 4.23D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.167D-03-0.152D-01 0.802D-01 0.265D+00 0.669D+00

Coeff: 0.167D-03-0.152D-01 0.802D-01 0.265D+00 0.669D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.70D-07 MaxDP=9.00D-06 DE=-1.02D-07 OVMax= 4.82D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.25D-07 CP: 1.00D+00 1.10D+00 9.45D-01 7.99D-01 7.78D-01

E= -1914.33331813703 Delta-E= -0.000000011298 Rises=F Damp=F

DIIS: error= 2.17D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33331813703 IErMin= 6 ErrMin= 2.17D-06

ErrMax= 2.17D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.25D-08 BMatP= 4.32D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.103D-02-0.183D-01 0.317D-02 0.109D+00 0.427D+00 0.479D+00

Coeff: 0.103D-02-0.183D-01 0.317D-02 0.109D+00 0.427D+00 0.479D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=8.22D-08 MaxDP=6.29D-06 DE=-1.13D-08 OVMax= 5.45D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 6.66D-08 CP: 1.00D+00 1.10D+00 9.53D-01 8.00D-01 9.09D-01

CP: 8.57D-01

E= -1914.33331814136 Delta-E= -0.000000004327 Rises=F Damp=F

DIIS: error= 8.35D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33331814136 IErMin= 7 ErrMin= 8.35D-07

ErrMax= 8.35D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D-09 BMatP= 1.25D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.373D-03-0.508D-02-0.804D-02 0.101D-01 0.783D-01 0.195D+00

Coeff-Com: 0.730D+00

Coeff: 0.373D-03-0.508D-02-0.804D-02 0.101D-01 0.783D-01 0.195D+00

Coeff: 0.730D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.14D-08 MaxDP=3.25D-06 DE=-4.33D-09 OVMax= 4.14D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.72D-08 CP: 1.00D+00 1.10D+00 9.56D-01 8.15D-01 9.59D-01

CP: 1.11D+00 1.32D+00

E= -1914.33331814236 Delta-E= -0.000000001007 Rises=F Damp=F

DIIS: error= 7.06D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33331814236 IErMin= 8 ErrMin= 7.06D-07

ErrMax= 7.06D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.87D-10 BMatP= 1.09D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.406D-03 0.856D-02-0.794D-02-0.647D-01-0.234D+00-0.163D+00

Coeff-Com: 0.531D+00 0.931D+00

Coeff: -0.406D-03 0.856D-02-0.794D-02-0.647D-01-0.234D+00-0.163D+00

Coeff: 0.531D+00 0.931D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.78D-08 MaxDP=6.17D-06 DE=-1.01D-09 OVMax= 7.70D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.24D-08 CP: 1.00D+00 1.10D+00 9.59D-01 8.27D-01 1.06D+00

CP: 1.44D+00 2.08D+00 1.43D+00

E= -1914.33331814339 Delta-E= -0.000000001024 Rises=F Damp=F

DIIS: error= 4.12D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33331814339 IErMin= 9 ErrMin= 4.12D-07

ErrMax= 4.12D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.48D-10 BMatP= 5.87D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.229D-03 0.430D-02-0.134D-02-0.262D-01-0.111D+00-0.925D-01

Coeff-Com: 0.546D-01 0.408D+00 0.765D+00

Coeff: -0.229D-03 0.430D-02-0.134D-02-0.262D-01-0.111D+00-0.925D-01

Coeff: 0.546D-01 0.408D+00 0.765D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.56D-08 MaxDP=2.69D-06 DE=-1.02D-09 OVMax= 3.64D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 9.74D-09 CP: 1.00D+00 1.10D+00 9.60D-01 8.32D-01 1.09D+00

CP: 1.59D+00 2.39D+00 1.87D+00 1.49D+00

E= -1914.33331814369 Delta-E= -0.000000000302 Rises=F Damp=F

DIIS: error= 3.43D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33331814369 IErMin=10 ErrMin= 3.43D-07

ErrMax= 3.43D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.08D-11 BMatP= 1.48D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.733D-04-0.195D-02 0.359D-02 0.197D-01 0.547D-01 0.377D-01

Coeff-Com: -0.277D+00-0.205D+00 0.473D+00 0.895D+00

Coeff: 0.733D-04-0.195D-02 0.359D-02 0.197D-01 0.547D-01 0.377D-01

Coeff: -0.277D+00-0.205D+00 0.473D+00 0.895D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.76D-08 MaxDP=3.12D-06 DE=-3.02D-10 OVMax= 4.09D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.49D-09 CP: 1.00D+00 1.10D+00 9.61D-01 8.36D-01 1.13D+00

CP: 1.73D+00 2.71D+00 2.35D+00 2.29D+00 1.29D+00

E= -1914.33331814389 Delta-E= -0.000000000197 Rises=F Damp=F

DIIS: error= 2.06D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33331814389 IErMin=11 ErrMin= 2.06D-07

ErrMax= 2.06D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.74D-11 BMatP= 7.08D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.103D-03-0.218D-02 0.182D-02 0.171D-01 0.572D-01 0.509D-01

Coeff-Com: -0.158D+00-0.198D+00-0.670D-01 0.427D+00 0.871D+00

Coeff: 0.103D-03-0.218D-02 0.182D-02 0.171D-01 0.572D-01 0.509D-01

Coeff: -0.158D+00-0.198D+00-0.670D-01 0.427D+00 0.871D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.46D-08 MaxDP=1.94D-06 DE=-1.97D-10 OVMax= 2.69D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 3.99D-09 CP: 1.00D+00 1.10D+00 9.62D-01 8.38D-01 1.15D+00

CP: 1.81D+00 2.91D+00 2.70D+00 2.82D+00 1.88D+00

CP: 1.39D+00

E= -1914.33331814388 Delta-E= 0.000000000007 Rises=F Damp=F

DIIS: error= 1.34D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=11 EnMin= -1914.33331814389 IErMin=12 ErrMin= 1.34D-07

ErrMax= 1.34D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.38D-11 BMatP= 2.74D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.280D-04-0.351D-03-0.987D-03 0.600D-03 0.669D-02 0.175D-01

Coeff-Com: 0.432D-01 0.122D-02-0.335D+00-0.199D+00 0.594D+00 0.872D+00

Coeff: 0.280D-04-0.351D-03-0.987D-03 0.600D-03 0.669D-02 0.175D-01

Coeff: 0.432D-01 0.122D-02-0.335D+00-0.199D+00 0.594D+00 0.872D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.02D-08 MaxDP=1.73D-06 DE= 7.28D-12 OVMax= 2.24D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 8.10D-09 CP: 1.00D+00 1.10D+00 9.62D-01 8.40D-01 1.17D+00

CP: 1.87D+00 3.00D+00 2.97D+00 3.00D+00 2.32D+00

CP: 2.10D+00 1.17D+00

E= -1914.33331814392 Delta-E= -0.000000000045 Rises=F Damp=F

DIIS: error= 6.46D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1914.33331814392 IErMin=13 ErrMin= 6.46D-08

ErrMax= 6.46D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.95D-12 BMatP= 1.38D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.172D-04 0.500D-03-0.116D-02-0.484D-02-0.150D-01-0.530D-02

Coeff-Com: 0.679D-01 0.664D-01-0.170D+00-0.233D+00 0.491D-01 0.468D+00

Coeff-Com: 0.777D+00

Coeff: -0.172D-04 0.500D-03-0.116D-02-0.484D-02-0.150D-01-0.530D-02

Coeff: 0.679D-01 0.664D-01-0.170D+00-0.233D+00 0.491D-01 0.468D+00

Coeff: 0.777D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.02D-08 MaxDP=8.62D-07 DE=-4.46D-11 OVMax= 1.13D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 3.84D-09 CP: 1.00D+00 1.10D+00 9.62D-01 8.41D-01 1.17D+00

CP: 1.90D+00 3.00D+00 3.00D+00 3.00D+00 2.56D+00

CP: 2.44D+00 1.58D+00 1.85D+00

E= -1914.33331814396 Delta-E= -0.000000000040 Rises=F Damp=F

DIIS: error= 3.41D-08 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1914.33331814396 IErMin=14 ErrMin= 3.41D-08

ErrMax= 3.41D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.45D-12 BMatP= 3.95D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.178D-04 0.378D-03-0.309D-03-0.268D-02-0.105D-01-0.768D-02

Coeff-Com: 0.221D-01 0.393D-01 0.848D-02-0.604D-01-0.164D+00-0.200D-01

Coeff-Com: 0.439D+00 0.756D+00

Coeff: -0.178D-04 0.378D-03-0.309D-03-0.268D-02-0.105D-01-0.768D-02

Coeff: 0.221D-01 0.393D-01 0.848D-02-0.604D-01-0.164D+00-0.200D-01

Coeff: 0.439D+00 0.756D+00

Gap= 0.048 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.74D-09 MaxDP=4.03D-07 DE=-4.00D-11 OVMax= 5.23D-06

Error on total polarization charges = 0.08257

SCF Done: E(UB3LYP) = -1914.33331814 A.U. after 14 cycles

NFock= 14 Conv=0.47D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0182

<L.S>= 0.000000000000E+00

KE= 1.906379454358D+03 PE=-1.516298988332D+04 EE= 5.985594425941D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0551, after 2.0017

Leave Link 502 at Thu Aug 29 02:37:32 2019, MaxMem= 4294967296 cpu: 5732.0

(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: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48359268D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64214166D-01

Leave Link 801 at Thu Aug 29 02:37:32 2019, MaxMem= 4294967296 cpu: 1.0

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Thu Aug 29 02:37:39 2019, MaxMem= 4294967296 cpu: 111.0

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Thu Aug 29 02:37:39 2019, MaxMem= 4294967296 cpu: 2.5

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 190

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 Thu Aug 29 02:57:29 2019, MaxMem= 4294967296 cpu: 19033.5

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 590000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.41D+03 4.52D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.54D+02 3.64D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.56D+00 4.69D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.03D-01 3.99D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.59D-04 2.11D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.60D-06 1.35D-04.

189 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 1.99D-08 1.02D-05.

80 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.33D-11 6.24D-07.

41 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.20D-13 3.96D-08.

3 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 8.83D-15 4.42D-09.

2 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 4.58D-15 2.53D-09.

InvSVY: IOpt=1 It= 1 EMax= 1.28D-13

Solved reduced A of dimension 1722 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1126.63 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 Thu Aug 29 06:48:40 2019, MaxMem= 4294967296 cpu: 221873.5

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 190

Leave Link 701 at Thu Aug 29 06:50:09 2019, MaxMem= 4294967296 cpu: 1427.0

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Thu Aug 29 06:50:09 2019, MaxMem= 4294967296 cpu: 0.5

(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=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

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= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Thu Aug 29 07:08:23 2019, MaxMem= 4294967296 cpu: 17492.5

(Enter /home/kira/g09/l716.exe)

Dipole =-2.49067321D-04-5.25903481D-03-4.78097575D-01

Polarizability= 1.25699800D+03-2.79616977D+01 1.66780030D+03

6.57250187D-03-8.69613908D-02 4.55095842D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000182414 0.000039355 0.000236967

2 6 0.000219896 -0.000094081 -0.000288791

3 7 0.000065912 -0.000005615 0.000006759

4 6 0.000224104 -0.000101668 0.000289115

5 6 -0.000165227 0.000043011 -0.000244216

6 6 -0.000294026 0.000083670 -0.000292256

7 6 0.000238245 -0.000078161 0.000184933

8 7 0.000038292 0.000009640 0.000035997

9 6 -0.000299268 -0.000085572 0.000193277

10 6 0.000206373 0.000009678 -0.000128015

11 6 -0.000203367 0.000025357 -0.000109472

12 6 -0.000341248 0.000083864 0.000303607

13 6 0.000299008 -0.000082157 -0.000192470

14 6 -0.000206150 0.000010351 0.000128471

15 6 0.000203070 0.000025546 0.000109793

16 6 -0.000237382 -0.000081382 -0.000185880

17 7 -0.000045589 0.000014816 -0.000034097

18 6 0.000291551 0.000086382 0.000292827

19 6 -0.000222700 -0.000101415 -0.000289090

20 6 0.000165071 0.000040461 0.000244403

21 6 0.000184142 0.000037729 -0.000236249

22 6 -0.000223141 -0.000094332 0.000287281

23 7 -0.000068262 -0.000001525 0.000000364

24 6 0.000341687 0.000087050 -0.000304158

25 6 -0.000000117 -0.000000226 0.000024601

26 6 -0.000017715 0.000000278 -0.000024918

27 6 -0.000000631 0.000002902 0.000026092

28 6 -0.000017934 -0.000004135 -0.000011490

29 6 0.000029545 0.000001458 -0.000006728

30 6 -0.000010938 0.000005986 -0.000008030

31 6 0.000004320 -0.000018716 0.000007127

32 6 -0.000005603 0.000010118 0.000003296

33 6 0.000035227 -0.000002726 -0.000004235

34 6 -0.000020319 0.000039079 0.000002124

35 6 0.000004045 -0.000008126 -0.000032445

36 6 -0.000005165 0.000017309 0.000016590

37 6 0.000020005 0.000038776 -0.000003517

38 6 -0.000002372 -0.000008837 0.000030353

39 6 0.000005050 0.000016698 -0.000016869

40 6 -0.000004583 -0.000020488 -0.000006706

41 6 0.000004145 0.000007332 -0.000001659

42 6 -0.000034904 -0.000002217 0.000003260

43 6 -0.000000079 0.000000928 -0.000025119

44 6 0.000012008 0.000005714 0.000007935

45 6 -0.000029549 0.000001473 0.000007014

46 6 0.000018234 -0.000005330 0.000010689

47 6 0.000000649 0.000002555 -0.000025820

48 6 0.000018218 -0.000004090 0.000022978

49 1 0.000007121 0.000003333 -0.000005122

50 1 0.000000018 -0.000002159 0.000000229

51 1 -0.000008169 0.000002117 -0.000006127

52 1 -0.000010174 0.000005620 -0.000004166

53 1 0.000007915 0.000002378 0.000006298

54 1 0.000009761 0.000005534 0.000003834

55 1 -0.000002006 -0.000001041 0.000002676

56 1 -0.000005789 0.000001094 0.000005617

57 1 0.000009016 0.000002593 -0.000001394

58 1 -0.000000309 0.000002271 -0.000002219

59 1 0.000003967 -0.000000189 0.000004467

60 1 -0.000004407 0.000003286 -0.000002981

61 1 -0.000005852 -0.000003649 0.000000536

62 1 -0.000003800 0.000000416 0.000001659

63 1 0.000000333 0.000000010 -0.000003016

64 1 -0.000008238 -0.000009144 -0.000005242

65 1 0.000001582 -0.000001349 -0.000002280

66 1 0.000000780 -0.000000557 0.000000416

67 1 -0.000000442 -0.000001255 0.000003113

68 1 -0.000000564 -0.000001511 -0.000000334

69 1 0.000003724 -0.000000732 -0.000001860

70 1 -0.000000566 -0.000001024 0.000003010

71 1 0.000007969 -0.000010996 0.000005364

72 1 0.000006455 -0.000003913 0.000000015

73 1 0.000004670 0.000002713 0.000003208

74 1 -0.000004166 -0.000001028 -0.000004274

75 1 -0.000000328 0.000001070 0.000001702

76 1 -0.000009107 0.000001125 0.000000641

77 1 0.000008987 0.000024074 0.000017232

78 1 0.000001501 0.000034199 -0.000024625

-------------------------------------------------------------------

Cartesian Forces: Max 0.000341687 RMS 0.000102217

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Thu Aug 29 07:08:23 2019, MaxMem= 4294967296 cpu: 2.0

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000275142 RMS 0.000044567

Search for a local minimum.

Step number 19 out of a maximum of 452

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= 7.09D-07 DEPred=-8.05D-07 R=-8.81D-01

Trust test=-8.81D-01 RLast= 1.95D-02 DXMaxT set to 6.38D-02

ITU= -1 1 1 -1 -1 1 0 -1 1 1 -1 1 -1 -1 1 1 -1 1 0

Eigenvalues --- 0.00066 0.00221 0.00420 0.00601 0.00726

Eigenvalues --- 0.00823 0.00927 0.01044 0.01056 0.01118

Eigenvalues --- 0.01134 0.01168 0.01264 0.01281 0.01302

Eigenvalues --- 0.01306 0.01323 0.01423 0.01433 0.01529

Eigenvalues --- 0.01542 0.01557 0.01589 0.01671 0.01711

Eigenvalues --- 0.01716 0.01728 0.01737 0.01753 0.01759

Eigenvalues --- 0.01760 0.01782 0.01802 0.01803 0.01885

Eigenvalues --- 0.01934 0.01983 0.01994 0.02008 0.02167

Eigenvalues --- 0.02170 0.02257 0.02289 0.02294 0.02305

Eigenvalues --- 0.02331 0.02395 0.02467 0.02478 0.02524

Eigenvalues --- 0.02538 0.02543 0.02590 0.02625 0.02628

Eigenvalues --- 0.02644 0.02647 0.02769 0.02779 0.02797

Eigenvalues --- 0.02805 0.02869 0.02873 0.02874 0.02875

Eigenvalues --- 0.02956 0.02981 0.03909 0.04090 0.04194

Eigenvalues --- 0.04319 0.04369 0.04462 0.04539 0.04567

Eigenvalues --- 0.08118 0.09637 0.09687 0.09724 0.09868

Eigenvalues --- 0.09892 0.10266 0.10438 0.10561 0.10691

Eigenvalues --- 0.10692 0.10704 0.10731 0.10733 0.10933

Eigenvalues --- 0.11391 0.11393 0.11409 0.11414 0.11987

Eigenvalues --- 0.11992 0.11996 0.12002 0.12272 0.12272

Eigenvalues --- 0.12319 0.12320 0.12767 0.12769 0.12774

Eigenvalues --- 0.12778 0.15711 0.15911 0.16292 0.16829

Eigenvalues --- 0.17211 0.17272 0.17572 0.17825 0.17976

Eigenvalues --- 0.18030 0.18240 0.18309 0.19241 0.19282

Eigenvalues --- 0.19356 0.19358 0.19368 0.19405 0.19410

Eigenvalues --- 0.19428 0.19551 0.19551 0.19555 0.19556

Eigenvalues --- 0.20291 0.21489 0.22042 0.22701 0.22871

Eigenvalues --- 0.23260 0.23780 0.24242 0.24755 0.24986

Eigenvalues --- 0.26277 0.26399 0.26670 0.27158 0.28517

Eigenvalues --- 0.28549 0.28742 0.29003 0.29768 0.31030

Eigenvalues --- 0.31695 0.31979 0.32821 0.33072 0.33142

Eigenvalues --- 0.33326 0.34112 0.34709 0.35042 0.35563

Eigenvalues --- 0.35624 0.35625 0.35633 0.35639 0.35755

Eigenvalues --- 0.35758 0.35762 0.35806 0.35923 0.35924

Eigenvalues --- 0.35929 0.35932 0.35989 0.35992 0.36007

Eigenvalues --- 0.36011 0.36193 0.36204 0.36241 0.36245

Eigenvalues --- 0.36993 0.37058 0.37241 0.37381 0.37394

Eigenvalues --- 0.37492 0.38152 0.38426 0.38512 0.38592

Eigenvalues --- 0.39443 0.40396 0.40721 0.41031 0.41044

Eigenvalues --- 0.41099 0.41182 0.41245 0.41322 0.41346

Eigenvalues --- 0.41557 0.41778 0.42304 0.42700 0.44552

Eigenvalues --- 0.45275 0.45884 0.45918 0.45924 0.45983

Eigenvalues --- 0.45999 0.46133 0.46252 0.46258 0.46309

Eigenvalues --- 0.46320 0.48284 0.48921 0.49340 0.49571

Eigenvalues --- 0.50752 0.50754 0.50780 0.50783 0.51844

Eigenvalues --- 0.52213 0.57122 0.57687

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.17203 0.55215 -0.01850 0.15506 -0.22241

DIIS coeff's: 0.35542 0.00625

Cosine: 0.864 > 0.500

Length: 0.839

GDIIS step was calculated using 7 of the last 19 vectors.

Iteration 1 RMS(Cart)= 0.00264190 RMS(Int)= 0.00000169

Iteration 2 RMS(Cart)= 0.00000315 RMS(Int)= 0.00000106

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000106

ITry= 1 IFail=0 DXMaxC= 1.16D-02 DCOld= 1.00D+10 DXMaxT= 6.38D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.65743 -0.00018 -0.00049 -0.00017 -0.00066 2.65678

R2 2.64040 0.00018 0.00059 0.00009 0.00068 2.64108

R3 2.03709 0.00000 0.00002 0.00000 0.00002 2.03711

R4 2.59919 -0.00006 -0.00008 -0.00005 -0.00012 2.59907

R5 2.71527 0.00022 0.00070 0.00019 0.00089 2.71616

R6 2.59899 -0.00003 -0.00007 -0.00004 -0.00011 2.59889

R7 1.91001 -0.00000 -0.00003 -0.00006 -0.00009 1.90992

R8 2.65711 -0.00018 -0.00058 0.00002 -0.00056 2.65654

R9 2.71618 0.00024 0.00081 0.00004 0.00086 2.71704

R10 2.03714 0.00000 0.00001 0.00000 0.00001 2.03715

R11 2.64161 -0.00023 -0.00071 0.00021 -0.00050 2.64111

R12 2.80409 -0.00001 -0.00007 -0.00000 -0.00007 2.80402

R13 2.59626 -0.00000 0.00009 -0.00023 -0.00014 2.59611

R14 2.76141 0.00013 0.00052 0.00008 0.00061 2.76202

R15 2.59431 0.00003 -0.00010 0.00030 0.00020 2.59451

R16 2.76178 0.00012 0.00054 -0.00001 0.00053 2.76231

R17 2.64355 -0.00028 -0.00048 -0.00037 -0.00085 2.64270

R18 2.55485 -0.00018 -0.00042 -0.00005 -0.00047 2.55438

R19 2.03917 0.00001 -0.00000 -0.00000 -0.00000 2.03917

R20 2.03907 -0.00000 0.00001 -0.00002 -0.00001 2.03906

R21 2.64367 -0.00027 -0.00049 -0.00035 -0.00084 2.64283

R22 2.80364 -0.00001 -0.00005 -0.00003 -0.00008 2.80355

R23 2.76181 0.00013 0.00053 -0.00000 0.00053 2.76233

R24 2.59424 0.00003 -0.00010 0.00030 0.00020 2.59444

R25 2.55486 -0.00018 -0.00042 -0.00005 -0.00047 2.55439

R26 2.03917 0.00001 0.00000 -0.00001 -0.00000 2.03917

R27 2.76140 0.00013 0.00053 0.00008 0.00061 2.76201

R28 2.03907 -0.00000 0.00001 -0.00002 -0.00001 2.03906

R29 2.59630 -0.00001 0.00009 -0.00024 -0.00015 2.59615

R30 2.64148 -0.00024 -0.00071 0.00020 -0.00051 2.64097

R31 2.71604 0.00023 0.00082 0.00003 0.00085 2.71688

R32 2.80446 -0.00001 -0.00005 -0.00000 -0.00005 2.80440

R33 2.65726 -0.00018 -0.00056 0.00001 -0.00055 2.65670

R34 2.59911 -0.00002 -0.00006 -0.00004 -0.00009 2.59901

R35 2.64029 0.00018 0.00057 0.00009 0.00067 2.64095

R36 2.03711 0.00000 0.00001 -0.00000 0.00001 2.03712

R37 2.65754 -0.00018 -0.00047 -0.00018 -0.00065 2.65689

R38 2.03705 0.00000 0.00002 -0.00000 0.00002 2.03707

R39 2.59927 -0.00005 -0.00005 -0.00006 -0.00011 2.59916

R40 2.71512 0.00022 0.00072 0.00018 0.00089 2.71601

R41 1.91020 0.00001 -0.00000 -0.00007 -0.00007 1.91013

R42 2.80397 -0.00001 -0.00002 -0.00004 -0.00006 2.80391

R43 2.65130 -0.00001 0.00003 0.00001 0.00004 2.65135

R44 2.64995 0.00001 0.00000 0.00004 0.00004 2.64999

R45 2.62865 -0.00002 -0.00004 -0.00000 -0.00004 2.62861

R46 2.04848 0.00000 -0.00000 -0.00001 -0.00001 2.04847

R47 2.63627 0.00000 0.00003 0.00001 0.00003 2.63631

R48 2.05017 0.00000 0.00000 -0.00000 -0.00000 2.05017

R49 2.63413 -0.00001 -0.00002 0.00000 -0.00002 2.63411

R50 2.05006 -0.00000 0.00000 -0.00000 -0.00000 2.05006

R51 2.63091 0.00002 0.00003 -0.00001 0.00002 2.63093

R52 2.05014 -0.00000 -0.00000 -0.00000 -0.00000 2.05014

R53 2.04859 0.00001 -0.00000 0.00000 -0.00000 2.04858

R54 2.63630 0.00002 0.00003 0.00001 0.00004 2.63633

R55 2.63426 -0.00001 -0.00002 -0.00000 -0.00003 2.63423

R56 2.05007 -0.00000 0.00000 -0.00000 -0.00000 2.05006

R57 2.62887 0.00001 -0.00003 -0.00002 -0.00004 2.62883

R58 2.05018 -0.00000 -0.00000 0.00000 -0.00000 2.05018

R59 2.65146 0.00001 0.00002 0.00002 0.00004 2.65150

R60 2.04848 -0.00000 -0.00001 -0.00001 -0.00002 2.04846

R61 2.65017 -0.00001 0.00001 0.00002 0.00002 2.65019

R62 2.63060 0.00000 0.00003 -0.00001 0.00002 2.63062

R63 2.04854 0.00000 0.00000 -0.00001 -0.00001 2.04853

R64 2.05016 0.00000 0.00000 -0.00000 -0.00000 2.05015

R65 2.65003 -0.00001 0.00000 0.00001 0.00001 2.65005

R66 2.65134 0.00001 0.00002 0.00002 0.00004 2.65138

R67 2.63064 0.00000 0.00004 -0.00001 0.00003 2.63066

R68 2.04856 0.00000 0.00001 -0.00001 -0.00000 2.04856

R69 2.63425 -0.00001 -0.00002 -0.00001 -0.00003 2.63422

R70 2.05016 0.00000 0.00000 -0.00000 -0.00000 2.05015

R71 2.63627 0.00002 0.00003 0.00001 0.00004 2.63631

R72 2.05007 -0.00000 0.00000 -0.00000 -0.00000 2.05007

R73 2.62893 0.00001 -0.00003 -0.00001 -0.00004 2.62889

R74 2.05019 -0.00000 -0.00000 0.00000 0.00000 2.05019

R75 2.04849 -0.00000 -0.00002 -0.00000 -0.00002 2.04847

R76 2.64981 0.00001 -0.00000 0.00003 0.00003 2.64984

R77 2.65117 -0.00001 0.00003 0.00000 0.00004 2.65120

R78 2.63096 0.00002 0.00003 -0.00001 0.00003 2.63098

R79 2.04861 0.00001 -0.00001 0.00001 0.00000 2.04862

R80 2.63413 -0.00001 -0.00002 0.00000 -0.00002 2.63411

R81 2.05014 0.00000 -0.00000 0.00000 -0.00000 2.05014

R82 2.63625 0.00000 0.00002 0.00001 0.00003 2.63628

R83 2.05006 -0.00000 0.00000 -0.00000 -0.00000 2.05006

R84 2.62871 -0.00002 -0.00004 0.00000 -0.00004 2.62867

R85 2.05017 0.00000 0.00000 -0.00000 -0.00000 2.05017

R86 2.04849 0.00000 -0.00000 -0.00001 -0.00001 2.04848

A1 1.88164 -0.00001 -0.00010 -0.00001 -0.00011 1.88153

A2 2.18756 0.00001 0.00011 0.00002 0.00012 2.18769

A3 2.21397 -0.00000 -0.00000 -0.00001 -0.00001 2.21395

A4 1.86782 -0.00000 0.00009 0.00003 0.00012 1.86794

A5 2.22213 0.00005 0.00008 0.00016 0.00024 2.22237

A6 2.19282 -0.00005 -0.00019 -0.00018 -0.00037 2.19245

A7 1.92527 0.00004 -0.00003 0.00004 0.00001 1.92528

A8 2.17760 -0.00004 0.00002 -0.00026 -0.00024 2.17736

A9 2.17959 -0.00000 0.00003 0.00021 0.00024 2.17984

A10 1.86796 -0.00000 0.00011 -0.00006 0.00005 1.86802

A11 2.19430 -0.00001 -0.00010 -0.00005 -0.00014 2.19416

A12 2.22054 0.00002 -0.00001 0.00009 0.00008 2.22062

A13 1.88173 -0.00002 -0.00007 -0.00001 -0.00008 1.88165

A14 2.21417 0.00001 -0.00001 -0.00001 -0.00002 2.21416

A15 2.18725 0.00001 0.00008 0.00002 0.00010 2.18735

A16 2.18650 0.00000 -0.00011 0.00006 -0.00005 2.18645

A17 2.02309 -0.00000 -0.00020 -0.00003 -0.00023 2.02286

A18 2.07354 -0.00000 0.00031 -0.00003 0.00028 2.07382

A19 2.19174 0.00001 -0.00001 0.00018 0.00017 2.19191

A20 2.16528 -0.00002 0.00012 -0.00020 -0.00009 2.16519

A21 1.92614 0.00001 -0.00011 0.00002 -0.00009 1.92605

A22 1.84703 -0.00004 0.00009 0.00001 0.00009 1.84712

A23 1.92658 0.00001 -0.00007 -0.00007 -0.00014 1.92644

A24 2.19197 0.00004 0.00018 -0.00013 0.00005 2.19203

A25 2.16462 -0.00005 -0.00011 0.00020 0.00009 2.16471

A26 1.86198 0.00001 0.00006 -0.00000 0.00006 1.86204

A27 2.19700 -0.00001 -0.00007 0.00000 -0.00007 2.19693

A28 2.22381 -0.00000 0.00001 0.00000 0.00001 2.22382

A29 1.86204 0.00002 0.00003 0.00004 0.00007 1.86211

A30 2.19691 0.00000 -0.00004 -0.00001 -0.00004 2.19687

A31 2.22389 -0.00002 0.00001 -0.00004 -0.00003 2.22386

A32 2.18511 0.00001 -0.00000 -0.00022 -0.00021 2.18489

A33 2.02536 0.00003 -0.00020 -0.00000 -0.00020 2.02516

A34 2.07267 -0.00004 0.00020 0.00022 0.00041 2.07308

A35 2.16479 -0.00005 -0.00014 0.00023 0.00009 2.16487

A36 2.19181 0.00004 0.00021 -0.00015 0.00006 2.19187

A37 1.92657 0.00001 -0.00006 -0.00008 -0.00014 1.92643

A38 1.86199 0.00001 0.00006 0.00000 0.00006 1.86205

A39 2.19698 -0.00001 -0.00009 0.00001 -0.00008 2.19691

A40 2.22381 -0.00000 0.00002 -0.00001 0.00001 2.22383

A41 1.86202 0.00001 0.00003 0.00004 0.00007 1.86209

A42 2.22390 -0.00002 -0.00001 -0.00002 -0.00004 2.22386

A43 2.19692 0.00000 -0.00002 -0.00002 -0.00003 2.19689

A44 1.92613 0.00001 -0.00011 0.00002 -0.00009 1.92604

A45 2.16518 -0.00001 0.00014 -0.00021 -0.00008 2.16511

A46 2.19185 0.00000 -0.00003 0.00019 0.00016 2.19201

A47 1.84704 -0.00004 0.00008 0.00001 0.00009 1.84714

A48 2.18703 0.00000 -0.00010 0.00006 -0.00003 2.18700

A49 2.07290 0.00001 0.00025 -0.00002 0.00023 2.07313

A50 2.02322 -0.00001 -0.00016 -0.00005 -0.00021 2.02301

A51 2.22049 0.00001 -0.00002 0.00008 0.00006 2.22056

A52 2.19430 -0.00001 -0.00010 -0.00004 -0.00014 2.19416

A53 1.86795 -0.00000 0.00011 -0.00006 0.00006 1.86800

A54 1.88176 -0.00002 -0.00007 -0.00001 -0.00007 1.88169

A55 2.18742 0.00001 0.00009 0.00002 0.00011 2.18753

A56 2.21398 0.00001 -0.00002 -0.00001 -0.00003 2.21395

A57 1.88165 -0.00001 -0.00009 -0.00001 -0.00011 1.88154

A58 2.21385 -0.00000 -0.00003 0.00000 -0.00003 2.21382

A59 2.18768 0.00001 0.00012 0.00001 0.00014 2.18781

A60 1.86784 0.00000 0.00009 0.00004 0.00012 1.86797

A61 2.22212 0.00005 0.00006 0.00017 0.00023 2.22235

A62 2.19272 -0.00005 -0.00018 -0.00019 -0.00037 2.19235

A63 1.92520 0.00003 -0.00004 0.00004 0.00000 1.92521

A64 2.17956 0.00001 0.00002 0.00023 0.00025 2.17981

A65 2.17742 -0.00004 -0.00000 -0.00026 -0.00026 2.17715

A66 2.18557 -0.00000 0.00003 -0.00023 -0.00019 2.18538

A67 2.07203 -0.00004 0.00015 0.00024 0.00039 2.07242

A68 2.02555 0.00004 -0.00018 -0.00002 -0.00019 2.02536

A69 2.10460 -0.00002 -0.00025 0.00017 -0.00007 2.10453

A70 2.10694 0.00003 0.00028 -0.00014 0.00014 2.10707

A71 2.07164 -0.00001 -0.00003 -0.00003 -0.00006 2.07158

A72 2.10511 0.00001 0.00003 0.00001 0.00004 2.10515

A73 2.08505 0.00000 -0.00000 -0.00001 -0.00001 2.08504

A74 2.09285 -0.00001 -0.00004 0.00000 -0.00003 2.09282

A75 2.09776 -0.00000 -0.00001 0.00001 0.00000 2.09776

A76 2.08896 0.00000 -0.00000 0.00001 0.00000 2.08896

A77 2.09647 -0.00000 0.00002 -0.00002 -0.00000 2.09646

A78 2.08903 0.00000 -0.00001 -0.00000 -0.00001 2.08902

A79 2.09692 -0.00001 0.00000 -0.00001 -0.00000 2.09691

A80 2.09724 0.00000 0.00000 0.00001 0.00001 2.09725

A81 2.09761 -0.00000 0.00002 -0.00001 0.00001 2.09762

A82 2.09704 0.00000 -0.00000 0.00001 0.00001 2.09705

A83 2.08852 -0.00000 -0.00002 -0.00000 -0.00002 2.08851

A84 2.10508 -0.00001 -0.00001 0.00003 0.00002 2.10511

A85 2.08423 0.00000 -0.00000 -0.00002 -0.00002 2.08421

A86 2.09372 0.00000 0.00001 -0.00001 0.00000 2.09372

A87 2.08897 -0.00000 -0.00000 -0.00001 -0.00001 2.08896

A88 2.09698 0.00000 0.00000 -0.00000 0.00000 2.09698

A89 2.09724 -0.00000 0.00000 0.00001 0.00001 2.09725

A90 2.09798 0.00000 -0.00001 0.00001 0.00001 2.09798

A91 2.09646 0.00000 0.00000 -0.00001 -0.00000 2.09646

A92 2.08874 -0.00000 0.00000 -0.00001 -0.00000 2.08874

A93 2.10491 -0.00001 0.00002 0.00000 0.00002 2.10493

A94 2.09322 0.00002 0.00002 -0.00000 0.00002 2.09324

A95 2.08486 -0.00001 -0.00005 -0.00000 -0.00005 2.08481

A96 2.10682 0.00005 0.00003 -0.00012 -0.00010 2.10672

A97 2.10490 -0.00005 -0.00001 0.00015 0.00014 2.10504

A98 2.07147 -0.00000 -0.00002 -0.00002 -0.00004 2.07142

A99 2.10544 0.00001 0.00000 0.00001 0.00002 2.10545

A100 2.08381 -0.00001 -0.00002 0.00002 0.00000 2.08382

A101 2.09380 -0.00000 0.00001 -0.00003 -0.00002 2.09378

A102 2.09748 -0.00000 0.00000 0.00000 0.00001 2.09748

A103 2.09704 0.00000 0.00000 -0.00000 0.00000 2.09705

A104 2.08866 0.00000 -0.00001 -0.00000 -0.00001 2.08865

A105 2.10469 -0.00005 0.00006 0.00009 0.00015 2.10484

A106 2.10691 0.00005 -0.00004 -0.00007 -0.00011 2.10680

A107 2.07158 0.00000 -0.00002 -0.00002 -0.00004 2.07154

A108 2.10539 0.00001 -0.00000 0.00002 0.00001 2.10541

A109 2.08378 -0.00001 -0.00002 0.00002 -0.00000 2.08377

A110 2.09389 -0.00000 0.00003 -0.00004 -0.00001 2.09388

A111 2.09746 -0.00000 0.00001 -0.00000 0.00001 2.09747

A112 2.08867 0.00000 -0.00001 0.00000 -0.00001 2.08867

A113 2.09704 0.00000 0.00000 0.00000 0.00000 2.09704

A114 2.08898 -0.00000 -0.00000 -0.00001 -0.00001 2.08896

A115 2.09724 -0.00000 0.00000 0.00001 0.00001 2.09725

A116 2.09697 0.00000 0.00000 -0.00000 -0.00000 2.09697

A117 2.09797 0.00000 -0.00001 0.00001 0.00000 2.09797

A118 2.09648 0.00000 0.00001 -0.00001 0.00000 2.09648

A119 2.08873 -0.00000 -0.00000 -0.00000 -0.00000 2.08873

A120 2.10486 -0.00001 0.00003 -0.00001 0.00002 2.10488

A121 2.08489 -0.00001 -0.00005 -0.00000 -0.00005 2.08484

A122 2.09324 0.00002 0.00002 0.00000 0.00002 2.09327

A123 2.10674 0.00002 0.00030 -0.00018 0.00012 2.10686

A124 2.10468 -0.00002 -0.00027 0.00021 -0.00006 2.10462

A125 2.07176 -0.00000 -0.00003 -0.00002 -0.00006 2.07170

A126 2.10504 -0.00001 -0.00001 0.00003 0.00002 2.10506

A127 2.08419 0.00000 -0.00000 -0.00003 -0.00003 2.08417

A128 2.09381 0.00000 0.00001 -0.00000 0.00001 2.09382

A129 2.09759 -0.00000 0.00002 -0.00001 0.00001 2.09760

A130 2.08854 -0.00000 -0.00002 0.00000 -0.00002 2.08853

A131 2.09705 0.00000 -0.00000 0.00001 0.00001 2.09706

A132 2.08904 0.00000 -0.00001 -0.00000 -0.00001 2.08903

A133 2.09724 0.00000 0.00000 0.00001 0.00001 2.09725

A134 2.09691 -0.00000 0.00000 -0.00001 -0.00001 2.09690

A135 2.09776 -0.00000 -0.00001 0.00001 -0.00000 2.09776

A136 2.09649 -0.00000 0.00002 -0.00002 -0.00000 2.09648

A137 2.08894 0.00000 -0.00001 0.00001 0.00000 2.08895

A138 2.10505 0.00001 0.00004 0.00000 0.00004 2.10509

A139 2.08509 0.00000 0.00000 -0.00001 -0.00001 2.08508

A140 2.09287 -0.00001 -0.00005 0.00002 -0.00003 2.09284

D1 0.01552 -0.00000 0.00006 -0.00010 -0.00005 0.01547

D2 -3.09619 0.00000 0.00044 -0.00022 0.00022 -3.09597

D3 -3.12014 -0.00000 -0.00012 -0.00009 -0.00021 -3.12035

D4 0.05133 0.00000 0.00026 -0.00021 0.00006 0.05139

D5 -0.00060 -0.00000 -0.00016 0.00021 0.00005 -0.00056

D6 -3.13415 0.00000 -0.00022 0.00006 -0.00016 -3.13431

D7 3.13494 0.00000 0.00001 0.00020 0.00021 3.13516

D8 0.00139 0.00000 -0.00004 0.00005 0.00001 0.00140

D9 -0.02524 0.00000 0.00008 -0.00005 0.00003 -0.02521

D10 3.07691 0.00001 0.00067 -0.00015 0.00053 3.07743

D11 3.08711 -0.00000 -0.00029 0.00007 -0.00022 3.08689

D12 -0.09393 0.00001 0.00031 -0.00003 0.00028 -0.09365

D13 -2.94908 0.00001 0.00085 0.00132 0.00217 -2.94691

D14 0.18204 0.00000 0.00078 0.00115 0.00193 0.18397

D15 0.22767 0.00002 0.00129 0.00118 0.00248 0.23015

D16 -2.92439 0.00001 0.00123 0.00101 0.00223 -2.92216

D17 0.02487 -0.00000 -0.00018 0.00018 -0.00000 0.02487

D18 -3.08888 -0.00000 -0.00036 0.00084 0.00048 -3.08840

D19 -3.07722 -0.00001 -0.00077 0.00029 -0.00049 -3.07771

D20 0.09221 -0.00001 -0.00096 0.00096 -0.00001 0.09221

D21 -0.01455 0.00000 0.00021 -0.00024 -0.00003 -0.01458

D22 3.11916 0.00000 0.00026 -0.00009 0.00017 3.11933

D23 3.09865 -0.00000 0.00040 -0.00092 -0.00052 3.09813

D24 -0.05082 -0.00000 0.00045 -0.00077 -0.00032 -0.05114

D25 -0.23774 -0.00003 -0.00226 -0.00004 -0.00230 -0.24004

D26 2.91491 -0.00002 -0.00209 -0.00001 -0.00210 2.91281

D27 2.93729 -0.00002 -0.00249 0.00077 -0.00172 2.93557

D28 -0.19324 -0.00002 -0.00232 0.00079 -0.00152 -0.19477

D29 -0.12631 0.00001 0.00119 -0.00096 0.00023 -0.12608

D30 3.02445 0.00001 0.00102 -0.00082 0.00019 3.02464

D31 3.00393 0.00001 0.00101 -0.00098 0.00002 3.00396

D32 -0.12850 0.00001 0.00084 -0.00085 -0.00001 -0.12851

D33 -0.99603 -0.00000 0.00060 0.00055 0.00115 -0.99488

D34 2.14185 0.00000 0.00082 0.00028 0.00109 2.14295

D35 2.15586 0.00000 0.00076 0.00058 0.00134 2.15720

D36 -0.98943 0.00001 0.00098 0.00030 0.00128 -0.98815

D37 -3.09171 0.00001 -0.00010 0.00034 0.00024 -3.09147

D38 0.04178 0.00000 0.00005 0.00022 0.00027 0.04205

D39 3.10657 -0.00001 -0.00004 -0.00014 -0.00019 3.10639

D40 -0.06166 -0.00001 -0.00005 -0.00028 -0.00033 -0.06199

D41 -0.02707 -0.00001 -0.00019 -0.00003 -0.00022 -0.02729

D42 3.08788 -0.00000 -0.00019 -0.00017 -0.00036 3.08752

D43 -0.04105 0.00000 0.00010 -0.00033 -0.00023 -0.04128

D44 3.09581 -0.00000 0.00073 -0.00075 -0.00003 3.09578

D45 0.02507 -0.00000 -0.00022 0.00031 0.00009 0.02516

D46 -3.08820 -0.00000 0.00002 0.00030 0.00032 -3.08788

D47 -3.11188 -0.00000 -0.00084 0.00073 -0.00010 -3.11198

D48 0.05804 0.00000 -0.00060 0.00072 0.00012 0.05816

D49 0.13514 -0.00000 -0.00034 -0.00050 -0.00084 0.13430

D50 -2.99819 0.00001 -0.00071 -0.00007 -0.00078 -2.99897

D51 -3.01181 -0.00001 0.00037 -0.00098 -0.00061 -3.01242

D52 0.13805 0.00000 -0.00000 -0.00055 -0.00055 0.13750

D53 0.00117 0.00001 0.00024 -0.00017 0.00007 0.00124

D54 -3.11324 0.00000 0.00024 -0.00003 0.00022 -3.11302

D55 3.11386 0.00000 -0.00001 -0.00015 -0.00016 3.11370

D56 -0.00055 -0.00000 -0.00000 -0.00001 -0.00001 -0.00056

D57 -3.01277 -0.00001 0.00051 -0.00112 -0.00061 -3.01338

D58 0.13500 -0.00001 -0.00013 -0.00062 -0.00074 0.13425

D59 0.13956 -0.00000 0.00058 -0.00094 -0.00036 0.13920

D60 -2.99586 0.00000 -0.00006 -0.00044 -0.00049 -2.99635

D61 0.99106 -0.00000 -0.00052 -0.00072 -0.00124 0.98982

D62 -2.14698 -0.00000 -0.00036 -0.00073 -0.00109 -2.14807

D63 -2.16029 -0.00001 -0.00059 -0.00089 -0.00147 -2.16176

D64 0.98485 -0.00001 -0.00042 -0.00090 -0.00132 0.98353

D65 -3.11093 -0.00000 -0.00081 0.00080 -0.00001 -3.11094

D66 0.05901 0.00000 -0.00053 0.00074 0.00021 0.05922

D67 0.02531 -0.00000 -0.00026 0.00036 0.00011 0.02542

D68 -3.08794 -0.00000 0.00002 0.00031 0.00033 -3.08761

D69 3.09495 -0.00000 0.00066 -0.00079 -0.00013 3.09482

D70 -0.04119 -0.00000 0.00010 -0.00035 -0.00025 -0.04143

D71 0.00093 0.00001 0.00029 -0.00022 0.00007 0.00100

D72 -3.11364 0.00000 0.00029 -0.00008 0.00020 -3.11343

D73 3.11361 0.00000 0.00001 -0.00016 -0.00016 3.11345

D74 -0.00096 -0.00000 -0.00000 -0.00002 -0.00002 -0.00098

D75 -0.02690 -0.00001 -0.00025 0.00002 -0.00023 -0.02713

D76 3.10720 -0.00001 -0.00007 -0.00011 -0.00018 3.10702

D77 3.08820 -0.00000 -0.00024 -0.00012 -0.00036 3.08784

D78 -0.06088 -0.00001 -0.00006 -0.00025 -0.00031 -0.06119

D79 0.04177 0.00001 0.00009 0.00021 0.00029 0.04206

D80 -3.09219 0.00001 -0.00010 0.00034 0.00024 -3.09195

D81 3.02396 0.00001 0.00112 -0.00089 0.00023 3.02419

D82 -0.12677 0.00001 0.00133 -0.00116 0.00016 -0.12660

D83 -0.12626 0.00001 0.00133 -0.00104 0.00029 -0.12598

D84 3.00619 0.00000 0.00154 -0.00131 0.00023 3.00642

D85 2.94721 -0.00003 -0.00136 0.00031 -0.00105 2.94616

D86 -0.23074 -0.00003 -0.00167 -0.00022 -0.00189 -0.23263

D87 -0.18547 -0.00002 -0.00157 0.00057 -0.00100 -0.18647

D88 2.91976 -0.00002 -0.00187 0.00004 -0.00183 2.91793

D89 -0.99449 0.00001 0.00084 0.00024 0.00108 -0.99341

D90 2.15013 0.00001 0.00042 0.00061 0.00103 2.15116

D91 2.13881 0.00000 0.00103 -0.00001 0.00102 2.13983

D92 -0.99976 0.00000 0.00061 0.00037 0.00098 -0.99878

D93 3.09599 0.00000 -0.00015 -0.00062 -0.00077 3.09522

D94 -0.05229 -0.00000 0.00009 -0.00056 -0.00047 -0.05276

D95 -0.01473 0.00001 0.00011 -0.00017 -0.00006 -0.01479

D96 3.12017 0.00000 0.00036 -0.00011 0.00025 3.12042

D97 -3.08611 -0.00000 0.00023 0.00051 0.00074 -3.08537

D98 0.10185 -0.00001 0.00060 0.00029 0.00089 0.10273

D99 0.02520 -0.00001 -0.00003 0.00008 0.00005 0.02525

D100 -3.07002 -0.00002 0.00034 -0.00015 0.00019 -3.06983

D101 -0.00063 -0.00000 -0.00015 0.00020 0.00005 -0.00058

D102 3.13614 -0.00000 0.00017 0.00013 0.00031 3.13645

D103 -3.13540 0.00000 -0.00040 0.00014 -0.00026 -3.13566

D104 0.00137 0.00000 -0.00008 0.00007 -0.00000 0.00137

D105 0.01575 -0.00000 0.00013 -0.00015 -0.00002 0.01573

D106 -3.09332 0.00000 0.00096 -0.00048 0.00048 -3.09283

D107 -3.12111 -0.00000 -0.00018 -0.00009 -0.00027 -3.12139

D108 0.05301 0.00000 0.00064 -0.00041 0.00023 0.05324

D109 -0.02559 0.00001 -0.00007 0.00005 -0.00002 -0.02561

D110 3.06971 0.00002 -0.00043 0.00029 -0.00015 3.06956

D111 3.08417 0.00000 -0.00086 0.00037 -0.00049 3.08368

D112 -0.10372 0.00001 -0.00123 0.00061 -0.00062 -0.10434

D113 -2.95886 0.00002 -0.00021 0.00179 0.00157 -2.95729

D114 0.17466 0.00001 0.00015 0.00137 0.00152 0.17618

D115 0.22101 0.00002 0.00075 0.00140 0.00215 0.22316

D116 -2.92866 0.00001 0.00111 0.00099 0.00210 -2.92656

D117 0.98945 -0.00002 -0.00018 -0.00091 -0.00108 0.98837

D118 -2.15463 -0.00002 -0.00016 -0.00103 -0.00119 -2.15582

D119 -2.14463 -0.00001 -0.00051 -0.00052 -0.00103 -2.14566

D120 0.99448 -0.00001 -0.00050 -0.00064 -0.00114 0.99334

D121 -3.13050 -0.00000 0.00063 -0.00066 -0.00002 -3.13052

D122 -0.00867 0.00000 0.00039 -0.00037 0.00002 -0.00865

D123 0.01472 -0.00001 0.00042 -0.00039 0.00003 0.01476

D124 3.13655 -0.00000 0.00017 -0.00010 0.00008 3.13663

D125 -3.14015 -0.00000 -0.00066 0.00064 -0.00002 -3.14017

D126 -0.01700 -0.00000 -0.00053 0.00044 -0.00009 -0.01709

D127 -0.00219 0.00000 -0.00045 0.00037 -0.00007 -0.00227

D128 3.12096 0.00000 -0.00032 0.00017 -0.00015 3.12081

D129 -0.01633 0.00000 -0.00017 0.00020 0.00003 -0.01630

D130 3.12471 0.00000 -0.00013 0.00014 0.00001 3.12472

D131 -3.13808 -0.00000 0.00008 -0.00009 -0.00001 -3.13809

D132 0.00297 -0.00000 0.00012 -0.00015 -0.00004 0.00293

D133 0.00518 -0.00000 -0.00007 0.00001 -0.00006 0.00513

D134 -3.13368 0.00000 -0.00007 0.00009 0.00002 -3.13367

D135 -3.13586 0.00000 -0.00010 0.00007 -0.00003 -3.13589

D136 0.00846 0.00000 -0.00010 0.00014 0.00004 0.00850

D137 0.00730 0.00000 0.00004 -0.00002 0.00001 0.00732

D138 -3.13184 -0.00000 0.00009 -0.00008 0.00001 -3.13184

D139 -3.13701 -0.00000 0.00004 -0.00010 -0.00006 -3.13707

D140 0.00702 -0.00000 0.00009 -0.00016 -0.00007 0.00696

D141 -0.00877 -0.00000 0.00022 -0.00017 0.00005 -0.00872

D142 -3.13183 -0.00000 0.00009 0.00003 0.00013 -3.13170

D143 3.13039 0.00000 0.00017 -0.00011 0.00006 3.13045

D144 0.00733 0.00000 0.00004 0.00009 0.00014 0.00747

D145 -0.00542 0.00000 0.00004 0.00002 0.00006 -0.00536

D146 3.13567 0.00000 0.00005 0.00007 0.00012 3.13578

D147 3.13463 0.00000 -0.00005 0.00003 -0.00002 3.13461

D148 -0.00747 0.00000 -0.00004 0.00008 0.00004 -0.00742

D149 -0.00651 0.00000 -0.00005 0.00002 -0.00003 -0.00655

D150 3.13187 -0.00000 0.00001 -0.00015 -0.00014 3.13173

D151 3.13662 0.00000 0.00003 0.00001 0.00004 3.13666

D152 -0.00818 -0.00000 0.00009 -0.00016 -0.00007 -0.00825

D153 0.01653 0.00000 -0.00000 0.00015 0.00015 0.01668

D154 3.13674 -0.00000 0.00009 -0.00007 0.00002 3.13676

D155 -3.12456 0.00000 -0.00001 0.00010 0.00009 -3.12447

D156 -0.00435 -0.00000 0.00008 -0.00012 -0.00004 -0.00440

D157 3.12965 -0.00001 0.00014 -0.00036 -0.00022 3.12943

D158 -0.01542 -0.00001 -0.00002 -0.00035 -0.00037 -0.01579

D159 0.00935 -0.00000 0.00005 -0.00014 -0.00009 0.00926

D160 -3.13573 -0.00001 -0.00011 -0.00013 -0.00024 -3.13597

D161 3.14156 0.00001 -0.00015 0.00040 0.00025 -3.14138

D162 0.01757 0.00000 -0.00008 0.00029 0.00021 0.01778

D163 0.00344 0.00001 0.00001 0.00038 0.00039 0.00384

D164 -3.12055 0.00000 0.00008 0.00028 0.00036 -3.12018

D165 0.00746 -0.00001 0.00003 -0.00022 -0.00020 0.00727

D166 -3.13094 -0.00001 -0.00003 -0.00006 -0.00009 -3.13102

D167 3.13135 -0.00000 -0.00005 -0.00012 -0.00016 3.13119

D168 -0.00705 0.00000 -0.00010 0.00005 -0.00005 -0.00710

D169 -3.14081 0.00001 0.00007 0.00020 0.00028 -3.14054

D170 0.01791 0.00000 0.00006 0.00016 0.00022 0.01813

D171 0.00321 0.00001 0.00006 0.00033 0.00038 0.00360

D172 -3.12125 0.00000 0.00004 0.00028 0.00033 -3.12092

D173 3.12891 -0.00001 -0.00006 -0.00018 -0.00024 3.12867

D174 0.00862 -0.00000 -0.00012 -0.00000 -0.00012 0.00850

D175 -0.01512 -0.00001 -0.00004 -0.00030 -0.00034 -0.01547

D176 -3.13541 -0.00001 -0.00010 -0.00013 -0.00023 -3.13564

D177 0.00751 -0.00001 -0.00002 -0.00019 -0.00021 0.00730

D178 -3.13110 -0.00001 -0.00007 -0.00003 -0.00010 -3.13119

D179 3.13187 -0.00000 -0.00001 -0.00015 -0.00015 3.13171

D180 -0.00674 0.00000 -0.00005 0.00001 -0.00004 -0.00678

D181 -0.00643 0.00000 -0.00003 0.00002 -0.00001 -0.00644

D182 3.13654 0.00000 0.00003 0.00002 0.00005 3.13659

D183 3.13216 -0.00000 0.00001 -0.00014 -0.00013 3.13204

D184 -0.00805 -0.00000 0.00008 -0.00014 -0.00006 -0.00812

D185 -0.00544 0.00000 0.00005 -0.00000 0.00005 -0.00539

D186 3.13549 0.00000 0.00004 0.00006 0.00011 3.13560

D187 3.13477 0.00000 -0.00001 0.00000 -0.00001 3.13476

D188 -0.00748 0.00000 -0.00002 0.00007 0.00005 -0.00744

D189 0.01636 0.00000 -0.00002 0.00015 0.00013 0.01649

D190 3.13654 -0.00000 0.00005 -0.00003 0.00001 3.13656

D191 -3.12458 0.00000 -0.00000 0.00008 0.00008 -3.12450

D192 -0.00439 -0.00000 0.00006 -0.00010 -0.00004 -0.00443

D193 -3.14060 0.00000 -0.00089 0.00078 -0.00011 -3.14071

D194 -0.01707 0.00000 -0.00066 0.00052 -0.00014 -0.01721

D195 -0.00197 0.00000 -0.00048 0.00041 -0.00007 -0.00205

D196 3.12156 0.00000 -0.00025 0.00015 -0.00010 3.12146

D197 -3.13011 -0.00000 0.00083 -0.00077 0.00007 -3.13004

D198 -0.00825 0.00000 0.00057 -0.00046 0.00011 -0.00814

D199 0.01444 -0.00001 0.00042 -0.00040 0.00003 0.01447

D200 3.13631 -0.00000 0.00016 -0.00009 0.00007 3.13638

D201 -0.00878 -0.00000 0.00027 -0.00022 0.00005 -0.00873

D202 3.13049 0.00000 0.00023 -0.00015 0.00008 3.13057

D203 -3.13221 -0.00000 0.00004 0.00004 0.00008 -3.13213

D204 0.00705 0.00000 -0.00000 0.00011 0.00011 0.00717

D205 0.00716 0.00000 0.00001 0.00000 0.00002 0.00718

D206 -3.13698 -0.00000 0.00005 -0.00010 -0.00005 -3.13703

D207 -3.13210 -0.00000 0.00005 -0.00006 -0.00001 -3.13211

D208 0.00695 -0.00000 0.00008 -0.00017 -0.00008 0.00687

D209 0.00527 -0.00000 -0.00007 0.00001 -0.00006 0.00520

D210 -3.13570 -0.00000 -0.00009 0.00006 -0.00004 -3.13574

D211 -3.13378 0.00000 -0.00010 0.00011 0.00000 -3.13378

D212 0.00844 0.00000 -0.00013 0.00016 0.00003 0.00847

D213 -0.01620 0.00000 -0.00015 0.00019 0.00004 -0.01616

D214 -3.13798 -0.00000 0.00011 -0.00011 -0.00000 -3.13798

D215 3.12477 0.00000 -0.00013 0.00014 0.00002 3.12479

D216 0.00300 -0.00000 0.00013 -0.00016 -0.00003 0.00297

Item Value Threshold Converged?

Maximum Force 0.000275 0.000450 YES

RMS Force 0.000045 0.000300 YES

Maximum Displacement 0.011606 0.001800 NO

RMS Displacement 0.002642 0.001200 NO

Predicted change in Energy=-1.785824D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

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Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=1 Diff= 1.83D-02

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 1.006933 -4.104298 0.556757

2 6 0 1.342027 -2.786215 0.200464

3 7 0 0.160875 -2.109431 0.004317

4 6 0 -0.909235 -2.953024 0.190302

5 6 0 -0.386826 -4.207589 0.549993

6 6 0 -2.292710 -2.606596 0.007991

7 6 0 -2.789049 -1.306382 -0.120156

8 7 0 -2.061569 -0.152923 0.046111

9 6 0 -2.954637 0.878549 -0.107198

10 6 0 -4.280980 0.358918 -0.435099

11 6 0 -4.178479 -0.988879 -0.444108

12 6 0 2.659480 -2.238019 0.028061

13 6 0 2.954718 -0.877972 -0.109734

14 6 0 4.280993 -0.357662 -0.436877

15 6 0 4.178450 0.990151 -0.443325

16 6 0 2.788986 1.306966 -0.118862

17 7 0 2.061595 0.153136 0.045346

18 6 0 2.292549 2.606895 0.010985

19 6 0 0.909263 2.953725 0.193322

20 6 0 0.386621 4.211077 0.543142

21 6 0 -1.007073 4.107806 0.550221

22 6 0 -1.342040 2.786955 0.203964

23 7 0 -0.160784 2.108556 0.013750

24 6 0 -2.659284 2.238367 0.031884

25 6 0 -3.246014 -3.743064 -0.029107

26 6 0 -3.090028 -4.775271 -0.966505

27 6 0 -3.990791 -5.834313 -1.010556

28 6 0 -5.051821 -5.890979 -0.106546

29 6 0 -5.209159 -4.877855 0.837812

30 6 0 -4.317073 -3.809586 0.873609

31 6 0 5.891129 -5.060474 -0.021935

32 6 0 4.841777 -5.180620 -0.933361

33 6 0 3.787765 -4.273012 -0.910766

34 6 0 3.774789 -3.216193 0.012104

35 6 0 4.835330 -3.104879 0.922953

36 6 0 5.882220 -4.022289 0.908258

37 6 0 -3.775070 3.216257 0.014254

38 6 0 -4.834250 3.107257 0.926850

39 6 0 -5.882065 4.023615 0.910097

40 6 0 -5.893173 5.058299 -0.023959

41 6 0 -4.845196 5.175966 -0.937266

42 6 0 -3.790311 4.269377 -0.912703

43 6 0 3.246373 3.743155 -0.027306

44 6 0 4.315363 3.811694 0.877584

45 6 0 5.208330 4.879217 0.840420

46 6 0 5.053847 5.889440 -0.107507

47 6 0 3.994926 5.830575 -1.013821

48 6 0 3.093328 4.772258 -0.968481

49 1 0 1.711840 -4.884085 0.795712

50 1 0 -0.971587 -5.082514 0.783821

51 1 0 -5.155917 0.951388 -0.653919

52 1 0 -4.954035 -1.703890 -0.671186

53 1 0 5.155903 -0.949700 -0.656974

54 1 0 4.954038 1.705625 -0.668845

55 1 0 0.971057 5.088204 0.769335

56 1 0 -1.711992 4.889767 0.781842

57 1 0 -2.269124 -4.734140 -1.673250

58 1 0 -3.864850 -6.616360 -1.751874

59 1 0 -5.749600 -6.721084 -0.136842

60 1 0 -6.026315 -4.919063 1.550231

61 1 0 -4.437433 -3.028350 1.615485

62 1 0 6.709392 -5.772609 -0.036169

63 1 0 4.844317 -5.982762 -1.663834

64 1 0 2.976911 -4.367830 -1.623911

65 1 0 4.826975 -2.304548 1.654073

66 1 0 6.689786 -3.927144 1.626437

67 1 0 -4.824328 2.309335 1.660601

68 1 0 -6.688706 3.930279 1.629552

69 1 0 -6.712169 5.769557 -0.039840

70 1 0 -4.849525 5.975259 -1.670851

71 1 0 -2.980598 4.362110 -1.627424

72 1 0 4.433632 3.032460 1.621921

73 1 0 6.023983 4.922046 1.554466

74 1 0 5.752313 6.718927 -0.138899

75 1 0 3.871288 6.610271 -1.758003

76 1 0 2.274111 4.729320 -1.677081

77 1 0 0.090076 -1.124258 -0.209934

78 1 0 -0.089851 1.120320 -0.186417

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0587911 0.0582605 0.0300936

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(Enter /home/kira/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5356.9364728017 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122095537 Hartrees.

Nuclear repulsion after empirical dispersion term = 5356.7242632480 Hartrees.

Force inversion solution in PCM.

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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 : Matrix inversion.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5796

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.34D-11

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 322

GePol: Fraction of low-weight points (<1% of avg) = 5.56%

GePol: Cavity surface area = 610.574 Ang\*\*2

GePol: Cavity volume = 628.046 Ang\*\*3

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Atomic radii for non-electrostatic terms: SMD-CDS.

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PCM non-electrostatic energy = -0.0021018479 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5356.7221614001 Hartrees.

Leave Link 301 at Thu Aug 29 07:08:23 2019, MaxMem= 4294967296 cpu: 2.5

(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.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Thu Aug 29 07:08:25 2019, MaxMem= 4294967296 cpu: 27.0

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Thu Aug 29 07:08:25 2019, MaxMem= 4294967296 cpu: 2.5

(Enter /home/kira/g09/l401.exe)

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= -0.000000 -0.000000 -0.000000

Rot= 0.999979 0.000002 0.000001 -0.006457 Ang= 0.74 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0182

Leave Link 401 at Thu Aug 29 07:08:28 2019, MaxMem= 4294967296 cpu: 44.5

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 590000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 100780848.

Iteration 1 A\*A^-1 deviation from unit magnitude is 4.44D-15 for 5768.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.92D-15 for 3601 329.

Iteration 1 A^-1\*A deviation from unit magnitude is 4.22D-15 for 5763.

Iteration 1 A^-1\*A deviation from orthogonality is 2.64D-06 for 5693 5675.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.44D-15 for 2740.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.89D-15 for 5377 382.

Iteration 2 A^-1\*A deviation from unit magnitude is 8.88D-16 for 432.

Iteration 2 A^-1\*A deviation from orthogonality is 3.76D-16 for 3439 1010.

E= -1914.33327217156

DIIS: error= 1.73D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.33327217156 IErMin= 1 ErrMin= 1.73D-04

ErrMax= 1.73D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.30D-05 BMatP= 8.30D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.73D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.640 Goal= None Shift= 0.000

Gap= 0.706 Goal= None Shift= 0.000

RMSDP=6.63D-06 MaxDP=2.06D-04 OVMax= 9.53D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.63D-06 CP: 1.00D+00

E= -1914.33331242904 Delta-E= -0.000040257477 Rises=F Damp=F

DIIS: error= 2.54D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33331242904 IErMin= 2 ErrMin= 2.54D-05

ErrMax= 2.54D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.28D-06 BMatP= 8.30D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.601D-01 0.106D+01

Coeff: -0.601D-01 0.106D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.37D-06 MaxDP=4.47D-05 DE=-4.03D-05 OVMax= 2.96D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.29D-06 CP: 1.00D+00 1.07D+00

E= -1914.33331291946 Delta-E= -0.000000490422 Rises=F Damp=F

DIIS: error= 2.34D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33331291946 IErMin= 3 ErrMin= 2.34D-05

ErrMax= 2.34D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.57D-07 BMatP= 1.28D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.361D-01 0.507D+00 0.529D+00

Coeff: -0.361D-01 0.507D+00 0.529D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.57D-07 MaxDP=4.47D-05 DE=-4.90D-07 OVMax= 2.01D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.31D-07 CP: 1.00D+00 1.09D+00 5.96D-01

E= -1914.33331308487 Delta-E= -0.000000165414 Rises=F Damp=F

DIIS: error= 1.01D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33331308487 IErMin= 4 ErrMin= 1.01D-05

ErrMax= 1.01D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.16D-07 BMatP= 8.57D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.111D-01 0.122D+00 0.336D+00 0.553D+00

Coeff: -0.111D-01 0.122D+00 0.336D+00 0.553D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.35D-07 MaxDP=2.37D-05 DE=-1.65D-07 OVMax= 1.17D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.90D-07 CP: 1.00D+00 1.09D+00 7.49D-01 6.43D-01

E= -1914.33331313707 Delta-E= -0.000000052198 Rises=F Damp=F

DIIS: error= 2.21D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33331313707 IErMin= 5 ErrMin= 2.21D-06

ErrMax= 2.21D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.56D-08 BMatP= 2.16D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.240D-02 0.142D-01 0.126D+00 0.285D+00 0.578D+00

Coeff: -0.240D-02 0.142D-01 0.126D+00 0.285D+00 0.578D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.01D-07 MaxDP=5.63D-06 DE=-5.22D-08 OVMax= 4.56D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 8.23D-08 CP: 1.00D+00 1.09D+00 7.48D-01 7.39D-01 8.81D-01

E= -1914.33331314151 Delta-E= -0.000000004440 Rises=F Damp=F

DIIS: error= 1.18D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33331314151 IErMin= 6 ErrMin= 1.18D-06

ErrMax= 1.18D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.11D-09 BMatP= 1.56D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.964D-03-0.184D-01 0.160D-03 0.388D-01 0.325D+00 0.654D+00

Coeff: 0.964D-03-0.184D-01 0.160D-03 0.388D-01 0.325D+00 0.654D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=6.91D-08 MaxDP=5.23D-06 DE=-4.44D-09 OVMax= 6.45D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 4.85D-08 CP: 1.00D+00 1.09D+00 7.66D-01 7.60D-01 1.09D+00

CP: 1.18D+00

E= -1914.33331314323 Delta-E= -0.000000001719 Rises=F Damp=F

DIIS: error= 7.87D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33331314323 IErMin= 7 ErrMin= 7.87D-07

ErrMax= 7.87D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.23D-10 BMatP= 3.11D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.633D-03-0.966D-02-0.904D-02-0.489D-02 0.105D+00 0.316D+00

Coeff-Com: 0.602D+00

Coeff: 0.633D-03-0.966D-02-0.904D-02-0.489D-02 0.105D+00 0.316D+00

Coeff: 0.602D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.95D-08 MaxDP=2.93D-06 DE=-1.72D-09 OVMax= 3.78D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.70D-08 CP: 1.00D+00 1.09D+00 7.72D-01 7.73D-01 1.19D+00

CP: 1.47D+00 1.32D+00

E= -1914.33331314382 Delta-E= -0.000000000587 Rises=F Damp=F

DIIS: error= 7.65D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33331314382 IErMin= 8 ErrMin= 7.65D-07

ErrMax= 7.65D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.22D-10 BMatP= 5.23D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.352D-03 0.854D-02-0.511D-02-0.329D-01-0.192D+00-0.297D+00

Coeff-Com: 0.301D+00 0.122D+01

Coeff: -0.352D-03 0.854D-02-0.511D-02-0.329D-01-0.192D+00-0.297D+00

Coeff: 0.301D+00 0.122D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=8.79D-08 MaxDP=6.98D-06 DE=-5.87D-10 OVMax= 9.42D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.50D-08 CP: 1.00D+00 1.09D+00 7.83D-01 8.00D-01 1.41D+00

CP: 2.10D+00 2.34D+00 1.64D+00

E= -1914.33331314469 Delta-E= -0.000000000878 Rises=F Damp=F

DIIS: error= 4.24D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33331314469 IErMin= 9 ErrMin= 4.24D-07

ErrMax= 4.24D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.62D-10 BMatP= 2.22D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.470D-03 0.932D-02-0.451D-03-0.190D-01-0.172D+00-0.314D+00

Coeff-Com: -0.682D-01 0.874D+00 0.691D+00

Coeff: -0.470D-03 0.932D-02-0.451D-03-0.190D-01-0.172D+00-0.314D+00

Coeff: -0.682D-01 0.874D+00 0.691D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.29D-08 MaxDP=3.96D-06 DE=-8.78D-10 OVMax= 5.59D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 9.29D-09 CP: 1.00D+00 1.09D+00 7.89D-01 8.16D-01 1.54D+00

CP: 2.48D+00 2.94D+00 2.37D+00 1.28D+00

E= -1914.33331314500 Delta-E= -0.000000000304 Rises=F Damp=F

DIIS: error= 2.87D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33331314500 IErMin=10 ErrMin= 2.87D-07

ErrMax= 2.87D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.44D-11 BMatP= 1.62D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.701D-04 0.501D-03 0.219D-02 0.950D-02 0.501D-02-0.458D-02

Coeff-Com: -0.224D+00-0.898D-01 0.355D+00 0.947D+00

Coeff: -0.701D-04 0.501D-03 0.219D-02 0.950D-02 0.501D-02-0.458D-02

Coeff: -0.224D+00-0.898D-01 0.355D+00 0.947D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.00D-08 MaxDP=3.28D-06 DE=-3.04D-10 OVMax= 4.44D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.02D-08 CP: 1.00D+00 1.09D+00 7.92D-01 8.29D-01 1.63D+00

CP: 2.76D+00 3.00D+00 2.87D+00 1.99D+00 1.38D+00

E= -1914.33331314525 Delta-E= -0.000000000255 Rises=F Damp=F

DIIS: error= 1.37D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33331314525 IErMin=11 ErrMin= 1.37D-07

ErrMax= 1.37D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.83D-11 BMatP= 4.44D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.127D-03-0.303D-02 0.905D-03 0.124D-01 0.615D-01 0.116D+00

Coeff-Com: -0.109D+00-0.338D+00-0.821D-01 0.487D+00 0.854D+00

Coeff: 0.127D-03-0.303D-02 0.905D-03 0.124D-01 0.615D-01 0.116D+00

Coeff: -0.109D+00-0.338D+00-0.821D-01 0.487D+00 0.854D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.25D-08 MaxDP=1.80D-06 DE=-2.55D-10 OVMax= 2.48D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 5.01D-09 CP: 1.00D+00 1.09D+00 7.94D-01 8.36D-01 1.68D+00

CP: 2.90D+00 3.00D+00 3.00D+00 2.43D+00 1.85D+00

CP: 1.60D+00

E= -1914.33331314520 Delta-E= 0.000000000058 Rises=F Damp=F

DIIS: error= 7.17D-08 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=11 EnMin= -1914.33331314525 IErMin=12 ErrMin= 7.17D-08

ErrMax= 7.17D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.69D-12 BMatP= 1.83D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.936D-04-0.174D-02-0.626D-03 0.286D-02 0.280D-01 0.654D-01

Coeff-Com: 0.235D-01-0.122D+00-0.188D+00-0.115D+00 0.433D+00 0.875D+00

Coeff: 0.936D-04-0.174D-02-0.626D-03 0.286D-02 0.280D-01 0.654D-01

Coeff: 0.235D-01-0.122D+00-0.188D+00-0.115D+00 0.433D+00 0.875D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.20D-08 MaxDP=1.02D-06 DE= 5.82D-11 OVMax= 1.33D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 2.49D-09 CP: 1.00D+00 1.09D+00 7.94D-01 8.40D-01 1.70D+00

CP: 2.98D+00 3.00D+00 3.00D+00 2.71D+00 2.15D+00

CP: 1.92D+00 1.45D+00

E= -1914.33331314523 Delta-E= -0.000000000030 Rises=F Damp=F

DIIS: error= 2.87D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=11 EnMin= -1914.33331314525 IErMin=13 ErrMin= 2.87D-08

ErrMax= 2.87D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.90D-12 BMatP= 5.69D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.134D-04-0.422D-04-0.720D-03-0.214D-02-0.332D-02 0.210D-02

Coeff-Com: 0.436D-01 0.389D-01-0.876D-01-0.208D+00-0.221D-01 0.494D+00

Coeff-Com: 0.746D+00

Coeff: 0.134D-04-0.422D-04-0.720D-03-0.214D-02-0.332D-02 0.210D-02

Coeff: 0.436D-01 0.389D-01-0.876D-01-0.208D+00-0.221D-01 0.494D+00

Coeff: 0.746D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.34D-09 MaxDP=4.59D-07 DE=-3.00D-11 OVMax= 5.83D-06

Error on total polarization charges = 0.08258

SCF Done: E(UB3LYP) = -1914.33331315 A.U. after 13 cycles

NFock= 13 Conv=0.53D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0183

<L.S>= 0.000000000000E+00

KE= 1.906380182065D+03 PE=-1.516306993907D+04 EE= 5.985634282463D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0551, after 2.0017

Leave Link 502 at Thu Aug 29 07:14:14 2019, MaxMem= 4294967296 cpu: 5468.5

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48635814D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64292936D-01

Leave Link 801 at Thu Aug 29 07:14:15 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Thu Aug 29 07:14:22 2019, MaxMem= 4294967296 cpu: 111.5

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Thu Aug 29 07:14:22 2019, MaxMem= 4294967296 cpu: 2.0

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 188

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 Thu Aug 29 07:34:11 2019, MaxMem= 4294967296 cpu: 19027.5

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 590000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.39D+03 4.50D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.52D+02 3.64D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.52D+00 4.65D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.02D-01 3.96D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.58D-04 2.10D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.58D-06 1.35D-04.

190 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 1.98D-08 1.01D-05.

77 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.28D-11 6.18D-07.

36 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.16D-13 3.87D-08.

3 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 8.84D-15 4.56D-09.

2 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 3.29D-15 1.65D-09.

InvSVY: IOpt=1 It= 1 EMax= 1.42D-14

Solved reduced A of dimension 1715 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1125.95 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 Thu Aug 29 11:26:10 2019, MaxMem= 4294967296 cpu: 222641.5

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 188

Leave Link 701 at Thu Aug 29 11:27:39 2019, MaxMem= 4294967296 cpu: 1422.5

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Thu Aug 29 11:27:39 2019, MaxMem= 4294967296 cpu: 0.0

(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=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

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= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Thu Aug 29 11:46:12 2019, MaxMem= 4294967296 cpu: 17809.5

(Enter /home/kira/g09/l716.exe)

Dipole =-1.56427346D-04-5.58773507D-03-4.82634895D-01

Polarizability= 1.25677673D+03-3.31490791D+01 1.66630867D+03

-4.97739847D-03-9.39350333D-02 4.54773440D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000010044 0.000001133 -0.000000337

2 6 -0.000006350 0.000003075 0.000017109

3 7 -0.000013290 -0.000007787 0.000007216

4 6 0.000009977 -0.000009785 -0.000032753

5 6 -0.000003983 -0.000000654 -0.000006113

6 6 0.000004189 -0.000002971 0.000019265

7 6 0.000008648 0.000000075 -0.000001827

8 7 0.000056893 -0.000041108 0.000001107

9 6 -0.000006706 0.000001329 0.000014390

10 6 0.000006069 0.000008894 0.000004984

11 6 0.000001098 0.000005356 -0.000008308

12 6 0.000007534 -0.000014075 -0.000002527

13 6 0.000006366 0.000001658 -0.000014116

14 6 -0.000006017 0.000008189 -0.000003915

15 6 -0.000001173 0.000007154 0.000008363

16 6 -0.000007874 -0.000000265 0.000001552

17 7 -0.000058067 -0.000035148 -0.000001173

18 6 -0.000005971 -0.000004139 -0.000019321

19 6 -0.000008914 -0.000009046 0.000034269

20 6 0.000004843 -0.000001675 0.000006740

21 6 0.000010330 -0.000000523 0.000000411

22 6 0.000003094 0.000002366 -0.000018648

23 7 0.000010861 -0.000007356 -0.000003862

24 6 -0.000006918 -0.000013985 0.000001861

25 6 -0.000011485 0.000002119 0.000029252

26 6 -0.000018300 0.000017062 -0.000033547

27 6 0.000001790 -0.000007482 0.000007670

28 6 -0.000016745 0.000007377 -0.000007071

29 6 0.000006916 -0.000012240 0.000009247

30 6 -0.000008340 0.000019958 0.000013090

31 6 0.000012329 -0.000008641 -0.000004167

32 6 0.000004989 -0.000002175 0.000010515

33 6 0.000013822 0.000007497 -0.000001326

34 6 -0.000018561 0.000023440 -0.000013124

35 6 0.000012758 0.000003077 -0.000024056

36 6 -0.000018253 0.000003168 -0.000001948

37 6 0.000018142 0.000020828 0.000014874

38 6 -0.000011051 0.000002953 0.000022292

39 6 0.000017754 0.000001554 0.000003578

40 6 -0.000011731 -0.000009594 0.000003125

41 6 -0.000006145 -0.000005478 -0.000009428

42 6 -0.000012745 0.000007301 0.000000903

43 6 0.000013333 0.000002301 -0.000029595

44 6 0.000008478 0.000020459 -0.000013858

45 6 -0.000006798 -0.000012873 -0.000009055

46 6 0.000016277 0.000006120 0.000006462

47 6 -0.000001239 -0.000008575 -0.000007384

48 6 0.000019385 0.000013679 0.000032527

49 1 0.000008060 0.000006432 -0.000014088

50 1 -0.000004927 -0.000014842 0.000022555

51 1 0.000003763 -0.000001858 -0.000006109

52 1 0.000001733 -0.000011480 0.000000410

53 1 -0.000004257 -0.000001603 0.000006156

54 1 -0.000002404 -0.000011735 -0.000000393

55 1 0.000002632 -0.000013339 -0.000021397

56 1 -0.000006184 0.000006196 0.000012789

57 1 0.000012121 0.000011833 -0.000008167

58 1 -0.000002276 0.000000794 -0.000006557

59 1 0.000000377 -0.000002400 0.000002841

60 1 0.000000325 0.000000209 0.000000118

61 1 0.000007560 -0.000012778 -0.000016449

62 1 -0.000006323 0.000000352 0.000002052

63 1 -0.000000359 -0.000000382 -0.000001502

64 1 -0.000000056 0.000005124 0.000001293

65 1 0.000010090 -0.000008655 0.000010152

66 1 0.000003441 -0.000001744 -0.000002210

67 1 -0.000009739 -0.000009139 -0.000009229

68 1 -0.000003027 -0.000002778 0.000002144

69 1 0.000006063 -0.000001199 -0.000002011

70 1 0.000000218 -0.000001296 0.000001146

71 1 -0.000000304 0.000004268 -0.000001600

72 1 -0.000008066 -0.000013883 0.000016781

73 1 -0.000000198 -0.000000541 -0.000000046

74 1 -0.000000618 -0.000003364 -0.000002891

75 1 0.000001643 -0.000000250 0.000006060

76 1 -0.000012111 0.000011290 0.000007798

77 1 -0.000103184 0.000027895 -0.000009412

78 1 0.000106830 0.000056322 0.000006421

-------------------------------------------------------------------

Cartesian Forces: Max 0.000106830 RMS 0.000016119

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Thu Aug 29 11:46:13 2019, MaxMem= 4294967296 cpu: 2.0

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000115881 RMS 0.000023418

Search for a local minimum.

Step number 20 out of a maximum of 452

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= 5.00D-06 DEPred=-1.79D-06 R=-2.80D+00

Trust test=-2.80D+00 RLast= 1.01D-02 DXMaxT set to 5.00D-02

ITU= -1 -1 1 1 -1 -1 1 0 -1 1 1 -1 1 -1 -1 1 1 -1 1 0

Eigenvalues --- 0.00126 0.00239 0.00385 0.00594 0.00719

Eigenvalues --- 0.00793 0.00911 0.01044 0.01058 0.01117

Eigenvalues --- 0.01134 0.01156 0.01261 0.01280 0.01301

Eigenvalues --- 0.01301 0.01321 0.01421 0.01427 0.01549

Eigenvalues --- 0.01561 0.01564 0.01603 0.01675 0.01711

Eigenvalues --- 0.01717 0.01727 0.01737 0.01756 0.01761

Eigenvalues --- 0.01763 0.01780 0.01797 0.01801 0.01884

Eigenvalues --- 0.01937 0.01992 0.02006 0.02012 0.02165

Eigenvalues --- 0.02170 0.02252 0.02288 0.02296 0.02304

Eigenvalues --- 0.02329 0.02392 0.02468 0.02473 0.02523

Eigenvalues --- 0.02542 0.02548 0.02586 0.02629 0.02630

Eigenvalues --- 0.02647 0.02650 0.02765 0.02778 0.02797

Eigenvalues --- 0.02804 0.02865 0.02870 0.02873 0.02874

Eigenvalues --- 0.02924 0.02949 0.03928 0.04087 0.04189

Eigenvalues --- 0.04319 0.04362 0.04466 0.04545 0.04574

Eigenvalues --- 0.08309 0.09660 0.09675 0.09767 0.09846

Eigenvalues --- 0.09868 0.10300 0.10429 0.10565 0.10697

Eigenvalues --- 0.10704 0.10706 0.10738 0.10739 0.11006

Eigenvalues --- 0.11398 0.11402 0.11411 0.11415 0.11984

Eigenvalues --- 0.11990 0.11997 0.12004 0.12284 0.12286

Eigenvalues --- 0.12328 0.12328 0.12770 0.12772 0.12774

Eigenvalues --- 0.12777 0.15721 0.15929 0.16305 0.16642

Eigenvalues --- 0.17203 0.17360 0.17598 0.17852 0.18022

Eigenvalues --- 0.18024 0.18299 0.18376 0.19240 0.19282

Eigenvalues --- 0.19358 0.19361 0.19373 0.19408 0.19416

Eigenvalues --- 0.19428 0.19552 0.19552 0.19554 0.19555

Eigenvalues --- 0.20299 0.21486 0.22044 0.22799 0.22900

Eigenvalues --- 0.23213 0.23771 0.24246 0.24744 0.25368

Eigenvalues --- 0.26259 0.26391 0.26663 0.27103 0.28523

Eigenvalues --- 0.28554 0.28754 0.29013 0.29781 0.31026

Eigenvalues --- 0.31696 0.32007 0.32860 0.33075 0.33292

Eigenvalues --- 0.33327 0.34187 0.34407 0.35039 0.35566

Eigenvalues --- 0.35626 0.35628 0.35635 0.35642 0.35758

Eigenvalues --- 0.35761 0.35767 0.35813 0.35927 0.35927

Eigenvalues --- 0.35933 0.35936 0.35987 0.35991 0.36008

Eigenvalues --- 0.36011 0.36194 0.36202 0.36249 0.36255

Eigenvalues --- 0.36965 0.37053 0.37240 0.37386 0.37389

Eigenvalues --- 0.37476 0.38147 0.38418 0.38492 0.38515

Eigenvalues --- 0.39471 0.40354 0.40746 0.41057 0.41077

Eigenvalues --- 0.41121 0.41197 0.41258 0.41356 0.41371

Eigenvalues --- 0.41575 0.41823 0.42257 0.42588 0.44493

Eigenvalues --- 0.45178 0.45829 0.45915 0.45925 0.45990

Eigenvalues --- 0.46008 0.46109 0.46260 0.46264 0.46315

Eigenvalues --- 0.46326 0.48479 0.49000 0.49376 0.49588

Eigenvalues --- 0.50750 0.50752 0.50778 0.50780 0.51861

Eigenvalues --- 0.52191 0.57160 0.57697

Cut down GDIIS temporarily because of the coefficient check. E 4

DIIS coeff's: 0.66879 -0.05431 0.42389 -0.03837

Cosine: 0.879 > 0.500

Length: 0.594

GDIIS step was calculated using 4 of the last 20 vectors.

Iteration 1 RMS(Cart)= 0.00468162 RMS(Int)= 0.00000363

Iteration 2 RMS(Cart)= 0.00000694 RMS(Int)= 0.00000032

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000032

ITry= 1 IFail=0 DXMaxC= 2.35D-02 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.65678 -0.00000 -0.00003 0.00008 0.00006 2.65683

R2 2.64108 -0.00004 -0.00001 -0.00008 -0.00009 2.64099

R3 2.03711 -0.00000 -0.00001 -0.00001 -0.00003 2.03708

R4 2.59907 0.00005 0.00004 0.00008 0.00012 2.59918

R5 2.71616 -0.00003 -0.00002 -0.00017 -0.00019 2.71597

R6 2.59889 0.00007 0.00010 0.00003 0.00014 2.59902

R7 1.90992 0.00011 0.00012 0.00008 0.00019 1.91011

R8 2.65654 -0.00002 -0.00004 0.00002 -0.00002 2.65652

R9 2.71704 -0.00005 -0.00010 -0.00003 -0.00013 2.71691

R10 2.03715 -0.00001 -0.00002 -0.00001 -0.00002 2.03713

R11 2.64111 -0.00010 -0.00016 -0.00015 -0.00031 2.64080

R12 2.80402 -0.00001 0.00011 0.00007 0.00017 2.80419

R13 2.59611 -0.00006 -0.00004 0.00012 0.00009 2.59620

R14 2.76202 -0.00001 0.00002 -0.00006 -0.00003 2.76199

R15 2.59451 -0.00001 0.00004 -0.00017 -0.00013 2.59438

R16 2.76231 0.00001 0.00007 0.00000 0.00007 2.76238

R17 2.64270 -0.00003 -0.00011 0.00020 0.00009 2.64279

R18 2.55438 -0.00001 -0.00005 0.00004 -0.00001 2.55437

R19 2.03917 0.00000 0.00000 0.00001 0.00002 2.03919

R20 2.03906 -0.00000 0.00000 -0.00000 0.00000 2.03906

R21 2.64283 -0.00002 -0.00015 0.00013 -0.00001 2.64282

R22 2.80355 -0.00001 0.00012 0.00004 0.00016 2.80371

R23 2.76233 0.00002 0.00007 -0.00001 0.00006 2.76239

R24 2.59444 -0.00001 0.00006 -0.00014 -0.00008 2.59436

R25 2.55439 -0.00001 -0.00005 0.00003 -0.00002 2.55437

R26 2.03917 0.00000 0.00001 0.00001 0.00002 2.03919

R27 2.76201 -0.00001 0.00003 -0.00006 -0.00003 2.76198

R28 2.03906 -0.00000 0.00000 -0.00000 -0.00000 2.03906

R29 2.59615 -0.00006 -0.00005 0.00010 0.00006 2.59620

R30 2.64097 -0.00010 -0.00013 -0.00008 -0.00021 2.64076

R31 2.71688 -0.00005 -0.00006 0.00004 -0.00002 2.71686

R32 2.80440 -0.00002 0.00002 -0.00013 -0.00011 2.80430

R33 2.65670 -0.00002 -0.00007 -0.00006 -0.00013 2.65657

R34 2.59901 0.00007 0.00007 -0.00002 0.00005 2.59906

R35 2.64095 -0.00005 0.00001 -0.00001 -0.00000 2.64095

R36 2.03712 -0.00001 -0.00001 0.00001 -0.00000 2.03712

R37 2.65689 -0.00001 -0.00005 0.00002 -0.00003 2.65686

R38 2.03707 -0.00000 -0.00001 0.00000 -0.00000 2.03707

R39 2.59916 0.00006 0.00002 0.00003 0.00005 2.59921

R40 2.71601 -0.00003 0.00001 -0.00009 -0.00008 2.71593

R41 1.91013 0.00012 0.00008 -0.00003 0.00005 1.91018

R42 2.80391 -0.00001 0.00004 -0.00014 -0.00010 2.80381

R43 2.65135 0.00002 -0.00008 -0.00003 -0.00010 2.65124

R44 2.64999 0.00000 -0.00007 -0.00003 -0.00010 2.64989

R45 2.62861 -0.00000 0.00002 0.00001 0.00003 2.62864

R46 2.04847 0.00000 0.00002 0.00001 0.00003 2.04850

R47 2.63631 -0.00001 -0.00001 -0.00001 -0.00002 2.63628

R48 2.05017 -0.00000 0.00000 -0.00000 0.00000 2.05017

R49 2.63411 -0.00002 -0.00001 -0.00001 -0.00002 2.63409

R50 2.05006 -0.00000 0.00000 -0.00000 -0.00000 2.05006

R51 2.63093 -0.00001 0.00003 0.00001 0.00004 2.63097

R52 2.05014 -0.00000 0.00000 -0.00000 0.00000 2.05014

R53 2.04858 0.00000 0.00003 0.00001 0.00003 2.04862

R54 2.63633 0.00000 -0.00001 -0.00001 -0.00001 2.63632

R55 2.63423 -0.00001 -0.00001 0.00000 -0.00001 2.63423

R56 2.05006 -0.00000 -0.00000 -0.00000 -0.00001 2.05006

R57 2.62883 0.00001 0.00004 0.00003 0.00008 2.62890

R58 2.05018 -0.00000 0.00000 -0.00000 0.00000 2.05018

R59 2.65150 0.00002 -0.00005 -0.00001 -0.00006 2.65144

R60 2.04846 0.00000 0.00002 0.00000 0.00002 2.04848

R61 2.65019 -0.00000 -0.00006 -0.00002 -0.00008 2.65011

R62 2.63062 -0.00002 0.00001 -0.00001 -0.00001 2.63061

R63 2.04853 -0.00000 0.00001 0.00001 0.00001 2.04855

R64 2.05015 0.00000 0.00000 0.00000 0.00000 2.05016

R65 2.65005 -0.00000 -0.00003 0.00005 0.00002 2.65007

R66 2.65138 0.00002 -0.00002 0.00005 0.00003 2.65140

R67 2.63066 -0.00002 -0.00001 -0.00004 -0.00004 2.63062

R68 2.04856 -0.00000 0.00000 -0.00001 -0.00001 2.04855

R69 2.63422 -0.00001 -0.00000 0.00000 0.00000 2.63422

R70 2.05015 0.00000 0.00000 0.00000 0.00000 2.05016

R71 2.63631 0.00000 0.00000 0.00000 0.00001 2.63631

R72 2.05007 -0.00000 -0.00000 -0.00000 -0.00001 2.05006

R73 2.62889 0.00001 0.00003 0.00000 0.00003 2.62892

R74 2.05019 -0.00000 -0.00000 -0.00000 -0.00000 2.05018

R75 2.04847 0.00000 0.00001 0.00000 0.00001 2.04848

R76 2.64984 0.00001 -0.00004 0.00004 0.00001 2.64985

R77 2.65120 0.00001 -0.00005 0.00005 -0.00000 2.65120

R78 2.63098 -0.00001 0.00002 -0.00001 0.00001 2.63099

R79 2.04862 0.00000 0.00002 -0.00001 0.00001 2.04863

R80 2.63411 -0.00002 -0.00001 -0.00001 -0.00002 2.63409

R81 2.05014 -0.00000 0.00000 -0.00000 0.00000 2.05014

R82 2.63628 -0.00001 -0.00001 0.00000 -0.00000 2.63627

R83 2.05006 -0.00000 -0.00000 -0.00000 -0.00000 2.05006

R84 2.62867 -0.00000 0.00001 -0.00002 -0.00001 2.62866

R85 2.05017 -0.00000 0.00000 -0.00000 -0.00000 2.05017

R86 2.04848 0.00000 0.00002 0.00000 0.00002 2.04850

A1 1.88153 0.00002 0.00001 0.00002 0.00002 1.88155

A2 2.18769 0.00000 0.00007 0.00008 0.00015 2.18784

A3 2.21395 -0.00003 -0.00008 -0.00009 -0.00017 2.21378

A4 1.86794 0.00001 0.00006 -0.00002 0.00004 1.86797

A5 2.22237 -0.00009 -0.00021 0.00005 -0.00016 2.22221

A6 2.19245 0.00008 0.00017 -0.00006 0.00011 2.19256

A7 1.92528 -0.00006 -0.00010 -0.00004 -0.00014 1.92514

A8 2.17736 0.00004 0.00006 -0.00007 -0.00000 2.17736

A9 2.17984 0.00002 0.00002 0.00005 0.00006 2.17990

A10 1.86802 0.00002 0.00005 0.00002 0.00008 1.86809

A11 2.19416 -0.00001 0.00012 0.00010 0.00022 2.19438

A12 2.22062 -0.00002 -0.00017 -0.00013 -0.00030 2.22032

A13 1.88165 0.00000 -0.00001 0.00002 0.00001 1.88166

A14 2.21416 -0.00002 -0.00008 -0.00004 -0.00012 2.21404

A15 2.18735 0.00002 0.00009 0.00003 0.00011 2.18746

A16 2.18645 -0.00008 0.00016 0.00007 0.00024 2.18669

A17 2.02286 0.00011 0.00003 -0.00001 0.00002 2.02288

A18 2.07382 -0.00002 -0.00019 -0.00006 -0.00025 2.07357

A19 2.19191 -0.00007 0.00001 -0.00014 -0.00013 2.19178

A20 2.16519 0.00003 -0.00006 0.00015 0.00008 2.16528

A21 1.92605 0.00004 0.00006 -0.00001 0.00005 1.92609

A22 1.84712 -0.00002 -0.00003 -0.00000 -0.00003 1.84709

A23 1.92644 0.00001 -0.00001 0.00004 0.00003 1.92647

A24 2.19203 -0.00001 0.00008 -0.00004 0.00004 2.19207

A25 2.16471 0.00000 -0.00007 -0.00000 -0.00008 2.16463

A26 1.86204 -0.00001 0.00001 -0.00001 0.00001 1.86205

A27 2.19693 0.00001 -0.00001 -0.00000 -0.00001 2.19692

A28 2.22382 -0.00000 0.00000 0.00001 0.00001 2.22382

A29 1.86211 -0.00002 -0.00002 -0.00002 -0.00004 1.86207

A30 2.19687 0.00001 -0.00003 0.00004 0.00001 2.19688

A31 2.22386 0.00001 0.00006 -0.00002 0.00004 2.22390

A32 2.18489 0.00002 0.00023 0.00006 0.00029 2.18519

A33 2.02516 -0.00003 -0.00011 0.00023 0.00012 2.02528

A34 2.07308 0.00000 -0.00012 -0.00029 -0.00041 2.07267

A35 2.16487 0.00000 -0.00010 -0.00009 -0.00019 2.16468

A36 2.19187 -0.00001 0.00011 0.00005 0.00015 2.19202

A37 1.92643 0.00000 -0.00000 0.00004 0.00004 1.92647

A38 1.86205 -0.00001 0.00001 -0.00001 -0.00000 1.86205

A39 2.19691 0.00001 -0.00000 0.00001 0.00000 2.19691

A40 2.22383 -0.00000 -0.00000 0.00000 0.00000 2.22383

A41 1.86209 -0.00002 -0.00002 -0.00001 -0.00003 1.86206

A42 2.22386 0.00002 0.00006 -0.00002 0.00004 2.22390

A43 2.19689 0.00001 -0.00003 0.00003 -0.00001 2.19688

A44 1.92604 0.00004 0.00006 -0.00001 0.00005 1.92609

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A47 1.84714 -0.00002 -0.00003 -0.00001 -0.00004 1.84709

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A49 2.07313 -0.00002 -0.00004 0.00029 0.00025 2.07338

A50 2.02301 0.00010 -0.00001 -0.00009 -0.00010 2.02292

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A52 2.19416 -0.00000 0.00012 0.00011 0.00023 2.19439

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D3 -3.12035 0.00000 -0.00016 -0.00017 -0.00033 -3.12068

D4 0.05139 -0.00001 -0.00054 0.00076 0.00021 0.05160

D5 -0.00056 0.00001 0.00002 -0.00010 -0.00009 -0.00064

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D11 3.08689 0.00001 0.00049 -0.00107 -0.00058 3.08631

D12 -0.09365 0.00001 -0.00001 -0.00268 -0.00270 -0.09635

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D14 0.18397 0.00000 -0.00146 -0.00252 -0.00398 0.17998

D15 0.23015 0.00001 -0.00171 -0.00205 -0.00376 0.22639

D16 -2.92216 -0.00000 -0.00191 -0.00143 -0.00334 -2.92550

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D18 -3.08840 -0.00001 -0.00022 0.00045 0.00023 -3.08818

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D28 -0.19477 0.00000 0.00174 0.00071 0.00245 -0.19231

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D31 3.00396 0.00001 0.00104 0.00089 0.00192 3.00588

D32 -0.12851 0.00000 0.00056 0.00111 0.00167 -0.12684

D33 -0.99488 -0.00004 -0.00238 -0.00105 -0.00343 -0.99831

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D35 2.15720 -0.00004 -0.00253 -0.00130 -0.00383 2.15337

D36 -0.98815 -0.00003 -0.00241 -0.00110 -0.00350 -0.99166

D37 -3.09147 -0.00002 -0.00077 0.00025 -0.00052 -3.09199

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D52 0.13750 0.00002 -0.00035 0.00166 0.00131 0.13881

D53 0.00124 0.00000 -0.00012 0.00015 0.00004 0.00127

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D87 -0.18647 -0.00000 0.00010 -0.00353 -0.00344 -0.18990

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D91 2.13983 -0.00004 -0.00163 0.00073 -0.00089 2.13894

D92 -0.99878 -0.00004 -0.00153 0.00091 -0.00062 -0.99940

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D179 3.13171 -0.00001 -0.00007 -0.00017 -0.00024 3.13147

D180 -0.00678 -0.00000 -0.00002 -0.00007 -0.00009 -0.00686

D181 -0.00644 0.00000 0.00003 0.00001 0.00004 -0.00641

D182 3.13659 -0.00000 -0.00002 -0.00002 -0.00004 3.13655

D183 3.13204 -0.00000 -0.00003 -0.00009 -0.00012 3.13192

D184 -0.00812 -0.00000 -0.00007 -0.00012 -0.00019 -0.00831

D185 -0.00539 -0.00000 0.00002 -0.00001 0.00001 -0.00538

D186 3.13560 -0.00000 0.00003 0.00005 0.00008 3.13568

D187 3.13476 0.00000 0.00007 0.00002 0.00008 3.13485

D188 -0.00744 0.00000 0.00007 0.00008 0.00015 -0.00728

D189 0.01649 0.00000 -0.00001 0.00006 0.00005 0.01654

D190 3.13656 0.00000 0.00009 0.00001 0.00010 3.13665

D191 -3.12450 0.00000 -0.00001 -0.00001 -0.00002 -3.12452

D192 -0.00443 -0.00000 0.00008 -0.00005 0.00003 -0.00441

D193 -3.14071 0.00000 0.00022 0.00017 0.00038 -3.14033

D194 -0.01721 -0.00001 0.00018 -0.00004 0.00014 -0.01707

D195 -0.00205 0.00001 0.00012 -0.00001 0.00011 -0.00193

D196 3.12146 0.00000 0.00009 -0.00022 -0.00013 3.12133

D197 -3.13004 0.00000 -0.00020 -0.00010 -0.00031 -3.13035

D198 -0.00814 0.00000 -0.00005 -0.00005 -0.00011 -0.00824

D199 0.01447 -0.00001 -0.00011 0.00008 -0.00004 0.01443

D200 3.13638 -0.00001 0.00004 0.00012 0.00016 3.13654

D201 -0.00873 -0.00001 -0.00007 -0.00008 -0.00015 -0.00888

D202 3.13057 -0.00001 -0.00005 -0.00008 -0.00012 3.13044

D203 -3.13213 -0.00000 -0.00004 0.00013 0.00009 -3.13204

D204 0.00717 0.00000 -0.00001 0.00013 0.00012 0.00728

D205 0.00718 0.00000 -0.00000 0.00012 0.00012 0.00729

D206 -3.13703 0.00000 -0.00005 -0.00002 -0.00007 -3.13710

D207 -3.13211 0.00000 -0.00002 0.00011 0.00009 -3.13202

D208 0.00687 -0.00000 -0.00008 -0.00002 -0.00010 0.00677

D209 0.00520 -0.00000 0.00001 -0.00005 -0.00004 0.00516

D210 -3.13574 0.00000 0.00003 -0.00006 -0.00003 -3.13577

D211 -3.13378 0.00000 0.00006 0.00008 0.00014 -3.13363

D212 0.00847 0.00000 0.00008 0.00007 0.00015 0.00862

D213 -0.01616 0.00000 0.00005 -0.00004 0.00000 -0.01616

D214 -3.13798 0.00000 -0.00011 -0.00009 -0.00020 -3.13818

D215 3.12479 -0.00000 0.00003 -0.00004 -0.00001 3.12478

D216 0.00297 -0.00000 -0.00012 -0.00008 -0.00021 0.00276

Item Value Threshold Converged?

Maximum Force 0.000116 0.000450 YES

RMS Force 0.000023 0.000300 YES

Maximum Displacement 0.023524 0.001800 NO

RMS Displacement 0.004682 0.001200 NO

Predicted change in Energy=-1.191630D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

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(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=1 Diff= 7.52D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 0.984365 -4.111068 0.552013

2 6 0 1.326750 -2.793587 0.200342

3 7 0 0.149335 -2.109689 0.005964

4 6 0 -0.925368 -2.948276 0.188600

5 6 0 -0.409876 -4.206852 0.544195

6 6 0 -2.306911 -2.594281 0.006721

7 6 0 -2.796503 -1.291591 -0.120416

8 7 0 -2.062518 -0.142085 0.045009

9 6 0 -2.950077 0.894171 -0.107395

10 6 0 -4.279728 0.381761 -0.433418

11 6 0 -4.184611 -0.966571 -0.442492

12 6 0 2.647211 -2.252346 0.029841

13 6 0 2.950107 -0.894015 -0.108187

14 6 0 4.279749 -0.381420 -0.433976

15 6 0 4.184624 0.966918 -0.442340

16 6 0 2.796500 1.291749 -0.120145

17 7 0 2.062532 0.142145 0.044683

18 6 0 2.306879 2.594358 0.007488

19 6 0 0.925390 2.948465 0.189379

20 6 0 0.409846 4.207842 0.542152

21 6 0 -0.984375 4.112068 0.550105

22 6 0 -1.326741 2.793797 0.201328

23 7 0 -0.149307 2.109431 0.008610

24 6 0 -2.647150 2.252444 0.030960

25 6 0 -3.266341 -3.725660 -0.031677

26 6 0 -3.118267 -4.755470 -0.972904

27 6 0 -4.024799 -5.809547 -1.018144

28 6 0 -5.083835 -5.863511 -0.111654

29 6 0 -5.233387 -4.852679 0.836400

30 6 0 -4.335508 -3.789285 0.873403

31 6 0 5.865109 -5.090641 -0.014169

32 6 0 4.818175 -5.204419 -0.929174

33 6 0 3.768457 -4.291736 -0.908744

34 6 0 3.757595 -3.236262 0.015643

35 6 0 4.815642 -3.131367 0.930082

36 6 0 5.858195 -4.053726 0.917452

37 6 0 -3.757671 3.236276 0.016272

38 6 0 -4.815373 3.132003 0.931152

39 6 0 -5.858196 4.054060 0.917913

40 6 0 -5.865704 5.090013 -0.014771

41 6 0 -4.819121 5.203122 -0.930254

42 6 0 -3.769152 4.290728 -0.909246

43 6 0 3.266453 3.725679 -0.031202

44 6 0 4.335016 3.789863 0.874518

45 6 0 5.233116 4.853069 0.837201

46 6 0 5.084360 5.863121 -0.111809

47 6 0 4.025943 5.808544 -1.018977

48 6 0 3.119203 4.754647 -0.973446

49 1 0 1.684814 -4.895633 0.788363

50 1 0 -0.999328 -5.079499 0.774675

51 1 0 -5.151740 0.979004 -0.650983

52 1 0 -4.964429 -1.677382 -0.668160

53 1 0 5.151758 -0.978548 -0.651875

54 1 0 4.964457 1.677857 -0.667555

55 1 0 0.999217 5.081123 0.770410

56 1 0 -1.684816 4.897255 0.784377

57 1 0 -2.298878 -4.716511 -1.681551

58 1 0 -3.904955 -6.589790 -1.762371

59 1 0 -5.786077 -6.689809 -0.142880

60 1 0 -6.049021 -4.891805 1.550680

61 1 0 -4.450006 -3.009753 1.618020

62 1 0 6.680052 -5.806599 -0.026846

63 1 0 4.819227 -6.005514 -1.660798

64 1 0 2.959476 -4.381570 -1.624672

65 1 0 4.808864 -2.331947 1.662226

66 1 0 6.663911 -3.963444 1.638335

67 1 0 -4.808172 2.333248 1.664022

68 1 0 -6.663680 3.964263 1.639116

69 1 0 -6.680861 5.805719 -0.027932

70 1 0 -4.820657 6.003430 -1.662740

71 1 0 -2.960470 4.379994 -1.625586

72 1 0 4.448924 3.010878 1.619802

73 1 0 6.048306 4.892645 1.551962

74 1 0 5.786772 6.689265 -0.143284

75 1 0 3.906740 6.588152 -1.763974

76 1 0 2.300305 4.715189 -1.682635

77 1 0 0.083919 -1.122954 -0.203234

78 1 0 -0.083880 1.121805 -0.196515

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0587908 0.0582551 0.0300941

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(Enter /home/kira/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5356.8913583296 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122021580 Hartrees.

Nuclear repulsion after empirical dispersion term = 5356.6791561716 Hartrees.

Force inversion solution in PCM.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5786

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.69D-10

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 303

GePol: Fraction of low-weight points (<1% of avg) = 5.24%

GePol: Cavity surface area = 610.624 Ang\*\*2

GePol: Cavity volume = 628.014 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0020999876 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5356.6770561840 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.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

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(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Thu Aug 29 11:46:15 2019, MaxMem= 4294967296 cpu: 3.0

(Enter /home/kira/g09/l401.exe)

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= -0.000000 0.000000 0.000000

Rot= 0.999996 -0.000034 -0.000004 0.002664 Ang= -0.31 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0182

Generating alternative initial guess.

ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= 2001

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= -1914.30504424447

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(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 590000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 100433388.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.55D-15 for 5781.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.77D-15 for 5774 4722.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.33D-15 for 5775.

Iteration 1 A^-1\*A deviation from orthogonality is 2.24D-10 for 3129 3113.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.44D-15 for 2737.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.49D-15 for 4444 3482.

Iteration 2 A^-1\*A deviation from unit magnitude is 8.88D-16 for 782.

Iteration 2 A^-1\*A deviation from orthogonality is 4.01D-16 for 3437 1005.

E= -1914.33321305258

DIIS: error= 2.04D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.33321305258 IErMin= 1 ErrMin= 2.04D-04

ErrMax= 2.04D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.10D-04 BMatP= 2.10D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.04D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.640 Goal= None Shift= 0.000

Gap= 0.706 Goal= None Shift= 0.000

RMSDP=1.50D-05 MaxDP=6.87D-04 OVMax= 1.46D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.50D-05 CP: 1.00D+00

E= -1914.33331500352 Delta-E= -0.000101950940 Rises=F Damp=F

DIIS: error= 2.96D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33331500352 IErMin= 2 ErrMin= 2.96D-05

ErrMax= 2.96D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.72D-06 BMatP= 2.10D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.636D-01 0.106D+01

Coeff: -0.636D-01 0.106D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.90D-06 MaxDP=7.99D-05 DE=-1.02D-04 OVMax= 2.90D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.69D-06 CP: 1.00D+00 1.06D+00

E= -1914.33331646321 Delta-E= -0.000001459699 Rises=F Damp=F

DIIS: error= 1.66D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33331646321 IErMin= 3 ErrMin= 1.66D-05

ErrMax= 1.66D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.64D-07 BMatP= 2.72D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.298D-01 0.397D+00 0.632D+00

Coeff: -0.298D-01 0.397D+00 0.632D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=6.84D-07 MaxDP=7.38D-05 DE=-1.46D-06 OVMax= 1.94D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.21D-07 CP: 1.00D+00 1.06D+00 8.32D-01

E= -1914.33331660276 Delta-E= -0.000000139544 Rises=F Damp=F

DIIS: error= 1.08D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33331660276 IErMin= 4 ErrMin= 1.08D-05

ErrMax= 1.08D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.29D-07 BMatP= 8.64D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.899D-02 0.925D-01 0.383D+00 0.533D+00

Coeff: -0.899D-02 0.925D-01 0.383D+00 0.533D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.06D-07 MaxDP=3.37D-05 DE=-1.40D-07 OVMax= 1.03D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.25D-07 CP: 1.00D+00 1.06D+00 8.91D-01 7.14D-01

E= -1914.33331668295 Delta-E= -0.000000080195 Rises=F Damp=F

DIIS: error= 2.18D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33331668295 IErMin= 5 ErrMin= 2.18D-06

ErrMax= 2.18D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.70D-08 BMatP= 3.29D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.649D-03-0.529D-02 0.914D-01 0.227D+00 0.688D+00

Coeff: -0.649D-03-0.529D-02 0.914D-01 0.227D+00 0.688D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.17D-07 MaxDP=7.07D-06 DE=-8.02D-08 OVMax= 5.12D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.58D-08 CP: 1.00D+00 1.06D+00 9.08D-01 7.95D-01 8.61D-01

E= -1914.33331668705 Delta-E= -0.000000004095 Rises=F Damp=F

DIIS: error= 1.60D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33331668705 IErMin= 6 ErrMin= 1.60D-06

ErrMax= 1.60D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.51D-09 BMatP= 1.70D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.930D-03-0.177D-01 0.501D-03 0.659D-01 0.449D+00 0.502D+00

Coeff: 0.930D-03-0.177D-01 0.501D-03 0.659D-01 0.449D+00 0.502D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=6.37D-08 MaxDP=5.04D-06 DE=-4.10D-09 OVMax= 4.34D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.32D-08 CP: 1.00D+00 1.06D+00 9.17D-01 7.95D-01 9.87D-01

CP: 8.71D-01

E= -1914.33331668967 Delta-E= -0.000000002617 Rises=F Damp=F

DIIS: error= 5.98D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33331668967 IErMin= 7 ErrMin= 5.98D-07

ErrMax= 5.98D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.66D-10 BMatP= 7.51D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.421D-03-0.666D-02-0.635D-02 0.105D-01 0.129D+00 0.222D+00

Coeff-Com: 0.651D+00

Coeff: 0.421D-03-0.666D-02-0.635D-02 0.105D-01 0.129D+00 0.222D+00

Coeff: 0.651D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.62D-08 MaxDP=2.81D-06 DE=-2.62D-09 OVMax= 3.09D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.82D-08 CP: 1.00D+00 1.06D+00 9.19D-01 8.09D-01 1.03D+00

CP: 1.10D+00 1.33D+00

E= -1914.33331669024 Delta-E= -0.000000000578 Rises=F Damp=F

DIIS: error= 6.02D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1914.33331669024 IErMin= 7 ErrMin= 5.98D-07

ErrMax= 6.02D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.83D-10 BMatP= 5.66D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.402D-03 0.875D-02-0.534D-02-0.428D-01-0.257D+00-0.205D+00

Coeff-Com: 0.442D+00 0.106D+01

Coeff: -0.402D-03 0.875D-02-0.534D-02-0.428D-01-0.257D+00-0.205D+00

Coeff: 0.442D+00 0.106D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=6.91D-08 MaxDP=6.04D-06 DE=-5.78D-10 OVMax= 6.94D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.65D-08 CP: 1.00D+00 1.06D+00 9.24D-01 8.22D-01 1.15D+00

CP: 1.49D+00 2.21D+00 1.54D+00

E= -1914.33331669091 Delta-E= -0.000000000664 Rises=F Damp=F

DIIS: error= 3.45D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1914.33331669091 IErMin= 9 ErrMin= 3.45D-07

ErrMax= 3.45D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-10 BMatP= 2.83D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.296D-03 0.569D-02-0.154D-03-0.206D-01-0.150D+00-0.146D+00

Coeff-Com: -0.361D-01 0.521D+00 0.826D+00

Coeff: -0.296D-03 0.569D-02-0.154D-03-0.206D-01-0.150D+00-0.146D+00

Coeff: -0.361D-01 0.521D+00 0.826D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.90D-08 MaxDP=3.31D-06 DE=-6.64D-10 OVMax= 3.98D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 8.57D-09 CP: 1.00D+00 1.06D+00 9.26D-01 8.30D-01 1.20D+00

CP: 1.72D+00 2.68D+00 2.13D+00 1.50D+00

E= -1914.33331669119 Delta-E= -0.000000000281 Rises=F Damp=F

DIIS: error= 2.60D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1914.33331669119 IErMin=10 ErrMin= 2.60D-07

ErrMax= 2.60D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.49D-11 BMatP= 1.03D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.179D-04-0.933D-03 0.276D-02 0.975D-02 0.373D-01 0.163D-01

Coeff-Com: -0.283D+00-0.164D+00 0.527D+00 0.856D+00

Coeff: 0.179D-04-0.933D-03 0.276D-02 0.975D-02 0.373D-01 0.163D-01

Coeff: -0.283D+00-0.164D+00 0.527D+00 0.856D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.28D-08 MaxDP=2.89D-06 DE=-2.81D-10 OVMax= 3.56D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.72D-09 CP: 1.00D+00 1.06D+00 9.28D-01 8.35D-01 1.25D+00

CP: 1.89D+00 3.00D+00 2.62D+00 2.24D+00 1.26D+00

E= -1914.33331669123 Delta-E= -0.000000000039 Rises=F Damp=F

DIIS: error= 1.33D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1914.33331669123 IErMin=11 ErrMin= 1.33D-07

ErrMax= 1.33D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.71D-11 BMatP= 4.49D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.808D-04-0.187D-02 0.143D-02 0.104D-01 0.563D-01 0.456D-01

Coeff-Com: -0.161D+00-0.194D+00 0.598D-01 0.491D+00 0.692D+00

Coeff: 0.808D-04-0.187D-02 0.143D-02 0.104D-01 0.563D-01 0.456D-01

Coeff: -0.161D+00-0.194D+00 0.598D-01 0.491D+00 0.692D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.45D-08 MaxDP=1.17D-06 DE=-3.91D-11 OVMax= 1.56D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 6.99D-09 CP: 1.00D+00 1.06D+00 9.28D-01 8.37D-01 1.26D+00

CP: 1.95D+00 3.00D+00 2.87D+00 2.60D+00 1.65D+00

CP: 1.89D+00

E= -1914.33331669130 Delta-E= -0.000000000074 Rises=F Damp=F

DIIS: error= 1.02D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1914.33331669130 IErMin=12 ErrMin= 1.02D-07

ErrMax= 1.02D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.92D-12 BMatP= 1.71D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.387D-04-0.613D-03-0.753D-03 0.116D-02 0.136D-01 0.204D-01

Coeff-Com: 0.436D-01-0.169D-02-0.265D+00-0.133D+00 0.377D+00 0.945D+00

Coeff: 0.387D-04-0.613D-03-0.753D-03 0.116D-02 0.136D-01 0.204D-01

Coeff: 0.436D-01-0.169D-02-0.265D+00-0.133D+00 0.377D+00 0.945D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.25D-08 MaxDP=1.08D-06 DE=-7.37D-11 OVMax= 1.40D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 2.35D-09 CP: 1.00D+00 1.06D+00 9.29D-01 8.38D-01 1.28D+00

CP: 2.00D+00 3.00D+00 3.00D+00 2.95D+00 2.02D+00

CP: 2.92D+00 1.50D+00

E= -1914.33331669129 Delta-E= 0.000000000014 Rises=F Damp=F

DIIS: error= 5.11D-08 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=12 EnMin= -1914.33331669130 IErMin=13 ErrMin= 5.11D-08

ErrMax= 5.11D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.70D-12 BMatP= 5.92D-12

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.701D-05 0.328D-03-0.101D-02-0.298D-02-0.127D-01-0.441D-02

Coeff-Com: 0.764D-01 0.780D-01-0.184D+00-0.238D+00-0.600D-01 0.556D+00

Coeff-Com: 0.793D+00

Coeff: -0.701D-05 0.328D-03-0.101D-02-0.298D-02-0.127D-01-0.441D-02

Coeff: 0.764D-01 0.780D-01-0.184D+00-0.238D+00-0.600D-01 0.556D+00

Coeff: 0.793D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.56D-09 MaxDP=6.93D-07 DE= 1.36D-11 OVMax= 8.33D-06

Error on total polarization charges = 0.08258

SCF Done: E(UB3LYP) = -1914.33331669 A.U. after 13 cycles

NFock= 13 Conv=0.76D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0182

<L.S>= 0.000000000000E+00

KE= 1.906380711802D+03 PE=-1.516298094191D+04 EE= 5.985589857228D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0551, after 2.0017

Leave Link 502 at Thu Aug 29 11:52:04 2019, MaxMem= 4294967296 cpu: 5429.5

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48636716D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64280087D-01

Leave Link 801 at Thu Aug 29 11:52:04 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Thu Aug 29 11:52:11 2019, MaxMem= 4294967296 cpu: 110.5

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Thu Aug 29 11:52:12 2019, MaxMem= 4294967296 cpu: 2.5

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 189

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 Thu Aug 29 12:11:58 2019, MaxMem= 4294967296 cpu: 18972.5

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 590000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.39D+03 4.50D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.52D+02 3.62D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.52D+00 4.66D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.02D-01 3.97D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.57D-04 2.10D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.58D-06 1.35D-04.

191 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 1.98D-08 1.02D-05.

81 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.29D-11 6.19D-07.

43 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.16D-13 3.89D-08.

5 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 8.55D-15 5.63D-09.

4 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 4.13D-15 1.83D-09.

4 vectors produced by pass 11 Test12= 2.55D-13 1.00D-09 XBig12= 3.35D-15 2.08D-09.

4 vectors produced by pass 12 Test12= 2.55D-13 1.00D-09 XBig12= 7.13D-15 3.00D-09.

4 vectors produced by pass 13 Test12= 2.55D-13 1.00D-09 XBig12= 5.89D-15 2.56D-09.

4 vectors produced by pass 14 Test12= 2.55D-13 1.00D-09 XBig12= 1.13D-14 3.44D-09.

4 vectors produced by pass 15 Test12= 2.55D-13 1.00D-09 XBig12= 6.52D-15 2.48D-09.

4 vectors produced by pass 16 Test12= 2.55D-13 1.00D-09 XBig12= 1.01D-14 3.24D-09.

3 vectors produced by pass 17 Test12= 2.55D-13 1.00D-09 XBig12= 5.92D-15 3.03D-09.

3 vectors produced by pass 18 Test12= 2.55D-13 1.00D-09 XBig12= 7.61D-15 2.27D-09.

3 vectors produced by pass 19 Test12= 2.55D-13 1.00D-09 XBig12= 6.55D-15 2.55D-09.

3 vectors produced by pass 20 Test12= 2.55D-13 1.00D-09 XBig12= 5.54D-15 2.53D-09.

2 vectors produced by pass 21 Test12= 2.55D-13 1.00D-09 XBig12= 2.67D-15 1.56D-09.

InvSVY: IOpt=1 It= 1 EMax= 8.53D-14

Solved reduced A of dimension 1769 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1125.48 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 Thu Aug 29 16:06:05 2019, MaxMem= 4294967296 cpu: 224690.5

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 189

Leave Link 701 at Thu Aug 29 16:07:34 2019, MaxMem= 4294967296 cpu: 1415.5

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Thu Aug 29 16:07:34 2019, MaxMem= 4294967296 cpu: 1.0

(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=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

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= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Thu Aug 29 16:25:18 2019, MaxMem= 4294967296 cpu: 17028.5

(Enter /home/kira/g09/l716.exe)

Dipole =-1.21393861D-04-1.55882081D-03-4.79140231D-01

Polarizability= 1.25585449D+03-3.10611790D+01 1.66534786D+03

-7.23513675D-04-2.73277185D-02 4.55249424D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000000684 0.000000007 -0.000000174

2 6 0.000000054 0.000000150 0.000000678

3 7 -0.000000287 -0.000000288 -0.000000215

4 6 0.000000179 -0.000000638 -0.000002465

5 6 -0.000000283 0.000000213 -0.000001330

6 6 0.000000531 0.000000203 0.000001853

7 6 -0.000000744 0.000000028 -0.000000181

8 7 0.000013353 -0.000004892 0.000001102

9 6 -0.000001005 0.000000211 0.000001063

10 6 -0.000000231 0.000000582 0.000000212

11 6 -0.000000138 0.000000702 -0.000000686

12 6 0.000000004 -0.000000452 -0.000000515

13 6 0.000001109 0.000000340 -0.000001015

14 6 0.000000129 0.000000733 -0.000000110

15 6 0.000000119 0.000000848 0.000000805

16 6 0.000000759 -0.000000041 -0.000000097

17 7 -0.000013124 -0.000004955 -0.000001502

18 6 -0.000000597 0.000000261 -0.000001996

19 6 -0.000000307 -0.000000907 0.000002331

20 6 0.000000679 -0.000000136 0.000001746

21 6 0.000000658 -0.000000346 -0.000000049

22 6 -0.000000061 0.000000017 -0.000001155

23 7 0.000000311 -0.000001003 0.000000326

24 6 0.000000009 -0.000001145 0.000000639

25 6 -0.000001993 0.000000035 0.000001570

26 6 -0.000001746 0.000000534 -0.000002455

27 6 -0.000001119 -0.000000320 -0.000000344

28 6 -0.000001066 0.000000453 -0.000000760

29 6 -0.000000312 -0.000000231 -0.000000408

30 6 0.000000021 0.000000948 0.000000740

31 6 0.000001323 -0.000000135 -0.000000606

32 6 0.000001312 -0.000000492 -0.000000216

33 6 0.000000375 0.000000943 0.000000230

34 6 -0.000000359 0.000000979 -0.000001612

35 6 0.000000095 0.000000637 -0.000002092

36 6 -0.000000040 0.000000360 -0.000001082

37 6 0.000000704 0.000000863 0.000001579

38 6 -0.000000063 0.000000617 0.000002526

39 6 -0.000000054 -0.000000457 0.000001366

40 6 -0.000001089 -0.000000492 0.000000620

41 6 -0.000001267 -0.000000830 -0.000000035

42 6 -0.000000443 0.000000681 -0.000000271

43 6 0.000001561 -0.000000313 -0.000001702

44 6 0.000000130 0.000000764 -0.000000563

45 6 -0.000000083 -0.000000519 0.000000239

46 6 0.000001301 0.000000344 0.000001038

47 6 0.000001034 -0.000000516 0.000000148

48 6 0.000002025 0.000000514 0.000002898

49 1 0.000000577 0.000000313 -0.000001323

50 1 -0.000000105 -0.000000516 0.000000881

51 1 -0.000001086 -0.000000430 -0.000000757

52 1 0.000000099 -0.000000669 0.000000018

53 1 0.000000913 -0.000000382 0.000000674

54 1 -0.000000217 -0.000000771 -0.000000038

55 1 0.000000169 -0.000000710 -0.000001066

56 1 -0.000000544 0.000000196 0.000001157

57 1 0.000000477 0.000000852 -0.000000921

58 1 -0.000000470 0.000000243 -0.000000898

59 1 -0.000000566 -0.000000074 -0.000000329

60 1 -0.000000373 0.000000046 -0.000000407

61 1 0.000000173 -0.000001130 -0.000001213

62 1 0.000000021 0.000000243 -0.000000324

63 1 0.000000263 0.000000183 -0.000000585

64 1 0.000000249 0.000000498 -0.000000250

65 1 0.000001262 -0.000000504 0.000000437

66 1 0.000000676 -0.000000003 -0.000000405

67 1 -0.000001317 -0.000000694 -0.000000447

68 1 -0.000000626 -0.000000297 0.000000423

69 1 -0.000000049 -0.000000178 0.000000356

70 1 -0.000000366 -0.000000263 0.000000531

71 1 -0.000000421 0.000000382 0.000000246

72 1 0.000000180 -0.000001077 0.000001028

73 1 0.000000482 -0.000000032 0.000000492

74 1 0.000000518 -0.000000305 0.000000313

75 1 0.000000329 -0.000000048 0.000000885

76 1 -0.000000429 0.000000739 0.000000893

77 1 -0.000017580 0.000002183 -0.000002980

78 1 0.000017079 0.000008347 0.000003534

-------------------------------------------------------------------

Cartesian Forces: Max 0.000017580 RMS 0.000002310

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Thu Aug 29 16:25:18 2019, MaxMem= 4294967296 cpu: 2.0

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000019916 RMS 0.000003834

Search for a local minimum.

Step number 21 out of a maximum of 452

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -3.55D-06 DEPred=-1.19D-06 R= 2.98D+00

TightC=F SS= 1.41D+00 RLast= 1.91D-02 DXNew= 8.4090D-02 5.7407D-02

Trust test= 2.98D+00 RLast= 1.91D-02 DXMaxT set to 5.74D-02

ITU= 1 -1 -1 1 1 -1 -1 1 0 -1 1 1 -1 1 -1 -1 1 1 -1 1

ITU= 0

Eigenvalues --- 0.00073 0.00245 0.00398 0.00596 0.00721

Eigenvalues --- 0.00803 0.00916 0.01045 0.01059 0.01118

Eigenvalues --- 0.01135 0.01160 0.01263 0.01280 0.01302

Eigenvalues --- 0.01303 0.01322 0.01421 0.01427 0.01540

Eigenvalues --- 0.01554 0.01561 0.01596 0.01673 0.01710

Eigenvalues --- 0.01716 0.01727 0.01737 0.01755 0.01759

Eigenvalues --- 0.01762 0.01781 0.01799 0.01802 0.01885

Eigenvalues --- 0.01935 0.01989 0.01998 0.02012 0.02164

Eigenvalues --- 0.02170 0.02254 0.02288 0.02293 0.02304

Eigenvalues --- 0.02330 0.02391 0.02468 0.02469 0.02521

Eigenvalues --- 0.02539 0.02545 0.02585 0.02627 0.02629

Eigenvalues --- 0.02645 0.02648 0.02767 0.02779 0.02796

Eigenvalues --- 0.02803 0.02867 0.02871 0.02873 0.02874

Eigenvalues --- 0.02934 0.02959 0.03913 0.04087 0.04190

Eigenvalues --- 0.04317 0.04366 0.04465 0.04544 0.04573

Eigenvalues --- 0.08234 0.09657 0.09682 0.09745 0.09856

Eigenvalues --- 0.09880 0.10300 0.10434 0.10567 0.10697

Eigenvalues --- 0.10701 0.10704 0.10736 0.10736 0.11005

Eigenvalues --- 0.11398 0.11399 0.11410 0.11412 0.11983

Eigenvalues --- 0.11986 0.11997 0.12003 0.12281 0.12282

Eigenvalues --- 0.12325 0.12325 0.12770 0.12771 0.12773

Eigenvalues --- 0.12774 0.15719 0.15925 0.16302 0.16710

Eigenvalues --- 0.17206 0.17326 0.17586 0.17841 0.18007

Eigenvalues --- 0.18024 0.18276 0.18352 0.19241 0.19283

Eigenvalues --- 0.19358 0.19361 0.19371 0.19408 0.19414

Eigenvalues --- 0.19427 0.19551 0.19552 0.19554 0.19555

Eigenvalues --- 0.20296 0.21486 0.22042 0.22765 0.22888

Eigenvalues --- 0.23228 0.23769 0.24238 0.24749 0.25212

Eigenvalues --- 0.26276 0.26385 0.26662 0.27129 0.28524

Eigenvalues --- 0.28552 0.28749 0.29013 0.29785 0.31030

Eigenvalues --- 0.31698 0.32011 0.32854 0.33076 0.33226

Eigenvalues --- 0.33325 0.34147 0.34501 0.35052 0.35566

Eigenvalues --- 0.35625 0.35626 0.35634 0.35640 0.35757

Eigenvalues --- 0.35760 0.35765 0.35811 0.35925 0.35926

Eigenvalues --- 0.35931 0.35935 0.35986 0.35988 0.36007

Eigenvalues --- 0.36010 0.36191 0.36200 0.36246 0.36248

Eigenvalues --- 0.36975 0.37056 0.37240 0.37387 0.37393

Eigenvalues --- 0.37483 0.38141 0.38430 0.38504 0.38532

Eigenvalues --- 0.39458 0.40362 0.40735 0.41048 0.41067

Eigenvalues --- 0.41110 0.41194 0.41257 0.41353 0.41357

Eigenvalues --- 0.41569 0.41807 0.42269 0.42618 0.44516

Eigenvalues --- 0.45218 0.45893 0.45917 0.45927 0.45975

Eigenvalues --- 0.46010 0.46024 0.46258 0.46262 0.46316

Eigenvalues --- 0.46326 0.48433 0.49012 0.49405 0.49615

Eigenvalues --- 0.50751 0.50753 0.50779 0.50782 0.51864

Eigenvalues --- 0.52203 0.57174 0.57706

Cosine: 0.077 < 0.500

Cut down GDIIS temporarily because of the cosine check. E 7

DIIS coeff's: 1.19405 -0.19023 0.01264 -0.01855 -0.00364

DIIS coeff's: 0.00573

Cosine: 0.916 > 0.500

Length: 0.778

GDIIS step was calculated using 6 of the last 21 vectors.

Iteration 1 RMS(Cart)= 0.00071599 RMS(Int)= 0.00000017

Iteration 2 RMS(Cart)= 0.00000027 RMS(Int)= 0.00000005

ITry= 1 IFail=0 DXMaxC= 4.72D-03 DCOld= 1.00D+10 DXMaxT= 5.74D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.65683 0.00000 0.00002 -0.00001 0.00001 2.65685

R2 2.64099 -0.00001 -0.00002 0.00000 -0.00002 2.64097

R3 2.03708 -0.00000 -0.00000 -0.00000 -0.00001 2.03707

R4 2.59918 0.00001 0.00002 0.00001 0.00003 2.59921

R5 2.71597 -0.00000 -0.00005 0.00002 -0.00002 2.71595

R6 2.59902 0.00001 0.00002 0.00001 0.00003 2.59905

R7 1.91011 0.00002 0.00003 0.00002 0.00005 1.91016

R8 2.65652 -0.00000 0.00000 -0.00000 0.00000 2.65652

R9 2.71691 -0.00001 -0.00002 -0.00000 -0.00003 2.71688

R10 2.03713 -0.00000 -0.00000 0.00000 -0.00000 2.03713

R11 2.64080 -0.00002 -0.00005 0.00001 -0.00003 2.64076

R12 2.80419 -0.00000 0.00003 -0.00000 0.00003 2.80422

R13 2.59620 -0.00001 0.00002 -0.00003 -0.00001 2.59619

R14 2.76199 -0.00000 -0.00001 0.00001 -0.00001 2.76198

R15 2.59438 -0.00000 -0.00003 0.00003 -0.00000 2.59437

R16 2.76238 0.00000 0.00001 0.00000 0.00001 2.76239

R17 2.64279 -0.00000 0.00004 -0.00004 0.00000 2.64279

R18 2.55437 -0.00000 0.00001 -0.00000 0.00000 2.55437

R19 2.03919 0.00000 0.00000 0.00000 0.00000 2.03919

R20 2.03906 0.00000 0.00000 0.00000 0.00000 2.03906

R21 2.64282 -0.00000 0.00002 -0.00004 -0.00002 2.64280

R22 2.80371 -0.00000 0.00002 0.00002 0.00005 2.80376

R23 2.76239 0.00000 0.00000 0.00000 0.00001 2.76239

R24 2.59436 -0.00000 -0.00002 0.00003 0.00001 2.59437

R25 2.55437 -0.00000 0.00000 -0.00001 -0.00000 2.55437

R26 2.03919 0.00000 0.00000 -0.00000 0.00000 2.03919

R27 2.76198 -0.00000 -0.00001 0.00001 -0.00001 2.76198

R28 2.03906 0.00000 0.00000 -0.00000 0.00000 2.03906

R29 2.59620 -0.00001 0.00002 -0.00003 -0.00001 2.59619

R30 2.64076 -0.00002 -0.00003 0.00002 -0.00001 2.64075

R31 2.71686 -0.00001 -0.00000 0.00001 0.00000 2.71687

R32 2.80430 -0.00000 -0.00002 -0.00003 -0.00005 2.80425

R33 2.65657 -0.00000 -0.00002 -0.00002 -0.00003 2.65654

R34 2.59906 0.00001 0.00000 -0.00000 -0.00000 2.59906

R35 2.64095 -0.00001 -0.00001 0.00001 0.00001 2.64096

R36 2.03712 -0.00000 0.00000 0.00000 0.00000 2.03712

R37 2.65686 0.00000 0.00001 -0.00001 -0.00001 2.65686

R38 2.03707 -0.00000 0.00000 0.00000 0.00000 2.03707

R39 2.59921 0.00001 0.00001 -0.00000 0.00001 2.59922

R40 2.71593 -0.00000 -0.00002 0.00003 0.00000 2.71593

R41 1.91018 0.00002 0.00000 0.00000 0.00000 1.91018

R42 2.80381 -0.00000 -0.00002 0.00000 -0.00002 2.80379

R43 2.65124 0.00000 -0.00002 -0.00000 -0.00002 2.65123

R44 2.64989 0.00000 -0.00002 0.00000 -0.00001 2.64988

R45 2.62864 -0.00000 0.00000 0.00000 0.00001 2.62864

R46 2.04850 0.00000 0.00000 -0.00000 0.00000 2.04850

R47 2.63628 -0.00000 -0.00000 -0.00000 -0.00000 2.63628

R48 2.05017 0.00000 0.00000 0.00000 0.00000 2.05017

R49 2.63409 -0.00000 -0.00000 0.00000 -0.00000 2.63409

R50 2.05006 -0.00000 0.00000 -0.00000 -0.00000 2.05006

R51 2.63097 -0.00000 0.00001 -0.00000 0.00001 2.63098

R52 2.05014 0.00000 0.00000 0.00000 0.00000 2.05014

R53 2.04862 0.00000 0.00000 -0.00000 0.00000 2.04862

R54 2.63632 -0.00000 -0.00000 -0.00000 -0.00000 2.63632

R55 2.63423 -0.00000 0.00000 -0.00000 -0.00000 2.63422

R56 2.05006 -0.00000 -0.00000 0.00000 -0.00000 2.05006

R57 2.62890 0.00000 0.00001 -0.00000 0.00001 2.62891

R58 2.05018 -0.00000 0.00000 0.00000 0.00000 2.05018

R59 2.65144 0.00000 -0.00001 -0.00001 -0.00002 2.65142

R60 2.04848 0.00000 0.00000 -0.00000 0.00000 2.04848

R61 2.65011 -0.00000 -0.00001 -0.00001 -0.00002 2.65009

R62 2.63061 -0.00000 -0.00000 0.00001 0.00001 2.63061

R63 2.04855 -0.00000 0.00000 0.00000 0.00000 2.04855

R64 2.05016 0.00000 0.00000 -0.00000 0.00000 2.05016

R65 2.65007 -0.00000 0.00001 -0.00000 0.00000 2.65008

R66 2.65140 0.00000 0.00001 0.00000 0.00001 2.65141

R67 2.63062 -0.00000 -0.00001 0.00000 -0.00000 2.63062

R68 2.04855 -0.00000 -0.00000 -0.00000 -0.00000 2.04855

R69 2.63422 -0.00000 0.00000 -0.00000 -0.00000 2.63422

R70 2.05016 0.00000 0.00000 -0.00000 0.00000 2.05016

R71 2.63631 -0.00000 0.00000 0.00000 0.00000 2.63632

R72 2.05006 -0.00000 -0.00000 0.00000 -0.00000 2.05006

R73 2.62892 0.00000 0.00000 -0.00001 -0.00000 2.62892

R74 2.05018 -0.00000 -0.00000 -0.00000 -0.00000 2.05018

R75 2.04848 0.00000 0.00000 -0.00000 0.00000 2.04848

R76 2.64985 0.00000 0.00000 0.00001 0.00002 2.64986

R77 2.65120 -0.00000 0.00000 0.00001 0.00001 2.65121

R78 2.63099 -0.00000 0.00000 -0.00000 -0.00000 2.63098

R79 2.04863 0.00000 0.00000 -0.00000 -0.00000 2.04862

R80 2.63409 -0.00000 -0.00000 0.00000 -0.00000 2.63409

R81 2.05014 0.00000 -0.00000 -0.00000 -0.00000 2.05014

R82 2.63627 -0.00000 -0.00000 0.00000 0.00000 2.63628

R83 2.05006 -0.00000 -0.00000 -0.00000 -0.00000 2.05006

R84 2.62866 -0.00000 -0.00000 -0.00000 -0.00001 2.62865

R85 2.05017 0.00000 -0.00000 -0.00000 -0.00000 2.05017

R86 2.04850 0.00000 0.00000 -0.00000 0.00000 2.04850

A1 1.88155 0.00000 0.00000 0.00001 0.00001 1.88156

A2 2.18784 -0.00000 0.00002 -0.00001 0.00001 2.18785

A3 2.21378 -0.00000 -0.00003 0.00001 -0.00002 2.21376

A4 1.86797 0.00000 0.00000 0.00000 0.00001 1.86798

A5 2.22221 -0.00002 -0.00001 -0.00005 -0.00006 2.22215

A6 2.19256 0.00001 0.00000 0.00004 0.00004 2.19260

A7 1.92514 -0.00001 -0.00002 -0.00001 -0.00003 1.92511

A8 2.17736 0.00001 -0.00001 0.00006 0.00005 2.17741

A9 2.17990 0.00000 0.00001 -0.00006 -0.00005 2.17985

A10 1.86809 0.00001 0.00001 0.00001 0.00002 1.86811

A11 2.19438 -0.00000 0.00003 -0.00003 0.00000 2.19438

A12 2.22032 -0.00000 -0.00005 0.00002 -0.00003 2.22029

A13 1.88166 -0.00000 0.00000 -0.00001 -0.00000 1.88166

A14 2.21404 -0.00000 -0.00002 0.00000 -0.00001 2.21402

A15 2.18746 0.00000 0.00001 0.00001 0.00002 2.18748

A16 2.18669 -0.00002 0.00004 -0.00005 -0.00001 2.18668

A17 2.02288 0.00002 -0.00000 0.00006 0.00005 2.02293

A18 2.07357 0.00000 -0.00004 -0.00000 -0.00004 2.07353

A19 2.19178 -0.00002 -0.00003 -0.00003 -0.00005 2.19173

A20 2.16528 0.00001 0.00002 0.00001 0.00004 2.16532

A21 1.92609 0.00001 0.00000 0.00001 0.00002 1.92611

A22 1.84709 -0.00000 -0.00000 -0.00000 -0.00001 1.84708

A23 1.92647 0.00000 0.00001 -0.00001 -0.00000 1.92647

A24 2.19207 0.00000 0.00001 0.00001 0.00002 2.19209

A25 2.16463 -0.00000 -0.00001 -0.00000 -0.00002 2.16462

A26 1.86205 -0.00000 0.00000 0.00000 0.00000 1.86205

A27 2.19692 0.00000 -0.00000 -0.00001 -0.00001 2.19691

A28 2.22382 0.00000 0.00000 0.00001 0.00001 2.22384

A29 1.86207 -0.00000 -0.00001 -0.00000 -0.00001 1.86206

A30 2.19688 0.00000 0.00001 -0.00000 0.00000 2.19688

A31 2.22390 0.00000 0.00000 0.00001 0.00001 2.22391

A32 2.18519 0.00001 0.00005 0.00006 0.00010 2.18529

A33 2.02528 -0.00001 0.00003 -0.00003 -0.00000 2.02528

A34 2.07267 -0.00000 -0.00008 -0.00002 -0.00010 2.07257

A35 2.16468 -0.00000 -0.00004 -0.00001 -0.00005 2.16463

A36 2.19202 0.00000 0.00003 0.00002 0.00005 2.19207

A37 1.92647 0.00000 0.00001 -0.00001 0.00000 1.92647

A38 1.86205 -0.00000 -0.00000 0.00000 -0.00000 1.86205

A39 2.19691 0.00000 -0.00000 -0.00001 -0.00001 2.19690

A40 2.22383 0.00000 0.00000 0.00000 0.00001 2.22384

A41 1.86206 -0.00000 -0.00000 -0.00000 -0.00001 1.86206

A42 2.22390 0.00000 0.00000 0.00001 0.00001 2.22391

A43 2.19688 0.00000 0.00000 -0.00000 -0.00000 2.19688

A44 1.92609 0.00001 0.00001 0.00001 0.00002 1.92611

A45 2.16526 0.00001 0.00004 0.00001 0.00005 2.16531

A46 2.19180 -0.00002 -0.00004 -0.00002 -0.00007 2.19174

A47 1.84709 -0.00000 -0.00001 -0.00000 -0.00001 1.84708

A48 2.18685 -0.00002 -0.00003 -0.00009 -0.00012 2.18673

A49 2.07338 0.00000 0.00005 0.00004 0.00009 2.07347

A50 2.02292 0.00002 -0.00002 0.00005 0.00003 2.02294

A51 2.22029 -0.00000 -0.00004 0.00003 -0.00001 2.22028

A52 2.19439 -0.00000 0.00004 -0.00004 -0.00001 2.19438

A53 1.86809 0.00001 0.00001 0.00001 0.00002 1.86811

A54 1.88167 -0.00000 -0.00000 -0.00001 -0.00001 1.88166

A55 2.18751 0.00000 -0.00001 -0.00001 -0.00002 2.18749

A56 2.21398 -0.00000 0.00001 0.00002 0.00003 2.21401

A57 1.88155 0.00000 0.00000 0.00000 0.00001 1.88156

A58 2.21375 -0.00000 -0.00001 0.00002 0.00000 2.21375

A59 2.18787 -0.00000 0.00001 -0.00002 -0.00001 2.18786

A60 1.86798 0.00000 -0.00000 0.00000 -0.00000 1.86798

A61 2.22221 -0.00002 -0.00001 -0.00005 -0.00006 2.22215

A62 2.19253 0.00001 0.00002 0.00005 0.00007 2.19259

A63 1.92511 -0.00001 -0.00001 -0.00001 -0.00001 1.92510

A64 2.17991 0.00000 0.00002 -0.00007 -0.00006 2.17985

A65 2.17728 0.00001 0.00002 0.00009 0.00011 2.17739

A66 2.18532 0.00001 -0.00002 0.00003 0.00001 2.18533

A67 2.07249 -0.00000 0.00001 0.00002 0.00003 2.07252

A68 2.02534 -0.00001 0.00001 -0.00005 -0.00004 2.02530

A69 2.10454 0.00000 -0.00001 0.00001 -0.00000 2.10453

A70 2.10698 -0.00000 -0.00000 -0.00000 -0.00001 2.10698

A71 2.07166 -0.00000 0.00001 -0.00000 0.00001 2.07167

A72 2.10512 0.00000 -0.00000 0.00000 -0.00000 2.10511

A73 2.08514 0.00000 0.00001 -0.00001 0.00001 2.08515

A74 2.09276 -0.00000 -0.00001 0.00001 -0.00000 2.09276

A75 2.09776 0.00000 -0.00000 0.00000 -0.00000 2.09776

A76 2.08897 -0.00000 0.00000 -0.00000 -0.00000 2.08897

A77 2.09645 -0.00000 -0.00000 0.00000 0.00000 2.09646

A78 2.08903 -0.00000 0.00000 -0.00000 -0.00000 2.08903

A79 2.09689 0.00000 -0.00000 0.00000 -0.00000 2.09689

A80 2.09726 0.00000 0.00000 -0.00000 0.00000 2.09726

A81 2.09760 -0.00000 -0.00000 -0.00000 -0.00000 2.09760

A82 2.09706 -0.00000 0.00000 -0.00000 0.00000 2.09706

A83 2.08852 0.00000 0.00000 0.00000 0.00000 2.08852

A84 2.10507 0.00000 -0.00001 0.00000 -0.00000 2.10507

A85 2.08430 0.00000 0.00001 -0.00001 0.00000 2.08430

A86 2.09366 -0.00000 -0.00001 0.00001 0.00000 2.09366

A87 2.08896 -0.00000 0.00000 0.00000 0.00000 2.08896

A88 2.09700 0.00000 0.00000 -0.00000 0.00000 2.09700

A89 2.09723 -0.00000 -0.00000 0.00000 -0.00000 2.09723

A90 2.09801 -0.00000 0.00000 -0.00000 -0.00000 2.09800

A91 2.09647 0.00000 0.00000 0.00000 0.00000 2.09647

A92 2.08871 0.00000 -0.00000 0.00000 -0.00000 2.08871

A93 2.10487 -0.00000 -0.00001 0.00000 -0.00001 2.10486

A94 2.09330 -0.00000 0.00001 -0.00000 0.00001 2.09331

A95 2.08482 0.00000 -0.00000 0.00000 0.00000 2.08482

A96 2.10711 0.00000 0.00007 -0.00004 0.00003 2.10714

A97 2.10459 -0.00000 -0.00008 0.00003 -0.00005 2.10454

A98 2.07148 -0.00000 0.00001 0.00001 0.00002 2.07149

A99 2.10548 0.00000 0.00000 -0.00001 -0.00001 2.10547

A100 2.08384 0.00000 0.00000 -0.00000 -0.00000 2.08384

A101 2.09374 -0.00000 -0.00000 0.00001 0.00001 2.09375

A102 2.09746 0.00000 -0.00001 0.00000 -0.00000 2.09745

A103 2.09705 -0.00000 0.00000 -0.00000 -0.00000 2.09705

A104 2.08867 -0.00000 0.00000 -0.00000 0.00000 2.08868

A105 2.10454 -0.00000 -0.00005 0.00004 -0.00001 2.10453

A106 2.10713 0.00000 0.00006 -0.00004 0.00002 2.10715

A107 2.07151 -0.00000 -0.00001 0.00000 -0.00000 2.07150

A108 2.10546 0.00000 0.00001 -0.00001 0.00000 2.10547

A109 2.08383 0.00000 0.00001 -0.00000 0.00001 2.08384

A110 2.09376 -0.00000 -0.00002 0.00001 -0.00001 2.09375

A111 2.09745 0.00000 -0.00000 0.00000 -0.00000 2.09745

A112 2.08868 -0.00000 0.00000 -0.00000 -0.00000 2.08868

A113 2.09705 -0.00000 0.00000 -0.00000 0.00000 2.09705

A114 2.08896 -0.00000 -0.00000 0.00000 0.00000 2.08896

A115 2.09723 -0.00000 -0.00000 0.00000 -0.00000 2.09723

A116 2.09700 0.00000 0.00000 -0.00000 0.00000 2.09700

A117 2.09800 0.00000 0.00000 -0.00000 0.00000 2.09800

A118 2.09648 -0.00000 -0.00000 -0.00000 -0.00000 2.09647

A119 2.08871 0.00000 -0.00000 0.00000 0.00000 2.08871

A120 2.10485 -0.00000 -0.00000 0.00000 0.00000 2.10486

A121 2.08483 0.00000 -0.00000 0.00000 -0.00000 2.08482

A122 2.09331 -0.00000 0.00001 -0.00000 0.00000 2.09331

A123 2.10692 -0.00000 0.00003 0.00001 0.00003 2.10696

A124 2.10456 0.00000 -0.00002 0.00000 -0.00002 2.10454

A125 2.07169 -0.00000 -0.00000 -0.00001 -0.00001 2.07168

A126 2.10506 0.00000 -0.00000 0.00000 0.00000 2.10507

A127 2.08429 0.00000 0.00002 -0.00001 0.00001 2.08430

A128 2.09368 -0.00000 -0.00002 0.00001 -0.00001 2.09367

A129 2.09760 -0.00000 0.00000 0.00000 0.00000 2.09760

A130 2.08852 0.00000 -0.00000 0.00000 -0.00000 2.08852

A131 2.09706 -0.00000 0.00000 -0.00000 -0.00000 2.09706

A132 2.08903 -0.00000 0.00000 -0.00000 -0.00000 2.08903

A133 2.09726 0.00000 0.00000 -0.00000 0.00000 2.09726

A134 2.09689 0.00000 -0.00000 0.00000 -0.00000 2.09689

A135 2.09776 0.00000 -0.00000 0.00000 0.00000 2.09776

A136 2.09646 -0.00000 -0.00000 -0.00000 -0.00000 2.09646

A137 2.08897 -0.00000 0.00000 -0.00000 0.00000 2.08897

A138 2.10510 0.00000 0.00000 0.00000 0.00001 2.10511

A139 2.08515 0.00000 0.00001 -0.00001 -0.00000 2.08515

A140 2.09277 -0.00000 -0.00001 0.00001 -0.00001 2.09276

D1 0.01555 -0.00000 0.00003 0.00001 0.00003 0.01559

D2 -3.09534 -0.00000 0.00017 0.00016 0.00033 -3.09502

D3 -3.12068 0.00000 -0.00005 -0.00004 -0.00009 -3.12078

D4 0.05160 -0.00000 0.00009 0.00011 0.00020 0.05181

D5 -0.00064 0.00000 -0.00002 0.00000 -0.00002 -0.00066

D6 -3.13445 0.00000 -0.00004 -0.00009 -0.00013 -3.13458

D7 3.13549 0.00000 0.00006 0.00005 0.00011 3.13560

D8 0.00169 0.00000 0.00005 -0.00005 -0.00000 0.00168

D9 -0.02525 0.00000 -0.00002 -0.00002 -0.00004 -0.02529

D10 3.07528 -0.00000 -0.00039 -0.00037 -0.00076 3.07451

D11 3.08631 -0.00000 -0.00016 -0.00017 -0.00033 3.08599

D12 -0.09635 -0.00000 -0.00053 -0.00052 -0.00105 -0.09740

D13 -2.95131 0.00000 -0.00083 -0.00027 -0.00110 -2.95241

D14 0.17998 0.00000 -0.00072 -0.00014 -0.00087 0.17911

D15 0.22639 0.00000 -0.00066 -0.00009 -0.00076 0.22564

D16 -2.92550 0.00000 -0.00056 0.00004 -0.00052 -2.92602

D17 0.02486 0.00000 0.00001 0.00002 0.00002 0.02488

D18 -3.08818 -0.00000 0.00006 0.00014 0.00020 -3.08798

D19 -3.07560 0.00000 0.00038 0.00037 0.00075 -3.07485

D20 0.09456 -0.00000 0.00043 0.00049 0.00092 0.09548

D21 -0.01452 -0.00000 0.00001 -0.00001 -0.00000 -0.01452

D22 3.11944 -0.00000 0.00002 0.00008 0.00011 3.11955

D23 3.09796 0.00000 -0.00004 -0.00014 -0.00018 3.09779

D24 -0.05127 0.00000 -0.00003 -0.00004 -0.00007 -0.05134

D25 -0.23744 0.00000 0.00039 0.00036 0.00074 -0.23670

D26 2.91499 0.00000 0.00031 0.00024 0.00054 2.91553

D27 2.93844 0.00000 0.00045 0.00050 0.00095 2.93939

D28 -0.19231 0.00000 0.00037 0.00038 0.00075 -0.19157

D29 -0.12459 0.00000 0.00024 -0.00009 0.00015 -0.12445

D30 3.02588 0.00000 0.00023 -0.00015 0.00008 3.02596

D31 3.00588 0.00000 0.00032 0.00003 0.00035 3.00623

D32 -0.12684 0.00000 0.00031 -0.00003 0.00028 -0.12655

D33 -0.99831 -0.00000 -0.00053 0.00010 -0.00043 -0.99874

D34 2.13984 -0.00000 -0.00046 0.00014 -0.00033 2.13952

D35 2.15337 -0.00000 -0.00060 -0.00001 -0.00062 2.15276

D36 -0.99166 -0.00000 -0.00054 0.00002 -0.00051 -0.99217

D37 -3.09199 -0.00000 -0.00004 -0.00004 -0.00008 -3.09207

D38 0.04176 -0.00000 -0.00003 0.00001 -0.00002 0.04174

D39 3.10677 0.00000 0.00001 0.00006 0.00007 3.10684

D40 -0.06125 0.00000 0.00008 0.00003 0.00011 -0.06114

D41 -0.02712 0.00000 0.00001 0.00000 0.00001 -0.02711

D42 3.08805 0.00000 0.00008 -0.00003 0.00005 3.08810

D43 -0.04096 0.00000 0.00005 -0.00002 0.00002 -0.04093

D44 3.09607 0.00000 0.00004 -0.00007 -0.00003 3.09604

D45 0.02494 -0.00000 -0.00004 0.00002 -0.00002 0.02492

D46 -3.08818 -0.00000 -0.00004 0.00003 -0.00002 -3.08820

D47 -3.11218 -0.00000 -0.00004 0.00007 0.00004 -3.11214

D48 0.05789 -0.00000 -0.00004 0.00007 0.00003 0.05792

D49 0.13418 0.00000 0.00007 -0.00007 0.00000 0.13419

D50 -2.99762 0.00000 0.00030 0.00000 0.00031 -2.99732

D51 -3.01257 0.00000 0.00007 -0.00013 -0.00006 -3.01263

D52 0.13881 0.00000 0.00030 -0.00005 0.00024 0.13905

D53 0.00127 0.00000 0.00002 -0.00002 0.00000 0.00128

D54 -3.11336 0.00000 -0.00005 0.00001 -0.00004 -3.11339

D55 3.11382 -0.00000 0.00002 -0.00002 0.00000 3.11383

D56 -0.00081 -0.00000 -0.00005 0.00001 -0.00003 -0.00085

D57 -3.01290 0.00000 0.00019 -0.00002 0.00017 -3.01273

D58 0.13414 0.00000 0.00008 -0.00005 0.00003 0.13417

D59 0.13925 0.00000 0.00008 -0.00015 -0.00007 0.13918

D60 -2.99689 0.00000 -0.00003 -0.00018 -0.00021 -2.99710

D61 0.99223 0.00000 0.00036 0.00011 0.00047 0.99270

D62 -2.14574 0.00000 0.00033 0.00004 0.00037 -2.14537

D63 -2.15897 0.00000 0.00046 0.00023 0.00069 -2.15828

D64 0.98625 0.00000 0.00043 0.00016 0.00059 0.98684

D65 -3.11185 -0.00000 -0.00017 -0.00002 -0.00019 -3.11204

D66 0.05821 -0.00000 -0.00017 -0.00002 -0.00019 0.05802

D67 0.02502 -0.00000 -0.00008 0.00000 -0.00007 0.02494

D68 -3.08811 -0.00000 -0.00008 0.00001 -0.00007 -3.08818

D69 3.09577 0.00000 0.00016 0.00003 0.00018 3.09595

D70 -0.04101 0.00000 0.00006 -0.00000 0.00006 -0.04095

D71 0.00121 0.00000 0.00005 -0.00001 0.00005 0.00126

D72 -3.11348 0.00000 0.00000 0.00005 0.00005 -3.11343

D73 3.11376 -0.00000 0.00006 -0.00001 0.00005 3.11381

D74 -0.00093 -0.00000 0.00001 0.00004 0.00005 -0.00088

D75 -0.02709 0.00000 -0.00002 0.00001 -0.00001 -0.02710

D76 3.10692 0.00000 -0.00007 0.00004 -0.00003 3.10689

D77 3.08814 0.00000 0.00003 -0.00005 -0.00001 3.08813

D78 -0.06104 0.00000 -0.00003 -0.00001 -0.00003 -0.06107

D79 0.04177 -0.00000 -0.00003 -0.00000 -0.00003 0.04174

D80 -3.09209 -0.00000 0.00003 -0.00004 -0.00001 -3.09211

D81 3.02577 0.00000 0.00029 -0.00015 0.00014 3.02592

D82 -0.12630 0.00000 0.00007 -0.00017 -0.00010 -0.12640

D83 -0.12456 0.00000 0.00023 -0.00011 0.00012 -0.12444

D84 3.00655 0.00000 0.00000 -0.00013 -0.00013 3.00642

D85 2.94148 -0.00000 -0.00092 -0.00026 -0.00117 2.94031

D86 -0.23529 0.00000 -0.00057 -0.00019 -0.00076 -0.23605

D87 -0.18990 0.00000 -0.00070 -0.00023 -0.00093 -0.19084

D88 2.91651 0.00000 -0.00035 -0.00017 -0.00052 2.91599

D89 -0.99315 -0.00000 0.00015 0.00038 0.00052 -0.99262

D90 2.15170 -0.00000 0.00019 0.00036 0.00055 2.15225

D91 2.13894 -0.00000 -0.00005 0.00035 0.00030 2.13924

D92 -0.99940 -0.00000 -0.00001 0.00034 0.00033 -0.99907

D93 3.09716 0.00000 0.00034 0.00005 0.00039 3.09755

D94 -0.05169 0.00000 0.00018 0.00004 0.00023 -0.05146

D95 -0.01457 0.00000 0.00004 -0.00000 0.00004 -0.01453

D96 3.11977 -0.00000 -0.00012 -0.00001 -0.00012 3.11965

D97 -3.08734 -0.00000 -0.00033 -0.00006 -0.00039 -3.08773

D98 0.09759 -0.00000 -0.00091 -0.00029 -0.00120 0.09639

D99 0.02495 -0.00000 -0.00004 -0.00001 -0.00005 0.02490

D100 -3.07330 -0.00000 -0.00062 -0.00024 -0.00086 -3.07416

D101 -0.00065 0.00000 -0.00002 0.00001 -0.00001 -0.00067

D102 3.13585 -0.00000 -0.00011 -0.00004 -0.00015 3.13571

D103 -3.13485 0.00000 0.00014 0.00001 0.00015 -3.13470

D104 0.00166 0.00000 0.00005 -0.00003 0.00002 0.00167

D105 0.01562 -0.00000 -0.00000 -0.00001 -0.00002 0.01561

D106 -3.09444 -0.00000 -0.00023 -0.00008 -0.00031 -3.09475

D107 -3.12098 -0.00000 0.00008 0.00003 0.00011 -3.12086

D108 0.05214 -0.00000 -0.00014 -0.00003 -0.00017 0.05196

D109 -0.02536 0.00000 0.00003 0.00001 0.00004 -0.02531

D110 3.07297 0.00000 0.00061 0.00024 0.00085 3.07382

D111 3.08540 0.00000 0.00025 0.00007 0.00032 3.08572

D112 -0.09946 0.00000 0.00083 0.00030 0.00113 -0.09833

D113 -2.95426 0.00000 0.00051 0.00045 0.00096 -2.95330

D114 0.17778 0.00000 0.00029 0.00038 0.00067 0.17845

D115 0.22442 0.00000 0.00024 0.00038 0.00062 0.22504

D116 -2.92673 0.00000 0.00002 0.00031 0.00033 -2.92640

D117 0.98754 0.00000 -0.00021 -0.00009 -0.00030 0.98724

D118 -2.15735 0.00000 -0.00032 -0.00011 -0.00043 -2.15778

D119 -2.14515 0.00000 -0.00000 -0.00002 -0.00003 -2.14518

D120 0.99315 0.00000 -0.00012 -0.00004 -0.00016 0.99299

D121 -3.13045 0.00000 0.00003 0.00005 0.00007 -3.13037

D122 -0.00835 0.00000 0.00006 0.00002 0.00008 -0.00828

D123 0.01452 -0.00000 -0.00003 0.00001 -0.00002 0.01449

D124 3.13661 -0.00000 -0.00000 -0.00002 -0.00002 3.13659

D125 -3.14021 -0.00000 -0.00002 -0.00006 -0.00008 -3.14030

D126 -0.01706 -0.00000 -0.00000 -0.00004 -0.00004 -0.01710

D127 -0.00200 0.00000 0.00004 -0.00002 0.00002 -0.00198

D128 3.12116 0.00000 0.00006 0.00000 0.00006 3.12121

D129 -0.01619 -0.00000 0.00001 -0.00000 0.00001 -0.01618

D130 3.12476 -0.00000 0.00000 0.00000 0.00001 3.12476

D131 -3.13820 0.00000 -0.00002 0.00003 0.00001 -3.13819

D132 0.00275 0.00000 -0.00003 0.00003 0.00000 0.00275

D133 0.00513 0.00000 0.00000 0.00000 0.00000 0.00513

D134 -3.13361 0.00000 0.00001 -0.00002 -0.00001 -3.13362

D135 -3.13582 0.00000 0.00001 0.00000 0.00001 -3.13581

D136 0.00863 0.00000 0.00002 -0.00002 -0.00000 0.00863

D137 0.00734 0.00000 0.00000 -0.00002 -0.00001 0.00733

D138 -3.13195 0.00000 -0.00002 -0.00001 -0.00003 -3.13197

D139 -3.13711 0.00000 -0.00000 0.00000 0.00000 -3.13711

D140 0.00679 -0.00000 -0.00003 0.00001 -0.00001 0.00678

D141 -0.00889 -0.00000 -0.00002 0.00003 0.00000 -0.00888

D142 -3.13194 -0.00000 -0.00004 0.00000 -0.00004 -3.13198

D143 3.13042 -0.00000 -0.00000 0.00002 0.00001 3.13043

D144 0.00736 0.00000 -0.00002 -0.00001 -0.00003 0.00734

D145 -0.00538 0.00000 -0.00000 0.00000 0.00000 -0.00538

D146 3.13574 -0.00000 -0.00001 -0.00001 -0.00002 3.13571

D147 3.13480 0.00000 0.00003 -0.00000 0.00003 3.13483

D148 -0.00727 0.00000 0.00002 -0.00002 0.00001 -0.00727

D149 -0.00644 0.00000 0.00002 -0.00000 0.00001 -0.00642

D150 3.13183 -0.00000 0.00002 0.00002 0.00004 3.13187

D151 3.13657 -0.00000 -0.00002 0.00000 -0.00001 3.13656

D152 -0.00835 -0.00000 -0.00001 0.00002 0.00001 -0.00834

D153 0.01661 -0.00000 -0.00002 -0.00002 -0.00003 0.01657

D154 3.13672 -0.00000 -0.00001 -0.00001 -0.00002 3.13671

D155 -3.12451 -0.00000 -0.00001 -0.00000 -0.00001 -3.12452

D156 -0.00439 0.00000 -0.00000 0.00001 0.00001 -0.00439

D157 3.12942 0.00000 -0.00001 -0.00004 -0.00005 3.12937

D158 -0.01572 0.00000 0.00002 0.00003 0.00005 -0.01568

D159 0.00921 0.00000 -0.00002 -0.00005 -0.00007 0.00914

D160 -3.13594 -0.00000 0.00001 0.00002 0.00003 -3.13591

D161 -3.14127 -0.00000 0.00003 0.00004 0.00007 -3.14121

D162 0.01763 -0.00000 -0.00002 0.00003 0.00001 0.01764

D163 0.00387 -0.00000 -0.00000 -0.00003 -0.00003 0.00384

D164 -3.12041 0.00000 -0.00005 -0.00004 -0.00008 -3.12050

D165 0.00715 -0.00000 -0.00001 0.00002 0.00000 0.00715

D166 -3.13113 0.00000 -0.00002 -0.00000 -0.00002 -3.13116

D167 3.13133 -0.00000 0.00003 0.00002 0.00005 3.13139

D168 -0.00695 -0.00000 0.00003 0.00000 0.00003 -0.00692

D169 -3.14103 -0.00000 -0.00008 -0.00003 -0.00011 -3.14114

D170 0.01774 -0.00000 -0.00006 -0.00001 -0.00007 0.01768

D171 0.00380 -0.00000 0.00003 -0.00001 0.00002 0.00381

D172 -3.12062 0.00000 0.00005 0.00001 0.00006 -3.12056

D173 3.12920 0.00000 0.00009 0.00002 0.00010 3.12931

D174 0.00899 0.00000 0.00008 0.00000 0.00009 0.00907

D175 -0.01562 0.00000 -0.00002 -0.00000 -0.00002 -0.01565

D176 -3.13584 -0.00000 -0.00003 -0.00001 -0.00004 -3.13588

D177 0.00716 0.00000 -0.00002 0.00002 -0.00000 0.00715

D178 -3.13118 0.00000 0.00000 0.00001 0.00001 -3.13117

D179 3.13147 -0.00000 -0.00004 -0.00000 -0.00004 3.13143

D180 -0.00686 -0.00000 -0.00001 -0.00002 -0.00003 -0.00689

D181 -0.00641 -0.00000 0.00000 -0.00001 -0.00001 -0.00642

D182 3.13655 -0.00000 -0.00001 0.00001 -0.00000 3.13655

D183 3.13192 -0.00000 -0.00002 -0.00000 -0.00002 3.13189

D184 -0.00831 -0.00000 -0.00003 0.00002 -0.00002 -0.00833

D185 -0.00538 0.00000 0.00000 0.00000 0.00000 -0.00538

D186 3.13568 0.00000 0.00001 0.00001 0.00002 3.13570

D187 3.13485 0.00000 0.00001 -0.00002 -0.00000 3.13484

D188 -0.00728 0.00000 0.00003 -0.00001 0.00001 -0.00727

D189 0.01654 -0.00000 0.00001 0.00001 0.00001 0.01655

D190 3.13665 0.00000 0.00001 0.00002 0.00003 3.13669

D191 -3.12452 -0.00000 -0.00000 0.00000 -0.00000 -3.12452

D192 -0.00441 0.00000 0.00000 0.00002 0.00002 -0.00439

D193 -3.14033 -0.00000 0.00005 -0.00005 -0.00000 -3.14033

D194 -0.01707 -0.00000 0.00001 -0.00005 -0.00003 -0.01711

D195 -0.00193 0.00000 0.00001 -0.00004 -0.00003 -0.00196

D196 3.12133 0.00000 -0.00003 -0.00003 -0.00006 3.12127

D197 -3.13035 0.00000 -0.00004 0.00004 0.00001 -3.13034

D198 -0.00824 0.00000 -0.00001 0.00001 0.00000 -0.00824

D199 0.01443 -0.00000 0.00000 0.00003 0.00003 0.01447

D200 3.13654 -0.00000 0.00003 -0.00000 0.00003 3.13657

D201 -0.00888 -0.00000 -0.00002 0.00002 0.00000 -0.00888

D202 3.13044 -0.00000 -0.00002 0.00001 -0.00000 3.13044

D203 -3.13204 -0.00000 0.00002 0.00002 0.00003 -3.13201

D204 0.00728 0.00000 0.00002 0.00001 0.00003 0.00731

D205 0.00729 0.00000 0.00002 0.00000 0.00002 0.00731

D206 -3.13710 0.00000 -0.00001 0.00001 -0.00000 -3.13710

D207 -3.13202 -0.00000 0.00002 0.00001 0.00003 -3.13200

D208 0.00677 -0.00000 -0.00001 0.00002 0.00000 0.00677

D209 0.00516 0.00000 -0.00001 -0.00001 -0.00002 0.00514

D210 -3.13577 0.00000 -0.00001 -0.00001 -0.00002 -3.13579

D211 -3.13363 0.00000 0.00002 -0.00001 0.00001 -3.13362

D212 0.00862 0.00000 0.00002 -0.00001 0.00001 0.00863

D213 -0.01616 -0.00000 -0.00000 -0.00001 -0.00001 -0.01617

D214 -3.13818 0.00000 -0.00003 0.00002 -0.00001 -3.13818

D215 3.12478 -0.00000 -0.00000 -0.00001 -0.00001 3.12477

D216 0.00276 0.00000 -0.00003 0.00003 -0.00000 0.00275

Item Value Threshold Converged?

Maximum Force 0.000020 0.000450 YES

RMS Force 0.000004 0.000300 YES

Maximum Displacement 0.004717 0.001800 NO

RMS Displacement 0.000716 0.001200 YES

Predicted change in Energy=-3.211618D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

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Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=1 Diff= 7.23D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 0.963236 -4.116328 0.551246

2 6 0 1.312306 -2.800301 0.200677

3 7 0 0.138370 -2.110277 0.006808

4 6 0 -0.940563 -2.943608 0.188666

5 6 0 -0.431460 -4.205068 0.543247

6 6 0 -2.320270 -2.582576 0.006793

7 6 0 -2.803191 -1.277418 -0.120353

8 7 0 -2.063244 -0.131724 0.044909

9 6 0 -2.945432 0.909101 -0.107529

10 6 0 -4.277757 0.403551 -0.433376

11 6 0 -4.189627 -0.945257 -0.442330

12 6 0 2.635510 -2.265772 0.030376

13 6 0 2.945442 -0.909052 -0.107761

14 6 0 4.277763 -0.403449 -0.433543

15 6 0 4.189631 0.945362 -0.442287

16 6 0 2.803191 1.277467 -0.120273

17 7 0 2.063249 0.131744 0.044817

18 6 0 2.320261 2.582601 0.007018

19 6 0 0.940569 2.943666 0.188889

20 6 0 0.431452 4.205369 0.542615

21 6 0 -0.963239 4.116631 0.550653

22 6 0 -1.312303 2.800366 0.200958

23 7 0 -0.138362 2.110201 0.007590

24 6 0 -2.635491 2.265803 0.030702

25 6 0 -3.285496 -3.709023 -0.031861

26 6 0 -3.142952 -4.739132 -0.973603

27 6 0 -4.054930 -5.788490 -1.019135

28 6 0 -5.114037 -5.837400 -0.112444

29 6 0 -5.258165 -4.826246 0.836105

30 6 0 -4.354785 -3.767527 0.873411

31 6 0 5.839074 -5.120258 -0.013570

32 6 0 4.791938 -5.228400 -0.929024

33 6 0 3.746814 -4.310452 -0.908630

34 6 0 3.740894 -3.255341 0.016203

35 6 0 4.799097 -3.156120 0.931078

36 6 0 5.837013 -4.083698 0.918469

37 6 0 -3.740919 3.255345 0.016388

38 6 0 -4.799002 3.156316 0.931413

39 6 0 -5.837002 4.083803 0.918630

40 6 0 -5.839258 5.120067 -0.013736

41 6 0 -4.792243 5.228002 -0.929352

42 6 0 -3.747041 4.310142 -0.908793

43 6 0 3.285532 3.709029 -0.031719

44 6 0 4.354632 3.767702 0.873753

45 6 0 5.258080 4.826363 0.836359

46 6 0 5.114199 5.837280 -0.112480

47 6 0 4.055285 5.788185 -1.019385

48 6 0 3.143243 4.738881 -0.973771

49 1 0 1.659683 -4.904651 0.786904

50 1 0 -1.025311 -5.074956 0.772863

51 1 0 -5.146680 1.005294 -0.650911

52 1 0 -4.973141 -1.652049 -0.667824

53 1 0 5.146685 -1.005157 -0.651180

54 1 0 4.973149 1.652192 -0.667649

55 1 0 1.025278 5.075448 0.771562

56 1 0 -1.659682 4.905143 0.785683

57 1 0 -2.323529 -4.704075 -1.682415

58 1 0 -3.939281 -6.568993 -1.763754

59 1 0 -5.820550 -6.660040 -0.143907

60 1 0 -6.073851 -4.861474 1.550527

61 1 0 -4.465113 -2.987734 1.618386

62 1 0 6.650424 -5.840285 -0.026238

63 1 0 4.789252 -6.029182 -1.660987

64 1 0 2.937672 -4.395912 -1.624914

65 1 0 4.796072 -2.356937 1.663508

66 1 0 6.642912 -3.997740 1.639677

67 1 0 -4.795838 2.357337 1.664066

68 1 0 -6.642818 3.997995 1.639948

69 1 0 -6.650673 5.840018 -0.026543

70 1 0 -4.789716 6.028543 -1.661580

71 1 0 -2.938001 4.395428 -1.625213

72 1 0 4.464777 2.988075 1.618931

73 1 0 6.073628 4.861727 1.550932

74 1 0 5.820764 6.659873 -0.144014

75 1 0 3.939835 6.568494 -1.764238

76 1 0 2.323973 4.703673 -1.682753

77 1 0 0.077884 -1.122901 -0.200966

78 1 0 -0.077874 1.122555 -0.198956

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0587906 0.0582552 0.0300942

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Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5356.8941668025 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122019428 Hartrees.

Nuclear repulsion after empirical dispersion term = 5356.6819648597 Hartrees.

Force inversion solution in PCM.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5786

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.37D-10

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 305

GePol: Fraction of low-weight points (<1% of avg) = 5.27%

GePol: Cavity surface area = 610.634 Ang\*\*2

GePol: Cavity volume = 627.956 Ang\*\*3

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Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0020998563 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5356.6798650034 Hartrees.

Leave Link 301 at Thu Aug 29 16:25:19 2019, MaxMem= 4294967296 cpu: 2.0

(Enter /home/kira/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Thu Aug 29 16:25:20 2019, MaxMem= 4294967296 cpu: 27.5

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Thu Aug 29 16:25:21 2019, MaxMem= 4294967296 cpu: 3.0

(Enter /home/kira/g09/l401.exe)

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= 0.000000 0.000000 -0.000000

Rot= 0.999997 -0.000009 -0.000001 0.002558 Ang= -0.29 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0182

Leave Link 401 at Thu Aug 29 16:25:24 2019, MaxMem= 4294967296 cpu: 51.5

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 590000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 100433388.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.10D-15 for 5781.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.13D-15 for 2280 2168.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.99D-15 for 5781.

Iteration 1 A^-1\*A deviation from orthogonality is 8.07D-09 for 5389 5156.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.44D-15 for 555.

Iteration 2 A\*A^-1 deviation from orthogonality is 2.89D-15 for 5156 1341.

Iteration 2 A^-1\*A deviation from unit magnitude is 8.88D-16 for 541.

Iteration 2 A^-1\*A deviation from orthogonality is 2.86D-16 for 2717 209.

E= -1914.33331523161

DIIS: error= 5.91D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.33331523161 IErMin= 1 ErrMin= 5.91D-05

ErrMax= 5.91D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.36D-06 BMatP= 7.36D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.640 Goal= None Shift= 0.000

Gap= 0.706 Goal= None Shift= 0.000

RMSDP=3.78D-06 MaxDP=1.93D-04 OVMax= 3.75D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.77D-06 CP: 1.00D+00

E= -1914.33331880861 Delta-E= -0.000003577001 Rises=F Damp=F

DIIS: error= 6.76D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33331880861 IErMin= 2 ErrMin= 6.76D-06

ErrMax= 6.76D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.07D-07 BMatP= 7.36D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.569D-01 0.106D+01

Coeff: -0.569D-01 0.106D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.12D-07 MaxDP=2.21D-05 DE=-3.58D-06 OVMax= 6.65D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.72D-07 CP: 1.00D+00 1.05D+00

E= -1914.33331885810 Delta-E= -0.000000049487 Rises=F Damp=F

DIIS: error= 4.66D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33331885810 IErMin= 3 ErrMin= 4.66D-06

ErrMax= 4.66D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.25D-08 BMatP= 1.07D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.323D-01 0.452D+00 0.581D+00

Coeff: -0.323D-01 0.452D+00 0.581D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.88D-07 MaxDP=1.44D-05 DE=-4.95D-08 OVMax= 5.51D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.57D-07 CP: 1.00D+00 1.05D+00 7.25D-01

E= -1914.33331886662 Delta-E= -0.000000008524 Rises=F Damp=F

DIIS: error= 2.47D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33331886662 IErMin= 4 ErrMin= 2.47D-06

ErrMax= 2.47D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.84D-08 BMatP= 5.25D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.114D-01 0.123D+00 0.372D+00 0.516D+00

Coeff: -0.114D-01 0.123D+00 0.372D+00 0.516D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=8.29D-08 MaxDP=5.02D-06 DE=-8.52D-09 OVMax= 2.03D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 5.06D-08 CP: 1.00D+00 1.05D+00 8.18D-01 6.46D-01

E= -1914.33331887091 Delta-E= -0.000000004295 Rises=F Damp=F

DIIS: error= 4.22D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33331887091 IErMin= 5 ErrMin= 4.22D-07

ErrMax= 4.22D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.34D-10 BMatP= 1.84D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.215D-02 0.112D-01 0.112D+00 0.236D+00 0.643D+00

Coeff: -0.215D-02 0.112D-01 0.112D+00 0.236D+00 0.643D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.64D-08 MaxDP=2.19D-06 DE=-4.29D-09 OVMax= 9.98D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.97D-08 CP: 1.00D+00 1.05D+00 8.19D-01 7.35D-01 7.98D-01

E= -1914.33331887113 Delta-E= -0.000000000216 Rises=F Damp=F

DIIS: error= 2.84D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33331887113 IErMin= 6 ErrMin= 2.84D-07

ErrMax= 2.84D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.49D-10 BMatP= 9.34D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.865D-03-0.175D-01-0.404D-02 0.452D-01 0.417D+00 0.558D+00

Coeff: 0.865D-03-0.175D-01-0.404D-02 0.452D-01 0.417D+00 0.558D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.16D-08 MaxDP=7.88D-07 DE=-2.16D-10 OVMax= 4.08D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 7.53D-09 CP: 1.00D+00 1.05D+00 8.31D-01 7.32D-01 8.91D-01

CP: 6.93D-01

E= -1914.33331887119 Delta-E= -0.000000000062 Rises=F Damp=F

DIIS: error= 7.64D-08 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33331887119 IErMin= 7 ErrMin= 7.64D-08

ErrMax= 7.64D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.86D-11 BMatP= 3.49D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.489D-03-0.842D-02-0.657D-02 0.958D-02 0.163D+00 0.261D+00

Coeff-Com: 0.581D+00

Coeff: 0.489D-03-0.842D-02-0.657D-02 0.958D-02 0.163D+00 0.261D+00

Coeff: 0.581D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.14D-09 MaxDP=3.77D-07 DE=-6.18D-11 OVMax= 2.95D-06

Error on total polarization charges = 0.08258

SCF Done: E(UB3LYP) = -1914.33331887 A.U. after 7 cycles

NFock= 7 Conv=0.41D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0182

<L.S>= 0.000000000000E+00

KE= 1.906380760257D+03 PE=-1.516298667332D+04 EE= 5.985592729186D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0551, after 2.0017

Leave Link 502 at Thu Aug 29 16:28:49 2019, MaxMem= 4294967296 cpu: 3206.0

(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: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48636164D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64278119D-01

Leave Link 801 at Thu Aug 29 16:28:49 2019, MaxMem= 4294967296 cpu: 1.0

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Thu Aug 29 16:28:56 2019, MaxMem= 4294967296 cpu: 110.0

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Thu Aug 29 16:28:56 2019, MaxMem= 4294967296 cpu: 2.0

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 189

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 Thu Aug 29 16:51:49 2019, MaxMem= 4294967296 cpu: 19352.5

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 590000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.39D+03 4.50D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.52D+02 3.62D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.53D+00 4.67D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.02D-01 3.97D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.57D-04 2.10D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.58D-06 1.35D-04.

190 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 1.99D-08 1.02D-05.

82 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.29D-11 6.21D-07.

42 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.16D-13 3.90D-08.

4 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 8.29D-15 3.97D-09.

4 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 4.54D-15 2.29D-09.

4 vectors produced by pass 11 Test12= 2.55D-13 1.00D-09 XBig12= 8.21D-15 3.45D-09.

3 vectors produced by pass 12 Test12= 2.55D-13 1.00D-09 XBig12= 4.13D-15 1.63D-09.

3 vectors produced by pass 13 Test12= 2.55D-13 1.00D-09 XBig12= 4.98D-15 2.65D-09.

3 vectors produced by pass 14 Test12= 2.55D-13 1.00D-09 XBig12= 9.80D-15 3.08D-09.

3 vectors produced by pass 15 Test12= 2.55D-13 1.00D-09 XBig12= 1.02D-14 2.81D-09.

3 vectors produced by pass 16 Test12= 2.55D-13 1.00D-09 XBig12= 7.27D-15 2.29D-09.

3 vectors produced by pass 17 Test12= 2.55D-13 1.00D-09 XBig12= 8.22D-15 2.53D-09.

3 vectors produced by pass 18 Test12= 2.55D-13 1.00D-09 XBig12= 7.53D-15 2.39D-09.

3 vectors produced by pass 19 Test12= 2.55D-13 1.00D-09 XBig12= 6.86D-15 3.32D-09.

3 vectors produced by pass 20 Test12= 2.55D-13 1.00D-09 XBig12= 4.82D-15 2.05D-09.

3 vectors produced by pass 21 Test12= 2.55D-13 1.00D-09 XBig12= 5.21D-15 2.47D-09.

3 vectors produced by pass 22 Test12= 2.55D-13 1.00D-09 XBig12= 5.47D-15 3.50D-09.

3 vectors produced by pass 23 Test12= 2.55D-13 1.00D-09 XBig12= 4.38D-15 2.04D-09.

3 vectors produced by pass 24 Test12= 2.55D-13 1.00D-09 XBig12= 3.80D-15 1.76D-09.

3 vectors produced by pass 25 Test12= 2.55D-13 1.00D-09 XBig12= 7.38D-15 2.17D-09.

3 vectors produced by pass 26 Test12= 2.55D-13 1.00D-09 XBig12= 4.66D-15 1.79D-09.

3 vectors produced by pass 27 Test12= 2.55D-13 1.00D-09 XBig12= 4.39D-15 1.95D-09.

3 vectors produced by pass 28 Test12= 2.55D-13 1.00D-09 XBig12= 4.32D-15 2.61D-09.

3 vectors produced by pass 29 Test12= 2.55D-13 1.00D-09 XBig12= 5.60D-15 1.93D-09.

3 vectors produced by pass 30 Test12= 2.55D-13 1.00D-09 XBig12= 3.77D-15 1.82D-09.

3 vectors produced by pass 31 Test12= 2.55D-13 1.00D-09 XBig12= 3.90D-15 2.17D-09.

3 vectors produced by pass 32 Test12= 2.55D-13 1.00D-09 XBig12= 5.38D-15 2.25D-09.

3 vectors produced by pass 33 Test12= 2.55D-13 1.00D-09 XBig12= 5.34D-15 2.25D-09.

3 vectors produced by pass 34 Test12= 2.55D-13 1.00D-09 XBig12= 4.70D-15 1.89D-09.

3 vectors produced by pass 35 Test12= 2.55D-13 1.00D-09 XBig12= 5.53D-15 2.22D-09.

3 vectors produced by pass 36 Test12= 2.55D-13 1.00D-09 XBig12= 4.13D-15 2.08D-09.

3 vectors produced by pass 37 Test12= 2.55D-13 1.00D-09 XBig12= 6.43D-15 2.70D-09.

3 vectors produced by pass 38 Test12= 2.55D-13 1.00D-09 XBig12= 6.41D-15 2.41D-09.

2 vectors produced by pass 39 Test12= 2.55D-13 1.00D-09 XBig12= 4.15D-15 1.54D-09.

InvSVY: IOpt=1 It= 1 EMax= 5.68D-14

Solved reduced A of dimension 1816 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1125.44 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 Thu Aug 29 20:47:16 2019, MaxMem= 4294967296 cpu: 225922.0

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 189

Leave Link 701 at Thu Aug 29 20:48:46 2019, MaxMem= 4294967296 cpu: 1423.5

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Thu Aug 29 20:48:46 2019, MaxMem= 4294967296 cpu: 0.0

(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=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

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= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Thu Aug 29 21:07:21 2019, MaxMem= 4294967296 cpu: 17838.5

(Enter /home/kira/g09/l716.exe)

Dipole =-3.79534535D-05-4.59664914D-04-4.79025225D-01

Polarizability= 1.25549168D+03-2.88691160D+01 1.66556824D+03

2.14488033D-04-8.19593909D-03 4.55268616D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000000096 -0.000000748 -0.000001187

2 6 0.000001081 -0.000000131 -0.000004738

3 7 0.000002313 -0.000000113 0.000000241

4 6 -0.000000479 0.000001552 0.000006159

5 6 0.000001348 0.000000894 -0.000000201

6 6 -0.000000811 0.000003671 -0.000003215

7 6 -0.000002462 -0.000000681 -0.000001346

8 7 -0.000014070 0.000007880 -0.000001557

9 6 0.000000413 -0.000000787 -0.000002678

10 6 -0.000001450 -0.000002894 -0.000002824

11 6 -0.000000351 -0.000000815 0.000005198

12 6 -0.000002212 0.000003750 -0.000001377

13 6 -0.000001207 -0.000000643 0.000002503

14 6 0.000001402 -0.000002809 0.000002838

15 6 0.000000302 -0.000000832 -0.000005150

16 6 0.000001659 -0.000000857 0.000001438

17 7 0.000015141 0.000007990 0.000001414

18 6 0.000001368 0.000003721 0.000003131

19 6 0.000000812 0.000001861 -0.000006293

20 6 -0.000001509 0.000000644 0.000000273

21 6 -0.000000279 -0.000000989 0.000001201

22 6 -0.000000790 0.000000247 0.000004740

23 7 -0.000002217 -0.000000654 -0.000000066

24 6 0.000002788 0.000003653 0.000001494

25 6 0.000005250 -0.000003591 -0.000004065

26 6 -0.000000464 -0.000005253 0.000004918

27 6 0.000000184 0.000002133 0.000000083

28 6 0.000000875 -0.000000599 0.000001283

29 6 0.000001516 0.000002739 -0.000002736

30 6 0.000000215 -0.000004883 -0.000007170

31 6 -0.000000748 0.000001601 0.000000291

32 6 -0.000000501 0.000001435 -0.000000668

33 6 0.000001847 -0.000001380 -0.000001683

34 6 0.000002729 -0.000002250 0.000005185

35 6 -0.000002320 -0.000002338 0.000002115

36 6 0.000002582 0.000000902 0.000002260

37 6 -0.000002811 -0.000002237 -0.000005487

38 6 0.000002345 -0.000002362 -0.000002056

39 6 -0.000002639 0.000000822 -0.000002237

40 6 0.000000839 0.000001479 -0.000000195

41 6 0.000000535 0.000001266 0.000000587

42 6 -0.000001919 -0.000001541 0.000001748

43 6 -0.000005564 -0.000003579 0.000004197

44 6 -0.000000164 -0.000004885 0.000007185

45 6 -0.000001659 0.000002738 0.000002705

46 6 -0.000000718 -0.000000623 -0.000001292

47 6 -0.000000170 0.000002016 -0.000000056

48 6 0.000000544 -0.000005365 -0.000004899

49 1 -0.000000453 -0.000002348 0.000001622

50 1 0.000000785 0.000002721 -0.000006814

51 1 -0.000004351 0.000000442 0.000000362

52 1 -0.000002724 0.000003732 -0.000001640

53 1 0.000004297 0.000000450 -0.000000370

54 1 0.000002698 0.000003745 0.000001631

55 1 -0.000000829 0.000002638 0.000006828

56 1 0.000000448 -0.000002418 -0.000001672

57 1 -0.000001798 -0.000002136 0.000001640

58 1 0.000000356 0.000000411 0.000000775

59 1 0.000000198 0.000001083 -0.000000643

60 1 -0.000001528 0.000000492 -0.000001002

61 1 -0.000003995 0.000003341 0.000003864

62 1 0.000001433 0.000000230 -0.000000496

63 1 0.000000755 -0.000000068 -0.000000917

64 1 -0.000001861 -0.000002907 -0.000002001

65 1 -0.000002597 0.000002977 -0.000003662

66 1 -0.000000256 0.000000065 0.000000271

67 1 0.000002605 0.000002924 0.000003702

68 1 0.000000294 -0.000000028 -0.000000270

69 1 -0.000001442 0.000000104 0.000000511

70 1 -0.000000778 -0.000000193 0.000000907

71 1 0.000001826 -0.000002971 0.000002021

72 1 0.000004075 0.000003340 -0.000003883

73 1 0.000001565 0.000000459 0.000001013

74 1 -0.000000217 0.000001010 0.000000639

75 1 -0.000000410 0.000000319 -0.000000796

76 1 0.000001813 -0.000002197 -0.000001670

77 1 0.000034836 -0.000007728 0.000004354

78 1 -0.000035413 -0.000006639 -0.000004311

-------------------------------------------------------------------

Cartesian Forces: Max 0.000035413 RMS 0.000004411

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Thu Aug 29 21:07:21 2019, MaxMem= 4294967296 cpu: 2.5

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000035990 RMS 0.000007539

Search for a local minimum.

Step number 22 out of a maximum of 452

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -2.18D-06 DEPred=-3.21D-08 R= 6.79D+01

TightC=F SS= 1.41D+00 RLast= 4.75D-03 DXNew= 9.6546D-02 1.4241D-02

Trust test= 6.79D+01 RLast= 4.75D-03 DXMaxT set to 5.74D-02

ITU= 1 1 -1 -1 1 1 -1 -1 1 0 -1 1 1 -1 1 -1 -1 1 1 -1

ITU= 1 0

Eigenvalues --- 0.00047 0.00237 0.00412 0.00599 0.00723

Eigenvalues --- 0.00815 0.00922 0.01045 0.01057 0.01119

Eigenvalues --- 0.01135 0.01165 0.01264 0.01280 0.01302

Eigenvalues --- 0.01305 0.01322 0.01422 0.01429 0.01531

Eigenvalues --- 0.01547 0.01558 0.01590 0.01672 0.01711

Eigenvalues --- 0.01716 0.01728 0.01737 0.01754 0.01759

Eigenvalues --- 0.01761 0.01782 0.01802 0.01804 0.01885

Eigenvalues --- 0.01934 0.01985 0.01994 0.02011 0.02166

Eigenvalues --- 0.02169 0.02256 0.02289 0.02292 0.02304

Eigenvalues --- 0.02330 0.02393 0.02468 0.02471 0.02522

Eigenvalues --- 0.02538 0.02543 0.02587 0.02626 0.02628

Eigenvalues --- 0.02644 0.02647 0.02768 0.02779 0.02796

Eigenvalues --- 0.02804 0.02868 0.02872 0.02874 0.02875

Eigenvalues --- 0.02947 0.02972 0.03907 0.04088 0.04191

Eigenvalues --- 0.04317 0.04368 0.04463 0.04542 0.04570

Eigenvalues --- 0.08133 0.09639 0.09687 0.09724 0.09865

Eigenvalues --- 0.09889 0.10300 0.10437 0.10569 0.10695

Eigenvalues --- 0.10696 0.10703 0.10733 0.10734 0.11008

Eigenvalues --- 0.11395 0.11396 0.11410 0.11412 0.11985

Eigenvalues --- 0.11988 0.11996 0.12002 0.12276 0.12277

Eigenvalues --- 0.12322 0.12322 0.12769 0.12770 0.12774

Eigenvalues --- 0.12775 0.15714 0.15917 0.16294 0.16779

Eigenvalues --- 0.17208 0.17287 0.17576 0.17830 0.17987

Eigenvalues --- 0.18026 0.18258 0.18332 0.19242 0.19284

Eigenvalues --- 0.19358 0.19360 0.19370 0.19407 0.19412

Eigenvalues --- 0.19428 0.19551 0.19551 0.19554 0.19556

Eigenvalues --- 0.20292 0.21486 0.22040 0.22718 0.22876

Eigenvalues --- 0.23246 0.23765 0.24229 0.24751 0.25031

Eigenvalues --- 0.26283 0.26384 0.26661 0.27149 0.28523

Eigenvalues --- 0.28549 0.28745 0.29013 0.29784 0.31031

Eigenvalues --- 0.31697 0.32012 0.32844 0.33076 0.33155

Eigenvalues --- 0.33324 0.34111 0.34605 0.35057 0.35564

Eigenvalues --- 0.35624 0.35626 0.35633 0.35640 0.35756

Eigenvalues --- 0.35759 0.35763 0.35808 0.35924 0.35925

Eigenvalues --- 0.35930 0.35933 0.35987 0.35989 0.36007

Eigenvalues --- 0.36010 0.36191 0.36201 0.36243 0.36244

Eigenvalues --- 0.36985 0.37057 0.37239 0.37386 0.37396

Eigenvalues --- 0.37488 0.38134 0.38439 0.38516 0.38551

Eigenvalues --- 0.39443 0.40371 0.40724 0.41036 0.41053

Eigenvalues --- 0.41095 0.41187 0.41251 0.41338 0.41348

Eigenvalues --- 0.41563 0.41790 0.42276 0.42649 0.44537

Eigenvalues --- 0.45251 0.45899 0.45923 0.45928 0.45969

Eigenvalues --- 0.46002 0.46029 0.46255 0.46259 0.46314

Eigenvalues --- 0.46323 0.48383 0.49008 0.49422 0.49636

Eigenvalues --- 0.50751 0.50754 0.50780 0.50783 0.51864

Eigenvalues --- 0.52214 0.57179 0.57715

Cosine: 0.453 < 0.500

Cut down GDIIS temporarily because of the cosine check. E 6

DIIS coeff's: 0.22590 0.77410

Cosine: 0.942 > 0.500

Length: 0.116

GDIIS step was calculated using 2 of the last 22 vectors.

Iteration 1 RMS(Cart)= 0.00059693 RMS(Int)= 0.00000003

Iteration 2 RMS(Cart)= 0.00000008 RMS(Int)= 0.00000001

ITry= 1 IFail=0 DXMaxC= 2.71D-03 DCOld= 1.00D+10 DXMaxT= 5.74D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.65685 0.00000 -0.00001 0.00002 0.00001 2.65685

R2 2.64097 0.00001 0.00001 -0.00001 0.00000 2.64097

R3 2.03707 0.00000 0.00000 -0.00000 0.00000 2.03707

R4 2.59921 -0.00002 -0.00002 0.00002 -0.00000 2.59921

R5 2.71595 0.00001 0.00002 -0.00003 -0.00001 2.71594

R6 2.59905 -0.00002 -0.00002 0.00001 -0.00001 2.59904

R7 1.91016 -0.00004 -0.00004 0.00003 -0.00001 1.91015

R8 2.65652 0.00000 -0.00000 0.00000 0.00000 2.65653

R9 2.71688 0.00001 0.00002 -0.00000 0.00002 2.71690

R10 2.03713 0.00000 0.00000 -0.00000 0.00000 2.03713

R11 2.64076 0.00003 0.00003 -0.00003 -0.00001 2.64076

R12 2.80422 0.00000 -0.00002 0.00002 0.00000 2.80422

R13 2.59619 0.00002 0.00001 0.00001 0.00002 2.59621

R14 2.76198 0.00000 0.00001 -0.00000 0.00000 2.76198

R15 2.59437 0.00001 0.00000 -0.00003 -0.00002 2.59435

R16 2.76239 -0.00000 -0.00001 0.00001 0.00000 2.76239

R17 2.64279 0.00001 -0.00000 0.00003 0.00003 2.64282

R18 2.55437 0.00000 -0.00000 0.00000 0.00000 2.55437

R19 2.03919 0.00000 -0.00000 0.00000 0.00000 2.03919

R20 2.03906 0.00000 -0.00000 0.00000 0.00000 2.03906

R21 2.64280 0.00001 0.00002 0.00001 0.00002 2.64282

R22 2.80376 0.00000 -0.00004 0.00003 -0.00001 2.80375

R23 2.76239 -0.00000 -0.00000 0.00000 0.00000 2.76239

R24 2.59437 0.00000 -0.00001 -0.00001 -0.00002 2.59435

R25 2.55437 0.00000 0.00000 0.00000 0.00000 2.55437

R26 2.03919 0.00000 -0.00000 0.00000 0.00000 2.03919

R27 2.76198 0.00000 0.00001 -0.00001 0.00000 2.76198

R28 2.03906 0.00000 -0.00000 0.00000 0.00000 2.03906

R29 2.59619 0.00002 0.00001 0.00001 0.00002 2.59621

R30 2.64075 0.00003 0.00000 -0.00001 -0.00000 2.64075

R31 2.71687 0.00001 -0.00000 0.00002 0.00002 2.71689

R32 2.80425 0.00000 0.00004 -0.00005 -0.00001 2.80424

R33 2.65654 0.00000 0.00002 -0.00003 -0.00000 2.65654

R34 2.59906 -0.00002 0.00000 -0.00002 -0.00001 2.59905

R35 2.64096 0.00001 -0.00001 0.00001 0.00001 2.64096

R36 2.03712 0.00000 -0.00000 0.00000 0.00000 2.03713

R37 2.65686 0.00000 0.00001 -0.00000 0.00000 2.65686

R38 2.03707 0.00000 -0.00000 0.00000 0.00000 2.03707

R39 2.59922 -0.00002 -0.00000 0.00000 -0.00000 2.59921

R40 2.71593 0.00001 -0.00000 -0.00000 -0.00000 2.71593

R41 1.91018 -0.00004 -0.00000 -0.00001 -0.00002 1.91016

R42 2.80379 0.00000 0.00002 -0.00003 -0.00002 2.80377

R43 2.65123 -0.00001 0.00001 -0.00001 0.00000 2.65123

R44 2.64988 0.00000 0.00001 -0.00001 0.00000 2.64988

R45 2.62864 -0.00000 -0.00000 0.00000 -0.00000 2.62864

R46 2.04850 0.00000 -0.00000 0.00000 -0.00000 2.04850

R47 2.63628 0.00000 0.00000 -0.00000 0.00000 2.63628

R48 2.05017 0.00000 -0.00000 0.00000 -0.00000 2.05017

R49 2.63409 0.00000 0.00000 -0.00000 -0.00000 2.63409

R50 2.05006 0.00000 0.00000 0.00000 0.00000 2.05006

R51 2.63098 0.00001 -0.00001 0.00001 0.00000 2.63098

R52 2.05014 0.00000 -0.00000 -0.00000 -0.00000 2.05014

R53 2.04862 0.00000 -0.00000 0.00000 -0.00000 2.04862

R54 2.63632 0.00000 0.00000 -0.00000 -0.00000 2.63632

R55 2.63422 0.00000 0.00000 -0.00000 0.00000 2.63423

R56 2.05006 0.00000 0.00000 0.00000 0.00000 2.05006

R57 2.62891 -0.00000 -0.00001 0.00001 -0.00000 2.62891

R58 2.05018 0.00000 -0.00000 0.00000 -0.00000 2.05018

R59 2.65142 -0.00000 0.00001 -0.00001 0.00000 2.65142

R60 2.04848 -0.00000 -0.00000 0.00000 -0.00000 2.04848

R61 2.65009 -0.00000 0.00002 -0.00001 0.00000 2.65009

R62 2.63061 0.00000 -0.00000 0.00000 -0.00000 2.63061

R63 2.04855 0.00000 -0.00000 0.00000 -0.00000 2.04855

R64 2.05016 0.00000 -0.00000 0.00000 0.00000 2.05016

R65 2.65008 -0.00000 -0.00000 0.00001 0.00001 2.65009

R66 2.65141 -0.00000 -0.00001 0.00001 0.00000 2.65142

R67 2.63062 0.00000 0.00000 -0.00001 -0.00000 2.63061

R68 2.04855 0.00000 0.00000 -0.00000 -0.00000 2.04855

R69 2.63422 0.00000 0.00000 0.00000 0.00000 2.63423

R70 2.05016 0.00000 -0.00000 0.00000 0.00000 2.05016

R71 2.63632 0.00000 -0.00000 0.00000 0.00000 2.63632

R72 2.05006 0.00000 0.00000 -0.00000 0.00000 2.05006

R73 2.62892 -0.00000 0.00000 -0.00000 -0.00000 2.62892

R74 2.05018 0.00000 0.00000 -0.00000 -0.00000 2.05018

R75 2.04848 -0.00000 -0.00000 -0.00000 -0.00000 2.04848

R76 2.64986 0.00000 -0.00001 0.00002 0.00000 2.64987

R77 2.65121 -0.00001 -0.00001 0.00002 0.00001 2.65122

R78 2.63098 0.00001 0.00000 -0.00000 -0.00000 2.63098

R79 2.04862 0.00000 0.00000 -0.00000 -0.00000 2.04862

R80 2.63409 0.00000 0.00000 -0.00000 -0.00000 2.63408

R81 2.05014 0.00000 0.00000 -0.00000 -0.00000 2.05014

R82 2.63628 0.00000 -0.00000 0.00000 0.00000 2.63628

R83 2.05006 0.00000 0.00000 -0.00000 0.00000 2.05006

R84 2.62865 -0.00000 0.00001 -0.00001 -0.00000 2.62865

R85 2.05017 0.00000 0.00000 -0.00000 -0.00000 2.05017

R86 2.04850 0.00000 -0.00000 -0.00000 -0.00000 2.04850

A1 1.88156 -0.00001 -0.00001 0.00000 -0.00000 1.88156

A2 2.18785 0.00000 -0.00001 0.00002 0.00001 2.18786

A3 2.21376 0.00000 0.00002 -0.00002 -0.00000 2.21376

A4 1.86798 -0.00001 -0.00000 -0.00000 -0.00001 1.86797

A5 2.22215 0.00003 0.00004 -0.00000 0.00004 2.22219

A6 2.19260 -0.00003 -0.00003 -0.00001 -0.00004 2.19257

A7 1.92511 0.00002 0.00002 -0.00001 0.00001 1.92512

A8 2.17741 -0.00001 -0.00004 0.00001 -0.00003 2.17738

A9 2.17985 -0.00001 0.00004 -0.00002 0.00002 2.17987

A10 1.86811 -0.00001 -0.00001 0.00001 -0.00001 1.86811

A11 2.19438 0.00000 -0.00000 0.00001 0.00000 2.19438

A12 2.22029 0.00001 0.00002 -0.00002 -0.00000 2.22029

A13 1.88166 -0.00000 0.00000 -0.00000 0.00000 1.88166

A14 2.21402 0.00001 0.00001 -0.00001 0.00000 2.21403

A15 2.18748 -0.00000 -0.00001 0.00001 -0.00001 2.18747

A16 2.18668 0.00003 0.00001 0.00000 0.00001 2.18669

A17 2.02293 -0.00003 -0.00004 0.00002 -0.00002 2.02291

A18 2.07353 0.00001 0.00003 -0.00002 0.00001 2.07354

A19 2.19173 0.00002 0.00004 -0.00005 -0.00000 2.19173

A20 2.16532 -0.00001 -0.00003 0.00004 0.00002 2.16533

A21 1.92611 -0.00001 -0.00001 0.00000 -0.00001 1.92610

A22 1.84708 0.00001 0.00001 0.00000 0.00001 1.84709

A23 1.92647 -0.00000 0.00000 0.00000 0.00000 1.92648

A24 2.19209 0.00001 -0.00001 0.00001 -0.00001 2.19208

A25 2.16462 -0.00001 0.00001 -0.00001 0.00000 2.16462

A26 1.86205 0.00000 -0.00000 0.00000 -0.00000 1.86205

A27 2.19691 -0.00000 0.00001 -0.00001 -0.00000 2.19691

A28 2.22384 0.00000 -0.00001 0.00001 0.00000 2.22384

A29 1.86206 0.00001 0.00001 -0.00001 0.00000 1.86206

A30 2.19688 -0.00000 -0.00000 0.00001 0.00001 2.19689

A31 2.22391 -0.00001 -0.00001 -0.00000 -0.00001 2.22390

A32 2.18529 -0.00000 -0.00008 0.00006 -0.00002 2.18527

A33 2.02528 0.00002 0.00000 0.00004 0.00004 2.02532

A34 2.07257 -0.00001 0.00008 -0.00010 -0.00002 2.07255

A35 2.16463 -0.00001 0.00004 -0.00004 -0.00000 2.16463

A36 2.19207 0.00001 -0.00004 0.00003 -0.00000 2.19207

A37 1.92647 -0.00000 -0.00000 0.00001 0.00000 1.92648

A38 1.86205 0.00000 0.00000 -0.00000 -0.00000 1.86205

A39 2.19690 -0.00000 0.00001 -0.00000 0.00000 2.19691

A40 2.22384 0.00000 -0.00001 0.00001 -0.00000 2.22384

A41 1.86206 0.00001 0.00000 -0.00000 0.00000 1.86206

A42 2.22391 -0.00001 -0.00001 -0.00000 -0.00001 2.22390

A43 2.19688 -0.00000 0.00000 0.00001 0.00001 2.19689

A44 1.92611 -0.00001 -0.00001 0.00000 -0.00001 1.92610

A45 2.16531 -0.00001 -0.00004 0.00005 0.00001 2.16532

A46 2.19174 0.00002 0.00005 -0.00006 -0.00000 2.19173

A47 1.84708 0.00001 0.00001 -0.00000 0.00000 1.84709

A48 2.18673 0.00003 0.00009 -0.00010 -0.00000 2.18672

A49 2.07347 0.00001 -0.00007 0.00010 0.00003 2.07350

A50 2.02294 -0.00003 -0.00002 -0.00001 -0.00003 2.02291

A51 2.22028 0.00001 0.00000 0.00000 0.00001 2.22029

A52 2.19438 0.00000 0.00001 -0.00000 0.00000 2.19438

A53 1.86811 -0.00001 -0.00002 0.00001 -0.00000 1.86811

A54 1.88166 -0.00000 0.00001 -0.00001 0.00000 1.88166

A55 2.18749 -0.00000 0.00001 -0.00002 -0.00001 2.18748

A56 2.21401 0.00001 -0.00002 0.00003 0.00001 2.21401

A57 1.88156 -0.00001 -0.00000 0.00000 -0.00000 1.88156

A58 2.21375 0.00000 -0.00000 0.00001 0.00000 2.21375

A59 2.18786 0.00000 0.00001 -0.00001 -0.00000 2.18786

A60 1.86798 -0.00001 0.00000 -0.00001 -0.00001 1.86798

A61 2.22215 0.00003 0.00004 -0.00000 0.00004 2.22219

A62 2.19259 -0.00003 -0.00005 0.00002 -0.00003 2.19256

A63 1.92510 0.00002 0.00001 0.00000 0.00001 1.92511

A64 2.17985 -0.00001 0.00005 -0.00003 0.00001 2.17986

A65 2.17739 -0.00001 -0.00008 0.00006 -0.00002 2.17737

A66 2.18533 -0.00000 -0.00001 -0.00002 -0.00003 2.18530

A67 2.07252 -0.00001 -0.00002 0.00002 0.00000 2.07252

A68 2.02530 0.00002 0.00003 -0.00001 0.00003 2.02533

A69 2.10453 -0.00002 0.00000 -0.00002 -0.00002 2.10452

A70 2.10698 0.00002 0.00001 0.00001 0.00002 2.10700

A71 2.07167 0.00000 -0.00001 0.00001 -0.00000 2.07167

A72 2.10511 0.00000 0.00000 -0.00000 0.00000 2.10512

A73 2.08515 -0.00000 -0.00000 0.00000 -0.00000 2.08515

A74 2.09276 0.00000 0.00000 -0.00000 -0.00000 2.09276

A75 2.09776 -0.00000 0.00000 -0.00000 -0.00000 2.09776

A76 2.08897 0.00000 0.00000 -0.00000 0.00000 2.08897

A77 2.09646 0.00000 -0.00000 0.00000 0.00000 2.09646

A78 2.08903 0.00000 0.00000 0.00000 0.00000 2.08903

A79 2.09689 -0.00000 0.00000 -0.00000 -0.00000 2.09689

A80 2.09726 0.00000 -0.00000 0.00000 0.00000 2.09726

A81 2.09760 0.00000 0.00000 0.00000 0.00000 2.09760

A82 2.09706 0.00000 -0.00000 0.00000 -0.00000 2.09706

A83 2.08852 -0.00000 -0.00000 -0.00000 -0.00000 2.08852

A84 2.10507 -0.00001 0.00000 -0.00000 -0.00000 2.10507

A85 2.08430 -0.00000 -0.00000 0.00000 -0.00000 2.08430

A86 2.09366 0.00001 -0.00000 0.00000 0.00000 2.09367

A87 2.08896 0.00000 -0.00000 0.00000 0.00000 2.08896

A88 2.09700 -0.00000 -0.00000 -0.00000 -0.00000 2.09700

A89 2.09723 0.00000 0.00000 -0.00000 0.00000 2.09723

A90 2.09800 -0.00000 0.00000 -0.00000 0.00000 2.09801

A91 2.09647 0.00000 -0.00000 0.00000 -0.00000 2.09647

A92 2.08871 0.00000 0.00000 -0.00000 -0.00000 2.08871

A93 2.10486 -0.00000 0.00001 -0.00001 0.00000 2.10486

A94 2.09331 0.00000 -0.00000 0.00001 0.00000 2.09331

A95 2.08482 -0.00000 -0.00000 -0.00000 -0.00000 2.08482

A96 2.10714 -0.00000 -0.00003 0.00004 0.00001 2.10716

A97 2.10454 -0.00000 0.00004 -0.00005 -0.00001 2.10453

A98 2.07149 0.00000 -0.00001 0.00001 -0.00000 2.07149

A99 2.10547 -0.00000 0.00000 -0.00000 0.00000 2.10547

A100 2.08384 -0.00000 0.00000 -0.00001 -0.00000 2.08384

A101 2.09375 0.00001 -0.00001 0.00001 0.00000 2.09375

A102 2.09745 -0.00000 0.00000 -0.00000 -0.00000 2.09745

A103 2.09705 0.00000 0.00000 0.00000 0.00000 2.09705

A104 2.08868 0.00000 -0.00000 0.00000 0.00000 2.08868

A105 2.10453 -0.00000 0.00001 -0.00002 -0.00001 2.10452

A106 2.10715 -0.00000 -0.00001 0.00003 0.00001 2.10717

A107 2.07150 0.00000 0.00000 -0.00001 -0.00000 2.07150

A108 2.10547 -0.00000 -0.00000 0.00001 0.00000 2.10547

A109 2.08384 -0.00000 -0.00000 0.00000 -0.00000 2.08383

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A111 2.09745 -0.00000 0.00000 -0.00000 -0.00000 2.09745

A112 2.08868 0.00000 0.00000 0.00000 0.00000 2.08868

A113 2.09705 0.00000 -0.00000 0.00000 0.00000 2.09705

A114 2.08896 0.00000 -0.00000 0.00000 0.00000 2.08896

A115 2.09723 0.00000 0.00000 -0.00000 -0.00000 2.09723

A116 2.09700 -0.00000 -0.00000 0.00000 -0.00000 2.09700

A117 2.09800 -0.00000 -0.00000 0.00000 0.00000 2.09800

A118 2.09647 0.00000 0.00000 -0.00000 -0.00000 2.09647

A119 2.08871 0.00000 -0.00000 0.00000 0.00000 2.08871

A120 2.10486 -0.00000 -0.00000 0.00000 0.00000 2.10486

A121 2.08482 -0.00000 0.00000 -0.00001 -0.00000 2.08482

A122 2.09331 0.00000 -0.00000 0.00000 0.00000 2.09331

A123 2.10696 0.00002 -0.00003 0.00005 0.00002 2.10698

A124 2.10454 -0.00002 0.00002 -0.00004 -0.00002 2.10452

A125 2.07168 0.00000 0.00001 -0.00001 -0.00000 2.07168

A126 2.10507 -0.00001 -0.00000 0.00000 -0.00000 2.10507

A127 2.08430 -0.00000 -0.00000 0.00001 0.00000 2.08430

A128 2.09367 0.00001 0.00001 -0.00001 -0.00000 2.09367

A129 2.09760 0.00000 -0.00000 0.00000 0.00000 2.09760

A130 2.08852 -0.00000 0.00000 -0.00000 -0.00000 2.08852

A131 2.09706 0.00000 0.00000 -0.00000 -0.00000 2.09706

A132 2.08903 0.00000 0.00000 0.00000 0.00000 2.08903

A133 2.09726 0.00000 -0.00000 0.00000 0.00000 2.09726

A134 2.09689 -0.00000 0.00000 -0.00000 -0.00000 2.09689

A135 2.09776 -0.00000 -0.00000 -0.00000 -0.00000 2.09776

A136 2.09646 0.00000 0.00000 -0.00000 0.00000 2.09646

A137 2.08897 0.00000 -0.00000 0.00000 0.00000 2.08897

A138 2.10511 0.00000 -0.00001 0.00001 0.00000 2.10511

A139 2.08515 -0.00000 0.00000 -0.00000 -0.00000 2.08515

A140 2.09276 0.00000 0.00000 -0.00001 -0.00000 2.09276

D1 0.01559 0.00000 -0.00003 0.00006 0.00003 0.01562

D2 -3.09502 0.00001 -0.00025 0.00042 0.00017 -3.09485

D3 -3.12078 0.00000 0.00007 -0.00008 -0.00001 -3.12078

D4 0.05181 0.00000 -0.00016 0.00028 0.00013 0.05193

D5 -0.00066 -0.00000 0.00002 -0.00003 -0.00002 -0.00068

D6 -3.13458 -0.00000 0.00010 -0.00014 -0.00004 -3.13462

D7 3.13560 0.00000 -0.00008 0.00011 0.00002 3.13562

D8 0.00168 -0.00000 0.00000 0.00000 0.00000 0.00169

D9 -0.02529 -0.00000 0.00003 -0.00007 -0.00004 -0.02533

D10 3.07451 0.00000 0.00059 -0.00074 -0.00015 3.07436

D11 3.08599 -0.00001 0.00025 -0.00042 -0.00017 3.08582

D12 -0.09740 -0.00000 0.00082 -0.00110 -0.00028 -0.09768

D13 -2.95241 -0.00001 0.00085 -0.00111 -0.00026 -2.95267

D14 0.17911 -0.00000 0.00067 -0.00083 -0.00016 0.17895

D15 0.22564 -0.00000 0.00058 -0.00069 -0.00011 0.22553

D16 -2.92602 0.00000 0.00040 -0.00041 -0.00001 -2.92603

D17 0.02488 0.00000 -0.00002 0.00005 0.00003 0.02491

D18 -3.08798 0.00001 -0.00015 0.00023 0.00008 -3.08790

D19 -3.07485 -0.00000 -0.00058 0.00072 0.00014 -3.07470

D20 0.09548 0.00000 -0.00071 0.00091 0.00019 0.09567

D21 -0.01452 0.00000 0.00000 -0.00001 -0.00001 -0.01452

D22 3.11955 0.00000 -0.00008 0.00010 0.00001 3.11956

D23 3.09779 -0.00000 0.00014 -0.00020 -0.00006 3.09773

D24 -0.05134 -0.00000 0.00005 -0.00009 -0.00004 -0.05137

D25 -0.23670 -0.00001 -0.00058 0.00047 -0.00010 -0.23680

D26 2.91553 -0.00001 -0.00042 0.00029 -0.00013 2.91540

D27 2.93939 -0.00000 -0.00074 0.00069 -0.00004 2.93935

D28 -0.19157 -0.00000 -0.00058 0.00051 -0.00007 -0.19163

D29 -0.12445 -0.00000 -0.00011 0.00014 0.00003 -0.12442

D30 3.02596 -0.00000 -0.00006 0.00015 0.00009 3.02605

D31 3.00623 -0.00000 -0.00027 0.00033 0.00005 3.00629

D32 -0.12655 0.00000 -0.00022 0.00034 0.00012 -0.12643

D33 -0.99874 0.00001 0.00033 -0.00027 0.00006 -0.99868

D34 2.13952 0.00001 0.00025 -0.00018 0.00008 2.13959

D35 2.15276 0.00001 0.00048 -0.00044 0.00004 2.15280

D36 -0.99217 0.00001 0.00040 -0.00034 0.00005 -0.99212

D37 -3.09207 0.00001 0.00006 0.00003 0.00010 -3.09197

D38 0.04174 0.00000 0.00002 0.00002 0.00004 0.04178

D39 3.10684 -0.00001 -0.00006 -0.00005 -0.00011 3.10673

D40 -0.06114 -0.00001 -0.00008 -0.00001 -0.00009 -0.06123

D41 -0.02711 -0.00000 -0.00001 -0.00004 -0.00005 -0.02716

D42 3.08810 -0.00000 -0.00004 0.00000 -0.00004 3.08806

D43 -0.04093 -0.00000 -0.00002 0.00000 -0.00002 -0.04095

D44 3.09604 -0.00000 0.00002 -0.00004 -0.00001 3.09603

D45 0.02492 0.00000 0.00001 -0.00003 -0.00001 0.02491

D46 -3.08820 0.00000 0.00002 0.00000 0.00002 -3.08819

D47 -3.11214 0.00000 -0.00003 0.00001 -0.00002 -3.11216

D48 0.05792 0.00000 -0.00003 0.00004 0.00001 0.05793

D49 0.13419 0.00000 -0.00000 0.00019 0.00019 0.13438

D50 -2.99732 0.00000 -0.00024 0.00044 0.00020 -2.99711

D51 -3.01263 0.00000 0.00005 0.00015 0.00020 -3.01244

D52 0.13905 -0.00000 -0.00019 0.00040 0.00021 0.13926

D53 0.00128 0.00000 -0.00000 0.00004 0.00004 0.00132

D54 -3.11339 -0.00000 0.00003 -0.00000 0.00002 -3.11337

D55 3.11383 0.00000 -0.00000 0.00001 0.00001 3.11383

D56 -0.00085 -0.00000 0.00003 -0.00003 -0.00001 -0.00085

D57 -3.01273 0.00000 -0.00013 0.00035 0.00022 -3.01251

D58 0.13417 0.00000 -0.00002 0.00019 0.00017 0.13434

D59 0.13918 -0.00000 0.00006 0.00006 0.00011 0.13930

D60 -2.99710 -0.00000 0.00016 -0.00009 0.00007 -2.99704

D61 0.99270 -0.00001 -0.00036 0.00026 -0.00010 0.99260

D62 -2.14537 -0.00001 -0.00029 0.00014 -0.00014 -2.14552

D63 -2.15828 -0.00000 -0.00053 0.00052 -0.00001 -2.15829

D64 0.98684 -0.00001 -0.00046 0.00041 -0.00005 0.98679

D65 -3.11204 0.00000 0.00015 -0.00020 -0.00006 -3.11210

D66 0.05802 0.00000 0.00015 -0.00017 -0.00003 0.05799

D67 0.02494 0.00000 0.00006 -0.00007 -0.00002 0.02493

D68 -3.08818 0.00000 0.00005 -0.00004 0.00001 -3.08817

D69 3.09595 -0.00000 -0.00014 0.00017 0.00003 3.09598

D70 -0.04095 -0.00000 -0.00005 0.00004 -0.00001 -0.04096

D71 0.00126 0.00000 -0.00004 0.00007 0.00004 0.00129

D72 -3.11343 -0.00000 -0.00004 0.00007 0.00003 -3.11340

D73 3.11381 0.00000 -0.00004 0.00004 0.00001 3.11381

D74 -0.00088 -0.00000 -0.00004 0.00004 -0.00000 -0.00088

D75 -0.02710 -0.00000 0.00001 -0.00005 -0.00005 -0.02715

D76 3.10689 -0.00001 0.00002 -0.00015 -0.00013 3.10676

D77 3.08813 -0.00000 0.00001 -0.00005 -0.00004 3.08809

D78 -0.06107 -0.00001 0.00003 -0.00015 -0.00012 -0.06119

D79 0.04174 0.00000 0.00003 0.00001 0.00004 0.04177

D80 -3.09211 0.00001 0.00001 0.00011 0.00012 -3.09199

D81 3.02592 -0.00000 -0.00011 0.00021 0.00010 3.02602

D82 -0.12640 0.00000 0.00008 -0.00005 0.00003 -0.12637

D83 -0.12444 -0.00000 -0.00009 0.00010 0.00001 -0.12443

D84 3.00642 -0.00000 0.00010 -0.00016 -0.00006 3.00637

D85 2.94031 -0.00000 0.00091 -0.00133 -0.00042 2.93989

D86 -0.23605 -0.00001 0.00059 -0.00095 -0.00036 -0.23641

D87 -0.19084 -0.00000 0.00072 -0.00108 -0.00035 -0.19119

D88 2.91599 -0.00001 0.00040 -0.00070 -0.00030 2.91569

D89 -0.99262 0.00001 -0.00041 0.00061 0.00021 -0.99242

D90 2.15225 0.00001 -0.00043 0.00065 0.00022 2.15248

D91 2.13924 0.00001 -0.00023 0.00038 0.00014 2.13938

D92 -0.99907 0.00001 -0.00025 0.00041 0.00016 -0.99891

D93 3.09755 -0.00000 -0.00030 0.00036 0.00006 3.09761

D94 -0.05146 -0.00000 -0.00018 0.00021 0.00003 -0.05143

D95 -0.01453 0.00000 -0.00003 0.00004 0.00001 -0.01452

D96 3.11965 0.00000 0.00009 -0.00011 -0.00002 3.11963

D97 -3.08773 0.00001 0.00030 -0.00036 -0.00005 -3.08778

D98 0.09639 0.00000 0.00093 -0.00113 -0.00020 0.09619

D99 0.02490 0.00000 0.00004 -0.00004 -0.00001 0.02490

D100 -3.07416 -0.00000 0.00067 -0.00082 -0.00016 -3.07431

D101 -0.00067 -0.00000 0.00001 -0.00003 -0.00002 -0.00068

D102 3.13571 0.00000 0.00011 -0.00014 -0.00003 3.13568

D103 -3.13470 -0.00000 -0.00012 0.00013 0.00001 -3.13469

D104 0.00167 -0.00000 -0.00001 0.00002 0.00001 0.00168

D105 0.01561 0.00000 0.00001 -0.00000 0.00001 0.01562

D106 -3.09475 0.00001 0.00024 -0.00019 0.00004 -3.09471

D107 -3.12086 0.00000 -0.00009 0.00011 0.00002 -3.12084

D108 0.05196 0.00000 0.00013 -0.00008 0.00005 0.05202

D109 -0.02531 -0.00000 -0.00003 0.00003 -0.00000 -0.02532

D110 3.07382 0.00000 -0.00066 0.00080 0.00015 3.07397

D111 3.08572 -0.00001 -0.00025 0.00022 -0.00003 3.08569

D112 -0.09833 -0.00000 -0.00087 0.00099 0.00012 -0.09822

D113 -2.95330 -0.00001 -0.00074 0.00084 0.00010 -2.95320

D114 0.17845 -0.00000 -0.00052 0.00060 0.00009 0.17853

D115 0.22504 -0.00000 -0.00048 0.00061 0.00013 0.22517

D116 -2.92640 0.00000 -0.00025 0.00038 0.00012 -2.92628

D117 0.98724 -0.00001 0.00023 -0.00043 -0.00020 0.98704

D118 -2.15778 -0.00000 0.00033 -0.00053 -0.00020 -2.15798

D119 -2.14518 -0.00001 0.00002 -0.00021 -0.00019 -2.14537

D120 0.99299 -0.00001 0.00012 -0.00031 -0.00019 0.99280

D121 -3.13037 -0.00000 -0.00006 0.00008 0.00003 -3.13035

D122 -0.00828 0.00000 -0.00006 0.00008 0.00002 -0.00826

D123 0.01449 0.00000 0.00002 -0.00001 0.00001 0.01450

D124 3.13659 0.00000 0.00002 -0.00001 0.00000 3.13659

D125 -3.14030 0.00000 0.00006 -0.00009 -0.00002 -3.14032

D126 -0.01710 0.00000 0.00003 -0.00005 -0.00002 -0.01713

D127 -0.00198 -0.00000 -0.00001 0.00000 -0.00001 -0.00199

D128 3.12121 0.00000 -0.00004 0.00004 -0.00001 3.12121

D129 -0.01618 0.00000 -0.00001 0.00000 -0.00001 -0.01619

D130 3.12476 0.00000 -0.00000 -0.00000 -0.00000 3.12476

D131 -3.13819 -0.00000 -0.00001 0.00001 0.00000 -3.13819

D132 0.00275 -0.00000 -0.00000 0.00001 0.00000 0.00276

D133 0.00513 -0.00000 -0.00000 0.00000 -0.00000 0.00513

D134 -3.13362 -0.00000 0.00001 -0.00001 -0.00000 -3.13362

D135 -3.13581 -0.00000 -0.00001 0.00001 -0.00000 -3.13581

D136 0.00863 -0.00000 0.00000 -0.00000 -0.00000 0.00863

D137 0.00733 -0.00000 0.00001 -0.00001 0.00000 0.00733

D138 -3.13197 -0.00000 0.00002 -0.00002 0.00000 -3.13197

D139 -3.13711 -0.00000 -0.00000 0.00000 0.00000 -3.13710

D140 0.00678 -0.00000 0.00001 -0.00001 0.00000 0.00678

D141 -0.00888 0.00000 -0.00000 0.00001 0.00000 -0.00888

D142 -3.13198 -0.00000 0.00003 -0.00003 -0.00000 -3.13198

D143 3.13043 0.00000 -0.00001 0.00002 0.00001 3.13044

D144 0.00734 -0.00000 0.00002 -0.00002 0.00000 0.00734

D145 -0.00538 0.00000 -0.00000 0.00000 0.00000 -0.00538

D146 3.13571 0.00000 0.00002 -0.00002 -0.00000 3.13571

D147 3.13483 0.00000 -0.00002 0.00003 0.00000 3.13483

D148 -0.00727 0.00000 -0.00000 0.00001 0.00000 -0.00727

D149 -0.00642 -0.00000 -0.00001 0.00001 -0.00000 -0.00643

D150 3.13187 0.00000 -0.00003 0.00003 0.00000 3.13187

D151 3.13656 0.00000 0.00001 -0.00002 -0.00000 3.13655

D152 -0.00834 0.00000 -0.00001 0.00001 0.00000 -0.00834

D153 0.01657 -0.00000 0.00002 -0.00003 -0.00000 0.01657

D154 3.13671 -0.00000 0.00001 -0.00003 -0.00001 3.13669

D155 -3.12452 -0.00000 0.00001 -0.00000 0.00000 -3.12452

D156 -0.00439 -0.00000 -0.00001 -0.00001 -0.00001 -0.00440

D157 3.12937 -0.00000 0.00004 -0.00008 -0.00004 3.12933

D158 -0.01568 -0.00000 -0.00004 0.00004 0.00000 -0.01567

D159 0.00914 -0.00000 0.00005 -0.00008 -0.00002 0.00911

D160 -3.13591 -0.00000 -0.00002 0.00004 0.00002 -3.13590

D161 -3.14121 0.00000 -0.00005 0.00009 0.00004 -3.14117

D162 0.01764 0.00000 -0.00001 0.00004 0.00003 0.01767

D163 0.00384 0.00000 0.00002 -0.00003 -0.00000 0.00383

D164 -3.12050 -0.00000 0.00006 -0.00008 -0.00001 -3.12051

D165 0.00715 -0.00000 -0.00000 0.00001 0.00000 0.00716

D166 -3.13116 -0.00000 0.00002 -0.00002 -0.00000 -3.13116

D167 3.13139 0.00000 -0.00004 0.00005 0.00001 3.13140

D168 -0.00692 0.00000 -0.00002 0.00003 0.00001 -0.00691

D169 -3.14114 0.00000 0.00009 -0.00008 0.00001 -3.14113

D170 0.01768 0.00000 0.00005 -0.00004 0.00001 0.01769

D171 0.00381 0.00000 -0.00001 0.00002 0.00000 0.00382

D172 -3.12056 -0.00000 -0.00005 0.00005 0.00001 -3.12055

D173 3.12931 -0.00000 -0.00008 0.00007 -0.00001 3.12930

D174 0.00907 -0.00000 -0.00007 0.00007 0.00000 0.00907

D175 -0.01565 -0.00000 0.00002 -0.00003 -0.00001 -0.01565

D176 -3.13588 -0.00000 0.00003 -0.00003 0.00000 -3.13588

D177 0.00715 -0.00000 0.00000 0.00000 0.00000 0.00716

D178 -3.13117 -0.00000 -0.00001 0.00001 0.00000 -3.13117

D179 3.13143 0.00000 0.00003 -0.00004 -0.00000 3.13143

D180 -0.00689 0.00000 0.00002 -0.00003 -0.00000 -0.00690

D181 -0.00642 -0.00000 0.00001 -0.00001 -0.00000 -0.00642

D182 3.13655 0.00000 0.00000 -0.00000 -0.00000 3.13655

D183 3.13189 0.00000 0.00002 -0.00002 -0.00000 3.13189

D184 -0.00833 0.00000 0.00001 -0.00001 -0.00000 -0.00833

D185 -0.00538 0.00000 -0.00000 0.00000 0.00000 -0.00538

D186 3.13570 0.00000 -0.00002 0.00002 0.00000 3.13570

D187 3.13484 0.00000 0.00000 -0.00001 -0.00000 3.13484

D188 -0.00727 0.00000 -0.00001 0.00001 -0.00000 -0.00727

D189 0.01655 -0.00000 -0.00001 0.00002 0.00001 0.01656

D190 3.13669 -0.00000 -0.00003 0.00002 -0.00001 3.13668

D191 -3.12452 -0.00000 0.00000 0.00000 0.00000 -3.12452

D192 -0.00439 -0.00000 -0.00001 0.00000 -0.00001 -0.00440

D193 -3.14033 0.00000 0.00000 -0.00000 -0.00000 -3.14033

D194 -0.01711 0.00000 0.00003 -0.00003 -0.00001 -0.01711

D195 -0.00196 -0.00000 0.00002 -0.00004 -0.00002 -0.00198

D196 3.12127 0.00000 0.00005 -0.00007 -0.00002 3.12124

D197 -3.13034 -0.00000 -0.00000 0.00001 0.00000 -3.13034

D198 -0.00824 0.00000 -0.00000 -0.00000 -0.00000 -0.00824

D199 0.01447 0.00000 -0.00003 0.00005 0.00002 0.01449

D200 3.13657 0.00000 -0.00002 0.00004 0.00002 3.13658

D201 -0.00888 0.00000 -0.00000 0.00000 0.00000 -0.00888

D202 3.13044 0.00000 0.00000 -0.00000 0.00000 3.13044

D203 -3.13201 -0.00000 -0.00003 0.00004 0.00001 -3.13200

D204 0.00731 -0.00000 -0.00002 0.00003 0.00001 0.00732

D205 0.00731 -0.00000 -0.00002 0.00002 0.00001 0.00732

D206 -3.13710 -0.00000 0.00000 -0.00000 0.00000 -3.13710

D207 -3.13200 -0.00000 -0.00002 0.00003 0.00001 -3.13199

D208 0.00677 -0.00000 -0.00000 0.00000 0.00000 0.00677

D209 0.00514 -0.00000 0.00001 -0.00001 -0.00000 0.00514

D210 -3.13579 -0.00000 0.00001 -0.00002 -0.00001 -3.13580

D211 -3.13362 -0.00000 -0.00001 0.00001 0.00000 -3.13362

D212 0.00863 -0.00000 -0.00001 0.00000 -0.00000 0.00862

D213 -0.01617 0.00000 0.00001 -0.00002 -0.00001 -0.01618

D214 -3.13818 -0.00000 0.00000 -0.00001 -0.00001 -3.13819

D215 3.12477 0.00000 0.00001 -0.00001 -0.00000 3.12477

D216 0.00275 -0.00000 0.00000 -0.00000 0.00000 0.00275

Item Value Threshold Converged?

Maximum Force 0.000036 0.000450 YES

RMS Force 0.000008 0.000300 YES

Maximum Displacement 0.002705 0.001800 NO

RMS Displacement 0.000597 0.001200 YES

Predicted change in Energy=-5.322420D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Thu Aug 29 21:07:21 2019, MaxMem= 4294967296 cpu: 5.5

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=1 Diff= 2.31D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 0.969832 -4.114775 0.551628

2 6 0 1.316848 -2.798192 0.201096

3 7 0 0.141834 -2.110047 0.007084

4 6 0 -0.935790 -2.945099 0.188764

5 6 0 -0.424721 -4.205746 0.543415

6 6 0 -2.316052 -2.586293 0.006617

7 6 0 -2.801079 -1.281921 -0.120546

8 7 0 -2.063025 -0.135024 0.044921

9 6 0 -2.946891 0.904363 -0.107492

10 6 0 -4.278349 0.396678 -0.433560

11 6 0 -4.188008 -0.951985 -0.442687

12 6 0 2.639190 -2.261543 0.030794

13 6 0 2.946901 -0.904331 -0.107602

14 6 0 4.278357 -0.396616 -0.433635

15 6 0 4.188014 0.952048 -0.442657

16 6 0 2.801079 1.281953 -0.120515

17 7 0 2.063029 0.135040 0.044868

18 6 0 2.316049 2.586313 0.006710

19 6 0 0.935796 2.945148 0.188825

20 6 0 0.424715 4.205943 0.542950

21 6 0 -0.969834 4.114972 0.551187

22 6 0 -1.316844 2.798241 0.201191

23 7 0 -0.141826 2.110016 0.007469

24 6 0 -2.639176 2.261566 0.030942

25 6 0 -3.279414 -3.714326 -0.032351

26 6 0 -3.134903 -4.744142 -0.974115

27 6 0 -4.045144 -5.794992 -1.019985

28 6 0 -5.104433 -5.845698 -0.113605

29 6 0 -5.250495 -4.834845 0.834970

30 6 0 -4.348865 -3.774647 0.872610

31 6 0 5.847535 -5.110660 -0.012716

32 6 0 4.800540 -5.220751 -0.928100

33 6 0 3.753868 -4.304565 -0.907840

34 6 0 3.746208 -3.249281 0.016785

35 6 0 4.804287 -3.148092 0.931590

36 6 0 5.843767 -4.073920 0.919118

37 6 0 -3.746228 3.249280 0.016883

38 6 0 -4.804191 3.148204 0.931828

39 6 0 -5.843730 4.073966 0.919293

40 6 0 -5.847669 5.110520 -0.012747

41 6 0 -4.800791 5.220488 -0.928279

42 6 0 -3.754063 4.304365 -0.907962

43 6 0 3.279445 3.714330 -0.032281

44 6 0 4.348732 3.774766 0.872859

45 6 0 5.250403 4.834930 0.835201

46 6 0 5.104541 5.845628 -0.113570

47 6 0 4.045420 5.794794 -1.020137

48 6 0 3.135139 4.743976 -0.974255

49 1 0 1.667501 -4.901993 0.787369

50 1 0 -1.017216 -5.076587 0.772918

51 1 0 -5.148225 0.997028 -0.651138

52 1 0 -4.970339 -1.660020 -0.668388

53 1 0 5.148234 -0.996947 -0.651263

54 1 0 4.970348 1.660104 -0.668280

55 1 0 1.017194 5.076902 0.772048

56 1 0 -1.667504 4.902300 0.786548

57 1 0 -2.315333 -4.707694 -1.682687

58 1 0 -3.927996 -6.575254 -1.764621

59 1 0 -5.809589 -6.669492 -0.145331

60 1 0 -6.066331 -4.871459 1.549151

61 1 0 -4.460689 -2.995086 1.617605

62 1 0 6.660100 -5.829317 -0.025281

63 1 0 4.799174 -6.021681 -1.659905

64 1 0 2.944846 -4.391526 -1.624078

65 1 0 4.799950 -2.348762 1.663852

66 1 0 6.649554 -3.986455 1.640269

67 1 0 -4.799728 2.349002 1.664230

68 1 0 -6.649434 3.986591 1.640548

69 1 0 -6.660280 5.829124 -0.025364

70 1 0 -4.799563 6.021265 -1.660251

71 1 0 -2.945135 4.391221 -1.624320

72 1 0 4.460405 2.995314 1.617992

73 1 0 6.066116 4.871637 1.549519

74 1 0 5.809727 6.669395 -0.145309

75 1 0 3.928431 6.574931 -1.764931

76 1 0 2.315699 4.707427 -1.682972

77 1 0 0.079823 -1.122745 -0.200575

78 1 0 -0.079806 1.122556 -0.199466

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0587910 0.0582554 0.0300943

Leave Link 202 at Thu Aug 29 21:07:22 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5356.8998960227 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122021847 Hartrees.

Nuclear repulsion after empirical dispersion term = 5356.6876938380 Hartrees.

Force inversion solution in PCM.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5786

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.10D-09

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 308

GePol: Fraction of low-weight points (<1% of avg) = 5.32%

GePol: Cavity surface area = 610.624 Ang\*\*2

GePol: Cavity volume = 627.980 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0020999601 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5356.6855938779 Hartrees.

Leave Link 301 at Thu Aug 29 21:07:22 2019, MaxMem= 4294967296 cpu: 3.0

(Enter /home/kira/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Thu Aug 29 21:07:24 2019, MaxMem= 4294967296 cpu: 28.5

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Thu Aug 29 21:07:24 2019, MaxMem= 4294967296 cpu: 2.5

(Enter /home/kira/g09/l401.exe)

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= -0.000000 -0.000000 0.000000

Rot= 1.000000 -0.000001 -0.000000 -0.000817 Ang= -0.09 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0182

Leave Link 401 at Thu Aug 29 21:07:27 2019, MaxMem= 4294967296 cpu: 46.0

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 590000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 100433388.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.77D-15 for 5786.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.23D-15 for 3600 327.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.55D-15 for 5786.

Iteration 1 A^-1\*A deviation from orthogonality is 3.89D-11 for 4192 3931.

E= -1914.33331724717

DIIS: error= 2.72D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.33331724717 IErMin= 1 ErrMin= 2.72D-05

ErrMax= 2.72D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.04D-06 BMatP= 2.04D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.640 Goal= None Shift= 0.000

Gap= 0.706 Goal= None Shift= 0.000

RMSDP=1.11D-06 MaxDP=3.67D-05 OVMax= 1.20D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.11D-06 CP: 1.00D+00

E= -1914.33331818686 Delta-E= -0.000000939686 Rises=F Damp=F

DIIS: error= 3.18D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33331818686 IErMin= 2 ErrMin= 3.18D-06

ErrMax= 3.18D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.37D-08 BMatP= 2.04D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.640D-01 0.106D+01

Coeff: -0.640D-01 0.106D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.82D-07 MaxDP=6.43D-06 DE=-9.40D-07 OVMax= 2.94D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.67D-07 CP: 1.00D+00 1.07D+00

E= -1914.33331819846 Delta-E= -0.000000011602 Rises=F Damp=F

DIIS: error= 1.39D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33331819846 IErMin= 3 ErrMin= 1.39D-06

ErrMax= 1.39D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.07D-08 BMatP= 2.37D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.328D-01 0.463D+00 0.570D+00

Coeff: -0.328D-01 0.463D+00 0.570D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.76D-08 MaxDP=4.66D-06 DE=-1.16D-08 OVMax= 1.50D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.36D-08 CP: 1.00D+00 1.08D+00 7.43D-01

E= -1914.33331820040 Delta-E= -0.000000001936 Rises=F Damp=F

DIIS: error= 9.31D-07 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33331820040 IErMin= 4 ErrMin= 9.31D-07

ErrMax= 9.31D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.06D-09 BMatP= 1.07D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.798D-02 0.857D-01 0.347D+00 0.575D+00

Coeff: -0.798D-02 0.857D-01 0.347D+00 0.575D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.42D-08 MaxDP=2.21D-06 DE=-1.94D-09 OVMax= 1.03D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.28D-08 CP: 1.00D+00 1.08D+00 8.46D-01 7.10D-01

E= -1914.33331820118 Delta-E= -0.000000000783 Rises=F Damp=F

DIIS: error= 2.42D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33331820118 IErMin= 5 ErrMin= 2.42D-07

ErrMax= 2.42D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.05D-10 BMatP= 3.06D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.863D-03-0.253D-02 0.114D+00 0.275D+00 0.614D+00

Coeff: -0.863D-03-0.253D-02 0.114D+00 0.275D+00 0.614D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.40D-08 MaxDP=9.54D-07 DE=-7.83D-10 OVMax= 8.13D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.16D-08 CP: 1.00D+00 1.08D+00 8.50D-01 8.23D-01 8.88D-01

E= -1914.33331820128 Delta-E= -0.000000000102 Rises=F Damp=F

DIIS: error= 1.43D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33331820128 IErMin= 6 ErrMin= 1.43D-07

ErrMax= 1.43D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.78D-11 BMatP= 2.05D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.976D-03-0.185D-01 0.414D-02 0.628D-01 0.393D+00 0.557D+00

Coeff: 0.976D-03-0.185D-01 0.414D-02 0.628D-01 0.393D+00 0.557D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.89D-09 MaxDP=4.86D-07 DE=-1.02D-10 OVMax= 5.38D-06

Error on total polarization charges = 0.08258

SCF Done: E(UB3LYP) = -1914.33331820 A.U. after 6 cycles

NFock= 6 Conv=0.79D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0182

<L.S>= 0.000000000000E+00

KE= 1.906380727245D+03 PE=-1.516299810879D+04 EE= 5.985598469470D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0551, after 2.0017

Leave Link 502 at Thu Aug 29 21:10:23 2019, MaxMem= 4294967296 cpu: 2743.0

(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: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48636843D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64280774D-01

Leave Link 801 at Thu Aug 29 21:10:23 2019, MaxMem= 4294967296 cpu: 1.0

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Thu Aug 29 21:10:30 2019, MaxMem= 4294967296 cpu: 112.5

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Thu Aug 29 21:10:30 2019, MaxMem= 4294967296 cpu: 2.5

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 189

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 Thu Aug 29 21:30:11 2019, MaxMem= 4294967296 cpu: 18895.0

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 590000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.39D+03 4.50D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.52D+02 3.62D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.53D+00 4.66D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.02D-01 3.97D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.57D-04 2.10D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.58D-06 1.35D-04.

193 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 1.99D-08 1.02D-05.

85 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.28D-11 6.21D-07.

46 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.16D-13 3.89D-08.

4 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 8.15D-15 4.22D-09.

2 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 3.60D-15 1.89D-09.

InvSVY: IOpt=1 It= 1 EMax= 3.55D-14

Solved reduced A of dimension 1737 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1125.48 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Fri Aug 30 01:20:49 2019, MaxMem= 4294967296 cpu: 221335.0

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 189

Leave Link 701 at Fri Aug 30 01:22:18 2019, MaxMem= 4294967296 cpu: 1418.5

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Fri Aug 30 01:22:18 2019, MaxMem= 4294967296 cpu: 0.0

(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=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

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= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Fri Aug 30 01:40:57 2019, MaxMem= 4294967296 cpu: 17900.0

(Enter /home/kira/g09/l716.exe)

Dipole =-2.31492686D-05-2.78502472D-04-4.79377149D-01

Polarizability= 1.25563631D+03-2.95448281D+01 1.66558151D+03

1.01510345D-03-8.77392485D-03 4.55234409D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000000171 -0.000000044 -0.000000735

2 6 0.000000903 -0.000000976 -0.000002470

3 7 0.000001412 0.000000895 -0.000000313

4 6 -0.000001012 0.000000192 0.000002950

5 6 0.000000943 0.000000651 -0.000000344

6 6 0.000000525 0.000001851 -0.000001320

7 6 -0.000002900 0.000000146 -0.000000450

8 7 -0.000004261 0.000003790 0.000000176

9 6 -0.000001945 -0.000000946 -0.000001933

10 6 -0.000000987 -0.000001616 -0.000001455

11 6 -0.000000512 -0.000000400 0.000002813

12 6 -0.000002455 0.000002295 -0.000000648

13 6 0.000001896 0.000000145 0.000001854

14 6 0.000000943 -0.000001363 0.000001474

15 6 0.000000487 -0.000000529 -0.000002862

16 6 0.000002857 -0.000001037 0.000000620

17 7 0.000004408 0.000003794 0.000000060

18 6 -0.000000361 0.000001853 0.000001283

19 6 0.000000624 0.000001829 -0.000003129

20 6 -0.000000896 0.000000043 0.000000232

21 6 0.000000384 -0.000000526 0.000000826

22 6 -0.000001274 0.000000692 0.000002626

23 7 -0.000000979 -0.000001431 0.000000512

24 6 0.000002646 0.000002129 0.000000576

25 6 0.000002628 -0.000002119 -0.000002091

26 6 -0.000000738 -0.000002531 0.000002190

27 6 -0.000000069 0.000001008 -0.000000240

28 6 0.000000239 -0.000000321 0.000000370

29 6 0.000000534 0.000001381 -0.000001720

30 6 0.000000161 -0.000002590 -0.000003799

31 6 -0.000000123 0.000000862 -0.000000135

32 6 -0.000000010 0.000000661 -0.000000622

33 6 0.000000975 -0.000000621 -0.000000971

34 6 0.000001757 -0.000001427 0.000002687

35 6 -0.000001206 -0.000001371 0.000000696

36 6 0.000001662 0.000000581 0.000001044

37 6 -0.000001437 -0.000000872 -0.000003005

38 6 0.000001421 -0.000001141 -0.000000736

39 6 -0.000001676 0.000000497 -0.000001079

40 6 0.000000122 0.000000753 0.000000268

41 6 0.000000014 0.000000715 0.000000521

42 6 -0.000001371 -0.000000965 0.000001164

43 6 -0.000002667 -0.000001777 0.000002096

44 6 0.000000170 -0.000002389 0.000004194

45 6 -0.000000640 0.000001345 0.000001651

46 6 -0.000000144 -0.000000259 -0.000000301

47 6 -0.000000023 0.000000972 0.000000165

48 6 0.000000434 -0.000002815 -0.000002432

49 1 -0.000000215 -0.000001242 0.000000631

50 1 0.000000408 0.000001471 -0.000003809

51 1 -0.000002782 0.000000217 0.000000187

52 1 -0.000001679 0.000001919 -0.000000879

53 1 0.000002770 0.000000071 -0.000000191

54 1 0.000001677 0.000002051 0.000000807

55 1 -0.000000296 0.000001333 0.000003914

56 1 0.000000151 -0.000001401 -0.000000471

57 1 -0.000001069 -0.000001187 0.000000678

58 1 0.000000032 0.000000216 0.000000129

59 1 -0.000000155 0.000000549 -0.000000558

60 1 -0.000001084 0.000000254 -0.000000716

61 1 -0.000002341 0.000001760 0.000001879

62 1 0.000000996 0.000000123 -0.000000527

63 1 0.000000566 -0.000000036 -0.000000758

64 1 -0.000000853 -0.000001553 -0.000001250

65 1 -0.000001138 0.000001576 -0.000002059

66 1 0.000000120 0.000000028 -0.000000045

67 1 0.000001099 0.000001554 0.000002034

68 1 -0.000000139 -0.000000019 0.000000072

69 1 -0.000000970 0.000000097 0.000000510

70 1 -0.000000584 -0.000000138 0.000000783

71 1 0.000000858 -0.000001578 0.000001275

72 1 0.000002418 0.000001801 -0.000001992

73 1 0.000001095 0.000000256 0.000000723

74 1 0.000000147 0.000000538 0.000000566

75 1 -0.000000027 0.000000176 -0.000000127

76 1 0.000001101 -0.000001214 -0.000000689

77 1 0.000016985 -0.000003556 0.000002173

78 1 -0.000017381 -0.000003082 -0.000002555

-------------------------------------------------------------------

Cartesian Forces: Max 0.000017381 RMS 0.000002201

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Fri Aug 30 01:40:58 2019, MaxMem= 4294967296 cpu: 2.0

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000017624 RMS 0.000003773

Search for a local minimum.

Step number 23 out of a maximum of 452

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= 6.70D-07 DEPred=-5.32D-08 R=-1.26D+01

Trust test=-1.26D+01 RLast= 1.36D-03 DXMaxT set to 5.00D-02

ITU= -1 1 1 -1 -1 1 1 -1 -1 1 0 -1 1 1 -1 1 -1 -1 1 1

ITU= -1 1 0

Eigenvalues --- 0.00055 0.00241 0.00408 0.00598 0.00723

Eigenvalues --- 0.00812 0.00921 0.01045 0.01058 0.01119

Eigenvalues --- 0.01135 0.01164 0.01264 0.01280 0.01302

Eigenvalues --- 0.01305 0.01322 0.01422 0.01428 0.01534

Eigenvalues --- 0.01549 0.01559 0.01592 0.01672 0.01711

Eigenvalues --- 0.01716 0.01728 0.01737 0.01754 0.01759

Eigenvalues --- 0.01761 0.01782 0.01801 0.01803 0.01885

Eigenvalues --- 0.01935 0.01987 0.01996 0.02011 0.02165

Eigenvalues --- 0.02169 0.02256 0.02289 0.02293 0.02304

Eigenvalues --- 0.02330 0.02392 0.02468 0.02471 0.02521

Eigenvalues --- 0.02538 0.02544 0.02586 0.02626 0.02628

Eigenvalues --- 0.02645 0.02648 0.02768 0.02779 0.02796

Eigenvalues --- 0.02803 0.02868 0.02872 0.02873 0.02875

Eigenvalues --- 0.02943 0.02968 0.03909 0.04088 0.04190

Eigenvalues --- 0.04318 0.04368 0.04463 0.04543 0.04571

Eigenvalues --- 0.08163 0.09646 0.09685 0.09730 0.09862

Eigenvalues --- 0.09886 0.10301 0.10436 0.10569 0.10696

Eigenvalues --- 0.10698 0.10703 0.10734 0.10734 0.11008

Eigenvalues --- 0.11397 0.11397 0.11410 0.11412 0.11985

Eigenvalues --- 0.11987 0.11997 0.12003 0.12278 0.12279

Eigenvalues --- 0.12323 0.12324 0.12770 0.12771 0.12773

Eigenvalues --- 0.12775 0.15716 0.15919 0.16297 0.16757

Eigenvalues --- 0.17208 0.17298 0.17580 0.17835 0.17994

Eigenvalues --- 0.18025 0.18266 0.18341 0.19242 0.19283

Eigenvalues --- 0.19358 0.19360 0.19370 0.19408 0.19413

Eigenvalues --- 0.19428 0.19551 0.19552 0.19554 0.19555

Eigenvalues --- 0.20293 0.21486 0.22041 0.22731 0.22879

Eigenvalues --- 0.23240 0.23766 0.24231 0.24750 0.25075

Eigenvalues --- 0.26281 0.26383 0.26661 0.27143 0.28524

Eigenvalues --- 0.28550 0.28748 0.29014 0.29785 0.31031

Eigenvalues --- 0.31697 0.32012 0.32848 0.33076 0.33172

Eigenvalues --- 0.33324 0.34120 0.34567 0.35055 0.35564

Eigenvalues --- 0.35625 0.35626 0.35633 0.35640 0.35756

Eigenvalues --- 0.35760 0.35764 0.35809 0.35925 0.35925

Eigenvalues --- 0.35930 0.35934 0.35987 0.35988 0.36007

Eigenvalues --- 0.36010 0.36191 0.36201 0.36244 0.36245

Eigenvalues --- 0.36981 0.37057 0.37239 0.37386 0.37395

Eigenvalues --- 0.37486 0.38136 0.38436 0.38511 0.38544

Eigenvalues --- 0.39446 0.40367 0.40727 0.41040 0.41059

Eigenvalues --- 0.41100 0.41189 0.41254 0.41345 0.41350

Eigenvalues --- 0.41565 0.41795 0.42274 0.42639 0.44530

Eigenvalues --- 0.45241 0.45910 0.45922 0.45937 0.45949

Eigenvalues --- 0.46005 0.46015 0.46256 0.46260 0.46315

Eigenvalues --- 0.46324 0.48393 0.49008 0.49415 0.49627

Eigenvalues --- 0.50751 0.50754 0.50779 0.50783 0.51863

Eigenvalues --- 0.52210 0.57177 0.57710

Cut down GDIIS permanently because of the ratio check. E10

DIIS coeff's: 0.92347 0.03591 0.19173 -0.01844 -0.02220

DIIS coeff's: -0.11335 -0.00025 0.00507 0.03765 -0.04430

DIIS coeff's: -0.00643 0.00908 0.00300 -0.00012 -0.00080

Cosine: 0.936 > 0.500

Length: 0.363

GDIIS step was calculated using 15 of the last 23 vectors.

Iteration 1 RMS(Cart)= 0.00088652 RMS(Int)= 0.00000011

Iteration 2 RMS(Cart)= 0.00000020 RMS(Int)= 0.00000007

ITry= 1 IFail=0 DXMaxC= 4.19D-03 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.65685 0.00000 0.00001 -0.00000 0.00001 2.65686

R2 2.64097 0.00001 0.00000 0.00000 0.00000 2.64097

R3 2.03707 0.00000 0.00000 -0.00000 0.00000 2.03708

R4 2.59921 -0.00001 -0.00000 0.00000 -0.00000 2.59921

R5 2.71594 0.00000 -0.00001 0.00000 -0.00001 2.71593

R6 2.59904 -0.00001 -0.00002 0.00000 -0.00001 2.59903

R7 1.91015 -0.00002 -0.00001 0.00000 -0.00001 1.91014

R8 2.65653 0.00000 0.00000 -0.00000 0.00000 2.65653

R9 2.71690 0.00001 0.00002 -0.00000 0.00002 2.71692

R10 2.03713 0.00000 0.00000 0.00000 0.00000 2.03713

R11 2.64076 0.00002 -0.00000 -0.00000 -0.00000 2.64075

R12 2.80422 0.00000 -0.00000 0.00000 0.00000 2.80422

R13 2.59621 0.00001 0.00002 -0.00000 0.00002 2.59623

R14 2.76198 0.00000 -0.00000 0.00000 -0.00000 2.76198

R15 2.59435 0.00000 -0.00003 0.00000 -0.00002 2.59433

R16 2.76239 -0.00000 -0.00000 0.00000 -0.00000 2.76239

R17 2.64282 0.00000 0.00003 -0.00000 0.00003 2.64285

R18 2.55437 0.00000 0.00001 -0.00000 0.00000 2.55438

R19 2.03919 0.00000 0.00000 0.00000 0.00000 2.03920

R20 2.03906 0.00000 0.00000 -0.00000 -0.00000 2.03906

R21 2.64282 0.00000 0.00002 -0.00000 0.00002 2.64285

R22 2.80375 0.00000 -0.00001 0.00000 -0.00001 2.80375

R23 2.76239 -0.00000 -0.00000 0.00000 -0.00000 2.76239

R24 2.59435 0.00000 -0.00002 0.00000 -0.00002 2.59433

R25 2.55437 0.00000 0.00001 -0.00000 0.00000 2.55438

R26 2.03919 0.00000 0.00000 0.00000 0.00000 2.03920

R27 2.76198 0.00000 -0.00000 0.00000 -0.00000 2.76198

R28 2.03906 0.00000 0.00000 -0.00000 -0.00000 2.03906

R29 2.59621 0.00001 0.00002 -0.00000 0.00002 2.59623

R30 2.64075 0.00002 0.00001 -0.00000 0.00001 2.64075

R31 2.71689 0.00001 0.00003 -0.00000 0.00003 2.71692

R32 2.80424 0.00000 -0.00002 0.00000 -0.00002 2.80422

R33 2.65654 0.00000 -0.00001 -0.00000 -0.00001 2.65653

R34 2.59905 -0.00001 -0.00002 -0.00000 -0.00002 2.59902

R35 2.64096 0.00001 0.00001 0.00000 0.00001 2.64097

R36 2.03713 0.00000 0.00000 0.00000 0.00000 2.03713

R37 2.65686 0.00000 0.00000 -0.00000 0.00000 2.65686

R38 2.03707 0.00000 0.00000 -0.00000 0.00000 2.03708

R39 2.59921 -0.00001 -0.00001 -0.00000 -0.00001 2.59921

R40 2.71593 0.00000 -0.00000 0.00000 -0.00000 2.71593

R41 1.91016 -0.00002 -0.00002 0.00000 -0.00002 1.91014

R42 2.80377 0.00000 -0.00003 0.00000 -0.00003 2.80374

R43 2.65123 -0.00000 0.00000 -0.00000 0.00000 2.65123

R44 2.64988 0.00000 0.00000 0.00000 0.00000 2.64988

R45 2.62864 -0.00000 -0.00000 0.00000 -0.00000 2.62864

R46 2.04850 0.00000 -0.00000 -0.00000 -0.00000 2.04850

R47 2.63628 0.00000 0.00000 0.00000 0.00000 2.63628

R48 2.05017 0.00000 0.00000 0.00000 0.00000 2.05017

R49 2.63409 0.00000 -0.00000 0.00000 -0.00000 2.63408

R50 2.05006 0.00000 0.00000 -0.00000 0.00000 2.05006

R51 2.63098 0.00000 0.00000 0.00000 0.00000 2.63098

R52 2.05014 0.00000 -0.00000 -0.00000 -0.00000 2.05014

R53 2.04862 0.00000 -0.00000 0.00000 -0.00000 2.04862

R54 2.63632 0.00000 0.00000 0.00000 0.00000 2.63632

R55 2.63423 0.00000 0.00000 0.00000 0.00000 2.63423

R56 2.05006 0.00000 0.00000 -0.00000 0.00000 2.05006

R57 2.62891 -0.00000 0.00000 0.00000 0.00000 2.62891

R58 2.05018 0.00000 -0.00000 0.00000 -0.00000 2.05018

R59 2.65142 -0.00000 0.00000 -0.00000 0.00000 2.65142

R60 2.04848 -0.00000 -0.00000 0.00000 -0.00000 2.04848

R61 2.65009 -0.00000 0.00000 -0.00000 0.00000 2.65010

R62 2.63061 0.00000 -0.00000 0.00000 -0.00000 2.63061

R63 2.04855 0.00000 -0.00000 -0.00000 -0.00000 2.04855

R64 2.05016 0.00000 -0.00000 0.00000 0.00000 2.05016

R65 2.65009 -0.00000 0.00001 -0.00000 0.00001 2.65010

R66 2.65142 -0.00000 0.00001 -0.00000 0.00001 2.65143

R67 2.63061 0.00000 -0.00000 0.00000 -0.00000 2.63061

R68 2.04855 -0.00000 -0.00000 -0.00000 -0.00000 2.04855

R69 2.63423 0.00000 0.00000 0.00000 0.00000 2.63423

R70 2.05016 0.00000 -0.00000 0.00000 -0.00000 2.05016

R71 2.63632 0.00000 0.00000 0.00000 0.00000 2.63632

R72 2.05006 0.00000 0.00000 -0.00000 0.00000 2.05006

R73 2.62892 -0.00000 -0.00000 0.00000 -0.00000 2.62891

R74 2.05018 0.00000 -0.00000 0.00000 -0.00000 2.05018

R75 2.04848 -0.00000 -0.00000 0.00000 -0.00000 2.04848

R76 2.64987 0.00000 0.00001 0.00000 0.00001 2.64988

R77 2.65122 -0.00000 0.00001 -0.00000 0.00001 2.65123

R78 2.63098 0.00000 -0.00000 0.00000 -0.00000 2.63098

R79 2.04862 0.00000 -0.00000 0.00000 -0.00000 2.04862

R80 2.63408 0.00000 -0.00000 0.00000 -0.00000 2.63408

R81 2.05014 0.00000 -0.00000 -0.00000 -0.00000 2.05014

R82 2.63628 0.00000 0.00000 0.00000 0.00000 2.63628

R83 2.05006 0.00000 0.00000 -0.00000 -0.00000 2.05006

R84 2.62865 -0.00000 -0.00001 0.00000 -0.00001 2.62864

R85 2.05017 0.00000 -0.00000 0.00000 -0.00000 2.05017

R86 2.04850 0.00000 -0.00000 -0.00000 -0.00000 2.04850

A1 1.88156 -0.00000 -0.00000 -0.00000 -0.00000 1.88155

A2 2.18786 0.00000 0.00001 0.00000 0.00001 2.18786

A3 2.21376 0.00000 -0.00000 -0.00000 -0.00000 2.21375

A4 1.86797 -0.00000 -0.00001 0.00000 -0.00001 1.86797

A5 2.22219 0.00002 0.00006 -0.00000 0.00006 2.22225

A6 2.19257 -0.00001 -0.00006 -0.00000 -0.00006 2.19251

A7 1.92512 0.00001 0.00002 -0.00000 0.00001 1.92513

A8 2.17738 -0.00001 -0.00004 -0.00000 -0.00004 2.17733

A9 2.17987 -0.00000 0.00002 0.00000 0.00002 2.17989

A10 1.86811 -0.00000 -0.00001 0.00000 -0.00001 1.86810

A11 2.19438 0.00000 -0.00000 0.00000 -0.00000 2.19438

A12 2.22029 0.00000 0.00001 -0.00000 0.00001 2.22030

A13 1.88166 -0.00000 0.00000 0.00000 0.00000 1.88166

A14 2.21403 0.00000 0.00000 0.00000 0.00000 2.21403

A15 2.18747 -0.00000 -0.00001 -0.00000 -0.00001 2.18746

A16 2.18669 0.00001 0.00001 -0.00000 0.00000 2.18670

A17 2.02291 -0.00002 -0.00002 0.00000 -0.00002 2.02289

A18 2.07354 0.00001 0.00002 -0.00000 0.00001 2.07355

A19 2.19173 0.00001 -0.00001 -0.00000 -0.00001 2.19171

A20 2.16533 -0.00000 0.00002 0.00000 0.00002 2.16535

A21 1.92610 -0.00001 -0.00001 0.00000 -0.00001 1.92609

A22 1.84709 0.00000 0.00001 -0.00000 0.00001 1.84709

A23 1.92648 -0.00000 0.00000 -0.00000 0.00000 1.92648

A24 2.19208 0.00001 -0.00001 0.00000 -0.00001 2.19207

A25 2.16462 -0.00000 0.00001 -0.00000 0.00001 2.16463

A26 1.86205 0.00000 -0.00000 0.00000 -0.00000 1.86205

A27 2.19691 -0.00000 -0.00000 -0.00000 -0.00000 2.19690

A28 2.22384 0.00000 0.00000 0.00000 0.00000 2.22384

A29 1.86206 0.00000 0.00000 0.00000 0.00000 1.86206

A30 2.19689 -0.00000 0.00001 -0.00000 0.00001 2.19690

A31 2.22390 -0.00000 -0.00001 0.00000 -0.00001 2.22389

A32 2.18527 -0.00000 -0.00002 -0.00000 -0.00002 2.18526

A33 2.02532 0.00001 0.00005 0.00000 0.00005 2.02537

A34 2.07255 -0.00001 -0.00003 -0.00000 -0.00003 2.07252

A35 2.16463 -0.00000 -0.00000 -0.00000 -0.00000 2.16463

A36 2.19207 0.00000 0.00000 0.00000 0.00000 2.19207

A37 1.92648 -0.00000 0.00000 -0.00000 0.00000 1.92648

A38 1.86205 0.00000 -0.00000 0.00000 -0.00000 1.86205

A39 2.19691 -0.00000 -0.00000 -0.00000 -0.00000 2.19690

A40 2.22384 0.00000 0.00000 0.00000 0.00001 2.22384

A41 1.86206 0.00000 0.00000 0.00000 0.00000 1.86206

A42 2.22390 -0.00000 -0.00001 -0.00000 -0.00001 2.22389

A43 2.19689 -0.00000 0.00001 -0.00000 0.00001 2.19690

A44 1.92610 -0.00001 -0.00001 0.00000 -0.00001 1.92609

A45 2.16532 -0.00000 0.00003 -0.00000 0.00003 2.16535

A46 2.19173 0.00001 -0.00002 0.00000 -0.00002 2.19171

A47 1.84709 0.00000 0.00001 -0.00000 0.00000 1.84709

A48 2.18672 0.00001 -0.00003 -0.00000 -0.00003 2.18669

A49 2.07350 0.00001 0.00006 0.00000 0.00006 2.07356

A50 2.02291 -0.00002 -0.00003 -0.00000 -0.00003 2.02288

A51 2.22029 0.00000 0.00001 0.00000 0.00001 2.22030

A52 2.19438 0.00000 -0.00000 -0.00000 -0.00000 2.19438

A53 1.86811 -0.00000 -0.00001 -0.00000 -0.00001 1.86810

A54 1.88166 -0.00000 0.00000 -0.00000 0.00000 1.88166

A55 2.18748 -0.00000 -0.00002 -0.00000 -0.00002 2.18746

A56 2.21401 0.00000 0.00002 0.00000 0.00002 2.21403

A57 1.88156 -0.00000 -0.00000 -0.00000 -0.00000 1.88155

A58 2.21375 0.00000 0.00000 0.00000 0.00000 2.21376

A59 2.18786 0.00000 0.00000 -0.00000 0.00000 2.18786

A60 1.86798 -0.00000 -0.00001 0.00000 -0.00001 1.86797

A61 2.22219 0.00002 0.00006 0.00000 0.00006 2.22225

A62 2.19256 -0.00001 -0.00005 -0.00000 -0.00005 2.19251

A63 1.92511 0.00001 0.00002 -0.00000 0.00002 1.92513

A64 2.17986 -0.00000 0.00002 0.00000 0.00002 2.17989

A65 2.17737 -0.00001 -0.00003 -0.00000 -0.00003 2.17734

A66 2.18530 -0.00000 -0.00005 0.00000 -0.00005 2.18525

A67 2.07252 -0.00001 0.00001 -0.00000 0.00001 2.07253

A68 2.02533 0.00001 0.00003 0.00000 0.00004 2.02536

A69 2.10452 -0.00001 -0.00002 0.00000 -0.00002 2.10450

A70 2.10700 0.00001 0.00002 -0.00000 0.00002 2.10702

A71 2.07167 0.00000 -0.00000 0.00000 -0.00000 2.07166

A72 2.10512 0.00000 0.00000 -0.00000 0.00000 2.10512

A73 2.08515 -0.00000 -0.00000 -0.00000 -0.00000 2.08515

A74 2.09276 0.00000 -0.00000 0.00000 -0.00000 2.09276

A75 2.09776 -0.00000 -0.00000 0.00000 -0.00000 2.09775

A76 2.08897 0.00000 0.00000 -0.00000 0.00000 2.08897

A77 2.09646 0.00000 0.00000 -0.00000 0.00000 2.09646

A78 2.08903 0.00000 0.00000 0.00000 0.00000 2.08903

A79 2.09689 -0.00000 -0.00000 -0.00000 -0.00000 2.09689

A80 2.09726 0.00000 0.00000 0.00000 0.00000 2.09726

A81 2.09760 -0.00000 0.00000 -0.00000 0.00000 2.09760

A82 2.09706 0.00000 0.00000 0.00000 0.00000 2.09707

A83 2.08852 -0.00000 -0.00000 0.00000 -0.00000 2.08851

A84 2.10507 -0.00000 -0.00000 0.00000 -0.00000 2.10507

A85 2.08430 -0.00000 -0.00000 -0.00000 -0.00000 2.08430

A86 2.09367 0.00000 0.00000 -0.00000 0.00000 2.09367

A87 2.08896 0.00000 0.00000 -0.00000 0.00000 2.08896

A88 2.09700 -0.00000 -0.00000 0.00000 -0.00000 2.09700

A89 2.09723 0.00000 -0.00000 0.00000 0.00000 2.09723

A90 2.09801 -0.00000 0.00000 -0.00000 0.00000 2.09801

A91 2.09647 0.00000 -0.00000 -0.00000 -0.00000 2.09647

A92 2.08871 0.00000 -0.00000 0.00000 -0.00000 2.08871

A93 2.10486 -0.00000 -0.00000 0.00000 -0.00000 2.10486

A94 2.09331 0.00000 0.00000 0.00000 0.00000 2.09331

A95 2.08482 -0.00000 -0.00000 -0.00000 -0.00000 2.08481

A96 2.10716 -0.00000 0.00003 0.00000 0.00003 2.10718

A97 2.10453 -0.00000 -0.00002 -0.00000 -0.00002 2.10451

A98 2.07149 0.00000 -0.00000 0.00000 -0.00000 2.07149

A99 2.10547 -0.00000 0.00000 -0.00000 0.00000 2.10548

A100 2.08384 -0.00000 -0.00001 0.00000 -0.00001 2.08383

A101 2.09375 0.00000 0.00000 0.00000 0.00000 2.09375

A102 2.09745 -0.00000 -0.00000 0.00000 -0.00000 2.09745

A103 2.09705 0.00000 0.00000 -0.00000 0.00000 2.09705

A104 2.08868 0.00000 0.00000 -0.00000 0.00000 2.08868

A105 2.10452 -0.00000 -0.00001 -0.00000 -0.00001 2.10451

A106 2.10717 -0.00000 0.00002 0.00000 0.00002 2.10718

A107 2.07150 0.00000 -0.00001 0.00000 -0.00001 2.07149

A108 2.10547 -0.00000 0.00001 -0.00000 0.00001 2.10548

A109 2.08383 -0.00000 -0.00000 0.00000 -0.00000 2.08383

A110 2.09375 0.00000 -0.00000 0.00000 -0.00000 2.09375

A111 2.09745 -0.00000 -0.00000 0.00000 -0.00000 2.09745

A112 2.08868 0.00000 0.00000 -0.00000 0.00000 2.08868

A113 2.09705 0.00000 0.00000 -0.00000 0.00000 2.09705

A114 2.08896 0.00000 0.00000 -0.00000 0.00000 2.08896

A115 2.09723 0.00000 -0.00000 0.00000 0.00000 2.09723

A116 2.09700 -0.00000 -0.00000 -0.00000 -0.00000 2.09700

A117 2.09800 -0.00000 0.00000 -0.00000 0.00000 2.09801

A118 2.09647 0.00000 -0.00000 -0.00000 -0.00000 2.09647

A119 2.08871 0.00000 -0.00000 0.00000 0.00000 2.08871

A120 2.10486 -0.00000 0.00000 0.00000 0.00000 2.10486

A121 2.08482 -0.00000 -0.00000 -0.00000 -0.00001 2.08481

A122 2.09331 0.00000 0.00000 0.00000 0.00000 2.09331

A123 2.10698 0.00001 0.00003 0.00000 0.00003 2.10702

A124 2.10452 -0.00001 -0.00002 -0.00000 -0.00002 2.10450

A125 2.07168 0.00000 -0.00001 -0.00000 -0.00001 2.07166

A126 2.10507 -0.00000 0.00000 0.00000 0.00000 2.10507

A127 2.08430 -0.00000 -0.00000 -0.00000 -0.00000 2.08430

A128 2.09367 0.00000 -0.00000 -0.00000 -0.00000 2.09367

A129 2.09760 0.00000 0.00000 -0.00000 0.00000 2.09760

A130 2.08852 -0.00000 -0.00000 0.00000 -0.00000 2.08851

A131 2.09706 0.00000 0.00000 0.00000 0.00000 2.09707

A132 2.08903 0.00000 0.00000 -0.00000 0.00000 2.08903

A133 2.09726 0.00000 0.00000 0.00000 0.00000 2.09726

A134 2.09689 -0.00000 -0.00000 -0.00000 -0.00000 2.09689

A135 2.09776 -0.00000 -0.00000 0.00000 -0.00000 2.09775

A136 2.09646 0.00000 -0.00000 -0.00000 -0.00000 2.09646

A137 2.08897 0.00000 0.00000 -0.00000 0.00000 2.08897

A138 2.10511 0.00000 0.00001 0.00000 0.00001 2.10512

A139 2.08515 -0.00000 -0.00000 -0.00000 -0.00000 2.08514

A140 2.09276 0.00000 -0.00000 0.00000 -0.00000 2.09276

D1 0.01562 0.00000 0.00004 -0.00001 0.00004 0.01566

D2 -3.09485 0.00000 0.00025 0.00000 0.00025 -3.09460

D3 -3.12078 0.00000 -0.00001 -0.00001 -0.00002 -3.12080

D4 0.05193 0.00000 0.00019 0.00000 0.00019 0.05213

D5 -0.00068 -0.00000 -0.00002 -0.00000 -0.00002 -0.00071

D6 -3.13462 -0.00000 -0.00005 -0.00000 -0.00005 -3.13467

D7 3.13562 0.00000 0.00003 0.00000 0.00003 3.13566

D8 0.00169 -0.00000 0.00001 -0.00000 0.00000 0.00169

D9 -0.02533 -0.00000 -0.00005 0.00001 -0.00004 -0.02536

D10 3.07436 0.00000 -0.00021 -0.00004 -0.00025 3.07411

D11 3.08582 -0.00000 -0.00024 0.00000 -0.00024 3.08558

D12 -0.09768 -0.00000 -0.00041 -0.00005 -0.00045 -0.09813

D13 -2.95267 -0.00000 -0.00035 -0.00004 -0.00039 -2.95306

D14 0.17895 -0.00000 -0.00023 -0.00004 -0.00027 0.17868

D15 0.22553 -0.00000 -0.00011 -0.00003 -0.00014 0.22539

D16 -2.92603 0.00000 0.00001 -0.00003 -0.00002 -2.92605

D17 0.02491 0.00000 0.00003 -0.00001 0.00002 0.02493

D18 -3.08790 0.00000 0.00012 -0.00001 0.00011 -3.08779

D19 -3.07470 -0.00000 0.00020 0.00004 0.00023 -3.07447

D20 0.09567 0.00000 0.00029 0.00004 0.00032 0.09600

D21 -0.01452 0.00000 -0.00001 0.00001 0.00000 -0.01452

D22 3.11956 0.00000 0.00002 0.00001 0.00003 3.11959

D23 3.09773 -0.00000 -0.00009 0.00000 -0.00009 3.09764

D24 -0.05137 -0.00000 -0.00007 0.00001 -0.00006 -0.05143

D25 -0.23680 -0.00000 -0.00016 0.00001 -0.00015 -0.23695

D26 2.91540 -0.00000 -0.00018 0.00002 -0.00016 2.91524

D27 2.93935 -0.00000 -0.00006 0.00001 -0.00004 2.93931

D28 -0.19163 -0.00000 -0.00008 0.00003 -0.00005 -0.19169

D29 -0.12442 -0.00000 -0.00001 -0.00000 -0.00001 -0.12443

D30 3.02605 -0.00000 0.00010 0.00001 0.00011 3.02616

D31 3.00629 -0.00000 0.00001 -0.00002 -0.00000 3.00628

D32 -0.12643 0.00000 0.00013 -0.00000 0.00012 -0.12631

D33 -0.99868 0.00001 0.00011 -0.00002 0.00009 -0.99859

D34 2.13959 0.00001 0.00013 -0.00002 0.00010 2.13970

D35 2.15280 0.00001 0.00009 -0.00001 0.00008 2.15288

D36 -0.99212 0.00000 0.00011 -0.00001 0.00010 -0.99202

D37 -3.09197 0.00000 0.00017 0.00002 0.00018 -3.09179

D38 0.04178 0.00000 0.00007 0.00000 0.00007 0.04185

D39 3.10673 -0.00000 -0.00017 -0.00001 -0.00018 3.10655

D40 -0.06123 -0.00000 -0.00015 -0.00002 -0.00017 -0.06140

D41 -0.02716 -0.00000 -0.00007 -0.00000 -0.00007 -0.02723

D42 3.08806 -0.00000 -0.00005 -0.00000 -0.00005 3.08801

D43 -0.04095 -0.00000 -0.00004 -0.00001 -0.00004 -0.04099

D44 3.09603 -0.00000 -0.00005 -0.00000 -0.00005 3.09597

D45 0.02491 0.00000 -0.00001 0.00001 -0.00000 0.02490

D46 -3.08819 0.00000 0.00003 0.00000 0.00004 -3.08815

D47 -3.11216 0.00000 0.00000 0.00000 0.00001 -3.11215

D48 0.05793 0.00000 0.00005 0.00000 0.00005 0.05798

D49 0.13438 0.00000 0.00026 0.00001 0.00027 0.13465

D50 -2.99711 0.00000 0.00030 0.00001 0.00031 -2.99680

D51 -3.01244 0.00000 0.00025 0.00001 0.00026 -3.01217

D52 0.13926 -0.00000 0.00029 0.00001 0.00030 0.13956

D53 0.00132 0.00000 0.00005 -0.00000 0.00004 0.00136

D54 -3.11337 -0.00000 0.00003 -0.00000 0.00002 -3.11335

D55 3.11383 0.00000 0.00000 0.00000 0.00000 3.11383

D56 -0.00085 -0.00000 -0.00002 0.00000 -0.00002 -0.00087

D57 -3.01251 0.00000 0.00031 0.00002 0.00033 -3.01218

D58 0.13434 0.00000 0.00027 0.00003 0.00030 0.13464

D59 0.13930 -0.00000 0.00019 0.00002 0.00021 0.13951

D60 -2.99704 0.00000 0.00015 0.00002 0.00017 -2.99686

D61 0.99260 -0.00000 -0.00014 0.00001 -0.00013 0.99247

D62 -2.14552 -0.00000 -0.00019 0.00000 -0.00019 -2.14570

D63 -2.15829 -0.00000 -0.00003 0.00001 -0.00002 -2.15830

D64 0.98679 -0.00000 -0.00008 0.00000 -0.00007 0.98671

D65 -3.11210 0.00000 -0.00006 0.00001 -0.00005 -3.11216

D66 0.05799 0.00000 -0.00002 0.00000 -0.00002 0.05797

D67 0.02493 0.00000 -0.00003 0.00000 -0.00002 0.02491

D68 -3.08817 0.00000 0.00002 -0.00000 0.00001 -3.08815

D69 3.09598 -0.00000 0.00001 -0.00001 0.00000 3.09598

D70 -0.04096 -0.00000 -0.00003 -0.00000 -0.00003 -0.04099

D71 0.00129 0.00000 0.00006 0.00000 0.00006 0.00136

D72 -3.11340 -0.00000 0.00005 0.00000 0.00006 -3.11335

D73 3.11381 0.00000 0.00002 0.00001 0.00003 3.11384

D74 -0.00088 -0.00000 0.00001 0.00001 0.00002 -0.00087

D75 -0.02715 -0.00000 -0.00008 -0.00000 -0.00009 -0.02723

D76 3.10676 -0.00000 -0.00021 -0.00001 -0.00022 3.10654

D77 3.08809 -0.00000 -0.00007 -0.00001 -0.00008 3.08801

D78 -0.06119 -0.00000 -0.00020 -0.00001 -0.00021 -0.06141

D79 0.04177 0.00000 0.00007 0.00001 0.00007 0.04185

D80 -3.09199 0.00000 0.00020 0.00001 0.00021 -3.09178

D81 3.02602 0.00000 0.00013 0.00002 0.00015 3.02617

D82 -0.12637 0.00000 0.00000 0.00001 0.00002 -0.12635

D83 -0.12443 -0.00000 -0.00002 0.00002 -0.00000 -0.12444

D84 3.00637 -0.00000 -0.00015 0.00001 -0.00014 3.00623

D85 2.93989 -0.00000 -0.00072 -0.00001 -0.00073 2.93916

D86 -0.23641 -0.00000 -0.00063 -0.00001 -0.00063 -0.23705

D87 -0.19119 -0.00000 -0.00060 -0.00001 -0.00060 -0.19179

D88 2.91569 -0.00000 -0.00050 0.00000 -0.00050 2.91519

D89 -0.99242 0.00000 0.00044 -0.00000 0.00044 -0.99197

D90 2.15248 0.00001 0.00047 0.00001 0.00047 2.15295

D91 2.13938 0.00001 0.00033 -0.00001 0.00032 2.13971

D92 -0.99891 0.00001 0.00035 -0.00000 0.00035 -0.99856

D93 3.09761 -0.00000 0.00009 0.00000 0.00009 3.09769

D94 -0.05143 -0.00000 0.00003 0.00001 0.00003 -0.05140

D95 -0.01452 0.00000 0.00001 -0.00001 0.00000 -0.01452

D96 3.11963 0.00000 -0.00005 0.00000 -0.00005 3.11958

D97 -3.08778 0.00000 -0.00007 0.00000 -0.00006 -3.08785

D98 0.09619 0.00000 -0.00036 -0.00002 -0.00038 0.09581

D99 0.02490 0.00000 0.00001 0.00001 0.00002 0.02492

D100 -3.07431 -0.00000 -0.00028 -0.00001 -0.00029 -3.07460

D101 -0.00068 -0.00000 -0.00002 -0.00000 -0.00002 -0.00071

D102 3.13568 0.00000 -0.00005 0.00001 -0.00004 3.13564

D103 -3.13469 -0.00000 0.00004 -0.00001 0.00003 -3.13465

D104 0.00168 -0.00000 0.00001 -0.00000 0.00001 0.00169

D105 0.01562 0.00000 0.00003 0.00001 0.00003 0.01565

D106 -3.09471 0.00000 0.00005 0.00000 0.00006 -3.09465

D107 -3.12084 0.00000 0.00006 -0.00000 0.00006 -3.12079

D108 0.05202 0.00000 0.00008 -0.00000 0.00008 0.05209

D109 -0.02532 -0.00000 -0.00003 -0.00001 -0.00003 -0.02535

D110 3.07397 0.00000 0.00027 0.00001 0.00028 3.07424

D111 3.08569 -0.00000 -0.00004 -0.00001 -0.00005 3.08563

D112 -0.09822 -0.00000 0.00025 0.00001 0.00026 -0.09795

D113 -2.95320 -0.00000 0.00031 -0.00002 0.00029 -2.95291

D114 0.17853 -0.00000 0.00027 -0.00002 0.00025 0.17879

D115 0.22517 -0.00000 0.00034 -0.00002 0.00031 0.22549

D116 -2.92628 0.00000 0.00029 -0.00002 0.00028 -2.92600

D117 0.98704 -0.00000 -0.00038 0.00000 -0.00038 0.98666

D118 -2.15798 -0.00000 -0.00041 0.00001 -0.00040 -2.15838

D119 -2.14537 -0.00001 -0.00034 -0.00001 -0.00035 -2.14572

D120 0.99280 -0.00000 -0.00037 0.00000 -0.00037 0.99243

D121 -3.13035 -0.00000 0.00002 -0.00001 0.00001 -3.13033

D122 -0.00826 0.00000 0.00002 -0.00000 0.00002 -0.00824

D123 0.01450 0.00000 -0.00000 -0.00000 -0.00000 0.01450

D124 3.13659 0.00000 0.00000 0.00000 0.00000 3.13660

D125 -3.14032 0.00000 -0.00002 0.00000 -0.00001 -3.14034

D126 -0.01713 0.00000 -0.00002 0.00001 -0.00001 -0.01714

D127 -0.00199 -0.00000 0.00000 -0.00000 -0.00000 -0.00199

D128 3.12121 0.00000 0.00000 0.00000 0.00000 3.12121

D129 -0.01619 0.00000 0.00000 0.00000 0.00000 -0.01618

D130 3.12476 0.00000 0.00000 0.00000 0.00000 3.12476

D131 -3.13819 -0.00000 0.00000 -0.00000 -0.00000 -3.13819

D132 0.00276 -0.00000 -0.00000 -0.00000 -0.00000 0.00275

D133 0.00513 -0.00000 -0.00000 -0.00000 -0.00000 0.00513

D134 -3.13362 -0.00000 0.00000 -0.00000 0.00000 -3.13362

D135 -3.13581 -0.00000 -0.00000 -0.00000 -0.00000 -3.13581

D136 0.00863 -0.00000 0.00000 -0.00000 -0.00000 0.00862

D137 0.00733 -0.00000 0.00000 -0.00000 -0.00000 0.00733

D138 -3.13197 -0.00000 -0.00000 -0.00000 -0.00001 -3.13198

D139 -3.13710 -0.00000 -0.00000 -0.00000 -0.00000 -3.13710

D140 0.00678 -0.00000 -0.00001 -0.00000 -0.00001 0.00677

D141 -0.00888 0.00000 -0.00000 0.00000 0.00000 -0.00888

D142 -3.13198 -0.00000 -0.00000 0.00000 -0.00000 -3.13198

D143 3.13044 0.00000 0.00000 0.00000 0.00001 3.13044

D144 0.00734 -0.00000 0.00000 -0.00000 0.00000 0.00734

D145 -0.00538 0.00000 0.00000 0.00000 0.00000 -0.00537

D146 3.13571 0.00000 -0.00000 -0.00000 -0.00000 3.13571

D147 3.13483 0.00000 0.00001 0.00000 0.00001 3.13484

D148 -0.00727 0.00000 0.00000 0.00000 0.00000 -0.00726

D149 -0.00643 -0.00000 -0.00000 0.00000 0.00000 -0.00643

D150 3.13187 0.00000 0.00000 0.00000 0.00001 3.13188

D151 3.13655 0.00000 -0.00001 -0.00000 -0.00001 3.13655

D152 -0.00834 0.00000 -0.00000 0.00000 -0.00000 -0.00834

D153 0.01657 -0.00000 0.00000 -0.00000 -0.00000 0.01657

D154 3.13669 -0.00000 -0.00002 -0.00000 -0.00002 3.13667

D155 -3.12452 -0.00000 0.00000 -0.00000 0.00000 -3.12451

D156 -0.00440 -0.00000 -0.00002 0.00000 -0.00002 -0.00442

D157 3.12933 -0.00000 -0.00005 -0.00001 -0.00005 3.12928

D158 -0.01567 -0.00000 -0.00000 0.00000 0.00000 -0.01567

D159 0.00911 -0.00000 -0.00003 -0.00001 -0.00004 0.00908

D160 -3.13590 -0.00000 0.00002 0.00000 0.00002 -3.13587

D161 -3.14117 0.00000 0.00005 0.00001 0.00006 -3.14111

D162 0.01767 0.00000 0.00003 0.00001 0.00004 0.01771

D163 0.00383 0.00000 0.00000 -0.00000 0.00000 0.00383

D164 -3.12051 -0.00000 -0.00001 -0.00000 -0.00002 -3.12053

D165 0.00716 -0.00000 0.00000 -0.00000 -0.00000 0.00715

D166 -3.13116 -0.00000 -0.00000 -0.00000 -0.00001 -3.13117

D167 3.13140 0.00000 0.00002 0.00000 0.00002 3.13142

D168 -0.00691 0.00000 0.00001 0.00000 0.00001 -0.00690

D169 -3.14113 0.00000 -0.00001 0.00001 -0.00000 -3.14113

D170 0.01769 0.00000 0.00001 0.00001 0.00001 0.01770

D171 0.00382 0.00000 0.00002 -0.00000 0.00002 0.00383

D172 -3.12055 -0.00000 0.00003 0.00000 0.00003 -3.12052

D173 3.12930 -0.00000 0.00000 -0.00001 -0.00000 3.12930

D174 0.00907 -0.00000 0.00002 -0.00000 0.00002 0.00909

D175 -0.01565 -0.00000 -0.00002 0.00000 -0.00002 -0.01567

D176 -3.13588 -0.00000 -0.00000 0.00000 -0.00000 -3.13588

D177 0.00716 -0.00000 -0.00000 0.00000 -0.00000 0.00716

D178 -3.13117 -0.00000 0.00001 -0.00000 0.00001 -3.13116

D179 3.13143 0.00000 -0.00002 0.00000 -0.00002 3.13141

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D181 -0.00642 -0.00000 -0.00000 -0.00000 -0.00001 -0.00643

D182 3.13655 0.00000 -0.00000 -0.00000 -0.00000 3.13655

D183 3.13189 0.00000 -0.00002 0.00000 -0.00002 3.13187

D184 -0.00833 0.00000 -0.00001 0.00000 -0.00001 -0.00834

D185 -0.00538 0.00000 0.00000 0.00000 0.00000 -0.00537

D186 3.13570 0.00000 0.00001 -0.00000 0.00001 3.13571

D187 3.13484 0.00000 -0.00000 0.00000 -0.00000 3.13484

D188 -0.00727 0.00000 0.00001 -0.00000 0.00000 -0.00726

D189 0.01656 -0.00000 0.00001 -0.00000 0.00001 0.01657

D190 3.13668 -0.00000 -0.00001 -0.00000 -0.00001 3.13667

D191 -3.12452 -0.00000 0.00000 0.00000 0.00000 -3.12451

D192 -0.00440 -0.00000 -0.00002 0.00000 -0.00002 -0.00441

D193 -3.14033 0.00000 0.00001 0.00001 0.00002 -3.14032

D194 -0.01711 0.00000 -0.00001 0.00000 -0.00001 -0.01712

D195 -0.00198 -0.00000 -0.00001 -0.00000 -0.00001 -0.00199

D196 3.12124 0.00000 -0.00004 -0.00000 -0.00004 3.12120

D197 -3.13034 -0.00000 -0.00000 -0.00001 -0.00001 -3.13035

D198 -0.00824 0.00000 -0.00001 -0.00000 -0.00001 -0.00826

D199 0.01449 0.00000 0.00002 0.00000 0.00002 0.01450

D200 3.13658 0.00000 0.00001 0.00000 0.00002 3.13660

D201 -0.00888 0.00000 -0.00000 0.00000 -0.00000 -0.00888

D202 3.13044 0.00000 -0.00000 0.00000 -0.00000 3.13044

D203 -3.13200 -0.00000 0.00002 0.00000 0.00003 -3.13197

D204 0.00732 -0.00000 0.00002 0.00000 0.00003 0.00735

D205 0.00732 -0.00000 0.00001 -0.00000 0.00001 0.00733

D206 -3.13710 -0.00000 -0.00000 -0.00000 -0.00000 -3.13710

D207 -3.13199 -0.00000 0.00001 -0.00000 0.00001 -3.13198

D208 0.00677 -0.00000 -0.00000 -0.00000 -0.00000 0.00677

D209 0.00514 -0.00000 -0.00001 -0.00000 -0.00001 0.00513

D210 -3.13580 -0.00000 -0.00001 -0.00000 -0.00001 -3.13581

D211 -3.13362 -0.00000 0.00001 0.00000 0.00001 -3.13362

D212 0.00862 -0.00000 0.00000 -0.00000 0.00000 0.00863

D213 -0.01618 0.00000 -0.00001 -0.00000 -0.00001 -0.01619

D214 -3.13819 -0.00000 -0.00000 -0.00000 -0.00001 -3.13820

D215 3.12477 0.00000 -0.00001 0.00000 -0.00000 3.12476

D216 0.00275 -0.00000 -0.00000 -0.00000 -0.00000 0.00275

Item Value Threshold Converged?

Maximum Force 0.000018 0.000450 YES

RMS Force 0.000004 0.000300 YES

Maximum Displacement 0.004188 0.001800 NO

RMS Displacement 0.000887 0.001200 YES

Predicted change in Energy=-3.945979D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Aug 30 01:40:58 2019, MaxMem= 4294967296 cpu: 2.5

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=2 Diff= 2.30D-03

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 0.976334 -4.113220 0.552153

2 6 0 1.321335 -2.796097 0.201646

3 7 0 0.145266 -2.109823 0.007401

4 6 0 -0.931069 -2.946574 0.188857

5 6 0 -0.418072 -4.206404 0.543637

6 6 0 -2.311861 -2.589978 0.006304

7 6 0 -2.798955 -1.286387 -0.120930

8 7 0 -2.062791 -0.138311 0.044855

9 6 0 -2.948307 0.899660 -0.107533

10 6 0 -4.278873 0.389877 -0.433969

11 6 0 -4.186339 -0.958637 -0.443344

12 6 0 2.642815 -2.257352 0.031317

13 6 0 2.948308 -0.899669 -0.107495

14 6 0 4.278875 -0.389896 -0.433940

15 6 0 4.186341 0.958618 -0.443360

16 6 0 2.798956 1.286378 -0.120966

17 7 0 2.062790 0.138307 0.044853

18 6 0 2.311863 2.589974 0.006231

19 6 0 0.931069 2.946570 0.188769

20 6 0 0.418076 4.206364 0.543678

21 6 0 -0.976331 4.113179 0.552195

22 6 0 -1.321334 2.796091 0.201558

23 7 0 -0.145267 2.109841 0.007228

24 6 0 -2.642816 2.257347 0.031243

25 6 0 -3.273369 -3.719580 -0.033039

26 6 0 -3.126806 -4.749141 -0.974768

27 6 0 -4.035311 -5.801474 -1.021023

28 6 0 -5.094878 -5.853926 -0.115067

29 6 0 -5.242966 -4.843334 0.833471

30 6 0 -4.343082 -3.781666 0.871495

31 6 0 5.856008 -5.101008 -0.011405

32 6 0 4.809158 -5.213202 -0.926700

33 6 0 3.760910 -4.298815 -0.906689

34 6 0 3.751477 -3.243243 0.017593

35 6 0 4.809428 -3.139934 0.932312

36 6 0 5.850502 -4.063971 0.920091

37 6 0 -3.751475 3.243240 0.017554

38 6 0 -4.809417 3.139906 0.932280

39 6 0 -5.850479 4.063956 0.920110

40 6 0 -5.855984 5.101031 -0.011343

41 6 0 -4.809143 5.213251 -0.926645

42 6 0 -3.760905 4.298850 -0.906684

43 6 0 3.273369 3.719577 -0.033078

44 6 0 4.343074 3.781645 0.871467

45 6 0 5.242942 4.843327 0.833491

46 6 0 5.094847 5.853953 -0.115010

47 6 0 4.035289 5.801519 -1.020977

48 6 0 3.126798 4.749172 -0.974768

49 1 0 1.675196 -4.899338 0.788030

50 1 0 -1.009239 -5.078187 0.772998

51 1 0 -5.149669 0.988862 -0.651636

52 1 0 -4.967476 -1.667887 -0.669364

53 1 0 5.149674 -0.988887 -0.651580

54 1 0 4.967479 1.667862 -0.669399

55 1 0 1.009246 5.078118 0.773139

56 1 0 -1.675195 4.899266 0.788171

57 1 0 -2.307012 -4.711343 -1.683009

58 1 0 -3.916591 -6.581530 -1.765628

59 1 0 -5.798674 -6.678870 -0.147092

60 1 0 -6.059029 -4.881290 1.547322

61 1 0 -4.456473 -3.002303 1.616458

62 1 0 6.669812 -5.818265 -0.023782

63 1 0 4.809137 -6.014371 -1.658244

64 1 0 2.952013 -4.387389 -1.622868

65 1 0 4.803753 -2.340363 1.664300

66 1 0 6.656176 -3.974880 1.641169

67 1 0 -4.803741 2.340308 1.664241

68 1 0 -6.656145 3.974846 1.641195

69 1 0 -6.669779 5.818299 -0.023680

70 1 0 -4.809121 6.014450 -1.658156

71 1 0 -2.952013 4.387447 -1.622866

72 1 0 4.456466 3.002260 1.616407

73 1 0 6.058997 4.881270 1.547353

74 1 0 5.798630 6.678909 -0.146996

75 1 0 3.916563 6.581602 -1.765552

76 1 0 2.307008 4.711391 -1.683016

77 1 0 0.081761 -1.122587 -0.200093

78 1 0 -0.081762 1.122650 -0.200477

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0587918 0.0582559 0.0300944

Leave Link 202 at Fri Aug 30 01:40:58 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l301.exe)

Standard basis: 6-311G(d) (5D, 7F)

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 1002 symmetry adapted cartesian basis functions of A symmetry.

There are 954 symmetry adapted basis functions of A symmetry.

954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

162 alpha electrons 160 beta electrons

nuclear repulsion energy 5356.9133425289 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= 78 NActive= 78 NUniq= 78 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2122027433 Hartrees.

Nuclear repulsion after empirical dispersion term = 5356.7011397856 Hartrees.

Force inversion solution in PCM.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 78.

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 = 78

GePol: Total number of spheres = 78

GePol: Number of exposed spheres = 78 (100.00%)

GePol: Number of points = 5786

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.57D-10

GePol: Maximum weight of points = 0.17992

GePol: Number of points with low weight = 310

GePol: Fraction of low-weight points (<1% of avg) = 5.36%

GePol: Cavity surface area = 610.611 Ang\*\*2

GePol: Cavity volume = 628.005 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0021001626 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5356.6990396230 Hartrees.

Leave Link 301 at Fri Aug 30 01:40:58 2019, MaxMem= 4294967296 cpu: 2.0

(Enter /home/kira/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

NBasis= 954 RedAO= T EigKep= 1.29D-04 NBF= 954

NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 954

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= 940 940 940 940 940 MxSgAt= 78 MxSgA2= 78.

Leave Link 302 at Fri Aug 30 01:41:00 2019, MaxMem= 4294967296 cpu: 27.0

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Fri Aug 30 01:41:00 2019, MaxMem= 4294967296 cpu: 2.5

(Enter /home/kira/g09/l401.exe)

Initial guess from the checkpoint file: "TPP3C1.chk"

B after Tr= -0.000000 -0.000000 0.000000

Rot= 1.000000 -0.000003 -0.000000 -0.000813 Ang= -0.09 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0182

Leave Link 401 at Fri Aug 30 01:41:03 2019, MaxMem= 4294967296 cpu: 47.5

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3054046 IEndB= 3054046 NGot= 4294967296 MDV= 4292934897

LenX= 4292934897 LenY= 4291929891

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= 590000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Inv3: Mode=1 IEnd= 100433388.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.33D-15 for 5760.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.79D-15 for 3600 327.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.77D-15 for 5760.

Iteration 1 A^-1\*A deviation from orthogonality is 1.09D-09 for 1854 1852.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.89D-15 for 636.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.00D-15 for 4071 3001.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 3628.

Iteration 2 A^-1\*A deviation from orthogonality is 4.95D-16 for 3440 1005.

E= -1914.33331478880

DIIS: error= 3.81D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1914.33331478880 IErMin= 1 ErrMin= 3.81D-05

ErrMax= 3.81D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.56D-06 BMatP= 5.56D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.640 Goal= None Shift= 0.000

Gap= 0.706 Goal= None Shift= 0.000

RMSDP=1.88D-06 MaxDP=6.45D-05 OVMax= 2.23D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.88D-06 CP: 1.00D+00

E= -1914.33331746351 Delta-E= -0.000002674708 Rises=F Damp=F

DIIS: error= 5.65D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1914.33331746351 IErMin= 2 ErrMin= 5.65D-06

ErrMax= 5.65D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.87D-08 BMatP= 5.56D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.657D-01 0.107D+01

Coeff: -0.657D-01 0.107D+01

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.04D-07 MaxDP=1.27D-05 DE=-2.67D-06 OVMax= 4.35D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.75D-07 CP: 1.00D+00 1.07D+00

E= -1914.33331750031 Delta-E= -0.000000036802 Rises=F Damp=F

DIIS: error= 2.15D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1914.33331750031 IErMin= 3 ErrMin= 2.15D-06

ErrMax= 2.15D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.37D-08 BMatP= 6.87D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.309D-01 0.417D+00 0.614D+00

Coeff: -0.309D-01 0.417D+00 0.614D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.25D-07 MaxDP=8.29D-06 DE=-3.68D-08 OVMax= 2.41D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.06D-07 CP: 1.00D+00 1.08D+00 7.69D-01

E= -1914.33331750419 Delta-E= -0.000000003875 Rises=F Damp=F

DIIS: error= 1.72D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1914.33331750419 IErMin= 4 ErrMin= 1.72D-06

ErrMax= 1.72D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.19D-09 BMatP= 2.37D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.853D-02 0.883D-01 0.382D+00 0.539D+00

Coeff: -0.853D-02 0.883D-01 0.382D+00 0.539D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=5.92D-08 MaxDP=3.74D-06 DE=-3.88D-09 OVMax= 1.85D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.78D-08 CP: 1.00D+00 1.08D+00 8.64D-01 6.55D-01

E= -1914.33331750637 Delta-E= -0.000000002186 Rises=F Damp=F

DIIS: error= 4.15D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1914.33331750637 IErMin= 5 ErrMin= 4.15D-07

ErrMax= 4.15D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.47D-10 BMatP= 9.19D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.811D-03-0.369D-02 0.113D+00 0.252D+00 0.640D+00

Coeff: -0.811D-03-0.369D-02 0.113D+00 0.252D+00 0.640D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.22D-08 MaxDP=1.53D-06 DE=-2.19D-09 OVMax= 1.06D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.74D-08 CP: 1.00D+00 1.08D+00 8.69D-01 7.65D-01 8.24D-01

E= -1914.33331750649 Delta-E= -0.000000000119 Rises=F Damp=F

DIIS: error= 2.38D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1914.33331750649 IErMin= 6 ErrMin= 2.38D-07

ErrMax= 2.38D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.89D-10 BMatP= 5.47D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.946D-03-0.180D-01 0.439D-02 0.663D-01 0.410D+00 0.536D+00

Coeff: 0.946D-03-0.180D-01 0.439D-02 0.663D-01 0.410D+00 0.536D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.13D-08 MaxDP=6.83D-07 DE=-1.19D-10 OVMax= 6.99D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 8.78D-09 CP: 1.00D+00 1.08D+00 8.84D-01 7.60D-01 9.75D-01

CP: 9.62D-01

E= -1914.33331750655 Delta-E= -0.000000000057 Rises=F Damp=F

DIIS: error= 1.32D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1914.33331750655 IErMin= 7 ErrMin= 1.32D-07

ErrMax= 1.32D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.39D-11 BMatP= 1.89D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.379D-03-0.573D-02-0.689D-02 0.521D-02 0.909D-01 0.189D+00

Coeff-Com: 0.727D+00

Coeff: 0.379D-03-0.573D-02-0.689D-02 0.521D-02 0.909D-01 0.189D+00

Coeff: 0.727D+00

Gap= 0.049 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.56D-09 MaxDP=5.93D-07 DE=-5.73D-11 OVMax= 7.16D-06

Error on total polarization charges = 0.08258

SCF Done: E(UB3LYP) = -1914.33331751 A.U. after 7 cycles

NFock= 7 Conv=0.76D-08 -V/T= 2.0042

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0551 S= 1.0182

<L.S>= 0.000000000000E+00

KE= 1.906380698939D+03 PE=-1.516302510729D+04 EE= 5.985612051218D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.32

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0551, after 2.0017

Leave Link 502 at Fri Aug 30 01:44:26 2019, MaxMem= 4294967296 cpu: 3184.5

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 954

NBasis= 954 NAE= 162 NBE= 160 NFC= 0 NFV= 0

NROrb= 954 NOA= 162 NOB= 160 NVA= 792 NVB= 794

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.48637651D-01

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.64285274D-01

Leave Link 801 at Fri Aug 30 01:44:26 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 78.

Will process 79 centers per pass.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Fri Aug 30 01:44:33 2019, MaxMem= 4294967296 cpu: 111.5

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Fri Aug 30 01:44:34 2019, MaxMem= 4294967296 cpu: 2.5

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 78.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966568.

G2DrvN: will do 79 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=T 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= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

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 = 189

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Fri Aug 30 02:04:24 2019, MaxMem= 4294967296 cpu: 19050.5

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=11111111111111111111111111111111111111111111111111

IDoAtm=1111111111111111111111111111

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.

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= 4294964604 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= 590000000 NMat= 72 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

There are 237 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

237 vectors produced by pass 0 Test12= 2.55D-13 1.00D-09 XBig12= 5.39D+03 4.50D+01.

AX will form 72 AO Fock derivatives at one time.

234 vectors produced by pass 1 Test12= 2.55D-13 1.00D-09 XBig12= 4.52D+02 3.62D+00.

234 vectors produced by pass 2 Test12= 2.55D-13 1.00D-09 XBig12= 9.53D+00 4.66D-01.

234 vectors produced by pass 3 Test12= 2.55D-13 1.00D-09 XBig12= 1.02D-01 3.97D-02.

234 vectors produced by pass 4 Test12= 2.55D-13 1.00D-09 XBig12= 6.57D-04 2.10D-03.

234 vectors produced by pass 5 Test12= 2.55D-13 1.00D-09 XBig12= 4.58D-06 1.35D-04.

192 vectors produced by pass 6 Test12= 2.55D-13 1.00D-09 XBig12= 1.99D-08 1.02D-05.

82 vectors produced by pass 7 Test12= 2.55D-13 1.00D-09 XBig12= 8.29D-11 6.21D-07.

44 vectors produced by pass 8 Test12= 2.55D-13 1.00D-09 XBig12= 5.16D-13 3.93D-08.

3 vectors produced by pass 9 Test12= 2.55D-13 1.00D-09 XBig12= 8.33D-15 4.47D-09.

3 vectors produced by pass 10 Test12= 2.55D-13 1.00D-09 XBig12= 3.32D-15 1.83D-09.

3 vectors produced by pass 11 Test12= 2.55D-13 1.00D-09 XBig12= 5.14D-15 3.10D-09.

3 vectors produced by pass 12 Test12= 2.55D-13 1.00D-09 XBig12= 6.88D-15 2.50D-09.

3 vectors produced by pass 13 Test12= 2.55D-13 1.00D-09 XBig12= 5.45D-15 2.18D-09.

3 vectors produced by pass 14 Test12= 2.55D-13 1.00D-09 XBig12= 6.86D-15 2.78D-09.

3 vectors produced by pass 15 Test12= 2.55D-13 1.00D-09 XBig12= 5.66D-15 2.60D-09.

3 vectors produced by pass 16 Test12= 2.55D-13 1.00D-09 XBig12= 7.43D-15 2.30D-09.

3 vectors produced by pass 17 Test12= 2.55D-13 1.00D-09 XBig12= 5.21D-15 2.14D-09.

3 vectors produced by pass 18 Test12= 2.55D-13 1.00D-09 XBig12= 6.62D-15 2.39D-09.

3 vectors produced by pass 19 Test12= 2.55D-13 1.00D-09 XBig12= 8.41D-15 2.95D-09.

3 vectors produced by pass 20 Test12= 2.55D-13 1.00D-09 XBig12= 5.70D-15 2.20D-09.

3 vectors produced by pass 21 Test12= 2.55D-13 1.00D-09 XBig12= 7.14D-15 2.89D-09.

3 vectors produced by pass 22 Test12= 2.55D-13 1.00D-09 XBig12= 1.07D-14 5.11D-09.

2 vectors produced by pass 23 Test12= 2.55D-13 1.00D-09 XBig12= 3.99D-15 2.36D-09.

InvSVY: IOpt=1 It= 1 EMax= 2.13D-14

Solved reduced A of dimension 1769 with 237 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1125.56 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Fri Aug 30 05:56:37 2019, MaxMem= 4294967296 cpu: 222845.5

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 189

Leave Link 701 at Fri Aug 30 05:58:07 2019, MaxMem= 4294967296 cpu: 1420.0

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Fri Aug 30 05:58:07 2019, MaxMem= 4294967296 cpu: 1.0

(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=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

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= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Fri Aug 30 06:16:22 2019, MaxMem= 4294967296 cpu: 17512.0

(Enter /home/kira/g09/l716.exe)

Dipole =-4.23633617D-06 8.37069968D-05-4.79848253D-01

Polarizability= 1.25581355D+03-3.02127364D+01 1.66568995D+03

-3.70850505D-05-4.36424170D-04 4.55164100D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000000467 -0.000000097 -0.000000236

2 6 0.000000343 -0.000000151 -0.000000551

3 7 0.000000484 0.000000465 -0.000000289

4 6 -0.000000208 0.000000170 0.000000015

5 6 -0.000000112 -0.000000027 -0.000000397

6 6 -0.000000221 -0.000000176 -0.000000436

7 6 -0.000000845 -0.000000006 0.000000278

8 7 0.000000227 0.000000010 -0.000000428

9 6 0.000000124 0.000000042 0.000000149

10 6 -0.000000529 0.000000004 0.000000021

11 6 -0.000000428 0.000000148 -0.000000445

12 6 0.000000015 0.000000055 0.000000185

13 6 -0.000000045 0.000000039 -0.000000242

14 6 0.000000568 0.000000180 -0.000000081

15 6 0.000000436 -0.000000080 0.000000476

16 6 0.000000810 -0.000000057 -0.000000303

17 7 -0.000000046 -0.000000348 0.000000400

18 6 0.000000158 -0.000000066 0.000000551

19 6 0.000000284 0.000000261 -0.000000441

20 6 -0.000000068 -0.000000085 0.000000450

21 6 -0.000000464 0.000000088 0.000000243

22 6 -0.000000134 -0.000000018 0.000000734

23 7 -0.000000195 0.000000377 0.000000413

24 6 -0.000000188 0.000000155 -0.000000066

25 6 -0.000000665 0.000000010 -0.000000601

26 6 0.000000022 -0.000000435 -0.000000028

27 6 -0.000000691 0.000000170 -0.000000731

28 6 -0.000000234 -0.000000052 -0.000000327

29 6 -0.000000828 0.000000267 -0.000000464

30 6 -0.000000263 -0.000000175 -0.000000147

31 6 0.000000193 0.000000039 -0.000000504

32 6 0.000000389 0.000000093 -0.000000625

33 6 -0.000000059 -0.000000121 -0.000000275

34 6 0.000000573 -0.000000425 -0.000000608

35 6 0.000000449 0.000000049 0.000000043

36 6 0.000000937 -0.000000102 -0.000000779

37 6 -0.000000470 -0.000000333 0.000000276

38 6 -0.000000583 -0.000000079 -0.000000052

39 6 -0.000000868 0.000000050 0.000000575

40 6 -0.000000199 0.000000008 0.000000652

41 6 -0.000000302 0.000000244 0.000000552

42 6 -0.000000087 -0.000000199 0.000000440

43 6 0.000000560 0.000000010 0.000000678

44 6 0.000000243 -0.000000308 0.000000252

45 6 0.000000866 0.000000418 0.000000547

46 6 0.000000250 -0.000000007 0.000000246

47 6 0.000000683 0.000000223 0.000000748

48 6 -0.000000131 -0.000000388 -0.000000051

49 1 0.000000003 0.000000038 -0.000000322

50 1 -0.000000086 0.000000208 -0.000000502

51 1 -0.000000346 0.000000066 0.000000177

52 1 -0.000000267 0.000000001 -0.000000235

53 1 0.000000353 0.000000084 -0.000000165

54 1 0.000000287 0.000000054 0.000000198

55 1 0.000000202 0.000000101 0.000000604

56 1 -0.000000136 -0.000000085 0.000000384

57 1 -0.000000420 0.000000059 -0.000000424

58 1 -0.000000410 -0.000000007 -0.000000545

59 1 -0.000000654 -0.000000010 -0.000000735

60 1 -0.000000508 -0.000000080 -0.000000425

61 1 -0.000000282 -0.000000053 -0.000000196

62 1 0.000000697 -0.000000012 -0.000000609

63 1 0.000000404 0.000000020 -0.000000583

64 1 0.000000397 0.000000124 -0.000000397

65 1 0.000000399 -0.000000012 -0.000000277

66 1 0.000000552 0.000000044 -0.000000392

67 1 -0.000000353 0.000000037 0.000000238

68 1 -0.000000575 0.000000067 0.000000407

69 1 -0.000000665 0.000000035 0.000000609

70 1 -0.000000411 0.000000021 0.000000629

71 1 -0.000000428 0.000000051 0.000000410

72 1 0.000000367 0.000000064 0.000000201

73 1 0.000000524 -0.000000056 0.000000425

74 1 0.000000661 0.000000026 0.000000751

75 1 0.000000431 -0.000000001 0.000000544

76 1 0.000000389 0.000000014 0.000000411

77 1 -0.000001492 -0.000000009 -0.000000336

78 1 0.000001144 -0.000000629 0.000000338

-------------------------------------------------------------------

Cartesian Forces: Max 0.000001492 RMS 0.000000394

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Fri Aug 30 06:16:22 2019, MaxMem= 4294967296 cpu: 2.0

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000001458 RMS 0.000000285

Search for a local minimum.

Step number 24 out of a maximum of 452

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= 6.95D-07 DEPred=-3.95D-08 R=-1.76D+01

Trust test=-1.76D+01 RLast= 2.35D-03 DXMaxT set to 5.00D-02

ITU= -1 -1 1 1 -1 -1 1 1 -1 -1 1 0 -1 1 1 -1 1 -1 -1 1

ITU= 1 -1 1 0

Eigenvalues --- 0.00063 0.00245 0.00404 0.00597 0.00722

Eigenvalues --- 0.00809 0.00920 0.01045 0.01058 0.01120

Eigenvalues --- 0.01135 0.01162 0.01264 0.01280 0.01302

Eigenvalues --- 0.01304 0.01322 0.01422 0.01428 0.01536

Eigenvalues --- 0.01551 0.01560 0.01593 0.01673 0.01711

Eigenvalues --- 0.01716 0.01728 0.01737 0.01755 0.01759

Eigenvalues --- 0.01762 0.01781 0.01800 0.01803 0.01885

Eigenvalues --- 0.01935 0.01988 0.01997 0.02012 0.02165

Eigenvalues --- 0.02169 0.02255 0.02288 0.02293 0.02304

Eigenvalues --- 0.02330 0.02392 0.02468 0.02471 0.02522

Eigenvalues --- 0.02539 0.02544 0.02586 0.02626 0.02628

Eigenvalues --- 0.02645 0.02648 0.02767 0.02779 0.02796

Eigenvalues --- 0.02803 0.02868 0.02872 0.02873 0.02875

Eigenvalues --- 0.02940 0.02965 0.03911 0.04087 0.04190

Eigenvalues --- 0.04318 0.04367 0.04464 0.04544 0.04573

Eigenvalues --- 0.08199 0.09653 0.09684 0.09737 0.09860

Eigenvalues --- 0.09884 0.10301 0.10435 0.10568 0.10697

Eigenvalues --- 0.10700 0.10704 0.10735 0.10735 0.11009

Eigenvalues --- 0.11398 0.11399 0.11410 0.11413 0.11984

Eigenvalues --- 0.11987 0.11997 0.12003 0.12280 0.12281

Eigenvalues --- 0.12325 0.12325 0.12771 0.12772 0.12773

Eigenvalues --- 0.12775 0.15719 0.15922 0.16301 0.16738

Eigenvalues --- 0.17208 0.17312 0.17584 0.17841 0.18003

Eigenvalues --- 0.18025 0.18275 0.18351 0.19241 0.19284

Eigenvalues --- 0.19359 0.19361 0.19371 0.19408 0.19414

Eigenvalues --- 0.19428 0.19551 0.19552 0.19554 0.19555

Eigenvalues --- 0.20294 0.21486 0.22042 0.22747 0.22883

Eigenvalues --- 0.23234 0.23768 0.24234 0.24750 0.25131

Eigenvalues --- 0.26281 0.26385 0.26662 0.27137 0.28526

Eigenvalues --- 0.28553 0.28751 0.29017 0.29786 0.31031

Eigenvalues --- 0.31698 0.32012 0.32852 0.33077 0.33195

Eigenvalues --- 0.33325 0.34131 0.34535 0.35053 0.35565

Eigenvalues --- 0.35625 0.35626 0.35634 0.35640 0.35757

Eigenvalues --- 0.35760 0.35765 0.35810 0.35925 0.35926

Eigenvalues --- 0.35931 0.35934 0.35987 0.35988 0.36008

Eigenvalues --- 0.36010 0.36191 0.36201 0.36245 0.36246

Eigenvalues --- 0.36978 0.37056 0.37239 0.37386 0.37394

Eigenvalues --- 0.37484 0.38139 0.38434 0.38508 0.38538

Eigenvalues --- 0.39451 0.40365 0.40732 0.41045 0.41064

Eigenvalues --- 0.41105 0.41193 0.41257 0.41352 0.41353

Eigenvalues --- 0.41568 0.41801 0.42275 0.42632 0.44525

Eigenvalues --- 0.45232 0.45915 0.45918 0.45932 0.45956

Eigenvalues --- 0.46010 0.46011 0.46257 0.46261 0.46315

Eigenvalues --- 0.46325 0.48409 0.49009 0.49411 0.49621

Eigenvalues --- 0.50751 0.50753 0.50779 0.50782 0.51864

Eigenvalues --- 0.52207 0.57175 0.57706

Cut down GDIIS permanently because of the ratio check. E10

DIIS coeff's: 0.83543 -0.05954 0.18777 0.01194 0.03115

DIIS coeff's: -0.01163 0.00355 0.00099 0.00459 0.00652

DIIS coeff's: -0.00838 -0.00551 0.00453 -0.00134 -0.00006

Cosine: 0.665 > 0.500

Length: 1.233

GDIIS step was calculated using 15 of the last 16 vectors.

Iteration 1 RMS(Cart)= 0.00019425 RMS(Int)= 0.00000004

Iteration 2 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000004

ITry= 1 IFail=0 DXMaxC= 8.89D-04 DCOld= 1.00D+10 DXMaxT= 5.00D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.65686 -0.00000 -0.00000 -0.00000 -0.00000 2.65686

R2 2.64097 -0.00000 0.00000 -0.00000 0.00000 2.64097

R3 2.03708 -0.00000 0.00000 -0.00000 0.00000 2.03708

R4 2.59921 0.00000 -0.00000 0.00000 -0.00000 2.59921

R5 2.71593 0.00000 0.00000 0.00000 0.00000 2.71593

R6 2.59903 0.00000 -0.00000 0.00000 0.00000 2.59903

R7 1.91014 0.00000 -0.00000 0.00000 -0.00000 1.91014

R8 2.65653 0.00000 -0.00000 0.00000 -0.00000 2.65653

R9 2.71692 0.00000 -0.00000 -0.00000 -0.00000 2.71692

R10 2.03713 0.00000 -0.00000 0.00000 -0.00000 2.03713

R11 2.64075 -0.00000 0.00000 0.00000 0.00000 2.64076

R12 2.80422 -0.00000 -0.00000 -0.00000 -0.00000 2.80422

R13 2.59623 -0.00000 -0.00000 -0.00000 -0.00000 2.59622

R14 2.76198 0.00000 0.00000 0.00000 0.00000 2.76198

R15 2.59433 -0.00000 0.00000 0.00000 0.00000 2.59433

R16 2.76239 0.00000 -0.00000 0.00000 -0.00000 2.76239

R17 2.64285 0.00000 -0.00001 -0.00000 -0.00001 2.64284

R18 2.55438 0.00000 -0.00000 -0.00000 -0.00000 2.55438

R19 2.03920 -0.00000 -0.00000 0.00000 -0.00000 2.03919

R20 2.03906 0.00000 -0.00000 0.00000 -0.00000 2.03906

R21 2.64285 -0.00000 -0.00000 -0.00000 -0.00000 2.64284

R22 2.80375 -0.00000 -0.00000 0.00000 -0.00000 2.80374

R23 2.76239 0.00000 -0.00000 0.00000 -0.00000 2.76239

R24 2.59433 -0.00000 0.00000 0.00000 0.00000 2.59433

R25 2.55438 0.00000 -0.00000 -0.00000 -0.00000 2.55438

R26 2.03920 -0.00000 -0.00000 0.00000 -0.00000 2.03919

R27 2.76198 0.00000 0.00000 0.00000 0.00000 2.76198

R28 2.03906 0.00000 -0.00000 -0.00000 -0.00000 2.03906

R29 2.59623 -0.00000 -0.00000 -0.00000 -0.00000 2.59623

R30 2.64075 -0.00000 -0.00000 0.00000 -0.00000 2.64075

R31 2.71692 0.00000 -0.00000 0.00000 -0.00000 2.71691

R32 2.80422 -0.00000 0.00001 -0.00000 0.00001 2.80422

R33 2.65653 -0.00000 0.00000 -0.00000 0.00000 2.65653

R34 2.59902 0.00000 0.00000 -0.00000 0.00000 2.59903

R35 2.64097 -0.00000 -0.00000 0.00000 -0.00000 2.64097

R36 2.03713 0.00000 -0.00000 0.00000 -0.00000 2.03713

R37 2.65686 0.00000 0.00000 0.00000 0.00000 2.65686

R38 2.03708 0.00000 -0.00000 0.00000 -0.00000 2.03707

R39 2.59921 0.00000 0.00000 0.00000 0.00000 2.59921

R40 2.71593 0.00000 -0.00000 0.00000 -0.00000 2.71593

R41 1.91014 0.00000 0.00001 -0.00000 0.00000 1.91014

R42 2.80374 0.00000 0.00001 0.00000 0.00001 2.80375

R43 2.65123 -0.00000 0.00000 0.00000 0.00000 2.65123

R44 2.64988 -0.00000 0.00000 0.00000 0.00000 2.64988

R45 2.62864 -0.00000 -0.00000 -0.00000 -0.00000 2.62864

R46 2.04850 0.00000 -0.00000 0.00000 -0.00000 2.04850

R47 2.63628 -0.00000 0.00000 -0.00000 0.00000 2.63628

R48 2.05017 -0.00000 -0.00000 -0.00000 -0.00000 2.05017

R49 2.63408 0.00000 0.00000 0.00000 0.00000 2.63409

R50 2.05006 0.00000 -0.00000 0.00000 -0.00000 2.05006

R51 2.63098 -0.00000 -0.00000 0.00000 -0.00000 2.63098

R52 2.05014 0.00000 0.00000 0.00000 0.00000 2.05014

R53 2.04862 -0.00000 -0.00000 0.00000 -0.00000 2.04862

R54 2.63632 -0.00000 0.00000 0.00000 0.00000 2.63632

R55 2.63423 -0.00000 -0.00000 -0.00000 -0.00000 2.63423

R56 2.05006 0.00000 0.00000 -0.00000 0.00000 2.05006

R57 2.62891 -0.00000 -0.00000 0.00000 -0.00000 2.62891

R58 2.05018 0.00000 0.00000 -0.00000 0.00000 2.05018

R59 2.65142 -0.00000 0.00000 0.00000 0.00000 2.65143

R60 2.04848 0.00000 -0.00000 0.00000 0.00000 2.04848

R61 2.65010 0.00000 0.00000 0.00000 0.00000 2.65010

R62 2.63061 0.00000 -0.00000 -0.00000 -0.00000 2.63061

R63 2.04855 0.00000 -0.00000 0.00000 -0.00000 2.04855

R64 2.05016 -0.00000 -0.00000 -0.00000 -0.00000 2.05016

R65 2.65010 0.00000 -0.00000 0.00000 -0.00000 2.65009

R66 2.65143 -0.00000 -0.00000 -0.00000 -0.00000 2.65142

R67 2.63061 0.00000 0.00000 -0.00000 0.00000 2.63061

R68 2.04855 0.00000 0.00000 0.00000 0.00000 2.04855

R69 2.63423 -0.00000 -0.00000 -0.00000 -0.00000 2.63423

R70 2.05016 -0.00000 -0.00000 -0.00000 -0.00000 2.05016

R71 2.63632 -0.00000 -0.00000 -0.00000 -0.00000 2.63632

R72 2.05006 0.00000 0.00000 -0.00000 0.00000 2.05006

R73 2.62891 -0.00000 0.00000 0.00000 0.00000 2.62891

R74 2.05018 0.00000 0.00000 0.00000 0.00000 2.05018

R75 2.04848 0.00000 0.00000 0.00000 0.00000 2.04848

R76 2.64988 -0.00000 -0.00000 0.00000 -0.00000 2.64988

R77 2.65123 -0.00000 -0.00000 0.00000 -0.00000 2.65123

R78 2.63098 0.00000 0.00000 -0.00000 0.00000 2.63098

R79 2.04862 -0.00000 0.00000 -0.00000 0.00000 2.04862

R80 2.63408 0.00000 0.00000 -0.00000 0.00000 2.63408

R81 2.05014 0.00000 0.00000 0.00000 0.00000 2.05014

R82 2.63628 -0.00000 -0.00000 -0.00000 -0.00000 2.63628

R83 2.05006 0.00000 0.00000 0.00000 0.00000 2.05006

R84 2.62864 -0.00000 0.00000 -0.00000 0.00000 2.62864

R85 2.05017 -0.00000 0.00000 -0.00000 -0.00000 2.05017

R86 2.04850 0.00000 0.00000 0.00000 0.00000 2.04850

A1 1.88155 -0.00000 -0.00000 0.00000 -0.00000 1.88155

A2 2.18786 -0.00000 -0.00000 0.00000 -0.00000 2.18786

A3 2.21375 0.00000 0.00000 -0.00000 0.00000 2.21376

A4 1.86797 0.00000 0.00000 0.00000 0.00000 1.86797

A5 2.22225 -0.00000 -0.00001 -0.00000 -0.00001 2.22225

A6 2.19251 0.00000 0.00001 0.00000 0.00001 2.19251

A7 1.92513 -0.00000 -0.00000 -0.00000 -0.00000 1.92513

A8 2.17733 0.00000 0.00000 0.00000 0.00000 2.17734

A9 2.17989 0.00000 0.00000 -0.00000 -0.00000 2.17989

A10 1.86810 0.00000 -0.00000 0.00000 0.00000 1.86810

A11 2.19438 0.00000 0.00000 0.00000 0.00000 2.19438

A12 2.22030 -0.00000 0.00000 -0.00000 0.00000 2.22030

A13 1.88166 0.00000 -0.00000 0.00000 -0.00000 1.88166

A14 2.21403 -0.00000 0.00000 -0.00000 0.00000 2.21403

A15 2.18746 -0.00000 -0.00000 0.00000 -0.00000 2.18746

A16 2.18670 -0.00000 -0.00000 -0.00000 -0.00000 2.18670

A17 2.02289 -0.00000 -0.00000 -0.00000 -0.00000 2.02289

A18 2.07355 0.00000 0.00000 0.00000 0.00000 2.07355

A19 2.19171 -0.00000 0.00001 -0.00000 0.00001 2.19172

A20 2.16535 0.00000 -0.00001 0.00000 -0.00001 2.16535

A21 1.92609 0.00000 0.00000 0.00000 0.00000 1.92609

A22 1.84709 0.00000 -0.00000 0.00000 -0.00000 1.84709

A23 1.92648 0.00000 0.00000 -0.00000 -0.00000 1.92648

A24 2.19207 -0.00000 0.00000 0.00000 0.00000 2.19207

A25 2.16463 0.00000 -0.00000 0.00000 -0.00000 2.16462

A26 1.86205 -0.00000 -0.00000 0.00000 -0.00000 1.86205

A27 2.19690 0.00000 0.00000 0.00000 0.00000 2.19690

A28 2.22384 -0.00000 -0.00000 -0.00000 -0.00000 2.22384

A29 1.86206 -0.00000 0.00000 -0.00000 0.00000 1.86206

A30 2.19690 0.00000 -0.00000 0.00000 -0.00000 2.19690

A31 2.22389 0.00000 0.00000 -0.00000 0.00000 2.22389

A32 2.18526 0.00000 -0.00001 -0.00000 -0.00001 2.18525

A33 2.02537 -0.00000 -0.00001 0.00000 -0.00001 2.02536

A34 2.07252 0.00000 0.00002 -0.00000 0.00001 2.07253

A35 2.16463 0.00000 0.00000 -0.00000 0.00000 2.16463

A36 2.19207 -0.00000 -0.00000 -0.00000 -0.00000 2.19207

A37 1.92648 0.00000 -0.00000 0.00000 -0.00000 1.92648

A38 1.86205 -0.00000 0.00000 -0.00000 0.00000 1.86205

A39 2.19690 0.00000 0.00000 0.00000 0.00000 2.19690

A40 2.22384 -0.00000 -0.00000 -0.00000 -0.00000 2.22384

A41 1.86206 -0.00000 -0.00000 0.00000 0.00000 1.86206

A42 2.22389 0.00000 0.00000 -0.00000 0.00000 2.22389

A43 2.19690 0.00000 -0.00000 0.00000 -0.00000 2.19690

A44 1.92609 0.00000 0.00000 -0.00000 0.00000 1.92609

A45 2.16535 0.00000 -0.00001 -0.00000 -0.00001 2.16534

A46 2.19171 -0.00000 0.00001 0.00000 0.00001 2.19173

A47 1.84709 0.00000 -0.00000 0.00000 0.00000 1.84709

A48 2.18669 -0.00000 0.00002 -0.00000 0.00002 2.18671

A49 2.07356 -0.00000 -0.00002 0.00000 -0.00002 2.07354

A50 2.02288 0.00000 0.00000 -0.00000 0.00000 2.02289

A51 2.22030 -0.00000 -0.00000 0.00000 -0.00000 2.22030

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A56 2.21403 0.00000 -0.00001 0.00000 -0.00000 2.21403

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A61 2.22225 -0.00000 -0.00001 0.00000 -0.00001 2.22225

A62 2.19251 0.00000 0.00000 0.00000 0.00000 2.19251

A63 1.92513 -0.00000 -0.00000 0.00000 -0.00000 1.92513

A64 2.17989 0.00000 0.00000 -0.00000 0.00000 2.17989

A65 2.17734 0.00000 -0.00001 0.00000 -0.00000 2.17733

A66 2.18525 0.00000 0.00001 0.00000 0.00001 2.18526

A67 2.07253 0.00000 -0.00000 -0.00000 -0.00001 2.07252

A68 2.02536 -0.00000 -0.00000 0.00000 -0.00000 2.02536

A69 2.10450 -0.00000 0.00000 0.00000 0.00000 2.10450

A70 2.10702 0.00000 -0.00000 -0.00000 -0.00000 2.10701

A71 2.07166 0.00000 -0.00000 -0.00000 -0.00000 2.07166

A72 2.10512 0.00000 -0.00000 0.00000 -0.00000 2.10512

A73 2.08515 -0.00000 -0.00000 0.00000 -0.00000 2.08514

A74 2.09276 0.00000 0.00000 -0.00000 0.00000 2.09276

A75 2.09775 -0.00000 0.00000 -0.00000 0.00000 2.09775

A76 2.08897 -0.00000 -0.00000 0.00000 -0.00000 2.08897

A77 2.09646 0.00000 -0.00000 0.00000 -0.00000 2.09646

A78 2.08903 -0.00000 -0.00000 -0.00000 -0.00000 2.08903

A79 2.09689 0.00000 0.00000 0.00000 0.00000 2.09689

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A81 2.09760 0.00000 0.00000 0.00000 0.00000 2.09760

A82 2.09707 -0.00000 -0.00000 -0.00000 -0.00000 2.09707

A83 2.08851 0.00000 0.00000 -0.00000 0.00000 2.08851

A84 2.10507 -0.00000 0.00000 0.00000 0.00000 2.10507

A85 2.08430 0.00000 -0.00000 0.00000 0.00000 2.08430

A86 2.09367 0.00000 -0.00000 -0.00000 -0.00000 2.09367

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A88 2.09700 -0.00000 -0.00000 -0.00000 -0.00000 2.09700

A89 2.09723 0.00000 0.00000 -0.00000 0.00000 2.09723

A90 2.09801 -0.00000 -0.00000 -0.00000 -0.00000 2.09801

A91 2.09647 0.00000 -0.00000 0.00000 -0.00000 2.09647

A92 2.08871 0.00000 0.00000 -0.00000 0.00000 2.08871

A93 2.10486 0.00000 0.00000 -0.00000 0.00000 2.10486

A94 2.09331 -0.00000 -0.00000 -0.00000 -0.00000 2.09331

A95 2.08481 0.00000 0.00000 0.00000 0.00000 2.08482

A96 2.10718 -0.00000 -0.00001 0.00000 -0.00001 2.10717

A97 2.10451 0.00000 0.00001 -0.00000 0.00001 2.10452

A98 2.07149 -0.00000 -0.00000 -0.00000 -0.00000 2.07149

A99 2.10548 -0.00000 -0.00000 0.00000 -0.00000 2.10548

A100 2.08383 0.00000 0.00000 0.00000 0.00000 2.08383

A101 2.09375 0.00000 -0.00000 -0.00000 -0.00000 2.09375

A102 2.09745 0.00000 0.00000 -0.00000 0.00000 2.09745

A103 2.09705 -0.00000 -0.00000 0.00000 -0.00000 2.09705

A104 2.08868 -0.00000 -0.00000 -0.00000 -0.00000 2.08868

A105 2.10451 0.00000 0.00000 -0.00000 0.00000 2.10451

A106 2.10718 -0.00000 -0.00001 0.00000 -0.00001 2.10718

A107 2.07149 -0.00000 0.00000 -0.00000 0.00000 2.07149

A108 2.10548 -0.00000 -0.00000 0.00000 -0.00000 2.10547

A109 2.08383 0.00000 -0.00000 0.00000 -0.00000 2.08383

A110 2.09375 0.00000 0.00000 -0.00000 0.00000 2.09375

A111 2.09745 0.00000 0.00000 -0.00000 0.00000 2.09745

A112 2.08868 -0.00000 0.00000 -0.00000 0.00000 2.08868

A113 2.09705 -0.00000 -0.00000 0.00000 -0.00000 2.09705

A114 2.08896 0.00000 -0.00000 0.00000 0.00000 2.08896

A115 2.09723 0.00000 0.00000 -0.00000 0.00000 2.09723

A116 2.09700 -0.00000 -0.00000 -0.00000 -0.00000 2.09700

A117 2.09801 -0.00000 -0.00000 -0.00000 -0.00000 2.09801

A118 2.09647 0.00000 0.00000 0.00000 0.00000 2.09647

A119 2.08871 0.00000 -0.00000 -0.00000 -0.00000 2.08871

A120 2.10486 0.00000 -0.00000 -0.00000 -0.00000 2.10486

A121 2.08481 0.00000 0.00000 0.00000 0.00000 2.08482

A122 2.09331 -0.00000 -0.00000 -0.00000 -0.00000 2.09331

A123 2.10702 0.00000 -0.00001 0.00000 -0.00001 2.10701

A124 2.10450 -0.00000 0.00001 -0.00000 0.00000 2.10451

A125 2.07166 0.00000 0.00000 -0.00000 0.00000 2.07167

A126 2.10507 -0.00000 -0.00000 -0.00000 -0.00000 2.10507

A127 2.08430 0.00000 -0.00000 0.00000 -0.00000 2.08430

A128 2.09367 0.00000 0.00000 -0.00000 0.00000 2.09367

A129 2.09760 0.00000 -0.00000 0.00000 -0.00000 2.09760

A130 2.08851 -0.00000 0.00000 -0.00000 0.00000 2.08851

A131 2.09707 -0.00000 -0.00000 -0.00000 -0.00000 2.09707

A132 2.08903 -0.00000 -0.00000 -0.00000 -0.00000 2.08903

A133 2.09726 -0.00000 -0.00000 0.00000 -0.00000 2.09726

A134 2.09689 0.00000 0.00000 0.00000 0.00000 2.09689

A135 2.09775 -0.00000 0.00000 -0.00000 0.00000 2.09775

A136 2.09646 0.00000 0.00000 0.00000 0.00000 2.09646

A137 2.08897 -0.00000 -0.00000 0.00000 -0.00000 2.08897

A138 2.10512 0.00000 -0.00000 0.00000 -0.00000 2.10512

A139 2.08514 -0.00000 0.00000 0.00000 0.00000 2.08514

A140 2.09276 0.00000 0.00000 -0.00000 0.00000 2.09276

D1 0.01566 -0.00000 -0.00001 -0.00000 -0.00001 0.01565

D2 -3.09460 0.00000 -0.00007 0.00000 -0.00007 -3.09467

D3 -3.12080 -0.00000 0.00001 -0.00000 0.00001 -3.12079

D4 0.05213 0.00000 -0.00005 0.00000 -0.00005 0.05208

D5 -0.00071 -0.00000 0.00001 0.00000 0.00001 -0.00070

D6 -3.13467 -0.00000 0.00002 -0.00000 0.00002 -3.13465

D7 3.13566 0.00000 -0.00002 0.00000 -0.00002 3.13564

D8 0.00169 -0.00000 -0.00000 0.00000 -0.00000 0.00169

D9 -0.02536 0.00000 0.00001 0.00000 0.00001 -0.02535

D10 3.07411 -0.00000 0.00010 -0.00001 0.00010 3.07421

D11 3.08558 -0.00000 0.00007 -0.00000 0.00007 3.08565

D12 -0.09813 -0.00000 0.00017 -0.00001 0.00016 -0.09798

D13 -2.95306 -0.00000 0.00016 -0.00000 0.00015 -2.95291

D14 0.17868 0.00000 0.00012 -0.00000 0.00011 0.17880

D15 0.22539 -0.00000 0.00008 -0.00000 0.00008 0.22547

D16 -2.92605 0.00000 0.00004 0.00000 0.00004 -2.92601

D17 0.02493 -0.00000 -0.00001 -0.00000 -0.00001 0.02492

D18 -3.08779 -0.00000 -0.00004 0.00000 -0.00004 -3.08783

D19 -3.07447 0.00000 -0.00010 0.00001 -0.00009 -3.07456

D20 0.09600 0.00000 -0.00013 0.00001 -0.00013 0.09587

D21 -0.01452 0.00000 0.00000 0.00000 0.00000 -0.01452

D22 3.11959 0.00000 -0.00001 0.00000 -0.00001 3.11958

D23 3.09764 0.00000 0.00003 -0.00000 0.00003 3.09767

D24 -0.05143 0.00000 0.00002 -0.00000 0.00002 -0.05141

D25 -0.23695 0.00000 -0.00003 0.00000 -0.00003 -0.23698

D26 2.91524 0.00000 -0.00002 0.00000 -0.00001 2.91523

D27 2.93931 0.00000 -0.00007 0.00000 -0.00007 2.93924

D28 -0.19169 0.00000 -0.00006 0.00000 -0.00005 -0.19174

D29 -0.12443 -0.00000 -0.00001 -0.00000 -0.00001 -0.12444

D30 3.02616 -0.00000 -0.00003 -0.00000 -0.00003 3.02614

D31 3.00628 0.00000 -0.00003 -0.00000 -0.00003 3.00625

D32 -0.12631 -0.00000 -0.00004 -0.00000 -0.00005 -0.12635

D33 -0.99859 -0.00000 0.00003 -0.00000 0.00003 -0.99856

D34 2.13970 -0.00000 0.00002 -0.00000 0.00002 2.13971

D35 2.15288 -0.00000 0.00005 -0.00000 0.00005 2.15292

D36 -0.99202 -0.00000 0.00004 -0.00000 0.00003 -0.99199

D37 -3.09179 -0.00000 -0.00002 -0.00000 -0.00003 -3.09182

D38 0.04185 -0.00000 -0.00001 -0.00000 -0.00001 0.04184

D39 3.10655 0.00000 0.00002 0.00000 0.00003 3.10657

D40 -0.06140 0.00000 0.00002 0.00000 0.00002 -0.06138

D41 -0.02723 0.00000 0.00001 0.00000 0.00001 -0.02722

D42 3.08801 -0.00000 0.00000 0.00000 0.00000 3.08801

D43 -0.04099 0.00000 0.00001 -0.00000 0.00001 -0.04099

D44 3.09597 0.00000 0.00002 -0.00000 0.00002 3.09599

D45 0.02490 -0.00000 -0.00000 0.00000 0.00000 0.02491

D46 -3.08815 0.00000 -0.00000 0.00000 -0.00000 -3.08815

D47 -3.11215 -0.00000 -0.00001 0.00000 -0.00001 -3.11216

D48 0.05798 -0.00000 -0.00002 0.00000 -0.00001 0.05797

D49 0.13465 -0.00000 -0.00005 0.00000 -0.00005 0.13460

D50 -2.99680 -0.00000 -0.00009 0.00000 -0.00009 -2.99689

D51 -3.01217 0.00000 -0.00004 0.00000 -0.00004 -3.01221

D52 0.13956 -0.00000 -0.00008 0.00000 -0.00008 0.13948

D53 0.00136 -0.00000 -0.00001 -0.00000 -0.00001 0.00135

D54 -3.11335 0.00000 0.00000 -0.00000 0.00000 -3.11335

D55 3.11383 -0.00000 -0.00000 -0.00000 -0.00000 3.11383

D56 -0.00087 0.00000 0.00001 -0.00000 0.00001 -0.00087

D57 -3.01218 0.00000 -0.00007 0.00001 -0.00007 -3.01224

D58 0.13464 0.00000 -0.00006 0.00001 -0.00005 0.13459

D59 0.13951 0.00000 -0.00003 0.00001 -0.00003 0.13948

D60 -2.99686 -0.00000 -0.00002 0.00001 -0.00001 -2.99687

D61 0.99247 0.00000 -0.00002 0.00000 -0.00001 0.99245

D62 -2.14570 0.00000 -0.00000 0.00000 0.00000 -2.14570

D63 -2.15830 0.00000 -0.00006 0.00001 -0.00005 -2.15835

D64 0.98671 0.00000 -0.00004 0.00000 -0.00004 0.98668

D65 -3.11216 -0.00000 0.00002 0.00000 0.00002 -3.11213

D66 0.05797 -0.00000 0.00002 0.00000 0.00002 0.05799

D67 0.02491 -0.00000 0.00001 0.00000 0.00001 0.02492

D68 -3.08815 0.00000 0.00001 0.00000 0.00001 -3.08815

D69 3.09598 0.00000 -0.00002 0.00000 -0.00001 3.09597

D70 -0.04099 0.00000 -0.00000 0.00000 0.00000 -0.04099

D71 0.00136 -0.00000 -0.00001 -0.00000 -0.00001 0.00134

D72 -3.11335 0.00000 -0.00001 0.00000 -0.00001 -3.11336

D73 3.11384 -0.00000 -0.00001 -0.00000 -0.00001 3.11383

D74 -0.00087 0.00000 -0.00001 0.00000 -0.00001 -0.00087

D75 -0.02723 0.00000 0.00001 0.00000 0.00002 -0.02722

D76 3.10654 0.00000 0.00004 0.00001 0.00005 3.10659

D77 3.08801 -0.00000 0.00001 0.00000 0.00001 3.08802

D78 -0.06141 0.00000 0.00004 0.00001 0.00004 -0.06136

D79 0.04185 -0.00000 -0.00001 -0.00000 -0.00001 0.04184

D80 -3.09178 -0.00000 -0.00003 -0.00001 -0.00004 -3.09182

D81 3.02617 -0.00000 -0.00004 -0.00001 -0.00004 3.02613

D82 -0.12635 0.00000 0.00001 -0.00000 0.00001 -0.12634

D83 -0.12444 0.00000 -0.00001 0.00000 -0.00001 -0.12445

D84 3.00623 0.00000 0.00004 0.00001 0.00005 3.00627

D85 2.93916 0.00000 0.00025 -0.00000 0.00025 2.93941

D86 -0.23705 0.00000 0.00020 -0.00000 0.00019 -0.23685

D87 -0.19179 -0.00000 0.00021 -0.00001 0.00020 -0.19160

D88 2.91519 -0.00000 0.00015 -0.00001 0.00014 2.91533

D89 -0.99197 -0.00000 -0.00012 0.00000 -0.00012 -0.99210

D90 2.15295 -0.00000 -0.00013 0.00000 -0.00013 2.15282

D91 2.13971 0.00000 -0.00008 0.00000 -0.00007 2.13963

D92 -0.99856 0.00000 -0.00009 0.00001 -0.00008 -0.99864

D93 3.09769 -0.00000 -0.00005 -0.00000 -0.00005 3.09764

D94 -0.05140 -0.00000 -0.00002 -0.00000 -0.00003 -0.05142

D95 -0.01452 -0.00000 -0.00000 -0.00000 -0.00000 -0.01452

D96 3.11958 0.00000 0.00003 -0.00000 0.00002 3.11960

D97 -3.08785 0.00000 0.00005 0.00000 0.00005 -3.08780

D98 0.09581 0.00000 0.00019 0.00000 0.00019 0.09601

D99 0.02492 0.00000 -0.00000 0.00000 0.00000 0.02492

D100 -3.07460 0.00000 0.00015 -0.00000 0.00014 -3.07446

D101 -0.00071 -0.00000 0.00000 0.00000 0.00000 -0.00070

D102 3.13564 0.00000 0.00002 0.00000 0.00002 3.13566

D103 -3.13465 -0.00000 -0.00002 0.00000 -0.00002 -3.13468

D104 0.00169 -0.00000 -0.00001 0.00000 -0.00001 0.00169

D105 0.01565 0.00000 -0.00000 0.00000 -0.00000 0.01565

D106 -3.09465 0.00000 0.00002 0.00000 0.00002 -3.09463

D107 -3.12079 0.00000 -0.00002 0.00000 -0.00002 -3.12081

D108 0.05209 0.00000 0.00001 -0.00000 0.00000 0.05210

D109 -0.02535 -0.00000 0.00000 -0.00000 0.00000 -0.02535

D110 3.07424 -0.00000 -0.00014 0.00000 -0.00014 3.07410

D111 3.08563 -0.00000 -0.00002 -0.00000 -0.00002 3.08561

D112 -0.09795 -0.00000 -0.00017 0.00000 -0.00017 -0.09812

D113 -2.95291 -0.00000 -0.00016 -0.00000 -0.00016 -2.95307

D114 0.17879 -0.00000 -0.00012 -0.00000 -0.00012 0.17867

D115 0.22549 -0.00000 -0.00012 -0.00000 -0.00013 0.22536

D116 -2.92600 0.00000 -0.00009 -0.00000 -0.00009 -2.92609

D117 0.98666 0.00000 0.00010 0.00000 0.00010 0.98676

D118 -2.15838 0.00000 0.00012 0.00000 0.00012 -2.15826

D119 -2.14572 -0.00000 0.00006 0.00000 0.00007 -2.14565

D120 0.99243 -0.00000 0.00008 0.00000 0.00009 0.99252

D121 -3.13033 0.00000 -0.00001 -0.00000 -0.00001 -3.13034

D122 -0.00824 -0.00000 -0.00001 -0.00000 -0.00001 -0.00825

D123 0.01450 0.00000 0.00001 -0.00000 0.00000 0.01451

D124 3.13660 -0.00000 0.00000 -0.00000 0.00000 3.13660

D125 -3.14034 -0.00000 0.00001 0.00000 0.00001 -3.14033

D126 -0.01714 -0.00000 0.00000 0.00000 0.00001 -0.01713

D127 -0.00199 -0.00000 -0.00000 0.00000 -0.00000 -0.00200

D128 3.12121 -0.00000 -0.00001 0.00000 -0.00001 3.12120

D129 -0.01618 -0.00000 -0.00000 0.00000 -0.00000 -0.01619

D130 3.12476 -0.00000 -0.00000 0.00000 -0.00000 3.12476

D131 -3.13819 0.00000 0.00000 -0.00000 0.00000 -3.13819

D132 0.00275 0.00000 0.00000 -0.00000 0.00000 0.00275

D133 0.00513 0.00000 -0.00000 0.00000 0.00000 0.00513

D134 -3.13362 -0.00000 -0.00000 0.00000 -0.00000 -3.13362

D135 -3.13581 0.00000 -0.00000 0.00000 -0.00000 -3.13581

D136 0.00862 -0.00000 -0.00000 0.00000 -0.00000 0.00862

D137 0.00733 -0.00000 0.00000 -0.00000 0.00000 0.00733

D138 -3.13198 0.00000 0.00000 0.00000 0.00000 -3.13197

D139 -3.13710 0.00000 0.00000 -0.00000 0.00000 -3.13710

D140 0.00677 0.00000 0.00000 0.00000 0.00000 0.00677

D141 -0.00888 0.00000 0.00000 -0.00000 0.00000 -0.00888

D142 -3.13198 0.00000 0.00000 0.00000 0.00001 -3.13198

D143 3.13044 0.00000 -0.00000 -0.00000 -0.00000 3.13044

D144 0.00734 -0.00000 0.00000 0.00000 0.00000 0.00734

D145 -0.00537 -0.00000 -0.00000 -0.00000 -0.00000 -0.00538

D146 3.13571 0.00000 0.00000 -0.00000 0.00000 3.13571

D147 3.13484 -0.00000 -0.00001 0.00000 -0.00001 3.13483

D148 -0.00726 -0.00000 -0.00000 0.00000 -0.00000 -0.00727

D149 -0.00643 -0.00000 -0.00000 0.00000 -0.00000 -0.00643

D150 3.13188 0.00000 -0.00000 0.00000 -0.00000 3.13187

D151 3.13655 -0.00000 0.00000 -0.00000 0.00000 3.13655

D152 -0.00834 0.00000 0.00000 -0.00000 0.00000 -0.00834

D153 0.01657 0.00000 0.00000 0.00000 0.00000 0.01657

D154 3.13667 0.00000 0.00000 0.00000 0.00001 3.13667

D155 -3.12451 0.00000 0.00000 0.00000 0.00000 -3.12451

D156 -0.00442 0.00000 0.00000 -0.00000 0.00000 -0.00441

D157 3.12928 0.00000 0.00002 -0.00000 0.00001 3.12929

D158 -0.01567 0.00000 -0.00000 -0.00000 -0.00000 -0.01567

D159 0.00908 0.00000 0.00001 -0.00000 0.00001 0.00909

D160 -3.13587 0.00000 -0.00000 -0.00000 -0.00000 -3.13588

D161 -3.14111 -0.00000 -0.00002 0.00000 -0.00001 -3.14113

D162 0.01771 -0.00000 -0.00001 0.00000 -0.00001 0.01770

D163 0.00383 -0.00000 -0.00000 0.00000 0.00000 0.00383

D164 -3.12053 -0.00000 0.00001 -0.00000 0.00001 -3.12052

D165 0.00715 0.00000 0.00000 -0.00000 0.00000 0.00716

D166 -3.13117 0.00000 0.00000 -0.00000 0.00000 -3.13116

D167 3.13142 0.00000 -0.00001 0.00000 -0.00001 3.13141

D168 -0.00690 -0.00000 -0.00001 0.00000 -0.00000 -0.00691

D169 -3.14113 0.00000 0.00001 0.00000 0.00001 -3.14112

D170 0.01770 0.00000 0.00000 0.00000 0.00000 0.01771

D171 0.00383 -0.00000 -0.00001 0.00000 -0.00001 0.00382

D172 -3.12052 -0.00000 -0.00001 -0.00000 -0.00001 -3.12053

D173 3.12930 -0.00000 -0.00001 -0.00000 -0.00001 3.12928

D174 0.00909 -0.00000 -0.00001 -0.00000 -0.00001 0.00908

D175 -0.01567 -0.00000 0.00001 -0.00000 0.00001 -0.01567

D176 -3.13588 -0.00000 0.00001 -0.00000 0.00001 -3.13587

D177 0.00716 0.00000 0.00000 -0.00000 0.00000 0.00716

D178 -3.13116 -0.00000 -0.00000 -0.00000 -0.00000 -3.13116

D179 3.13141 0.00000 0.00001 0.00000 0.00001 3.13142

D180 -0.00691 0.00000 0.00000 0.00000 0.00001 -0.00690

D181 -0.00643 -0.00000 0.00000 -0.00000 0.00000 -0.00643

D182 3.13655 -0.00000 0.00000 -0.00000 0.00000 3.13655

D183 3.13187 0.00000 0.00001 -0.00000 0.00001 3.13188

D184 -0.00834 0.00000 0.00001 -0.00000 0.00000 -0.00833

D185 -0.00537 -0.00000 -0.00000 -0.00000 -0.00000 -0.00538

D186 3.13571 0.00000 -0.00001 0.00000 -0.00000 3.13571

D187 3.13484 -0.00000 -0.00000 0.00000 -0.00000 3.13484

D188 -0.00726 0.00000 -0.00000 0.00000 -0.00000 -0.00727

D189 0.01657 0.00000 -0.00000 0.00000 -0.00000 0.01657

D190 3.13667 0.00000 -0.00000 0.00000 -0.00000 3.13667

D191 -3.12451 0.00000 -0.00000 0.00000 -0.00000 -3.12451

D192 -0.00441 -0.00000 0.00000 -0.00000 0.00000 -0.00441

D193 -3.14032 -0.00000 -0.00001 0.00000 -0.00000 -3.14032

D194 -0.01712 -0.00000 0.00000 0.00000 0.00000 -0.01712

D195 -0.00199 -0.00000 0.00000 0.00000 0.00000 -0.00199

D196 3.12120 -0.00000 0.00001 0.00000 0.00001 3.12121

D197 -3.13035 0.00000 0.00000 -0.00000 0.00000 -3.13035

D198 -0.00826 0.00000 0.00000 -0.00000 0.00000 -0.00825

D199 0.01450 0.00000 -0.00000 -0.00000 -0.00001 0.01450

D200 3.13660 -0.00000 -0.00001 -0.00000 -0.00001 3.13659

D201 -0.00888 0.00000 0.00000 -0.00000 0.00000 -0.00888

D202 3.13044 0.00000 0.00000 -0.00000 0.00000 3.13044

D203 -3.13197 -0.00000 -0.00001 0.00000 -0.00001 -3.13198

D204 0.00735 -0.00000 -0.00001 -0.00000 -0.00001 0.00734

D205 0.00733 -0.00000 -0.00000 -0.00000 -0.00000 0.00733

D206 -3.13710 0.00000 0.00000 -0.00000 0.00000 -3.13710

D207 -3.13198 0.00000 -0.00000 0.00000 -0.00000 -3.13198

D208 0.00677 0.00000 0.00000 0.00000 0.00000 0.00677

D209 0.00513 0.00000 0.00000 -0.00000 0.00000 0.00513

D210 -3.13581 0.00000 0.00000 0.00000 0.00000 -3.13581

D211 -3.13362 -0.00000 -0.00000 0.00000 -0.00000 -3.13362

D212 0.00863 -0.00000 -0.00000 0.00000 -0.00000 0.00862

D213 -0.01619 -0.00000 0.00000 0.00000 0.00000 -0.01618

D214 -3.13820 0.00000 0.00000 0.00000 0.00000 -3.13819

D215 3.12476 -0.00000 0.00000 -0.00000 0.00000 3.12476

D216 0.00275 0.00000 0.00000 -0.00000 0.00000 0.00275

Item Value Threshold Converged?

Maximum Force 0.000001 0.000450 YES

RMS Force 0.000000 0.000300 YES

Maximum Displacement 0.000889 0.001800 YES

RMS Displacement 0.000194 0.001200 YES

Predicted change in Energy=-1.351313D-10

Optimization completed.

-- Stationary point found.

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! Optimized Parameters !

! (Angstroms and Degrees) !

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! Name Definition Value Derivative Info. !

--------------------------------------------------------------------------------

! R1 R(1,2) 1.4059 -DE/DX = 0.0 !

! R2 R(1,5) 1.3975 -DE/DX = 0.0 !

! R3 R(1,49) 1.078 -DE/DX = 0.0 !

! R4 R(2,3) 1.3754 -DE/DX = 0.0 !

! R5 R(2,12) 1.4372 -DE/DX = 0.0 !

! R6 R(3,4) 1.3753 -DE/DX = 0.0 !

! R7 R(3,77) 1.0108 -DE/DX = 0.0 !

! R8 R(4,5) 1.4058 -DE/DX = 0.0 !

! R9 R(4,6) 1.4377 -DE/DX = 0.0 !

! R10 R(5,50) 1.078 -DE/DX = 0.0 !

! R11 R(6,7) 1.3974 -DE/DX = 0.0 !

! R12 R(6,25) 1.4839 -DE/DX = 0.0 !

! R13 R(7,8) 1.3739 -DE/DX = 0.0 !

! R14 R(7,11) 1.4616 -DE/DX = 0.0 !

! R15 R(8,9) 1.3729 -DE/DX = 0.0 !

! R16 R(9,10) 1.4618 -DE/DX = 0.0 !

! R17 R(9,24) 1.3985 -DE/DX = 0.0 !

! R18 R(10,11) 1.3517 -DE/DX = 0.0 !

! R19 R(10,51) 1.0791 -DE/DX = 0.0 !

! R20 R(11,52) 1.079 -DE/DX = 0.0 !

! R21 R(12,13) 1.3985 -DE/DX = 0.0 !

! R22 R(12,34) 1.4837 -DE/DX = 0.0 !

! R23 R(13,14) 1.4618 -DE/DX = 0.0 !

! R24 R(13,17) 1.3729 -DE/DX = 0.0 !

! R25 R(14,15) 1.3517 -DE/DX = 0.0 !

! R26 R(14,53) 1.0791 -DE/DX = 0.0 !

! R27 R(15,16) 1.4616 -DE/DX = 0.0 !

! R28 R(15,54) 1.079 -DE/DX = 0.0 !

! R29 R(16,17) 1.3739 -DE/DX = 0.0 !

! R30 R(16,18) 1.3974 -DE/DX = 0.0 !

! R31 R(18,19) 1.4377 -DE/DX = 0.0 !

! R32 R(18,43) 1.4839 -DE/DX = 0.0 !

! R33 R(19,20) 1.4058 -DE/DX = 0.0 !

! R34 R(19,23) 1.3753 -DE/DX = 0.0 !

! R35 R(20,21) 1.3975 -DE/DX = 0.0 !

! R36 R(20,55) 1.078 -DE/DX = 0.0 !

! R37 R(21,22) 1.4059 -DE/DX = 0.0 !

! R38 R(21,56) 1.078 -DE/DX = 0.0 !

! R39 R(22,23) 1.3754 -DE/DX = 0.0 !

! R40 R(22,24) 1.4372 -DE/DX = 0.0 !

! R41 R(23,78) 1.0108 -DE/DX = 0.0 !

! R42 R(24,37) 1.4837 -DE/DX = 0.0 !

! R43 R(25,26) 1.403 -DE/DX = 0.0 !

! R44 R(25,30) 1.4023 -DE/DX = 0.0 !

! R45 R(26,27) 1.391 -DE/DX = 0.0 !

! R46 R(26,57) 1.084 -DE/DX = 0.0 !

! R47 R(27,28) 1.3951 -DE/DX = 0.0 !

! R48 R(27,58) 1.0849 -DE/DX = 0.0 !

! R49 R(28,29) 1.3939 -DE/DX = 0.0 !

! R50 R(28,59) 1.0848 -DE/DX = 0.0 !

! R51 R(29,30) 1.3923 -DE/DX = 0.0 !

! R52 R(29,60) 1.0849 -DE/DX = 0.0 !

! R53 R(30,61) 1.0841 -DE/DX = 0.0 !

! R54 R(31,32) 1.3951 -DE/DX = 0.0 !

! R55 R(31,36) 1.394 -DE/DX = 0.0 !

! R56 R(31,62) 1.0848 -DE/DX = 0.0 !

! R57 R(32,33) 1.3912 -DE/DX = 0.0 !

! R58 R(32,63) 1.0849 -DE/DX = 0.0 !

! R59 R(33,34) 1.4031 -DE/DX = 0.0 !

! R60 R(33,64) 1.084 -DE/DX = 0.0 !

! R61 R(34,35) 1.4024 -DE/DX = 0.0 !

! R62 R(35,36) 1.3921 -DE/DX = 0.0 !

! R63 R(35,65) 1.084 -DE/DX = 0.0 !

! R64 R(36,66) 1.0849 -DE/DX = 0.0 !

! R65 R(37,38) 1.4024 -DE/DX = 0.0 !

! R66 R(37,42) 1.4031 -DE/DX = 0.0 !

! R67 R(38,39) 1.3921 -DE/DX = 0.0 !

! R68 R(38,67) 1.084 -DE/DX = 0.0 !

! R69 R(39,40) 1.394 -DE/DX = 0.0 !

! R70 R(39,68) 1.0849 -DE/DX = 0.0 !

! R71 R(40,41) 1.3951 -DE/DX = 0.0 !

! R72 R(40,69) 1.0848 -DE/DX = 0.0 !

! R73 R(41,42) 1.3912 -DE/DX = 0.0 !

! R74 R(41,70) 1.0849 -DE/DX = 0.0 !

! R75 R(42,71) 1.084 -DE/DX = 0.0 !

! R76 R(43,44) 1.4023 -DE/DX = 0.0 !

! R77 R(43,48) 1.403 -DE/DX = 0.0 !

! R78 R(44,45) 1.3923 -DE/DX = 0.0 !

! R79 R(44,72) 1.0841 -DE/DX = 0.0 !

! R80 R(45,46) 1.3939 -DE/DX = 0.0 !

! R81 R(45,73) 1.0849 -DE/DX = 0.0 !

! R82 R(46,47) 1.3951 -DE/DX = 0.0 !

! R83 R(46,74) 1.0848 -DE/DX = 0.0 !

! R84 R(47,48) 1.391 -DE/DX = 0.0 !

! R85 R(47,75) 1.0849 -DE/DX = 0.0 !

! R86 R(48,76) 1.084 -DE/DX = 0.0 !

! A1 A(2,1,5) 107.8052 -DE/DX = 0.0 !

! A2 A(2,1,49) 125.3553 -DE/DX = 0.0 !

! A3 A(5,1,49) 126.8388 -DE/DX = 0.0 !

! A4 A(1,2,3) 107.0266 -DE/DX = 0.0 !

! A5 A(1,2,12) 127.3257 -DE/DX = 0.0 !

! A6 A(3,2,12) 125.6214 -DE/DX = 0.0 !

! A7 A(2,3,4) 110.3018 -DE/DX = 0.0 !

! A8 A(2,3,77) 124.7519 -DE/DX = 0.0 !

! A9 A(4,3,77) 124.8985 -DE/DX = 0.0 !

! A10 A(3,4,5) 107.0342 -DE/DX = 0.0 !

! A11 A(3,4,6) 125.7288 -DE/DX = 0.0 !

! A12 A(5,4,6) 127.2137 -DE/DX = 0.0 !

! A13 A(1,5,4) 107.8114 -DE/DX = 0.0 !

! A14 A(1,5,50) 126.8545 -DE/DX = 0.0 !

! A15 A(4,5,50) 125.3325 -DE/DX = 0.0 !

! A16 A(4,6,7) 125.2885 -DE/DX = 0.0 !

! A17 A(4,6,25) 115.903 -DE/DX = 0.0 !

! A18 A(7,6,25) 118.8058 -DE/DX = 0.0 !

! A19 A(6,7,8) 125.5759 -DE/DX = 0.0 !

! A20 A(6,7,11) 124.0657 -DE/DX = 0.0 !

! A21 A(8,7,11) 110.3567 -DE/DX = 0.0 !

! A22 A(7,8,9) 105.8305 -DE/DX = 0.0 !

! A23 A(8,9,10) 110.3791 -DE/DX = 0.0 !

! A24 A(8,9,24) 125.5964 -DE/DX = 0.0 !

! A25 A(10,9,24) 124.0239 -DE/DX = 0.0 !

! A26 A(9,10,11) 106.6873 -DE/DX = 0.0 !

! A27 A(9,10,51) 125.8731 -DE/DX = 0.0 !

! A28 A(11,10,51) 127.4168 -DE/DX = 0.0 !

! A29 A(7,11,10) 106.6883 -DE/DX = 0.0 !

! A30 A(7,11,52) 125.873 -DE/DX = 0.0 !

! A31 A(10,11,52) 127.4193 -DE/DX = 0.0 !

! A32 A(2,12,13) 125.206 -DE/DX = 0.0 !

! A33 A(2,12,34) 116.045 -DE/DX = 0.0 !

! A34 A(13,12,34) 118.7467 -DE/DX = 0.0 !

! A35 A(12,13,14) 124.0239 -DE/DX = 0.0 !

! A36 A(12,13,17) 125.5964 -DE/DX = 0.0 !

! A37 A(14,13,17) 110.3791 -DE/DX = 0.0 !

! A38 A(13,14,15) 106.6873 -DE/DX = 0.0 !

! A39 A(13,14,53) 125.8732 -DE/DX = 0.0 !

! A40 A(15,14,53) 127.4167 -DE/DX = 0.0 !

! A41 A(14,15,16) 106.6883 -DE/DX = 0.0 !

! A42 A(14,15,54) 127.4193 -DE/DX = 0.0 !

! A43 A(16,15,54) 125.8729 -DE/DX = 0.0 !

! A44 A(15,16,17) 110.3567 -DE/DX = 0.0 !

! A45 A(15,16,18) 124.0656 -DE/DX = 0.0 !

! A46 A(17,16,18) 125.576 -DE/DX = 0.0 !

! A47 A(13,17,16) 105.8305 -DE/DX = 0.0 !

! A48 A(16,18,19) 125.2882 -DE/DX = 0.0 !

! A49 A(16,18,43) 118.8063 -DE/DX = 0.0 !

! A50 A(19,18,43) 115.9028 -DE/DX = 0.0 !

! A51 A(18,19,20) 127.2138 -DE/DX = 0.0 !

! A52 A(18,19,23) 125.7288 -DE/DX = 0.0 !

! A53 A(20,19,23) 107.0342 -DE/DX = 0.0 !

! A54 A(19,20,21) 107.8114 -DE/DX = 0.0 !

! A55 A(19,20,55) 125.3324 -DE/DX = 0.0 !

! A56 A(21,20,55) 126.8546 -DE/DX = 0.0 !

! A57 A(20,21,22) 107.8051 -DE/DX = 0.0 !

! A58 A(20,21,56) 126.839 -DE/DX = 0.0 !

! A59 A(22,21,56) 125.3552 -DE/DX = 0.0 !

! A60 A(21,22,23) 107.0266 -DE/DX = 0.0 !

! A61 A(21,22,24) 127.3257 -DE/DX = 0.0 !

! A62 A(23,22,24) 125.6215 -DE/DX = 0.0 !

! A63 A(19,23,22) 110.3019 -DE/DX = 0.0 !

! A64 A(19,23,78) 124.8984 -DE/DX = 0.0 !

! A65 A(22,23,78) 124.7522 -DE/DX = 0.0 !

! A66 A(9,24,22) 125.2057 -DE/DX = 0.0 !

! A67 A(9,24,37) 118.7471 -DE/DX = 0.0 !

! A68 A(22,24,37) 116.0448 -DE/DX = 0.0 !

! A69 A(6,25,26) 120.579 -DE/DX = 0.0 !

! A70 A(6,25,30) 120.7231 -DE/DX = 0.0 !

! A71 A(26,25,30) 118.6977 -DE/DX = 0.0 !

! A72 A(25,26,27) 120.6145 -DE/DX = 0.0 !

! A73 A(25,26,57) 119.47 -DE/DX = 0.0 !

! A74 A(27,26,57) 119.9061 -DE/DX = 0.0 !

! A75 A(26,27,28) 120.1924 -DE/DX = 0.0 !

! A76 A(26,27,58) 119.6894 -DE/DX = 0.0 !

! A77 A(28,27,58) 120.1182 -DE/DX = 0.0 !

! A78 A(27,28,29) 119.6926 -DE/DX = 0.0 !

! A79 A(27,28,59) 120.1428 -DE/DX = 0.0 !

! A80 A(29,28,59) 120.1644 -DE/DX = 0.0 !

! A81 A(28,29,30) 120.1838 -DE/DX = 0.0 !

! A82 A(28,29,60) 120.153 -DE/DX = 0.0 !

! A83 A(30,29,60) 119.6631 -DE/DX = 0.0 !

! A84 A(25,30,29) 120.6115 -DE/DX = 0.0 !

! A85 A(25,30,61) 119.4216 -DE/DX = 0.0 !

! A86 A(29,30,61) 119.9585 -DE/DX = 0.0 !

! A87 A(32,31,36) 119.6884 -DE/DX = 0.0 !

! A88 A(32,31,62) 120.1491 -DE/DX = 0.0 !

! A89 A(36,31,62) 120.1624 -DE/DX = 0.0 !

! A90 A(31,32,33) 120.2069 -DE/DX = 0.0 !

! A91 A(31,32,63) 120.1189 -DE/DX = 0.0 !

! A92 A(33,32,63) 119.6741 -DE/DX = 0.0 !

! A93 A(32,33,34) 120.5995 -DE/DX = 0.0 !

! A94 A(32,33,64) 119.938 -DE/DX = 0.0 !

! A95 A(34,33,64) 119.4511 -DE/DX = 0.0 !

! A96 A(12,34,33) 120.7326 -DE/DX = 0.0 !

! A97 A(12,34,35) 120.5795 -DE/DX = 0.0 !

! A98 A(33,34,35) 118.6876 -DE/DX = 0.0 !

! A99 A(34,35,36) 120.6349 -DE/DX = 0.0 !

! A100 A(34,35,65) 119.3946 -DE/DX = 0.0 !

! A101 A(36,35,65) 119.9632 -DE/DX = 0.0 !

! A102 A(31,36,35) 120.1751 -DE/DX = 0.0 !

! A103 A(31,36,66) 120.1522 -DE/DX = 0.0 !

! A104 A(35,36,66) 119.6724 -DE/DX = 0.0 !

! A105 A(24,37,38) 120.5794 -DE/DX = 0.0 !

! A106 A(24,37,42) 120.7328 -DE/DX = 0.0 !

! A107 A(38,37,42) 118.6876 -DE/DX = 0.0 !

! A108 A(37,38,39) 120.6349 -DE/DX = 0.0 !

! A109 A(37,38,67) 119.3946 -DE/DX = 0.0 !

! A110 A(39,38,67) 119.9631 -DE/DX = 0.0 !

! A111 A(38,39,40) 120.1751 -DE/DX = 0.0 !

! A112 A(38,39,68) 119.6724 -DE/DX = 0.0 !

! A113 A(40,39,68) 120.1523 -DE/DX = 0.0 !

! A114 A(39,40,41) 119.6884 -DE/DX = 0.0 !

! A115 A(39,40,69) 120.1624 -DE/DX = 0.0 !

! A116 A(41,40,69) 120.1491 -DE/DX = 0.0 !

! A117 A(40,41,42) 120.2069 -DE/DX = 0.0 !

! A118 A(40,41,70) 120.1189 -DE/DX = 0.0 !

! A119 A(42,41,70) 119.6741 -DE/DX = 0.0 !

! A120 A(37,42,41) 120.5995 -DE/DX = 0.0 !

! A121 A(37,42,71) 119.4511 -DE/DX = 0.0 !

! A122 A(41,42,71) 119.9381 -DE/DX = 0.0 !

! A123 A(18,43,44) 120.7231 -DE/DX = 0.0 !

! A124 A(18,43,48) 120.579 -DE/DX = 0.0 !

! A125 A(44,43,48) 118.6976 -DE/DX = 0.0 !

! A126 A(43,44,45) 120.6115 -DE/DX = 0.0 !

! A127 A(43,44,72) 119.4217 -DE/DX = 0.0 !

! A128 A(45,44,72) 119.9584 -DE/DX = 0.0 !

! A129 A(44,45,46) 120.1838 -DE/DX = 0.0 !

! A130 A(44,45,73) 119.6631 -DE/DX = 0.0 !

! A131 A(46,45,73) 120.153 -DE/DX = 0.0 !

! A132 A(45,46,47) 119.6926 -DE/DX = 0.0 !

! A133 A(45,46,74) 120.1644 -DE/DX = 0.0 !

! A134 A(47,46,74) 120.1428 -DE/DX = 0.0 !

! A135 A(46,47,48) 120.1924 -DE/DX = 0.0 !

! A136 A(46,47,75) 120.1182 -DE/DX = 0.0 !

! A137 A(48,47,75) 119.6894 -DE/DX = 0.0 !

! A138 A(43,48,47) 120.6145 -DE/DX = 0.0 !

! A139 A(43,48,76) 119.47 -DE/DX = 0.0 !

! A140 A(47,48,76) 119.9061 -DE/DX = 0.0 !

! D1 D(5,1,2,3) 0.8973 -DE/DX = 0.0 !

! D2 D(5,1,2,12) -177.3074 -DE/DX = 0.0 !

! D3 D(49,1,2,3) -178.8086 -DE/DX = 0.0 !

! D4 D(49,1,2,12) 2.9867 -DE/DX = 0.0 !

! D5 D(2,1,5,4) -0.0404 -DE/DX = 0.0 !

! D6 D(2,1,5,50) -179.6035 -DE/DX = 0.0 !

! D7 D(49,1,5,4) 179.6599 -DE/DX = 0.0 !

! D8 D(49,1,5,50) 0.0968 -DE/DX = 0.0 !

! D9 D(1,2,3,4) -1.4533 -DE/DX = 0.0 !

! D10 D(1,2,3,77) 176.1336 -DE/DX = 0.0 !

! D11 D(12,2,3,4) 176.7905 -DE/DX = 0.0 !

! D12 D(12,2,3,77) -5.6226 -DE/DX = 0.0 !

! D13 D(1,2,12,13) -169.1981 -DE/DX = 0.0 !

! D14 D(1,2,12,34) 10.2378 -DE/DX = 0.0 !

! D15 D(3,2,12,13) 12.9138 -DE/DX = 0.0 !

! D16 D(3,2,12,34) -167.6504 -DE/DX = 0.0 !

! D17 D(2,3,4,5) 1.4284 -DE/DX = 0.0 !

! D18 D(2,3,4,6) -176.9172 -DE/DX = 0.0 !

! D19 D(77,3,4,5) -176.1541 -DE/DX = 0.0 !

! D20 D(77,3,4,6) 5.5002 -DE/DX = 0.0 !

! D21 D(3,4,5,1) -0.8321 -DE/DX = 0.0 !

! D22 D(3,4,5,50) 178.7394 -DE/DX = 0.0 !

! D23 D(6,4,5,1) 177.4816 -DE/DX = 0.0 !

! D24 D(6,4,5,50) -2.947 -DE/DX = 0.0 !

! D25 D(3,4,6,7) -13.5763 -DE/DX = 0.0 !

! D26 D(3,4,6,25) 167.0309 -DE/DX = 0.0 !

! D27 D(5,4,6,7) 168.41 -DE/DX = 0.0 !

! D28 D(5,4,6,25) -10.9828 -DE/DX = 0.0 !

! D29 D(4,6,7,8) -7.1295 -DE/DX = 0.0 !

! D30 D(4,6,7,11) 173.3864 -DE/DX = 0.0 !

! D31 D(25,6,7,8) 172.2472 -DE/DX = 0.0 !

! D32 D(25,6,7,11) -7.2369 -DE/DX = 0.0 !

! D33 D(4,6,25,26) -57.2149 -DE/DX = 0.0 !

! D34 D(4,6,25,30) 122.5956 -DE/DX = 0.0 !

! D35 D(7,6,25,26) 123.3507 -DE/DX = 0.0 !

! D36 D(7,6,25,30) -56.8388 -DE/DX = 0.0 !

! D37 D(6,7,8,9) -177.1466 -DE/DX = 0.0 !

! D38 D(11,7,8,9) 2.3976 -DE/DX = 0.0 !

! D39 D(6,7,11,10) 177.9921 -DE/DX = 0.0 !

! D40 D(6,7,11,52) -3.5178 -DE/DX = 0.0 !

! D41 D(8,7,11,10) -1.5604 -DE/DX = 0.0 !

! D42 D(8,7,11,52) 176.9297 -DE/DX = 0.0 !

! D43 D(7,8,9,10) -2.3487 -DE/DX = 0.0 !

! D44 D(7,8,9,24) 177.3862 -DE/DX = 0.0 !

! D45 D(8,9,10,11) 1.4269 -DE/DX = 0.0 !

! D46 D(8,9,10,51) -176.9379 -DE/DX = 0.0 !

! D47 D(24,9,10,11) -178.3131 -DE/DX = 0.0 !

! D48 D(24,9,10,51) 3.3221 -DE/DX = 0.0 !

! D49 D(8,9,24,22) 7.715 -DE/DX = 0.0 !

! D50 D(8,9,24,37) -171.7042 -DE/DX = 0.0 !

! D51 D(10,9,24,22) -172.5848 -DE/DX = 0.0 !

! D52 D(10,9,24,37) 7.996 -DE/DX = 0.0 !

! D53 D(9,10,11,7) 0.0779 -DE/DX = 0.0 !

! D54 D(9,10,11,52) -178.3816 -DE/DX = 0.0 !

! D55 D(51,10,11,7) 178.4096 -DE/DX = 0.0 !

! D56 D(51,10,11,52) -0.0499 -DE/DX = 0.0 !

! D57 D(2,12,13,14) -172.585 -DE/DX = 0.0 !

! D58 D(2,12,13,17) 7.7143 -DE/DX = 0.0 !

! D59 D(34,12,13,14) 7.9931 -DE/DX = 0.0 !

! D60 D(34,12,13,17) -171.7076 -DE/DX = 0.0 !

! D61 D(2,12,34,33) 56.8642 -DE/DX = 0.0 !

! D62 D(2,12,34,35) -122.9397 -DE/DX = 0.0 !

! D63 D(13,12,34,33) -123.6616 -DE/DX = 0.0 !

! D64 D(13,12,34,35) 56.5345 -DE/DX = 0.0 !

! D65 D(12,13,14,15) -178.3134 -DE/DX = 0.0 !

! D66 D(12,13,14,53) 3.3215 -DE/DX = 0.0 !

! D67 D(17,13,14,15) 1.427 -DE/DX = 0.0 !

! D68 D(17,13,14,53) -176.9381 -DE/DX = 0.0 !

! D69 D(12,13,17,16) 177.3867 -DE/DX = 0.0 !

! D70 D(14,13,17,16) -2.3487 -DE/DX = 0.0 !

! D71 D(13,14,15,16) 0.0778 -DE/DX = 0.0 !

! D72 D(13,14,15,54) -178.3816 -DE/DX = 0.0 !

! D73 D(53,14,15,16) 178.4097 -DE/DX = 0.0 !

! D74 D(53,14,15,54) -0.0497 -DE/DX = 0.0 !

! D75 D(14,15,16,17) -1.5604 -DE/DX = 0.0 !

! D76 D(14,15,16,18) 177.9916 -DE/DX = 0.0 !

! D77 D(54,15,16,17) 176.9297 -DE/DX = 0.0 !

! D78 D(54,15,16,18) -3.5183 -DE/DX = 0.0 !

! D79 D(15,16,17,13) 2.3976 -DE/DX = 0.0 !

! D80 D(18,16,17,13) -177.1461 -DE/DX = 0.0 !

! D81 D(15,16,18,19) 173.3866 -DE/DX = 0.0 !

! D82 D(15,16,18,43) -7.2393 -DE/DX = 0.0 !

! D83 D(17,16,18,19) -7.1298 -DE/DX = 0.0 !

! D84 D(17,16,18,43) 172.2443 -DE/DX = 0.0 !

! D85 D(16,18,19,20) 168.4012 -DE/DX = 0.0 !

! D86 D(16,18,19,23) -13.5817 -DE/DX = 0.0 !

! D87 D(43,18,19,20) -10.989 -DE/DX = 0.0 !

! D88 D(43,18,19,23) 167.028 -DE/DX = 0.0 !

! D89 D(16,18,43,44) -56.8359 -DE/DX = 0.0 !

! D90 D(16,18,43,48) 123.3548 -DE/DX = 0.0 !

! D91 D(19,18,43,44) 122.5961 -DE/DX = 0.0 !

! D92 D(19,18,43,48) -57.2131 -DE/DX = 0.0 !

! D93 D(18,19,20,21) 177.4848 -DE/DX = 0.0 !

! D94 D(18,19,20,55) -2.9449 -DE/DX = 0.0 !

! D95 D(23,19,20,21) -0.8317 -DE/DX = 0.0 !

! D96 D(23,19,20,55) 178.7386 -DE/DX = 0.0 !

! D97 D(18,19,23,22) -176.9206 -DE/DX = 0.0 !

! D98 D(18,19,23,78) 5.4898 -DE/DX = 0.0 !

! D99 D(20,19,23,22) 1.4278 -DE/DX = 0.0 !

! D100 D(20,19,23,78) -176.1618 -DE/DX = 0.0 !

! D101 D(19,20,21,22) -0.0405 -DE/DX = 0.0 !

! D102 D(19,20,21,56) 179.6588 -DE/DX = 0.0 !

! D103 D(55,20,21,22) -179.6024 -DE/DX = 0.0 !

! D104 D(55,20,21,56) 0.0969 -DE/DX = 0.0 !

! D105 D(20,21,22,23) 0.897 -DE/DX = 0.0 !

! D106 D(20,21,22,24) -177.3104 -DE/DX = 0.0 !

! D107 D(56,21,22,23) -178.8079 -DE/DX = 0.0 !

! D108 D(56,21,22,24) 2.9847 -DE/DX = 0.0 !

! D109 D(21,22,23,19) -1.4526 -DE/DX = 0.0 !

! D110 D(21,22,23,78) 176.1412 -DE/DX = 0.0 !

! D111 D(24,22,23,19) 176.7938 -DE/DX = 0.0 !

! D112 D(24,22,23,78) -5.6124 -DE/DX = 0.0 !

! D113 D(21,22,24,9) -169.1894 -DE/DX = 0.0 !

! D114 D(21,22,24,37) 10.2439 -DE/DX = 0.0 !

! D115 D(23,22,24,9) 12.9194 -DE/DX = 0.0 !

! D116 D(23,22,24,37) -167.6474 -DE/DX = 0.0 !

! D117 D(9,24,37,38) 56.5312 -DE/DX = 0.0 !

! D118 D(9,24,37,42) -123.6659 -DE/DX = 0.0 !

! D119 D(22,24,37,38) -122.9406 -DE/DX = 0.0 !

! D120 D(22,24,37,42) 56.8623 -DE/DX = 0.0 !

! D121 D(6,25,26,27) -179.3548 -DE/DX = 0.0 !

! D122 D(6,25,26,57) -0.4721 -DE/DX = 0.0 !

! D123 D(30,25,26,27) 0.8309 -DE/DX = 0.0 !

! D124 D(30,25,26,57) 179.7137 -DE/DX = 0.0 !

! D125 D(6,25,30,29) -179.9281 -DE/DX = 0.0 !

! D126 D(6,25,30,61) -0.9818 -DE/DX = 0.0 !

! D127 D(26,25,30,29) -0.1142 -DE/DX = 0.0 !

! D128 D(26,25,30,61) 178.8321 -DE/DX = 0.0 !

! D129 D(25,26,27,28) -0.9272 -DE/DX = 0.0 !

! D130 D(25,26,27,58) 179.0356 -DE/DX = 0.0 !

! D131 D(57,26,27,28) -179.8051 -DE/DX = 0.0 !

! D132 D(57,26,27,58) 0.1577 -DE/DX = 0.0 !

! D133 D(26,27,28,29) 0.294 -DE/DX = 0.0 !

! D134 D(26,27,28,59) -179.5431 -DE/DX = 0.0 !

! D135 D(58,27,28,29) -179.6687 -DE/DX = 0.0 !

! D136 D(58,27,28,59) 0.4942 -DE/DX = 0.0 !

! D137 D(27,28,29,30) 0.4202 -DE/DX = 0.0 !

! D138 D(27,28,29,60) -179.4492 -DE/DX = 0.0 !

! D139 D(59,28,29,30) -179.7428 -DE/DX = 0.0 !

! D140 D(59,28,29,60) 0.3879 -DE/DX = 0.0 !

! D141 D(28,29,30,25) -0.5087 -DE/DX = 0.0 !

! D142 D(28,29,30,61) -179.4494 -DE/DX = 0.0 !

! D143 D(60,29,30,25) 179.3612 -DE/DX = 0.0 !

! D144 D(60,29,30,61) 0.4206 -DE/DX = 0.0 !

! D145 D(36,31,32,33) -0.3079 -DE/DX = 0.0 !

! D146 D(36,31,32,63) 179.6629 -DE/DX = 0.0 !

! D147 D(62,31,32,33) 179.6131 -DE/DX = 0.0 !

! D148 D(62,31,32,63) -0.4161 -DE/DX = 0.0 !

! D149 D(32,31,36,35) -0.3682 -DE/DX = 0.0 !

! D150 D(32,31,36,66) 179.4434 -DE/DX = 0.0 !

! D151 D(62,31,36,35) 179.7108 -DE/DX = 0.0 !

! D152 D(62,31,36,66) -0.4776 -DE/DX = 0.0 !

! D153 D(31,32,33,34) 0.9494 -DE/DX = 0.0 !

! D154 D(31,32,33,64) 179.7179 -DE/DX = 0.0 !

! D155 D(63,32,33,34) -179.0215 -DE/DX = 0.0 !

! D156 D(63,32,33,64) -0.253 -DE/DX = 0.0 !

! D157 D(32,33,34,12) 179.2945 -DE/DX = 0.0 !

! D158 D(32,33,34,35) -0.8979 -DE/DX = 0.0 !

! D159 D(64,33,34,12) 0.52 -DE/DX = 0.0 !

! D160 D(64,33,34,35) -179.6724 -DE/DX = 0.0 !

! D161 D(12,34,35,36) -179.9725 -DE/DX = 0.0 !

! D162 D(12,34,35,65) 1.0148 -DE/DX = 0.0 !

! D163 D(33,34,35,36) 0.2196 -DE/DX = 0.0 !

! D164 D(33,34,35,65) -178.7931 -DE/DX = 0.0 !

! D165 D(34,35,36,31) 0.4099 -DE/DX = 0.0 !

! D166 D(34,35,36,66) -179.4025 -DE/DX = 0.0 !

! D167 D(65,35,36,31) 179.417 -DE/DX = 0.0 !

! D168 D(65,35,36,66) -0.3954 -DE/DX = 0.0 !

! D169 D(24,37,38,39) -179.9736 -DE/DX = 0.0 !

! D170 D(24,37,38,67) 1.0142 -DE/DX = 0.0 !

! D171 D(42,37,38,39) 0.2195 -DE/DX = 0.0 !

! D172 D(42,37,38,67) -178.7926 -DE/DX = 0.0 !

! D173 D(24,37,42,41) 179.2955 -DE/DX = 0.0 !

! D174 D(24,37,42,71) 0.5209 -DE/DX = 0.0 !

! D175 D(38,37,42,41) -0.898 -DE/DX = 0.0 !

! D176 D(38,37,42,71) -179.6726 -DE/DX = 0.0 !

! D177 D(37,38,39,40) 0.41 -DE/DX = 0.0 !

! D178 D(37,38,39,68) -179.4023 -DE/DX = 0.0 !

! D179 D(67,38,39,40) 179.4166 -DE/DX = 0.0 !

! D180 D(67,38,39,68) -0.3958 -DE/DX = 0.0 !

! D181 D(38,39,40,41) -0.3683 -DE/DX = 0.0 !

! D182 D(38,39,40,69) 179.7109 -DE/DX = 0.0 !

! D183 D(68,39,40,41) 179.4432 -DE/DX = 0.0 !

! D184 D(68,39,40,69) -0.4776 -DE/DX = 0.0 !

! D185 D(39,40,41,42) -0.3079 -DE/DX = 0.0 !

! D186 D(39,40,41,70) 179.6629 -DE/DX = 0.0 !

! D187 D(69,40,41,42) 179.6129 -DE/DX = 0.0 !

! D188 D(69,40,41,70) -0.4162 -DE/DX = 0.0 !

! D189 D(40,41,42,37) 0.9495 -DE/DX = 0.0 !

! D190 D(40,41,42,71) 179.7181 -DE/DX = 0.0 !

! D191 D(70,41,42,37) -179.0215 -DE/DX = 0.0 !

! D192 D(70,41,42,71) -0.2529 -DE/DX = 0.0 !

! D193 D(18,43,44,45) -179.9269 -DE/DX = 0.0 !

! D194 D(18,43,44,72) -0.9812 -DE/DX = 0.0 !

! D195 D(48,43,44,45) -0.1142 -DE/DX = 0.0 !

! D196 D(48,43,44,72) 178.8316 -DE/DX = 0.0 !

! D197 D(18,43,48,47) -179.3559 -DE/DX = 0.0 !

! D198 D(18,43,48,76) -0.473 -DE/DX = 0.0 !

! D199 D(44,43,48,47) 0.831 -DE/DX = 0.0 !

! D200 D(44,43,48,76) 179.7139 -DE/DX = 0.0 !

! D201 D(43,44,45,46) -0.5088 -DE/DX = 0.0 !

! D202 D(43,44,45,73) 179.361 -DE/DX = 0.0 !

! D203 D(72,44,45,46) -179.4489 -DE/DX = 0.0 !

! D204 D(72,44,45,73) 0.4209 -DE/DX = 0.0 !

! D205 D(44,45,46,47) 0.4202 -DE/DX = 0.0 !

! D206 D(44,45,46,74) -179.7429 -DE/DX = 0.0 !

! D207 D(73,45,46,47) -179.449 -DE/DX = 0.0 !

! D208 D(73,45,46,74) 0.388 -DE/DX = 0.0 !

! D209 D(45,46,47,48) 0.294 -DE/DX = 0.0 !

! D210 D(45,46,47,75) -179.6688 -DE/DX = 0.0 !

! D211 D(74,46,47,48) -179.5429 -DE/DX = 0.0 !

! D212 D(74,46,47,75) 0.4942 -DE/DX = 0.0 !

! D213 D(46,47,48,43) -0.9274 -DE/DX = 0.0 !

! D214 D(46,47,48,76) -179.8054 -DE/DX = 0.0 !

! D215 D(75,47,48,43) 179.0356 -DE/DX = 0.0 !

! D216 D(75,47,48,76) 0.1576 -DE/DX = 0.0 !

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Largest change from initial coordinates is atom 74 0.099 Angstoms.

Leave Link 103 at Fri Aug 30 06:16:22 2019, MaxMem= 4294967296 cpu: 1.5

(Enter /home/kira/g09/l202.exe)

Stoichiometry C44H30N4(3)

Framework group C1[X(C44H30N4)]

Deg. of freedom 228

Full point group C1 NOp 1

RotChk: IX=2 Diff= 1.56D-13

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 0.976334 -4.113220 0.552153

2 6 0 1.321335 -2.796097 0.201646

3 7 0 0.145266 -2.109823 0.007401

4 6 0 -0.931069 -2.946574 0.188857

5 6 0 -0.418072 -4.206404 0.543637

6 6 0 -2.311861 -2.589978 0.006304

7 6 0 -2.798955 -1.286387 -0.120930

8 7 0 -2.062791 -0.138311 0.044855

9 6 0 -2.948307 0.899660 -0.107533

10 6 0 -4.278873 0.389877 -0.433969

11 6 0 -4.186339 -0.958637 -0.443344

12 6 0 2.642815 -2.257352 0.031317

13 6 0 2.948308 -0.899669 -0.107495

14 6 0 4.278875 -0.389896 -0.433940

15 6 0 4.186341 0.958618 -0.443360

16 6 0 2.798956 1.286378 -0.120966

17 7 0 2.062790 0.138307 0.044853

18 6 0 2.311863 2.589974 0.006231

19 6 0 0.931069 2.946570 0.188769

20 6 0 0.418076 4.206364 0.543678

21 6 0 -0.976331 4.113179 0.552195

22 6 0 -1.321334 2.796091 0.201558

23 7 0 -0.145267 2.109841 0.007228

24 6 0 -2.642816 2.257347 0.031243

25 6 0 -3.273369 -3.719580 -0.033039

26 6 0 -3.126806 -4.749141 -0.974768

27 6 0 -4.035311 -5.801474 -1.021023

28 6 0 -5.094878 -5.853926 -0.115067

29 6 0 -5.242966 -4.843334 0.833471

30 6 0 -4.343082 -3.781666 0.871495

31 6 0 5.856008 -5.101008 -0.011405

32 6 0 4.809158 -5.213202 -0.926700

33 6 0 3.760910 -4.298815 -0.906689

34 6 0 3.751477 -3.243243 0.017593

35 6 0 4.809428 -3.139934 0.932312

36 6 0 5.850502 -4.063971 0.920091

37 6 0 -3.751475 3.243240 0.017554

38 6 0 -4.809417 3.139906 0.932280

39 6 0 -5.850479 4.063956 0.920110

40 6 0 -5.855984 5.101031 -0.011343

41 6 0 -4.809143 5.213251 -0.926645

42 6 0 -3.760905 4.298850 -0.906684

43 6 0 3.273369 3.719577 -0.033078

44 6 0 4.343074 3.781645 0.871467

45 6 0 5.242942 4.843327 0.833491

46 6 0 5.094847 5.853953 -0.115010

47 6 0 4.035289 5.801519 -1.020977

48 6 0 3.126798 4.749172 -0.974768

49 1 0 1.675196 -4.899338 0.788030

50 1 0 -1.009239 -5.078187 0.772998

51 1 0 -5.149669 0.988862 -0.651636

52 1 0 -4.967476 -1.667887 -0.669364

53 1 0 5.149674 -0.988887 -0.651580

54 1 0 4.967479 1.667862 -0.669399

55 1 0 1.009246 5.078118 0.773139

56 1 0 -1.675195 4.899266 0.788171

57 1 0 -2.307012 -4.711343 -1.683009

58 1 0 -3.916591 -6.581530 -1.765628

59 1 0 -5.798674 -6.678870 -0.147092

60 1 0 -6.059029 -4.881290 1.547322

61 1 0 -4.456473 -3.002303 1.616458

62 1 0 6.669812 -5.818265 -0.023782

63 1 0 4.809137 -6.014371 -1.658244

64 1 0 2.952013 -4.387389 -1.622868

65 1 0 4.803753 -2.340363 1.664300

66 1 0 6.656176 -3.974880 1.641169

67 1 0 -4.803741 2.340308 1.664241

68 1 0 -6.656145 3.974846 1.641195

69 1 0 -6.669779 5.818299 -0.023680

70 1 0 -4.809121 6.014450 -1.658156

71 1 0 -2.952013 4.387447 -1.622866

72 1 0 4.456466 3.002260 1.616407

73 1 0 6.058997 4.881270 1.547353

74 1 0 5.798630 6.678909 -0.146996

75 1 0 3.916563 6.581602 -1.765552

76 1 0 2.307008 4.711391 -1.683016

77 1 0 0.081761 -1.122587 -0.200093

78 1 0 -0.081762 1.122650 -0.200477

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Rotational constants (GHZ): 0.0587918 0.0582559 0.0300944

Leave Link 202 at Fri Aug 30 06:16:22 2019, MaxMem= 4294967296 cpu: 1.0

(Enter /home/kira/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 1 IROHF=0.

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Population analysis using the SCF density.

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Orbital symmetries:

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The electronic state is 3-A.

Alpha occ. eigenvalues -- -14.35883 -14.35883 -14.29973 -14.29973 -10.21772

Alpha occ. eigenvalues -- -10.21771 -10.21768 -10.21768 -10.20977 -10.20977

Alpha occ. eigenvalues -- -10.20962 -10.20962 -10.20752 -10.20752 -10.20739

Alpha occ. eigenvalues -- -10.20739 -10.19059 -10.19059 -10.19056 -10.19056

Alpha occ. eigenvalues -- -10.17703 -10.17703 -10.17694 -10.17693 -10.17687

Alpha occ. eigenvalues -- -10.17687 -10.17683 -10.17683 -10.17559 -10.17559

Alpha occ. eigenvalues -- -10.17554 -10.17554 -10.17434 -10.17434 -10.17430

Alpha occ. eigenvalues -- -10.17430 -10.17422 -10.17422 -10.17416 -10.17416

Alpha occ. eigenvalues -- -10.16860 -10.16860 -10.16827 -10.16827 -10.16808

Alpha occ. eigenvalues -- -10.16808 -10.16755 -10.16755 -0.99434 -0.99268

Alpha occ. eigenvalues -- -0.95347 -0.95053 -0.87499 -0.87084 -0.86996

Alpha occ. eigenvalues -- -0.86822 -0.83127 -0.81612 -0.81545 -0.80196

Alpha occ. eigenvalues -- -0.79056 -0.78436 -0.76905 -0.76507 -0.75321

Alpha occ. eigenvalues -- -0.75195 -0.75160 -0.75133 -0.74654 -0.74140

Alpha occ. eigenvalues -- -0.73831 -0.72703 -0.71586 -0.67787 -0.66312

Alpha occ. eigenvalues -- -0.62843 -0.61549 -0.61322 -0.61149 -0.60948

Alpha occ. eigenvalues -- -0.60439 -0.60329 -0.60240 -0.60092 -0.59795

Alpha occ. eigenvalues -- -0.59452 -0.57940 -0.57488 -0.56372 -0.55691

Alpha occ. eigenvalues -- -0.55098 -0.53228 -0.52484 -0.52466 -0.51418

Alpha occ. eigenvalues -- -0.51310 -0.50394 -0.50128 -0.49382 -0.46815

Alpha occ. eigenvalues -- -0.46762 -0.46397 -0.46204 -0.46106 -0.45558

Alpha occ. eigenvalues -- -0.45545 -0.45362 -0.44751 -0.44659 -0.44070

Alpha occ. eigenvalues -- -0.43713 -0.43227 -0.42868 -0.42834 -0.42553

Alpha occ. eigenvalues -- -0.42461 -0.42361 -0.42319 -0.42258 -0.42176

Alpha occ. eigenvalues -- -0.41729 -0.41127 -0.40757 -0.40082 -0.39920

Alpha occ. eigenvalues -- -0.39871 -0.38587 -0.38546 -0.38511 -0.37746

Alpha occ. eigenvalues -- -0.37223 -0.37136 -0.36653 -0.36480 -0.35603

Alpha occ. eigenvalues -- -0.35247 -0.35026 -0.35021 -0.34864 -0.34853

Alpha occ. eigenvalues -- -0.34850 -0.34560 -0.33060 -0.30087 -0.29962

Alpha occ. eigenvalues -- -0.28649 -0.28488 -0.27259 -0.26936 -0.26822

Alpha occ. eigenvalues -- -0.26289 -0.26246 -0.26235 -0.25974 -0.25638

Alpha occ. eigenvalues -- -0.25608 -0.25406 -0.25330 -0.25290 -0.21400

Alpha occ. eigenvalues -- -0.20981 -0.14386

Alpha virt. eigenvalues -- -0.09522 -0.05522 -0.01757 -0.01724 -0.01595

Alpha virt. eigenvalues -- -0.01370 -0.01246 -0.01216 -0.01192 -0.01185

Alpha virt. eigenvalues -- 0.02098 0.04760 0.05058 0.05262 0.05586

Alpha virt. eigenvalues -- 0.05637 0.05893 0.06875 0.07324 0.08148

Alpha virt. eigenvalues -- 0.08273 0.08366 0.09219 0.09370 0.09547

Alpha virt. eigenvalues -- 0.09762 0.09791 0.10020 0.10309 0.10467

Alpha virt. eigenvalues -- 0.10482 0.10519 0.10546 0.11070 0.11667

Alpha virt. eigenvalues -- 0.12559 0.12563 0.12750 0.12883 0.13092

Alpha virt. eigenvalues -- 0.13184 0.13193 0.13664 0.14147 0.14209

Alpha virt. eigenvalues -- 0.14272 0.14322 0.15046 0.15576 0.15638

Alpha virt. eigenvalues -- 0.16320 0.16577 0.17798 0.18128 0.20897

Alpha virt. eigenvalues -- 0.21579 0.21672 0.21935 0.23321 0.23382

Alpha virt. eigenvalues -- 0.23792 0.24011 0.24499 0.25292 0.25329

Alpha virt. eigenvalues -- 0.25547 0.26094 0.26242 0.26893 0.27454

Alpha virt. eigenvalues -- 0.27713 0.27770 0.27870 0.27878 0.28062

Alpha virt. eigenvalues -- 0.28711 0.28748 0.29441 0.29484 0.29491

Alpha virt. eigenvalues -- 0.29542 0.29752 0.30436 0.30661 0.31053

Alpha virt. eigenvalues -- 0.31126 0.31234 0.32070 0.32948 0.33688

Alpha virt. eigenvalues -- 0.34043 0.34637 0.34996 0.35209 0.35279

Alpha virt. eigenvalues -- 0.35703 0.35803 0.35868 0.36533 0.36549

Alpha virt. eigenvalues -- 0.36790 0.36925 0.37334 0.37657 0.37791

Alpha virt. eigenvalues -- 0.37955 0.38168 0.38562 0.38985 0.39111

Alpha virt. eigenvalues -- 0.39523 0.39932 0.40200 0.40300 0.40466

Alpha virt. eigenvalues -- 0.40656 0.40673 0.40775 0.40911 0.41070

Alpha virt. eigenvalues -- 0.41562 0.41580 0.41670 0.41892 0.41894

Alpha virt. eigenvalues -- 0.42482 0.42637 0.42731 0.42755 0.43169

Alpha virt. eigenvalues -- 0.43332 0.43435 0.43557 0.44077 0.44224

Alpha virt. eigenvalues -- 0.44548 0.44567 0.44642 0.45052 0.45305

Alpha virt. eigenvalues -- 0.45370 0.45426 0.45508 0.45633 0.45994

Alpha virt. eigenvalues -- 0.46921 0.47067 0.47076 0.47119 0.47174

Alpha virt. eigenvalues -- 0.47747 0.47814 0.48803 0.48807 0.49056

Alpha virt. eigenvalues -- 0.49276 0.50004 0.50259 0.50489 0.50639

Alpha virt. eigenvalues -- 0.51436 0.51688 0.52388 0.52716 0.52906

Alpha virt. eigenvalues -- 0.53193 0.53710 0.53884 0.54212 0.54280

Alpha virt. eigenvalues -- 0.54943 0.55321 0.55735 0.57313 0.57340

Alpha virt. eigenvalues -- 0.57515 0.57548 0.57696 0.57985 0.58005

Alpha virt. eigenvalues -- 0.59179 0.59477 0.59514 0.59815 0.59975

Alpha virt. eigenvalues -- 0.60049 0.60055 0.60199 0.60644 0.60686

Alpha virt. eigenvalues -- 0.60803 0.60943 0.61091 0.61368 0.61497

Alpha virt. eigenvalues -- 0.61512 0.61690 0.62010 0.62193 0.62453

Alpha virt. eigenvalues -- 0.62635 0.62924 0.63805 0.63918 0.64407

Alpha virt. eigenvalues -- 0.64625 0.64663 0.64827 0.65013 0.65065

Alpha virt. eigenvalues -- 0.65271 0.65448 0.65902 0.66020 0.66119

Alpha virt. eigenvalues -- 0.67129 0.67609 0.67967 0.68602 0.68887

Alpha virt. eigenvalues -- 0.68945 0.69604 0.69819 0.70052 0.70770

Alpha virt. eigenvalues -- 0.71746 0.71852 0.71909 0.72322 0.72751

Alpha virt. eigenvalues -- 0.72926 0.73422 0.73744 0.73948 0.74212

Alpha virt. eigenvalues -- 0.74227 0.75023 0.75146 0.75427 0.75929

Alpha virt. eigenvalues -- 0.76079 0.76410 0.76499 0.76938 0.77526

Alpha virt. eigenvalues -- 0.77656 0.77714 0.78336 0.78681 0.78739

Alpha virt. eigenvalues -- 0.78856 0.79353 0.80106 0.80126 0.80168

Alpha virt. eigenvalues -- 0.80505 0.80824 0.81397 0.81640 0.82531

Alpha virt. eigenvalues -- 0.82759 0.82866 0.83073 0.84355 0.84898

Alpha virt. eigenvalues -- 0.85006 0.85823 0.86732 0.86735 0.87003

Alpha virt. eigenvalues -- 0.88164 0.88300 0.88500 0.88549 0.89061

Alpha virt. eigenvalues -- 0.89279 0.90442 0.91177 0.91858 0.91917

Alpha virt. eigenvalues -- 0.92349 0.92699 0.93216 0.93628 0.93981

Alpha virt. eigenvalues -- 0.94897 0.95508 0.95530 0.95705 0.96597

Alpha virt. eigenvalues -- 0.96693 0.97185 0.98642 0.99053 0.99790

Alpha virt. eigenvalues -- 1.00313 1.01271 1.01322 1.01394 1.01658

Alpha virt. eigenvalues -- 1.02510 1.02813 1.02960 1.03112 1.04253

Alpha virt. eigenvalues -- 1.04911 1.05903 1.07151 1.07945 1.08535

Alpha virt. eigenvalues -- 1.08613 1.08799 1.08867 1.09911 1.10692

Alpha virt. eigenvalues -- 1.11995 1.12936 1.13080 1.13405 1.13532

Alpha virt. eigenvalues -- 1.14016 1.14521 1.14979 1.15138 1.15836

Alpha virt. eigenvalues -- 1.15977 1.16305 1.16526 1.17804 1.18692

Alpha virt. eigenvalues -- 1.18866 1.18976 1.19825 1.19957 1.20393

Alpha virt. eigenvalues -- 1.20455 1.20474 1.20535 1.20979 1.21222

Alpha virt. eigenvalues -- 1.21791 1.22926 1.23154 1.23537 1.24009

Alpha virt. eigenvalues -- 1.24394 1.24484 1.25116 1.25498 1.25589

Alpha virt. eigenvalues -- 1.25642 1.26284 1.26741 1.27489 1.27615

Alpha virt. eigenvalues -- 1.28640 1.29403 1.29569 1.31014 1.31972

Alpha virt. eigenvalues -- 1.32043 1.32101 1.32866 1.34128 1.35391

Alpha virt. eigenvalues -- 1.36521 1.37922 1.39407 1.39647 1.40529

Alpha virt. eigenvalues -- 1.40864 1.41446 1.41918 1.42149 1.43270

Alpha virt. eigenvalues -- 1.44706 1.44713 1.45270 1.45653 1.46681

Alpha virt. eigenvalues -- 1.47236 1.47255 1.47268 1.47595 1.47715

Alpha virt. eigenvalues -- 1.48240 1.48550 1.48829 1.49357 1.49360

Alpha virt. eigenvalues -- 1.51507 1.52660 1.52810 1.53016 1.53169

Alpha virt. eigenvalues -- 1.53516 1.53716 1.53772 1.55120 1.56714

Alpha virt. eigenvalues -- 1.57565 1.58661 1.61009 1.61137 1.61520

Alpha virt. eigenvalues -- 1.62132 1.62524 1.62815 1.64557 1.64757

Alpha virt. eigenvalues -- 1.67013 1.67106 1.67221 1.67882 1.68339

Alpha virt. eigenvalues -- 1.68743 1.69145 1.69691 1.70351 1.70718

Alpha virt. eigenvalues -- 1.71723 1.73276 1.73325 1.74016 1.74142

Alpha virt. eigenvalues -- 1.74997 1.75057 1.75132 1.75414 1.75992

Alpha virt. eigenvalues -- 1.76644 1.77359 1.78500 1.78520 1.78997

Alpha virt. eigenvalues -- 1.79589 1.79815 1.80428 1.80481 1.80965

Alpha virt. eigenvalues -- 1.81161 1.81506 1.81894 1.82484 1.82821

Alpha virt. eigenvalues -- 1.83376 1.83993 1.84162 1.85096 1.85121

Alpha virt. eigenvalues -- 1.85175 1.86739 1.87503 1.87633 1.87956

Alpha virt. eigenvalues -- 1.88148 1.88869 1.89375 1.89668 1.90411

Alpha virt. eigenvalues -- 1.91403 1.91483 1.91799 1.91891 1.92098

Alpha virt. eigenvalues -- 1.92309 1.92321 1.92693 1.92949 1.93176

Alpha virt. eigenvalues -- 1.93288 1.93469 1.94014 1.94115 1.94394

Alpha virt. eigenvalues -- 1.94470 1.95674 1.95722 1.95723 1.95836

Alpha virt. eigenvalues -- 1.96222 1.96856 1.96871 1.97341 1.99073

Alpha virt. eigenvalues -- 1.99174 2.00122 2.00957 2.01021 2.01882

Alpha virt. eigenvalues -- 2.05228 2.06298 2.06698 2.08082 2.08143

Alpha virt. eigenvalues -- 2.08819 2.09771 2.10378 2.12937 2.13336

Alpha virt. eigenvalues -- 2.14037 2.16704 2.18226 2.21498 2.23455

Alpha virt. eigenvalues -- 2.23533 2.23700 2.24302 2.24440 2.25120

Alpha virt. eigenvalues -- 2.25387 2.25498 2.26082 2.26210 2.26789

Alpha virt. eigenvalues -- 2.27166 2.27196 2.27486 2.27487 2.27634

Alpha virt. eigenvalues -- 2.27834 2.28083 2.29092 2.29355 2.29466

Alpha virt. eigenvalues -- 2.29999 2.30373 2.30854 2.31821 2.31874

Alpha virt. eigenvalues -- 2.32306 2.32854 2.32897 2.34485 2.34639

Alpha virt. eigenvalues -- 2.34665 2.35427 2.35592 2.36176 2.36287

Alpha virt. eigenvalues -- 2.37633 2.37868 2.37974 2.39384 2.39471

Alpha virt. eigenvalues -- 2.39695 2.40776 2.42542 2.43092 2.44169

Alpha virt. eigenvalues -- 2.44522 2.46810 2.47864 2.47988 2.50542

Alpha virt. eigenvalues -- 2.51008 2.51593 2.52193 2.52434 2.54057

Alpha virt. eigenvalues -- 2.54974 2.56737 2.57194 2.57658 2.57686

Alpha virt. eigenvalues -- 2.58471 2.59156 2.59200 2.59933 2.60271

Alpha virt. eigenvalues -- 2.61314 2.61384 2.62048 2.63295 2.64536

Alpha virt. eigenvalues -- 2.65516 2.65568 2.65923 2.67396 2.67522

Alpha virt. eigenvalues -- 2.69824 2.69931 2.70073 2.70342 2.70411

Alpha virt. eigenvalues -- 2.72186 2.72288 2.72361 2.73834 2.73845

Alpha virt. eigenvalues -- 2.74672 2.75002 2.76500 2.76705 2.77014

Alpha virt. eigenvalues -- 2.77888 2.78283 2.78452 2.78565 2.79580

Alpha virt. eigenvalues -- 2.82104 2.83174 2.83208 2.83348 2.83575

Alpha virt. eigenvalues -- 2.85126 2.85498 2.85862 2.86856 2.88105

Alpha virt. eigenvalues -- 2.89188 2.89851 2.90144 2.91987 2.93768

Alpha virt. eigenvalues -- 2.94929 2.95195 2.97044 2.97621 2.98437

Alpha virt. eigenvalues -- 2.98643 2.98953 3.00893 3.01501 3.02861

Alpha virt. eigenvalues -- 3.02879 3.04053 3.04701 3.05229 3.06963

Alpha virt. eigenvalues -- 3.06996 3.07357 3.07613 3.08178 3.09789

Alpha virt. eigenvalues -- 3.10713 3.11927 3.12252 3.14237 3.14989

Alpha virt. eigenvalues -- 3.15153 3.15365 3.16830 3.18815 3.18898

Alpha virt. eigenvalues -- 3.19470 3.21515 3.21872 3.23181 3.25158

Alpha virt. eigenvalues -- 3.25754 3.25946 3.26059 3.26447 3.28579

Alpha virt. eigenvalues -- 3.28963 3.29197 3.29219 3.29903 3.30228

Alpha virt. eigenvalues -- 3.30304 3.30560 3.30594 3.31122 3.31233

Alpha virt. eigenvalues -- 3.31536 3.31621 3.31652 3.32628 3.33206

Alpha virt. eigenvalues -- 3.33276 3.34077 3.35583 3.35675 3.36291

Alpha virt. eigenvalues -- 3.37309 3.38278 3.39402 3.40240 3.41312

Alpha virt. eigenvalues -- 3.42784 3.43140 3.44923 3.45005 3.48754

Alpha virt. eigenvalues -- 3.50731 3.50934 3.51427 3.56956 3.57834

Alpha virt. eigenvalues -- 3.58250 3.58457 3.58968 3.59651 3.60080

Alpha virt. eigenvalues -- 3.60769 3.61303 3.64259 3.65338 3.66599

Alpha virt. eigenvalues -- 3.71336 3.71377 3.72239 3.74377 3.76285

Alpha virt. eigenvalues -- 3.78638 3.79753 3.80197 3.83465 3.84408

Alpha virt. eigenvalues -- 3.85990 3.88651 3.91604 3.92527 3.93365

Alpha virt. eigenvalues -- 3.94011 3.95306 3.95514 3.96171 3.96477

Alpha virt. eigenvalues -- 3.98126 3.99148 4.02163 4.10366 4.28320

Alpha virt. eigenvalues -- 4.29474 4.35794 4.38914 4.47080 4.50893

Alpha virt. eigenvalues -- 4.54540 4.54670 4.62630 4.63256 4.66359

Alpha virt. eigenvalues -- 4.67293 4.78462 4.78473 4.78486 4.78500

Alpha virt. eigenvalues -- 5.08836 5.14668 5.16668 5.26452 23.24557

Alpha virt. eigenvalues -- 23.28038 23.28309 23.29981 23.45664 23.51372

Alpha virt. eigenvalues -- 23.53932 23.58410 23.73563 23.74318 23.78356

Alpha virt. eigenvalues -- 23.79139 23.80484 23.80596 23.80670 23.80882

Alpha virt. eigenvalues -- 23.85264 23.85870 23.86099 23.86674 23.87411

Alpha virt. eigenvalues -- 23.87636 23.98274 23.98436 23.98900 23.99454

Alpha virt. eigenvalues -- 24.00144 24.00300 24.04793 24.04892 24.04983

Alpha virt. eigenvalues -- 24.05055 24.07122 24.07459 24.07700 24.08062

Alpha virt. eigenvalues -- 24.10252 24.10351 24.15203 24.15203 24.15255

Alpha virt. eigenvalues -- 24.15265 24.16960 24.17131 35.55536 35.56356

Alpha virt. eigenvalues -- 35.62061 35.62624

Beta occ. eigenvalues -- -14.35808 -14.35808 -14.29439 -14.29439 -10.21744

Beta occ. eigenvalues -- -10.21744 -10.21742 -10.21742 -10.20913 -10.20913

Beta occ. eigenvalues -- -10.20897 -10.20897 -10.20458 -10.20458 -10.20436

Beta occ. eigenvalues -- -10.20436 -10.19108 -10.19108 -10.19104 -10.19104

Beta occ. eigenvalues -- -10.17646 -10.17646 -10.17638 -10.17638 -10.17630

Beta occ. eigenvalues -- -10.17630 -10.17625 -10.17625 -10.17522 -10.17522

Beta occ. eigenvalues -- -10.17518 -10.17518 -10.17450 -10.17450 -10.17445

Beta occ. eigenvalues -- -10.17445 -10.17430 -10.17430 -10.17425 -10.17425

Beta occ. eigenvalues -- -10.16846 -10.16846 -10.16773 -10.16773 -10.16746

Beta occ. eigenvalues -- -10.16746 -10.16694 -10.16694 -0.99190 -0.99039

Beta occ. eigenvalues -- -0.94823 -0.94554 -0.87220 -0.86894 -0.86802

Beta occ. eigenvalues -- -0.86668 -0.82635 -0.81024 -0.81012 -0.79735

Beta occ. eigenvalues -- -0.78757 -0.78018 -0.76668 -0.76267 -0.75247

Beta occ. eigenvalues -- -0.75129 -0.75091 -0.75062 -0.74535 -0.73947

Beta occ. eigenvalues -- -0.73722 -0.72615 -0.71019 -0.67193 -0.66106

Beta occ. eigenvalues -- -0.62645 -0.61435 -0.61227 -0.61069 -0.60859

Beta occ. eigenvalues -- -0.60275 -0.60202 -0.60129 -0.59869 -0.59667

Beta occ. eigenvalues -- -0.59339 -0.57739 -0.57325 -0.56198 -0.55648

Beta occ. eigenvalues -- -0.54978 -0.53060 -0.52399 -0.52367 -0.51322

Beta occ. eigenvalues -- -0.51201 -0.50264 -0.49940 -0.49130 -0.46700

Beta occ. eigenvalues -- -0.46580 -0.46003 -0.45930 -0.45925 -0.45376

Beta occ. eigenvalues -- -0.45358 -0.45250 -0.44657 -0.44386 -0.43992

Beta occ. eigenvalues -- -0.43210 -0.42785 -0.42716 -0.42716 -0.42469

Beta occ. eigenvalues -- -0.42430 -0.42189 -0.42172 -0.42134 -0.42044

Beta occ. eigenvalues -- -0.41597 -0.40722 -0.40297 -0.39793 -0.39754

Beta occ. eigenvalues -- -0.39426 -0.38524 -0.38414 -0.38327 -0.37624

Beta occ. eigenvalues -- -0.37074 -0.37016 -0.36551 -0.36257 -0.35490

Beta occ. eigenvalues -- -0.35124 -0.34901 -0.34802 -0.34780 -0.34771

Beta occ. eigenvalues -- -0.34731 -0.34415 -0.31480 -0.28603 -0.28510

Beta occ. eigenvalues -- -0.28111 -0.27940 -0.26724 -0.26340 -0.26268

Beta occ. eigenvalues -- -0.26118 -0.26066 -0.25654 -0.25608 -0.25405

Beta occ. eigenvalues -- -0.25254 -0.24934 -0.24469 -0.23896 -0.21104

Beta virt. eigenvalues -- -0.14675 -0.08689 -0.08343 -0.03716 -0.01583

Beta virt. eigenvalues -- -0.01570 -0.01412 -0.01265 -0.01095 -0.01065

Beta virt. eigenvalues -- -0.00951 -0.00828 0.03129 0.04996 0.05311

Beta virt. eigenvalues -- 0.05619 0.05659 0.05913 0.06035 0.07165

Beta virt. eigenvalues -- 0.07423 0.08165 0.08298 0.08381 0.09252

Beta virt. eigenvalues -- 0.09395 0.09561 0.09826 0.10048 0.10363

Beta virt. eigenvalues -- 0.10443 0.10504 0.10572 0.10708 0.11114

Beta virt. eigenvalues -- 0.11990 0.12255 0.12618 0.12781 0.12807

Beta virt. eigenvalues -- 0.12887 0.13166 0.13188 0.13275 0.13680

Beta virt. eigenvalues -- 0.14169 0.14238 0.14326 0.14351 0.15676

Beta virt. eigenvalues -- 0.16069 0.16172 0.16688 0.16752 0.17888

Beta virt. eigenvalues -- 0.18307 0.21100 0.21693 0.21963 0.22197

Beta virt. eigenvalues -- 0.23570 0.23787 0.23924 0.24116 0.24803

Beta virt. eigenvalues -- 0.25372 0.25413 0.25613 0.26140 0.26264

Beta virt. eigenvalues -- 0.26958 0.27658 0.27790 0.27854 0.27891

Beta virt. eigenvalues -- 0.27898 0.28082 0.28827 0.28843 0.29511

Beta virt. eigenvalues -- 0.29537 0.29551 0.29715 0.29845 0.30521

Beta virt. eigenvalues -- 0.30728 0.31114 0.31241 0.31429 0.32165

Beta virt. eigenvalues -- 0.32991 0.33858 0.34303 0.35001 0.35103

Beta virt. eigenvalues -- 0.35383 0.35445 0.35987 0.36114 0.36331

Beta virt. eigenvalues -- 0.36857 0.37019 0.37120 0.37148 0.37399

Beta virt. eigenvalues -- 0.37874 0.37934 0.38283 0.38390 0.38686

Beta virt. eigenvalues -- 0.39236 0.39336 0.39663 0.40064 0.40330

Beta virt. eigenvalues -- 0.40419 0.40525 0.40738 0.40825 0.40986

Beta virt. eigenvalues -- 0.41048 0.41186 0.41638 0.41733 0.41808

Beta virt. eigenvalues -- 0.41979 0.42004 0.42668 0.42738 0.42819

Beta virt. eigenvalues -- 0.42850 0.43260 0.43449 0.43550 0.43636

Beta virt. eigenvalues -- 0.44220 0.44376 0.44680 0.44686 0.44779

Beta virt. eigenvalues -- 0.45234 0.45384 0.45485 0.45508 0.45632

Beta virt. eigenvalues -- 0.45728 0.46239 0.47046 0.47210 0.47253

Beta virt. eigenvalues -- 0.47291 0.47415 0.47841 0.48043 0.48881

Beta virt. eigenvalues -- 0.48936 0.49134 0.49586 0.50094 0.50450

Beta virt. eigenvalues -- 0.50513 0.50789 0.51405 0.51870 0.52543

Beta virt. eigenvalues -- 0.52909 0.53201 0.53364 0.53865 0.53991

Beta virt. eigenvalues -- 0.54373 0.54395 0.55121 0.55439 0.55853

Beta virt. eigenvalues -- 0.57421 0.57542 0.57656 0.57695 0.57793

Beta virt. eigenvalues -- 0.58149 0.58282 0.59316 0.59538 0.59592

Beta virt. eigenvalues -- 0.59932 0.60017 0.60107 0.60215 0.60569

Beta virt. eigenvalues -- 0.60729 0.60762 0.60863 0.61043 0.61116

Beta virt. eigenvalues -- 0.61396 0.61568 0.61594 0.61916 0.62185

Beta virt. eigenvalues -- 0.62329 0.62639 0.62962 0.63271 0.63871

Beta virt. eigenvalues -- 0.64057 0.64478 0.64676 0.64757 0.64854

Beta virt. eigenvalues -- 0.65068 0.65277 0.65375 0.65517 0.66015

Beta virt. eigenvalues -- 0.66092 0.66213 0.67222 0.67980 0.67992

Beta virt. eigenvalues -- 0.68741 0.69103 0.69132 0.69829 0.69875

Beta virt. eigenvalues -- 0.70258 0.70924 0.71949 0.72000 0.72079

Beta virt. eigenvalues -- 0.72438 0.73072 0.73113 0.73725 0.73795

Beta virt. eigenvalues -- 0.74065 0.74307 0.74352 0.75174 0.75284

Beta virt. eigenvalues -- 0.75493 0.75973 0.76336 0.76454 0.76593

Beta virt. eigenvalues -- 0.77018 0.77744 0.78096 0.78267 0.78585

Beta virt. eigenvalues -- 0.78788 0.78809 0.78929 0.79474 0.80205

Beta virt. eigenvalues -- 0.80217 0.80250 0.80824 0.81014 0.81670

Beta virt. eigenvalues -- 0.81786 0.82602 0.82995 0.83139 0.83176

Beta virt. eigenvalues -- 0.84451 0.85035 0.85342 0.85865 0.86840

Beta virt. eigenvalues -- 0.86921 0.87118 0.88432 0.88450 0.88583

Beta virt. eigenvalues -- 0.88705 0.89096 0.89461 0.90599 0.91339

Beta virt. eigenvalues -- 0.91967 0.92085 0.92466 0.92924 0.93378

Beta virt. eigenvalues -- 0.93856 0.94188 0.95079 0.95600 0.95664

Beta virt. eigenvalues -- 0.95876 0.96713 0.96934 0.97267 0.98693

Beta virt. eigenvalues -- 0.99328 1.00021 1.00452 1.01337 1.01496

Beta virt. eigenvalues -- 1.01524 1.01850 1.02762 1.02971 1.03071

Beta virt. eigenvalues -- 1.03271 1.04342 1.05083 1.06049 1.07291

Beta virt. eigenvalues -- 1.08273 1.08781 1.08914 1.08933 1.09139

Beta virt. eigenvalues -- 1.10129 1.10916 1.12110 1.13060 1.13418

Beta virt. eigenvalues -- 1.13528 1.13805 1.14136 1.14662 1.15187

Beta virt. eigenvalues -- 1.15403 1.16019 1.16206 1.16391 1.16935

Beta virt. eigenvalues -- 1.17849 1.18793 1.18926 1.19012 1.19951

Beta virt. eigenvalues -- 1.20078 1.20554 1.20561 1.20584 1.20629

Beta virt. eigenvalues -- 1.21330 1.21434 1.21928 1.23045 1.23290

Beta virt. eigenvalues -- 1.23678 1.24110 1.24583 1.24660 1.25275

Beta virt. eigenvalues -- 1.25711 1.25728 1.25843 1.26491 1.26885

Beta virt. eigenvalues -- 1.27566 1.27797 1.28806 1.29772 1.29830

Beta virt. eigenvalues -- 1.31444 1.32122 1.32371 1.32435 1.32999

Beta virt. eigenvalues -- 1.34287 1.35477 1.36666 1.38112 1.39888

Beta virt. eigenvalues -- 1.39997 1.40836 1.41296 1.41506 1.41963

Beta virt. eigenvalues -- 1.42220 1.43560 1.44892 1.45009 1.45537

Beta virt. eigenvalues -- 1.46045 1.46871 1.47429 1.47451 1.47468

Beta virt. eigenvalues -- 1.47696 1.47879 1.48372 1.48743 1.48927

Beta virt. eigenvalues -- 1.49512 1.49514 1.51636 1.52797 1.52950

Beta virt. eigenvalues -- 1.53099 1.53313 1.53633 1.53892 1.54340

Beta virt. eigenvalues -- 1.55294 1.57216 1.58082 1.58750 1.61132

Beta virt. eigenvalues -- 1.61504 1.61612 1.62314 1.62829 1.62965

Beta virt. eigenvalues -- 1.64685 1.64971 1.67397 1.67425 1.67569

Beta virt. eigenvalues -- 1.68122 1.68447 1.69015 1.69258 1.70007

Beta virt. eigenvalues -- 1.70661 1.70918 1.71795 1.73760 1.73801

Beta virt. eigenvalues -- 1.74091 1.74499 1.75173 1.75228 1.75340

Beta virt. eigenvalues -- 1.75559 1.76074 1.76996 1.77648 1.78595

Beta virt. eigenvalues -- 1.78605 1.79426 1.79678 1.80006 1.80423

Beta virt. eigenvalues -- 1.80578 1.81142 1.81161 1.81663 1.81991

Beta virt. eigenvalues -- 1.82544 1.82981 1.83574 1.84066 1.84343

Beta virt. eigenvalues -- 1.85233 1.85256 1.85277 1.87026 1.87709

Beta virt. eigenvalues -- 1.87974 1.88210 1.88400 1.89168 1.89611

Beta virt. eigenvalues -- 1.89764 1.91126 1.91508 1.91588 1.91929

Beta virt. eigenvalues -- 1.91969 1.92203 1.92371 1.92414 1.92816

Beta virt. eigenvalues -- 1.93084 1.93305 1.93492 1.93535 1.94145

Beta virt. eigenvalues -- 1.94243 1.94519 1.94707 1.95885 1.95938

Beta virt. eigenvalues -- 1.96000 1.96156 1.96279 1.97064 1.97092

Beta virt. eigenvalues -- 1.97504 1.99294 1.99362 2.00347 2.01139

Beta virt. eigenvalues -- 2.01220 2.02020 2.05600 2.06636 2.07059

Beta virt. eigenvalues -- 2.08293 2.08402 2.09413 2.10016 2.10545

Beta virt. eigenvalues -- 2.13201 2.13654 2.14136 2.17397 2.18257

Beta virt. eigenvalues -- 2.21610 2.23605 2.23639 2.23850 2.24513

Beta virt. eigenvalues -- 2.24577 2.25422 2.25548 2.25557 2.26275

Beta virt. eigenvalues -- 2.26411 2.26868 2.27218 2.27396 2.27516

Beta virt. eigenvalues -- 2.27561 2.27683 2.27961 2.28167 2.29299

Beta virt. eigenvalues -- 2.29501 2.29527 2.30094 2.30409 2.31014

Beta virt. eigenvalues -- 2.31942 2.31988 2.32408 2.32903 2.33052

Beta virt. eigenvalues -- 2.34705 2.34805 2.34812 2.35678 2.35724

Beta virt. eigenvalues -- 2.36387 2.36496 2.37740 2.37962 2.38247

Beta virt. eigenvalues -- 2.39632 2.39819 2.40057 2.40885 2.42794

Beta virt. eigenvalues -- 2.43446 2.44551 2.44714 2.47090 2.48077

Beta virt. eigenvalues -- 2.48301 2.50983 2.51260 2.52484 2.52791

Beta virt. eigenvalues -- 2.52965 2.54206 2.55507 2.57061 2.57474

Beta virt. eigenvalues -- 2.58059 2.58080 2.58543 2.59229 2.60044

Beta virt. eigenvalues -- 2.60290 2.61203 2.61462 2.61882 2.62123

Beta virt. eigenvalues -- 2.63662 2.64634 2.65572 2.65654 2.65973

Beta virt. eigenvalues -- 2.67708 2.67740 2.69922 2.70081 2.70138

Beta virt. eigenvalues -- 2.70416 2.70622 2.72307 2.72601 2.72631

Beta virt. eigenvalues -- 2.74102 2.74294 2.74837 2.75169 2.76789

Beta virt. eigenvalues -- 2.77120 2.77365 2.78123 2.78414 2.78633

Beta virt. eigenvalues -- 2.78733 2.79856 2.82219 2.83239 2.83274

Beta virt. eigenvalues -- 2.83517 2.83876 2.85309 2.85545 2.86001

Beta virt. eigenvalues -- 2.86969 2.88211 2.89346 2.89952 2.90291

Beta virt. eigenvalues -- 2.92027 2.93833 2.95004 2.95272 2.97300

Beta virt. eigenvalues -- 2.98541 2.98904 2.99182 2.99761 3.01036

Beta virt. eigenvalues -- 3.01583 3.03069 3.03875 3.04851 3.04903

Beta virt. eigenvalues -- 3.05283 3.07317 3.07425 3.07538 3.07829

Beta virt. eigenvalues -- 3.08266 3.10551 3.10836 3.12016 3.12318

Beta virt. eigenvalues -- 3.14320 3.15107 3.15198 3.15599 3.16932

Beta virt. eigenvalues -- 3.18893 3.19001 3.19526 3.21544 3.21990

Beta virt. eigenvalues -- 3.23253 3.25248 3.25779 3.25972 3.26084

Beta virt. eigenvalues -- 3.26578 3.28683 3.29020 3.29246 3.29289

Beta virt. eigenvalues -- 3.29963 3.30297 3.30375 3.30576 3.30607

Beta virt. eigenvalues -- 3.31246 3.31309 3.31586 3.31685 3.31697

Beta virt. eigenvalues -- 3.32664 3.33315 3.33394 3.34305 3.35714

Beta virt. eigenvalues -- 3.35743 3.36479 3.37399 3.38379 3.39465

Beta virt. eigenvalues -- 3.40316 3.41425 3.42849 3.43185 3.45040

Beta virt. eigenvalues -- 3.45076 3.48847 3.50790 3.51026 3.51493

Beta virt. eigenvalues -- 3.56994 3.57916 3.58282 3.58582 3.59053

Beta virt. eigenvalues -- 3.59635 3.60108 3.60910 3.61339 3.64379

Beta virt. eigenvalues -- 3.65425 3.66665 3.71450 3.71453 3.72300

Beta virt. eigenvalues -- 3.74444 3.76484 3.78723 3.79916 3.80361

Beta virt. eigenvalues -- 3.83774 3.84566 3.88165 3.90696 3.91832

Beta virt. eigenvalues -- 3.92706 3.93519 3.94118 3.95485 3.95580

Beta virt. eigenvalues -- 3.96206 3.96515 3.98284 3.99271 4.02378

Beta virt. eigenvalues -- 4.10549 4.28696 4.29879 4.36196 4.39345

Beta virt. eigenvalues -- 4.47466 4.51337 4.54709 4.54975 4.63027

Beta virt. eigenvalues -- 4.63730 4.66621 4.67460 4.78511 4.78522

Beta virt. eigenvalues -- 4.78534 4.78549 5.09042 5.14834 5.17001

Beta virt. eigenvalues -- 5.26754 23.24592 23.28063 23.28336 23.30004

Beta virt. eigenvalues -- 23.45737 23.51382 23.54066 23.58458 23.73714

Beta virt. eigenvalues -- 23.74463 23.78500 23.79297 23.80518 23.80623

Beta virt. eigenvalues -- 23.80697 23.80907 23.85289 23.85906 23.86128

Beta virt. eigenvalues -- 23.86702 23.87483 23.87705 23.98402 23.98557

Beta virt. eigenvalues -- 23.99004 23.99530 24.00182 24.00323 24.04816

Beta virt. eigenvalues -- 24.04917 24.05008 24.05083 24.07239 24.07584

Beta virt. eigenvalues -- 24.07825 24.08192 24.10362 24.10460 24.15238

Beta virt. eigenvalues -- 24.15239 24.15291 24.15301 24.16938 24.17110

Beta virt. eigenvalues -- 35.55618 35.56436 35.62624 35.63188

Condensed to atoms (all electrons):

Atomic-Atomic Spin Densities.

Mulliken charges and spin densities:

1 2

1 C -0.287244 0.078035

2 C 0.316340 0.007730

3 N -0.672465 0.033904

4 C 0.315675 0.011793

5 C -0.286966 0.074309

6 C -0.065826 0.363472

7 C 0.195959 -0.108487

8 N -0.482708 0.258372

9 C 0.195185 -0.109773

10 C -0.248507 -0.011549

11 C -0.248503 -0.012439

12 C -0.065944 0.368255

13 C 0.195211 -0.109772

14 C -0.248500 -0.011548

15 C -0.248511 -0.012440

16 C 0.195937 -0.108488

17 N -0.482710 0.258372

18 C -0.065792 0.363474

19 C 0.315663 0.011792

20 C -0.286969 0.074307

21 C -0.287247 0.078032

22 C 0.316326 0.007730

23 N -0.672445 0.033904

24 C -0.065906 0.368258

25 C -0.101242 -0.040609

26 C -0.206704 0.031493

27 C -0.217879 -0.014201

28 C -0.216030 0.032412

29 C -0.216692 -0.014361

30 C -0.213708 0.036033

31 C -0.216073 0.033208

32 C -0.218051 -0.014682

33 C -0.208908 0.032221

34 C -0.099256 -0.041320

35 C -0.213997 0.036771

36 C -0.215963 -0.014730

37 C -0.099252 -0.041319

38 C -0.213996 0.036772

39 C -0.215964 -0.014729

40 C -0.216072 0.033209

41 C -0.218052 -0.014680

42 C -0.208906 0.032222

43 C -0.101237 -0.040607

44 C -0.213707 0.036033

45 C -0.216692 -0.014359

46 C -0.216030 0.032413

47 C -0.217879 -0.014199

48 C -0.206703 0.031492

49 H 0.243041 -0.004383

50 H 0.242931 -0.004223

51 H 0.241327 0.000983

52 H 0.241579 0.001031

53 H 0.241328 0.000983

54 H 0.241579 0.001031

55 H 0.242929 -0.004223

56 H 0.243039 -0.004383

57 H 0.230593 -0.001695

58 H 0.228062 0.001152

59 H 0.228285 -0.001740

60 H 0.228220 0.001005

61 H 0.232065 -0.001838

62 H 0.228310 -0.001782

63 H 0.228015 0.001179

64 H 0.230967 -0.001730

65 H 0.231983 -0.001878

66 H 0.228265 0.001023

67 H 0.231985 -0.001878

68 H 0.228265 0.001023

69 H 0.228310 -0.001782

70 H 0.228015 0.001178

71 H 0.230967 -0.001730

72 H 0.232066 -0.001838

73 H 0.228220 0.001005

74 H 0.228285 -0.001740

75 H 0.228063 0.001151

76 H 0.230592 -0.001695

77 H 0.415825 -0.002968

78 H 0.415832 -0.002966

Sum of Mulliken charges = -0.00000 2.00000

Mulliken charges and spin densities with hydrogens summed into heavy atoms:

1 2

1 C -0.044204 0.073652

2 C 0.316340 0.007730

3 N -0.256640 0.030936

4 C 0.315675 0.011793

5 C -0.044035 0.070086

6 C -0.065826 0.363472

7 C 0.195959 -0.108487

8 N -0.482708 0.258372

9 C 0.195185 -0.109773

10 C -0.007180 -0.010566

11 C -0.006924 -0.011408

12 C -0.065944 0.368255

13 C 0.195211 -0.109772

14 C -0.007172 -0.010565

15 C -0.006932 -0.011409

16 C 0.195937 -0.108488

17 N -0.482710 0.258372

18 C -0.065792 0.363474

19 C 0.315663 0.011792

20 C -0.044039 0.070084

21 C -0.044208 0.073650

22 C 0.316326 0.007730

23 N -0.256613 0.030938

24 C -0.065906 0.368258

25 C -0.101242 -0.040609

26 C 0.023888 0.029798

27 C 0.010184 -0.013050

28 C 0.012255 0.030673

29 C 0.011528 -0.013356

30 C 0.018357 0.034195

31 C 0.012237 0.031426

32 C 0.009963 -0.013503

33 C 0.022060 0.030491

34 C -0.099256 -0.041320

35 C 0.017986 0.034893

36 C 0.012302 -0.013707

37 C -0.099252 -0.041319

38 C 0.017989 0.034894

39 C 0.012301 -0.013706

40 C 0.012238 0.031428

41 C 0.009963 -0.013502

42 C 0.022061 0.030492

43 C -0.101237 -0.040607

44 C 0.018359 0.034195

45 C 0.011528 -0.013355

46 C 0.012256 0.030673

47 C 0.010184 -0.013048

48 C 0.023889 0.029797

APT charges:

1

1 C 0.165266

2 C -0.942006

3 N -0.107377

4 C -0.947441

5 C 0.168277

6 C 0.949263

7 C -0.018537

8 N -0.809601

9 C -0.003354

10 C 0.091420

11 C 0.105223

12 C 0.930953

13 C -0.003401

14 C 0.091426

15 C 0.105214

16 C -0.018505

17 N -0.809596

18 C 0.949230

19 C -0.947363

20 C 0.168270

21 C 0.165256

22 C -0.941925

23 N -0.107410

24 C 0.930910

25 C 0.012614

26 C -0.040384

27 C -0.087901

28 C -0.060634

29 C -0.102316

30 C -0.093899

31 C -0.061857

32 C -0.089556

33 C -0.036605

34 C 0.011244

35 C -0.096328

36 C -0.100486

37 C 0.011230

38 C -0.096327

39 C -0.100494

40 C -0.061860

41 C -0.089559

42 C -0.036595

43 C 0.012603

44 C -0.093897

45 C -0.102324

46 C -0.060635

47 C -0.087903

48 C -0.040381

49 H 0.098541

50 H 0.100577

51 H 0.082791

52 H 0.082864

53 H 0.082791

54 H 0.082865

55 H 0.100573

56 H 0.098536

57 H 0.056968

58 H 0.025681

59 H 0.033524

60 H 0.030932

61 H 0.066499

62 H 0.034074

63 H 0.027152

64 H 0.057286

65 H 0.066983

66 H 0.030682

67 H 0.066985

68 H 0.030681

69 H 0.034073

70 H 0.027151

71 H 0.057287

72 H 0.066500

73 H 0.030933

74 H 0.033523

75 H 0.025680

76 H 0.056969

77 H 0.369483

78 H 0.369476

Sum of APT charges = 0.00000

APT charges with hydrogens summed into heavy atoms:

1

1 C 0.263807

2 C -0.942006

3 N 0.262106

4 C -0.947441

5 C 0.268854

6 C 0.949263

7 C -0.018537

8 N -0.809601

9 C -0.003354

10 C 0.174211

11 C 0.188087

12 C 0.930953

13 C -0.003401

14 C 0.174216

15 C 0.188079

16 C -0.018505

17 N -0.809596

18 C 0.949230

19 C -0.947363

20 C 0.268843

21 C 0.263792

22 C -0.941925

23 N 0.262066

24 C 0.930910

25 C 0.012614

26 C 0.016584

27 C -0.062220

28 C -0.027110

29 C -0.071385

30 C -0.027401

31 C -0.027783

32 C -0.062404

33 C 0.020680

34 C 0.011244

35 C -0.029345

36 C -0.069804

37 C 0.011230

38 C -0.029343

39 C -0.069812

40 C -0.027787

41 C -0.062408

42 C 0.020692

43 C 0.012603

44 C -0.027397

45 C -0.071391

46 C -0.027112

47 C -0.062223

48 C 0.016588

Electronic spatial extent (au): <R\*\*2>= 33214.8553

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -0.0000 Y= 0.0002 Z= -1.2197 Tot= 1.2197

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -219.2316 YY= -218.0644 ZZ= -274.5123

XY= -0.0397 XZ= -0.0000 YZ= 0.0009

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 18.0378 YY= 19.2050 ZZ= -37.2429

XY= -0.0397 XZ= -0.0000 YZ= 0.0009

Octapole moment (field-independent basis, Debye-Ang\*\*2):

XXX= -0.0002 YYY= 0.0099 ZZZ= -3.1461 XYY= -0.0004

XXY= -0.0005 XXZ= 97.5783 XZZ= 0.0001 YZZ= 0.0005

YYZ= -101.0716 XYZ= 11.1328

Hexadecapole moment (field-independent basis, Debye-Ang\*\*3):

XXXX= -20644.1228 YYYY= -20510.2384 ZZZZ= -1003.6196 XXXY= -260.0634

XXXZ= -0.0040 YYYX= 259.2914 YYYZ= 0.0377 ZZZX= -0.0001

ZZZY= 0.0057 XXYY= -5602.0163 XXZZ= -3933.8175 YYZZ= -3876.3865

XXYZ= 0.0242 YYXZ= 0.0009 ZZXY= 1.0213

N-N= 5.356699039623D+03 E-N=-1.516302510312D+04 KE= 1.906380698939D+03

Exact polarizability:1255.814 -30.2131665.690 -0.000 -0.000 455.164

Approx polarizability:1220.997 -30.0141624.756 0.000 -0.002 534.414

Isotropic Fermi Contact Couplings

Atom a.u. MegaHertz Gauss 10(-4) cm-1

1 C(13) 0.00133 0.74478 0.26576 0.24843

2 C(13) -0.01190 -6.68668 -2.38597 -2.23044

3 N(14) 0.00119 0.19223 0.06859 0.06412

4 C(13) -0.01149 -6.45831 -2.30449 -2.15426

5 C(13) 0.00100 0.56018 0.19989 0.18686

6 C(13) 0.02096 11.77924 4.20312 3.92913

7 C(13) -0.02147 -12.07062 -4.30710 -4.02632

8 N(14) 0.02641 4.26653 1.52240 1.42316

9 C(13) -0.02173 -12.21349 -4.35808 -4.07398

10 C(13) 0.00040 0.22683 0.08094 0.07566

11 C(13) 0.00032 0.18182 0.06488 0.06065

12 C(13) 0.02136 12.00372 4.28322 4.00401

13 C(13) -0.02173 -12.21367 -4.35814 -4.07404

14 C(13) 0.00040 0.22689 0.08096 0.07568

15 C(13) 0.00032 0.18176 0.06486 0.06063

16 C(13) -0.02147 -12.07043 -4.30703 -4.02626

17 N(14) 0.02641 4.26654 1.52241 1.42316

18 C(13) 0.02096 11.77906 4.20306 3.92907

19 C(13) -0.01149 -6.45835 -2.30450 -2.15427

20 C(13) 0.00100 0.56033 0.19994 0.18691

21 C(13) 0.00133 0.74487 0.26579 0.24846

22 C(13) -0.01190 -6.68669 -2.38598 -2.23044

23 N(14) 0.00119 0.19228 0.06861 0.06414

24 C(13) 0.02135 12.00354 4.28316 4.00395

25 C(13) -0.01247 -7.00892 -2.50096 -2.33792

26 C(13) 0.00966 5.42824 1.93693 1.81067

27 C(13) -0.00108 -0.60766 -0.21683 -0.20269

28 C(13) 0.00208 1.16742 0.41656 0.38941

29 C(13) -0.00069 -0.38618 -0.13780 -0.12882

30 C(13) 0.01215 6.83160 2.43769 2.27878

31 C(13) 0.00213 1.19711 0.42716 0.39931

32 C(13) -0.00116 -0.65283 -0.23295 -0.21776

33 C(13) 0.00967 5.43679 1.93998 1.81352

34 C(13) -0.01268 -7.12649 -2.54291 -2.37714

35 C(13) 0.01236 6.94815 2.47927 2.31765

36 C(13) -0.00071 -0.39743 -0.14181 -0.13257

37 C(13) -0.01268 -7.12622 -2.54281 -2.37705

38 C(13) 0.01236 6.94759 2.47907 2.31747

39 C(13) -0.00071 -0.39731 -0.14177 -0.13253

40 C(13) 0.00213 1.19692 0.42709 0.39925

41 C(13) -0.00116 -0.65267 -0.23289 -0.21771

42 C(13) 0.00967 5.43633 1.93982 1.81336

43 C(13) -0.01247 -7.00858 -2.50084 -2.33781

44 C(13) 0.01215 6.83100 2.43747 2.27858

45 C(13) -0.00069 -0.38601 -0.13774 -0.12876

46 C(13) 0.00208 1.16717 0.41647 0.38932

47 C(13) -0.00108 -0.60744 -0.21675 -0.20262

48 C(13) 0.00966 5.42778 1.93677 1.81051

49 H(1) -0.00137 -3.05497 -1.09009 -1.01903

50 H(1) -0.00132 -2.95278 -1.05362 -0.98494

51 H(1) 0.00025 0.56746 0.20248 0.18928

52 H(1) 0.00027 0.59321 0.21167 0.19787

53 H(1) 0.00025 0.56742 0.20247 0.18927

54 H(1) 0.00027 0.59326 0.21169 0.19789

55 H(1) -0.00132 -2.95271 -1.05360 -0.98492

56 H(1) -0.00137 -3.05487 -1.09005 -1.01899

57 H(1) -0.00047 -1.04933 -0.37443 -0.35002

58 H(1) 0.00036 0.80904 0.28869 0.26987

59 H(1) -0.00046 -1.02531 -0.36586 -0.34201

60 H(1) 0.00031 0.69997 0.24977 0.23348

61 H(1) -0.00055 -1.21902 -0.43498 -0.40662

62 H(1) -0.00047 -1.04971 -0.37456 -0.35015

63 H(1) 0.00037 0.82694 0.29507 0.27584

64 H(1) -0.00048 -1.07429 -0.38333 -0.35835

65 H(1) -0.00055 -1.23812 -0.44179 -0.41299

66 H(1) 0.00032 0.71218 0.25412 0.23756

67 H(1) -0.00055 -1.23805 -0.44177 -0.41297

68 H(1) 0.00032 0.71203 0.25407 0.23751

69 H(1) -0.00047 -1.04965 -0.37454 -0.35012

70 H(1) 0.00037 0.82677 0.29501 0.27578

71 H(1) -0.00048 -1.07420 -0.38330 -0.35831

72 H(1) -0.00055 -1.21891 -0.43494 -0.40659

73 H(1) 0.00031 0.69979 0.24970 0.23342

74 H(1) -0.00046 -1.02520 -0.36582 -0.34197

75 H(1) 0.00036 0.80884 0.28861 0.26980

76 H(1) -0.00047 -1.04920 -0.37438 -0.34998

77 H(1) -0.00063 -1.41578 -0.50519 -0.47225

78 H(1) -0.00063 -1.41598 -0.50526 -0.47232

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Center ---- Spin Dipole Couplings ----

3XX-RR 3YY-RR 3ZZ-RR

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1 Atom -0.048976 -0.031139 0.080115

2 Atom -0.015586 -0.020436 0.036022

3 Atom -0.037050 -0.027462 0.064512

4 Atom -0.016311 -0.023653 0.039963

5 Atom -0.046464 -0.030006 0.076470

6 Atom -0.201360 -0.207783 0.409143

7 Atom 0.030419 0.063549 -0.093968

8 Atom -0.255528 -0.290827 0.546355

9 Atom 0.032894 0.062366 -0.095260

10 Atom 0.011938 0.010229 -0.022167

11 Atom 0.012466 0.010363 -0.022829

12 Atom -0.206233 -0.208621 0.414854

13 Atom 0.032895 0.062365 -0.095259

14 Atom 0.011938 0.010229 -0.022167

15 Atom 0.012467 0.010363 -0.022830

16 Atom 0.030420 0.063550 -0.093970

17 Atom -0.255532 -0.290826 0.546357

18 Atom -0.201366 -0.207785 0.409150

19 Atom -0.016310 -0.023649 0.039959

20 Atom -0.046462 -0.029991 0.076453

21 Atom -0.048975 -0.031122 0.080097

22 Atom -0.015585 -0.020433 0.036019

23 Atom -0.037050 -0.027441 0.064491

24 Atom -0.206238 -0.208623 0.414861

25 Atom -0.000412 0.002642 -0.002229

26 Atom -0.005286 0.019881 -0.014595

27 Atom 0.000638 0.002444 -0.003082

28 Atom -0.001111 -0.002932 0.004043

29 Atom 0.002993 0.000952 -0.003944

30 Atom 0.026127 -0.014132 -0.011995

31 Atom -0.004569 0.000063 0.004506

32 Atom 0.002949 0.000311 -0.003260

33 Atom -0.010142 0.024801 -0.014660

34 Atom 0.003075 -0.000627 -0.002448

35 Atom 0.022548 -0.010476 -0.012071

36 Atom 0.005323 -0.001161 -0.004162

37 Atom 0.003075 -0.000626 -0.002449

38 Atom 0.022549 -0.010478 -0.012071

39 Atom 0.005323 -0.001160 -0.004163

40 Atom -0.004569 0.000061 0.004508

41 Atom 0.002948 0.000312 -0.003261

42 Atom -0.010141 0.024801 -0.014660

43 Atom -0.000413 0.002643 -0.002230

44 Atom 0.026129 -0.014134 -0.011995

45 Atom 0.002992 0.000953 -0.003945

46 Atom -0.001110 -0.002934 0.004045

47 Atom 0.000637 0.002445 -0.003082

48 Atom -0.005285 0.019880 -0.014595

49 Atom -0.001385 0.004541 -0.003156

50 Atom -0.002816 0.006050 -0.003233

51 Atom 0.001908 0.000372 -0.002280

52 Atom 0.002427 -0.000141 -0.002286

53 Atom 0.001908 0.000372 -0.002280

54 Atom 0.002427 -0.000141 -0.002286

55 Atom -0.002816 0.006049 -0.003233

56 Atom -0.001385 0.004541 -0.003156

57 Atom -0.000267 0.000803 -0.000536

58 Atom 0.000121 0.000649 -0.000770

59 Atom 0.000646 0.001323 -0.001969

60 Atom 0.000506 0.000131 -0.000636

61 Atom 0.002161 -0.000754 -0.001407

62 Atom 0.001370 0.000628 -0.001999

63 Atom 0.000509 0.000286 -0.000795

64 Atom -0.000083 0.000707 -0.000624

65 Atom 0.002015 -0.000603 -0.001411

66 Atom 0.000814 -0.000170 -0.000644

67 Atom 0.002015 -0.000603 -0.001412

68 Atom 0.000814 -0.000170 -0.000644

69 Atom 0.001370 0.000628 -0.001999

70 Atom 0.000508 0.000286 -0.000795

71 Atom -0.000083 0.000707 -0.000624

72 Atom 0.002161 -0.000754 -0.001407

73 Atom 0.000506 0.000131 -0.000636

74 Atom 0.000646 0.001323 -0.001969

75 Atom 0.000121 0.000649 -0.000770

76 Atom -0.000267 0.000803 -0.000536

77 Atom 0.003834 0.005153 -0.008987

78 Atom 0.003833 0.005152 -0.008986

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XY XZ YZ

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1 Atom 0.000394 -0.002447 0.048614

2 Atom 0.006065 -0.000248 0.016209

3 Atom -0.000744 -0.003354 0.047334

4 Atom -0.005347 -0.002610 0.017788

5 Atom -0.003464 -0.005754 0.047037

6 Atom -0.002118 -0.071440 0.035823

7 Atom 0.004077 0.030318 -0.003314

8 Atom 0.003277 -0.204241 -0.017451

9 Atom -0.008698 0.029211 0.008847

10 Atom 0.001183 0.007404 0.000531

11 Atom -0.000982 0.007763 0.001003

12 Atom 0.002937 0.058710 0.052399

13 Atom -0.008699 -0.029209 -0.008850

14 Atom 0.001183 -0.007403 -0.000533

15 Atom -0.000982 -0.007763 -0.001004

16 Atom 0.004076 -0.030318 0.003312

17 Atom 0.003287 0.204234 0.017492

18 Atom -0.002117 0.071418 -0.035820

19 Atom -0.005347 0.002608 -0.017794

20 Atom -0.003466 0.005757 -0.047054

21 Atom 0.000394 0.002446 -0.048632

22 Atom 0.006065 0.000251 -0.016214

23 Atom -0.000746 0.003356 -0.047356

24 Atom 0.002935 -0.058689 -0.052394

25 Atom 0.013268 -0.012355 0.010223

26 Atom -0.019574 0.009761 -0.009744

27 Atom 0.008429 -0.006341 0.006965

28 Atom -0.012821 0.019079 -0.017679

29 Atom 0.008686 -0.006540 0.007143

30 Atom -0.012028 0.016237 -0.008714

31 Atom 0.012811 -0.017068 -0.020510

32 Atom -0.008506 0.005710 0.007872

33 Atom 0.015907 -0.008726 -0.011776

34 Atom -0.013321 0.011229 0.011994

35 Atom 0.017348 -0.015173 -0.011023

36 Atom -0.008242 0.005843 0.008067

37 Atom -0.013320 -0.011229 -0.011993

38 Atom 0.017348 0.015175 0.011023

39 Atom -0.008242 -0.005843 -0.008066

40 Atom 0.012812 0.017070 0.020511

41 Atom -0.008505 -0.005710 -0.007871

42 Atom 0.015909 0.008727 0.011779

43 Atom 0.013268 0.012355 -0.010222

44 Atom -0.012028 -0.016238 0.008713

45 Atom 0.008685 0.006540 -0.007142

46 Atom -0.012822 -0.019081 0.017679

47 Atom 0.008428 0.006340 -0.006964

48 Atom -0.019575 -0.009762 0.009746

49 Atom -0.006307 0.002218 -0.002487

50 Atom 0.005145 -0.001808 -0.002640

51 Atom 0.002153 0.000962 0.000771

52 Atom -0.001902 0.001035 -0.000618

53 Atom 0.002153 -0.000962 -0.000771

54 Atom -0.001902 -0.001034 0.000618

55 Atom 0.005144 0.001808 0.002640

56 Atom -0.006306 -0.002219 0.002488

57 Atom 0.000579 -0.000633 0.003356

58 Atom 0.001307 0.000061 0.000538

59 Atom 0.002410 0.000908 -0.000437

60 Atom 0.001171 -0.000392 0.000238

61 Atom -0.000021 -0.003662 0.001424

62 Atom -0.002458 -0.000784 -0.000642

63 Atom -0.001345 -0.000090 0.000488

64 Atom -0.000714 0.000220 0.003375

65 Atom 0.000465 0.003488 0.001955

66 Atom -0.001086 0.000383 0.000282

67 Atom 0.000466 -0.003488 -0.001955

68 Atom -0.001086 -0.000383 -0.000282

69 Atom -0.002458 0.000784 0.000642

70 Atom -0.001345 0.000090 -0.000488

71 Atom -0.000714 -0.000220 -0.003375

72 Atom -0.000021 0.003662 -0.001424

73 Atom 0.001171 0.000392 -0.000238

74 Atom 0.002410 -0.000908 0.000437

75 Atom 0.001307 -0.000061 -0.000538

76 Atom 0.000579 0.000633 -0.003356

77 Atom -0.000022 0.000178 -0.002458

78 Atom -0.000022 -0.000178 0.002458

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Anisotropic Spin Dipole Couplings in Principal Axis System

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Atom a.u. MegaHertz Gauss 10(-4) cm-1 Axes

Baa -0.0504 -6.769 -2.415 -2.258 -0.6507 0.7075 -0.2757

1 C(13) Bbb -0.0480 -6.435 -2.296 -2.146 0.7592 0.6132 -0.2183

Bcc 0.0984 13.204 4.711 4.404 -0.0146 0.3513 0.9362

Baa -0.0277 -3.713 -1.325 -1.239 -0.4409 0.8694 -0.2230

2 C(13) Bbb -0.0127 -1.705 -0.608 -0.569 0.8972 0.4204 -0.1353

Bcc 0.0404 5.418 1.933 1.807 0.0239 0.2597 0.9654

Baa -0.0475 -1.832 -0.654 -0.611 -0.0597 0.9189 -0.3901

3 N(14) Bbb -0.0371 -1.431 -0.511 -0.477 0.9978 0.0658 0.0023

Bcc 0.0846 3.263 1.164 1.089 -0.0278 0.3891 0.9208

Baa -0.0298 -4.002 -1.428 -1.335 0.3213 0.9204 -0.2226

4 C(13) Bbb -0.0150 -2.016 -0.719 -0.673 0.9448 -0.2958 0.1405

Bcc 0.0448 6.018 2.147 2.007 -0.0635 0.2555 0.9647

Baa -0.0486 -6.522 -2.327 -2.175 0.5490 0.7903 -0.2720

5 C(13) Bbb -0.0460 -6.170 -2.202 -2.058 0.8345 -0.5001 0.2313

Bcc 0.0946 12.692 4.529 4.234 -0.0468 0.3540 0.9341

Baa -0.2117 -28.411 -10.138 -9.477 -0.6780 0.7252 -0.1199

6 C(13) Bbb -0.2077 -27.873 -9.946 -9.298 0.7261 0.6862 0.0442

Bcc 0.4194 56.285 20.084 18.774 -0.1143 0.0570 0.9918

Baa -0.1011 -13.562 -4.839 -4.524 -0.2253 0.0252 0.9740

7 C(13) Bbb 0.0370 4.968 1.773 1.657 0.9665 -0.1202 0.2267

Bcc 0.0640 8.594 3.067 2.867 0.1228 0.9924 0.0027

Baa -0.3046 -11.748 -4.192 -3.919 0.9700 0.0659 0.2342

8 N(14) Bbb -0.2911 -11.228 -4.006 -3.745 -0.0687 0.9976 0.0040

Bcc 0.5957 22.976 8.198 7.664 -0.2333 -0.0200 0.9722

Baa -0.1023 -13.724 -4.897 -4.578 -0.2147 -0.0637 0.9746

9 C(13) Bbb 0.0375 5.036 1.797 1.680 0.9420 0.2501 0.2239

Bcc 0.0647 8.688 3.100 2.898 -0.2580 0.9661 0.0063

Baa -0.0237 -3.181 -1.135 -1.061 -0.2031 -0.0083 0.9791

10 C(13) Bbb 0.0098 1.314 0.469 0.438 -0.3202 0.9455 -0.0584

Bcc 0.0139 1.867 0.666 0.623 0.9253 0.3254 0.1947

Baa -0.0245 -3.288 -1.173 -1.097 -0.2063 -0.0339 0.9779

11 C(13) Bbb 0.0103 1.376 0.491 0.459 0.1816 0.9807 0.0723

Bcc 0.0142 1.912 0.682 0.638 0.9615 -0.1925 0.1961

Baa -0.2144 -28.770 -10.266 -9.597 0.5830 0.8034 -0.1213

12 C(13) Bbb -0.2103 -28.220 -10.070 -9.413 0.8072 -0.5897 -0.0264

Bcc 0.4247 56.990 20.336 19.010 0.0927 0.0825 0.9923

Baa -0.1023 -13.724 -4.897 -4.578 0.2147 0.0637 0.9746

13 C(13) Bbb 0.0375 5.036 1.797 1.680 0.9420 0.2501 -0.2239

Bcc 0.0647 8.688 3.100 2.898 -0.2580 0.9661 -0.0063

Baa -0.0237 -3.181 -1.135 -1.061 0.2031 0.0083 0.9791

14 C(13) Bbb 0.0098 1.314 0.469 0.438 -0.3202 0.9456 0.0584

Bcc 0.0139 1.867 0.666 0.623 0.9253 0.3254 -0.1947

Baa -0.0245 -3.288 -1.173 -1.097 0.2063 0.0340 0.9779

15 C(13) Bbb 0.0103 1.376 0.491 0.459 0.1816 0.9807 -0.0724

Bcc 0.0142 1.912 0.682 0.638 0.9615 -0.1925 -0.1961

Baa -0.1011 -13.563 -4.839 -4.524 0.2253 -0.0252 0.9740

16 C(13) Bbb 0.0370 4.968 1.773 1.657 0.9665 -0.1202 -0.2267

Bcc 0.0640 8.594 3.067 2.867 0.1228 0.9924 -0.0028

Baa -0.3046 -11.748 -4.192 -3.919 0.9700 0.0658 -0.2341

17 N(14) Bbb -0.2911 -11.228 -4.006 -3.745 -0.0687 0.9976 -0.0041

Bcc 0.5957 22.976 8.198 7.664 0.2333 0.0200 0.9722

Baa -0.2117 -28.411 -10.138 -9.477 -0.6780 0.7252 0.1198

18 C(13) Bbb -0.2077 -27.873 -9.946 -9.298 0.7261 0.6861 -0.0442

Bcc 0.4194 56.285 20.084 18.775 0.1143 -0.0570 0.9918

Baa -0.0298 -4.002 -1.428 -1.335 0.3213 0.9204 0.2227

19 C(13) Bbb -0.0150 -2.016 -0.719 -0.672 0.9448 -0.2958 -0.1405

Bcc 0.0448 6.018 2.147 2.007 0.0635 -0.2556 0.9647

Baa -0.0486 -6.521 -2.327 -2.175 0.5490 0.7903 0.2721

20 C(13) Bbb -0.0460 -6.170 -2.202 -2.058 0.8345 -0.5000 -0.2314

Bcc 0.0946 12.692 4.529 4.234 0.0468 -0.3541 0.9340

Baa -0.0504 -6.769 -2.415 -2.258 -0.6507 0.7075 0.2758

21 C(13) Bbb -0.0480 -6.435 -2.296 -2.146 0.7592 0.6131 0.2184

Bcc 0.0984 13.203 4.711 4.404 0.0146 -0.3514 0.9361

Baa -0.0277 -3.713 -1.325 -1.239 -0.4409 0.8694 0.2231

22 C(13) Bbb -0.0127 -1.705 -0.608 -0.569 0.8972 0.4204 0.1353

Bcc 0.0404 5.418 1.933 1.807 -0.0238 -0.2598 0.9654

Baa -0.0475 -1.832 -0.654 -0.611 -0.0597 0.9188 0.3903

23 N(14) Bbb -0.0371 -1.431 -0.511 -0.477 0.9978 0.0658 -0.0023

Bcc 0.0846 3.263 1.164 1.089 0.0278 -0.3893 0.9207

Baa -0.2144 -28.771 -10.266 -9.597 0.5829 0.8034 0.1213

24 C(13) Bbb -0.2103 -28.220 -10.070 -9.413 0.8072 -0.5897 0.0264

Bcc 0.4247 56.991 20.336 19.010 -0.0927 -0.0825 0.9923

Baa -0.0240 -3.224 -1.150 -1.075 0.6073 -0.5293 0.5925

25 C(13) Bbb 0.0095 1.276 0.455 0.426 -0.3772 0.4642 0.8014

Bcc 0.0145 1.948 0.695 0.650 0.6992 0.7102 -0.0823

Baa -0.0210 -2.819 -1.006 -0.940 -0.6219 -0.1130 0.7749

26 C(13) Bbb -0.0132 -1.767 -0.631 -0.590 0.6187 0.5358 0.5746

Bcc 0.0342 4.586 1.637 1.530 -0.4801 0.8368 -0.2633

Baa -0.0146 -1.958 -0.699 -0.653 0.5597 -0.5355 0.6324

27 C(13) Bbb 0.0045 0.599 0.214 0.200 -0.5553 0.3242 0.7659

Bcc 0.0101 1.359 0.485 0.453 0.6152 0.7798 0.1159

Baa -0.0188 -2.522 -0.900 -0.841 -0.4916 0.4401 0.7514

28 C(13) Bbb -0.0149 -1.996 -0.712 -0.666 0.6747 0.7380 0.0092

Bcc 0.0337 4.518 1.612 1.507 0.5505 -0.5115 0.6598

Baa -0.0151 -2.032 -0.725 -0.678 0.5054 -0.5629 0.6540

29 C(13) Bbb 0.0044 0.594 0.212 0.198 -0.4221 0.4998 0.7563

Bcc 0.0107 1.439 0.513 0.480 0.7526 0.6583 -0.0150

Baa -0.0220 -2.947 -1.052 -0.983 -0.0692 0.6926 0.7180

30 C(13) Bbb -0.0142 -1.909 -0.681 -0.637 0.4406 0.6670 -0.6009

Bcc 0.0362 4.857 1.733 1.620 0.8951 -0.2747 0.3513

Baa -0.0192 -2.581 -0.921 -0.861 0.4187 0.5163 0.7471

31 C(13) Bbb -0.0153 -2.049 -0.731 -0.684 0.7719 -0.6358 0.0068

Bcc 0.0345 4.630 1.652 1.544 -0.4785 -0.5738 0.6646

Baa -0.0150 -2.013 -0.718 -0.671 -0.4861 -0.5978 0.6374

32 C(13) Bbb 0.0047 0.629 0.224 0.210 0.4957 0.4120 0.7645

Bcc 0.0103 1.384 0.494 0.462 0.7197 -0.6876 -0.0960

Baa -0.0214 -2.875 -1.026 -0.959 0.6270 -0.0173 0.7789

33 C(13) Bbb -0.0136 -1.823 -0.650 -0.608 0.6875 -0.4579 -0.5636

Bcc 0.0350 4.697 1.676 1.567 0.3664 0.8889 -0.2751

Baa -0.0245 -3.284 -1.172 -1.095 0.5332 0.5986 -0.5978

34 C(13) Bbb 0.0097 1.308 0.467 0.436 0.3188 0.5124 0.7974

Bcc 0.0147 1.976 0.705 0.659 0.7837 -0.6157 0.0824

Baa -0.0223 -2.999 -1.070 -1.000 -0.0337 0.7060 0.7074

35 C(13) Bbb -0.0145 -1.948 -0.695 -0.650 0.5266 -0.5890 0.6130

Bcc 0.0369 4.947 1.765 1.650 0.8494 0.3932 -0.3519

Baa -0.0155 -2.082 -0.743 -0.694 -0.4291 -0.6172 0.6595

36 C(13) Bbb 0.0046 0.613 0.219 0.204 0.3432 0.5640 0.7511

Bcc 0.0109 1.469 0.524 0.490 0.8355 -0.5487 0.0302

Baa -0.0245 -3.284 -1.172 -1.095 0.5332 0.5986 0.5979

37 C(13) Bbb 0.0097 1.308 0.467 0.436 -0.3188 -0.5125 0.7974

Bcc 0.0147 1.976 0.705 0.659 0.7836 -0.6157 -0.0824

Baa -0.0224 -2.999 -1.070 -1.000 0.0337 -0.7060 0.7074

38 C(13) Bbb -0.0145 -1.948 -0.695 -0.650 -0.5266 0.5890 0.6130

Bcc 0.0369 4.947 1.765 1.650 0.8494 0.3932 0.3520

Baa -0.0155 -2.081 -0.743 -0.694 0.4291 0.6171 0.6596

39 C(13) Bbb 0.0046 0.613 0.219 0.204 -0.3432 -0.5640 0.7511

Bcc 0.0109 1.469 0.524 0.490 0.8355 -0.5487 -0.0302

Baa -0.0192 -2.581 -0.921 -0.861 -0.4187 -0.5163 0.7471

40 C(13) Bbb -0.0153 -2.049 -0.731 -0.684 0.7719 -0.6358 -0.0068

Bcc 0.0345 4.630 1.652 1.544 0.4785 0.5738 0.6647

Baa -0.0150 -2.013 -0.718 -0.671 0.4861 0.5978 0.6374

41 C(13) Bbb 0.0047 0.629 0.224 0.210 -0.4957 -0.4121 0.7645

Bcc 0.0103 1.384 0.494 0.462 0.7197 -0.6876 0.0960

Baa -0.0214 -2.875 -1.026 -0.959 -0.6269 0.0173 0.7789

42 C(13) Bbb -0.0136 -1.823 -0.650 -0.608 0.6875 -0.4579 0.5636

Bcc 0.0350 4.697 1.676 1.567 0.3664 0.8888 0.2752

Baa -0.0240 -3.224 -1.150 -1.075 0.6074 -0.5292 -0.5925

43 C(13) Bbb 0.0095 1.276 0.455 0.426 0.3772 -0.4642 0.8014

Bcc 0.0145 1.948 0.695 0.650 0.6992 0.7102 0.0823

Baa -0.0220 -2.947 -1.052 -0.983 0.0692 -0.6926 0.7180

44 C(13) Bbb -0.0142 -1.909 -0.681 -0.637 0.4406 0.6670 0.6009

Bcc 0.0362 4.857 1.733 1.620 0.8951 -0.2747 -0.3513

Baa -0.0151 -2.032 -0.725 -0.678 -0.5054 0.5629 0.6540

45 C(13) Bbb 0.0044 0.594 0.212 0.198 0.4221 -0.4999 0.7563

Bcc 0.0107 1.438 0.513 0.480 0.7526 0.6583 0.0151

Baa -0.0188 -2.522 -0.900 -0.841 0.4916 -0.4401 0.7514

46 C(13) Bbb -0.0149 -1.996 -0.712 -0.666 0.6747 0.7380 -0.0092

Bcc 0.0337 4.518 1.612 1.507 -0.5505 0.5115 0.6598

Baa -0.0146 -1.958 -0.699 -0.653 -0.5597 0.5355 0.6324

47 C(13) Bbb 0.0045 0.599 0.214 0.200 0.5553 -0.3242 0.7659

Bcc 0.0101 1.359 0.485 0.453 0.6151 0.7799 -0.1159

Baa -0.0210 -2.819 -1.006 -0.940 0.6218 0.1130 0.7750

48 C(13) Bbb -0.0132 -1.768 -0.631 -0.590 0.6187 0.5358 -0.5746

Bcc 0.0342 4.587 1.637 1.530 -0.4802 0.8367 0.2633

Baa -0.0056 -2.970 -1.060 -0.991 0.8388 0.4469 -0.3109

49 H(1) Bbb -0.0038 -2.049 -0.731 -0.684 0.1390 0.3763 0.9160

Bcc 0.0094 5.020 1.791 1.674 -0.5263 0.8116 -0.2536

Baa -0.0054 -2.871 -1.025 -0.958 0.8805 -0.3144 0.3547

50 H(1) Bbb -0.0038 -2.042 -0.729 -0.681 -0.2338 0.3629 0.9020

Bcc 0.0092 4.913 1.753 1.639 0.4123 0.8772 -0.2460

Baa -0.0025 -1.354 -0.483 -0.452 -0.1343 -0.1598 0.9780

51 H(1) Bbb -0.0011 -0.609 -0.217 -0.203 -0.5868 0.8081 0.0515

Bcc 0.0037 1.964 0.701 0.655 0.7986 0.5669 0.2023

Baa -0.0025 -1.351 -0.482 -0.450 -0.1543 0.1304 0.9794

52 H(1) Bbb -0.0011 -0.613 -0.219 -0.205 0.4785 0.8771 -0.0414

Bcc 0.0037 1.964 0.701 0.655 0.8644 -0.4622 0.1978

Baa -0.0025 -1.354 -0.483 -0.452 0.1343 0.1598 0.9780

53 H(1) Bbb -0.0011 -0.609 -0.217 -0.203 -0.5867 0.8081 -0.0515

Bcc 0.0037 1.964 0.701 0.655 0.7986 0.5669 -0.2023

Baa -0.0025 -1.351 -0.482 -0.450 0.1543 -0.1304 0.9794

54 H(1) Bbb -0.0011 -0.613 -0.219 -0.205 0.4785 0.8771 0.0414

Bcc 0.0037 1.964 0.701 0.655 0.8644 -0.4623 -0.1977

Baa -0.0054 -2.871 -1.025 -0.958 0.8805 -0.3143 -0.3548

55 H(1) Bbb -0.0038 -2.042 -0.729 -0.681 0.2339 -0.3630 0.9020

Bcc 0.0092 4.913 1.753 1.639 0.4123 0.8772 0.2461

Baa -0.0056 -2.970 -1.060 -0.991 0.8388 0.4468 0.3111

56 H(1) Bbb -0.0038 -2.049 -0.731 -0.684 -0.1391 -0.3765 0.9159

Bcc 0.0094 5.020 1.791 1.674 -0.5263 0.8116 0.2537

Baa -0.0035 -1.875 -0.669 -0.625 0.2552 -0.6145 0.7465

57 H(1) Bbb -0.0000 -0.022 -0.008 -0.007 0.9668 0.1522 -0.2052

Bcc 0.0036 1.897 0.677 0.633 0.0124 0.7741 0.6329

Baa -0.0012 -0.636 -0.227 -0.212 0.5284 -0.5610 0.6373

58 H(1) Bbb -0.0006 -0.324 -0.116 -0.108 -0.5920 0.2946 0.7502

Bcc 0.0018 0.960 0.343 0.320 0.6086 0.7736 0.1764

Baa -0.0027 -1.453 -0.518 -0.485 -0.4803 0.3720 0.7943

59 H(1) Bbb -0.0007 -0.379 -0.135 -0.126 0.5743 -0.5511 0.6054

Bcc 0.0034 1.831 0.653 0.611 0.6629 0.7469 0.0511

Baa -0.0012 -0.643 -0.229 -0.214 0.5373 -0.5800 0.6123

60 H(1) Bbb -0.0003 -0.165 -0.059 -0.055 -0.3502 0.5071 0.7876

Bcc 0.0015 0.808 0.288 0.269 0.7673 0.6376 -0.0693

Baa -0.0041 -2.203 -0.786 -0.735 0.4722 -0.3401 0.8132

61 H(1) Bbb -0.0004 -0.233 -0.083 -0.078 0.3051 0.9286 0.2112

Bcc 0.0046 2.437 0.869 0.813 0.8270 -0.1484 -0.5423

Baa -0.0028 -1.481 -0.529 -0.494 0.4160 0.4494 0.7906

62 H(1) Bbb -0.0007 -0.382 -0.136 -0.127 0.4964 0.6163 -0.6114

Bcc 0.0035 1.863 0.665 0.621 0.7620 -0.6468 -0.0333

Baa -0.0012 -0.642 -0.229 -0.214 -0.4533 -0.6196 0.6408

63 H(1) Bbb -0.0006 -0.323 -0.115 -0.108 0.5311 0.3896 0.7524

Bcc 0.0018 0.965 0.344 0.322 0.7158 -0.6814 -0.1525

Baa -0.0035 -1.874 -0.669 -0.625 -0.1800 -0.6328 0.7531

64 H(1) Bbb -0.0000 -0.009 -0.003 -0.003 0.9769 -0.0255 0.2121

Bcc 0.0035 1.883 0.672 0.628 -0.1150 0.7739 0.6228

Baa -0.0042 -2.232 -0.796 -0.744 -0.4294 -0.3892 0.8149

65 H(1) Bbb -0.0004 -0.222 -0.079 -0.074 -0.4386 0.8787 0.1885

Bcc 0.0046 2.454 0.876 0.819 0.7894 0.2765 0.5480

Baa -0.0012 -0.651 -0.232 -0.217 0.4577 0.6395 -0.6177

66 H(1) Bbb -0.0003 -0.165 -0.059 -0.055 0.2743 0.5593 0.7823

Bcc 0.0015 0.815 0.291 0.272 0.8457 -0.5275 0.0805

Baa -0.0042 -2.232 -0.796 -0.744 0.4294 0.3891 0.8150

67 H(1) Bbb -0.0004 -0.222 -0.079 -0.074 -0.4386 0.8787 -0.1884

Bcc 0.0046 2.454 0.876 0.819 0.7894 0.2765 -0.5480

Baa -0.0012 -0.651 -0.232 -0.217 0.4577 0.6395 0.6177

68 H(1) Bbb -0.0003 -0.165 -0.059 -0.055 -0.2743 -0.5593 0.7822

Bcc 0.0015 0.815 0.291 0.272 0.8458 -0.5274 -0.0806

Baa -0.0028 -1.481 -0.529 -0.494 -0.4160 -0.4494 0.7906

69 H(1) Bbb -0.0007 -0.382 -0.136 -0.127 0.4964 0.6162 0.6115

Bcc 0.0035 1.863 0.665 0.621 0.7620 -0.6468 0.0333

Baa -0.0012 -0.642 -0.229 -0.214 0.4533 0.6196 0.6408

70 H(1) Bbb -0.0006 -0.323 -0.115 -0.108 -0.5311 -0.3896 0.7524

Bcc 0.0018 0.965 0.344 0.322 0.7158 -0.6815 0.1525

Baa -0.0035 -1.874 -0.669 -0.625 0.1800 0.6328 0.7531

71 H(1) Bbb -0.0000 -0.009 -0.003 -0.003 0.9769 -0.0255 -0.2121

Bcc 0.0035 1.883 0.672 0.628 -0.1150 0.7739 -0.6228

Baa -0.0041 -2.203 -0.786 -0.735 -0.4722 0.3401 0.8132

72 H(1) Bbb -0.0004 -0.233 -0.083 -0.078 0.3052 0.9286 -0.2112

Bcc 0.0046 2.437 0.869 0.813 0.8270 -0.1484 0.5423

Baa -0.0012 -0.643 -0.229 -0.214 -0.5373 0.5800 0.6124

73 H(1) Bbb -0.0003 -0.165 -0.059 -0.055 0.3501 -0.5071 0.7875

Bcc 0.0015 0.808 0.288 0.269 0.7673 0.6375 0.0694

Baa -0.0027 -1.453 -0.518 -0.485 0.4803 -0.3720 0.7943

74 H(1) Bbb -0.0007 -0.379 -0.135 -0.126 -0.5743 0.5511 0.6054

Bcc 0.0034 1.831 0.653 0.611 0.6629 0.7469 -0.0511

Baa -0.0012 -0.636 -0.227 -0.212 -0.5284 0.5610 0.6373

75 H(1) Bbb -0.0006 -0.324 -0.116 -0.108 0.5920 -0.2946 0.7501

Bcc 0.0018 0.960 0.343 0.320 0.6085 0.7737 -0.1765

Baa -0.0035 -1.875 -0.669 -0.625 -0.2552 0.6145 0.7465

76 H(1) Bbb -0.0000 -0.022 -0.008 -0.007 0.9668 0.1522 0.2052

Bcc 0.0036 1.897 0.677 0.633 0.0124 0.7741 -0.6329

Baa -0.0094 -5.018 -1.790 -1.674 -0.0130 0.1664 0.9860

77 H(1) Bbb 0.0038 2.046 0.730 0.682 0.9995 0.0315 0.0079

Bcc 0.0056 2.972 1.060 0.991 -0.0298 0.9855 -0.1668

Baa -0.0094 -5.017 -1.790 -1.674 0.0130 -0.1665 0.9860

78 H(1) Bbb 0.0038 2.046 0.730 0.682 0.9995 0.0315 -0.0079

Bcc 0.0056 2.971 1.060 0.991 -0.0298 0.9855 0.1668

---------------------------------------------------------------------------------

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Fri Aug 30 06:16:25 2019, MaxMem= 4294967296 cpu: 44.0

(Enter /home/kira/g09/l716.exe)

Rotating derivatives to standard orientation.

Dipole =-4.23633617D-06 8.37069968D-05-4.79848253D-01

Polarizability= 1.25581355D+03-3.02127364D+01 1.66568995D+03

-3.70850505D-05-4.36424170D-04 4.55164100D+02

Full mass-weighted force constant matrix:

Low frequencies --- -11.2290 -3.5237 -2.4711 -0.0007 0.0003 0.0009

Low frequencies --- 6.9844 23.6156 26.6703

Diagonal vibrational polarizability:

102.8589823 162.4926195 173.0622385

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

A A A

Frequencies -- 6.8667 23.5260 25.3824

Red. masses -- 6.1513 4.9973 3.7901

Frc consts -- 0.0002 0.0016 0.0014

IR Inten -- 0.0042 1.9241 1.6047

Atom AN X Y Z X Y Z X Y Z

1 6 -0.02 -0.01 0.01 -0.00 0.03 0.14 0.00 -0.06 -0.12

2 6 -0.01 -0.00 0.02 0.00 0.01 0.09 -0.00 -0.02 0.02

3 7 0.00 0.00 -0.00 0.00 0.01 0.07 -0.00 0.00 0.10

4 6 -0.01 0.00 -0.03 0.00 0.01 0.09 -0.00 -0.02 0.01

5 6 -0.02 -0.00 -0.03 -0.00 0.02 0.14 0.00 -0.06 -0.12

6 6 -0.00 0.01 -0.05 0.00 0.00 0.04 0.00 -0.01 0.02

7 6 -0.00 0.01 -0.02 0.00 -0.00 0.02 0.00 -0.01 0.01

8 7 -0.00 0.01 -0.00 -0.01 -0.00 0.06 -0.00 -0.01 -0.01

9 6 0.00 0.01 0.03 0.00 -0.00 0.03 -0.00 -0.01 -0.03

10 6 -0.00 0.02 0.02 0.02 0.00 -0.03 -0.00 -0.02 -0.03

11 6 -0.00 0.02 -0.01 0.02 0.00 -0.04 -0.00 -0.02 0.01

12 6 -0.00 -0.01 0.04 0.00 0.00 0.05 -0.00 -0.01 0.04

13 6 -0.00 -0.01 0.03 -0.00 0.00 0.03 -0.00 -0.01 0.03

14 6 0.00 -0.02 0.02 -0.02 -0.00 -0.03 -0.00 -0.02 0.03

15 6 0.00 -0.02 -0.01 -0.02 -0.00 -0.04 -0.00 -0.02 -0.01

16 6 0.00 -0.01 -0.02 -0.00 0.00 0.02 0.00 -0.01 -0.01

17 7 0.00 -0.01 -0.00 0.01 0.00 0.06 -0.00 -0.01 0.01

18 6 0.00 -0.01 -0.05 -0.00 -0.00 0.04 0.00 -0.01 -0.02

19 6 0.01 -0.00 -0.03 -0.00 -0.01 0.09 -0.00 -0.02 -0.01

20 6 0.02 0.00 -0.03 0.00 -0.03 0.14 0.00 -0.06 0.12

21 6 0.02 0.01 0.01 0.00 -0.03 0.14 0.00 -0.06 0.12

22 6 0.01 0.00 0.02 -0.00 -0.01 0.09 -0.00 -0.02 -0.02

23 7 -0.00 -0.00 -0.00 -0.00 -0.01 0.07 -0.00 0.00 -0.10

24 6 0.00 0.01 0.04 -0.00 -0.00 0.05 -0.00 -0.01 -0.04

25 6 -0.00 0.01 -0.09 0.02 -0.01 -0.01 -0.01 -0.00 0.02

26 6 0.02 0.03 -0.11 0.08 -0.01 0.01 -0.07 0.04 -0.02

27 6 0.02 0.03 -0.15 0.09 -0.02 -0.04 -0.09 0.05 -0.02

28 6 0.01 0.00 -0.17 0.03 -0.01 -0.11 -0.04 0.03 0.03

29 6 -0.01 -0.02 -0.15 -0.04 -0.01 -0.13 0.02 -0.01 0.08

30 6 -0.01 -0.02 -0.10 -0.04 -0.00 -0.08 0.03 -0.02 0.07

31 6 0.01 0.01 0.18 -0.03 -0.03 -0.10 0.05 0.05 0.01

32 6 0.04 -0.02 0.15 -0.09 -0.04 -0.02 0.08 0.07 -0.04

33 6 0.03 -0.02 0.11 -0.08 -0.03 0.03 0.06 0.05 -0.03

34 6 0.00 -0.00 0.09 -0.01 -0.01 0.01 0.01 0.00 0.03

35 6 -0.02 0.02 0.11 0.05 0.00 -0.07 -0.03 -0.03 0.08

36 6 -0.02 0.02 0.16 0.04 -0.01 -0.12 -0.01 -0.00 0.06

37 6 -0.00 0.00 0.09 0.01 0.01 0.00 0.01 0.00 -0.03

38 6 0.02 -0.02 0.11 -0.05 -0.00 -0.07 -0.03 -0.03 -0.07

39 6 0.02 -0.02 0.16 -0.04 0.01 -0.12 -0.01 -0.00 -0.06

40 6 -0.01 -0.01 0.18 0.03 0.03 -0.10 0.05 0.05 -0.01

41 6 -0.04 0.02 0.15 0.09 0.04 -0.02 0.08 0.07 0.04

42 6 -0.03 0.02 0.11 0.08 0.03 0.03 0.06 0.05 0.03

43 6 0.00 -0.01 -0.09 -0.02 0.01 -0.01 -0.01 -0.00 -0.02

44 6 0.01 0.02 -0.10 0.04 0.00 -0.08 0.03 -0.02 -0.07

45 6 0.01 0.02 -0.15 0.04 0.01 -0.13 0.02 -0.01 -0.08

46 6 -0.01 -0.00 -0.17 -0.03 0.01 -0.11 -0.04 0.03 -0.03

47 6 -0.02 -0.03 -0.15 -0.09 0.02 -0.04 -0.09 0.05 0.02

48 6 -0.02 -0.03 -0.11 -0.08 0.01 0.01 -0.07 0.04 0.02

49 1 -0.03 -0.01 0.02 -0.00 0.03 0.17 0.00 -0.09 -0.22

50 1 -0.03 0.00 -0.04 -0.00 0.03 0.16 0.01 -0.09 -0.23

51 1 -0.00 0.02 0.04 0.02 0.00 -0.07 -0.00 -0.02 -0.04

52 1 -0.00 0.02 -0.03 0.03 0.00 -0.07 -0.00 -0.03 0.02

53 1 0.00 -0.02 0.04 -0.02 -0.00 -0.07 -0.00 -0.02 0.04

54 1 0.00 -0.02 -0.03 -0.03 -0.00 -0.07 -0.00 -0.03 -0.02

55 1 0.03 -0.00 -0.04 0.00 -0.03 0.16 0.01 -0.09 0.23

56 1 0.03 0.01 0.02 0.00 -0.03 0.17 0.00 -0.09 0.22

57 1 0.03 0.05 -0.10 0.13 -0.01 0.07 -0.11 0.06 -0.06

58 1 0.03 0.05 -0.17 0.14 -0.02 -0.03 -0.13 0.08 -0.06

59 1 0.01 0.00 -0.20 0.03 -0.02 -0.16 -0.05 0.04 0.03

60 1 -0.02 -0.04 -0.16 -0.09 -0.01 -0.18 0.05 -0.03 0.11

61 1 -0.03 -0.04 -0.09 -0.10 -0.00 -0.09 0.08 -0.05 0.11

62 1 0.02 0.01 0.21 -0.03 -0.03 -0.14 0.06 0.06 -0.00

63 1 0.06 -0.03 0.16 -0.14 -0.05 -0.01 0.13 0.11 -0.08

64 1 0.05 -0.04 0.09 -0.13 -0.04 0.08 0.09 0.08 -0.06

65 1 -0.05 0.03 0.10 0.11 0.02 -0.08 -0.07 -0.06 0.11

66 1 -0.04 0.04 0.18 0.09 0.00 -0.17 -0.03 -0.03 0.10

67 1 0.05 -0.03 0.10 -0.11 -0.02 -0.08 -0.07 -0.06 -0.11

68 1 0.04 -0.04 0.18 -0.09 -0.00 -0.17 -0.03 -0.03 -0.10

69 1 -0.02 -0.01 0.21 0.03 0.03 -0.14 0.06 0.06 0.00

70 1 -0.06 0.03 0.16 0.14 0.05 -0.01 0.13 0.11 0.08

71 1 -0.05 0.04 0.09 0.13 0.04 0.08 0.09 0.08 0.06

72 1 0.03 0.04 -0.09 0.10 0.00 -0.09 0.08 -0.05 -0.11

73 1 0.02 0.04 -0.16 0.09 0.01 -0.18 0.05 -0.03 -0.11

74 1 -0.01 -0.00 -0.20 -0.03 0.02 -0.16 -0.05 0.04 -0.03

75 1 -0.03 -0.05 -0.17 -0.14 0.02 -0.03 -0.13 0.08 0.06

76 1 -0.03 -0.05 -0.10 -0.13 0.01 0.07 -0.11 0.06 0.06

77 1 0.01 0.00 0.00 0.00 -0.00 0.03 -0.00 0.04 0.28

78 1 -0.01 -0.00 0.00 -0.00 0.00 0.03 -0.00 0.04 -0.28

4 5 6

A A A

Frequencies -- 27.7059 35.9174 41.1322

Red. masses -- 4.7468 5.3771 5.6331

Frc consts -- 0.0021 0.0041 0.0056

IR Inten -- 0.1672 0.0658 0.5952

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.03 -0.06 0.00 0.00 0.04 -0.01 0.01 0.09

2 6 0.00 -0.01 0.01 0.01 0.01 0.06 -0.01 0.02 0.14

3 7 0.00 0.00 0.05 0.01 0.01 0.04 -0.01 0.03 0.18

4 6 0.00 -0.01 0.01 0.01 0.00 0.01 -0.01 0.02 0.14

5 6 0.00 -0.03 -0.06 0.01 0.00 0.02 -0.01 0.01 0.09

6 6 -0.00 0.00 0.04 0.02 0.00 -0.03 -0.00 0.01 0.10

7 6 -0.01 0.00 0.09 0.03 0.00 -0.09 -0.01 0.00 0.06

8 7 -0.01 0.00 0.07 0.03 0.00 -0.09 -0.01 0.01 0.00

9 6 -0.01 0.00 0.09 0.03 0.00 -0.11 -0.01 0.00 -0.03

10 6 -0.02 -0.00 0.13 0.04 0.00 -0.15 -0.02 -0.01 0.01

11 6 -0.02 -0.00 0.13 0.04 0.00 -0.14 -0.01 -0.01 0.06

12 6 0.00 -0.00 0.04 0.02 0.00 0.08 -0.01 0.01 0.09

13 6 0.01 -0.00 0.09 0.03 0.00 0.11 -0.01 0.00 0.03

14 6 0.02 0.00 0.13 0.04 0.00 0.15 -0.02 -0.01 -0.01

15 6 0.02 0.00 0.13 0.04 0.00 0.14 -0.01 -0.01 -0.06

16 6 0.01 -0.00 0.09 0.03 0.00 0.09 -0.01 0.00 -0.06

17 7 0.01 -0.00 0.07 0.03 0.00 0.09 -0.01 0.01 -0.00

18 6 0.00 -0.00 0.04 0.02 0.00 0.03 -0.00 0.01 -0.10

19 6 -0.00 0.01 0.01 0.01 0.00 -0.01 -0.01 0.02 -0.14

20 6 -0.00 0.03 -0.06 0.01 0.00 -0.02 -0.01 0.01 -0.09

21 6 -0.00 0.03 -0.06 0.00 0.00 -0.04 -0.01 0.01 -0.09

22 6 -0.00 0.01 0.01 0.01 0.01 -0.06 -0.01 0.02 -0.14

23 7 -0.00 -0.00 0.05 0.01 0.01 -0.04 -0.01 0.03 -0.18

24 6 -0.00 0.00 0.04 0.02 0.00 -0.08 -0.01 0.01 -0.09

25 6 0.00 -0.00 0.00 0.00 0.02 -0.00 0.02 -0.01 0.04

26 6 -0.02 0.06 -0.07 0.00 -0.03 0.05 0.04 0.06 -0.02

27 6 -0.01 0.06 -0.12 -0.02 -0.02 0.08 0.06 0.05 -0.10

28 6 0.02 -0.01 -0.09 -0.04 0.05 0.06 0.05 -0.03 -0.12

29 6 0.04 -0.08 -0.01 -0.04 0.10 0.01 0.03 -0.09 -0.05

30 6 0.03 -0.07 0.03 -0.02 0.08 -0.02 0.01 -0.08 0.03

31 6 -0.01 -0.01 -0.10 -0.04 -0.06 -0.12 -0.02 0.00 -0.08

32 6 0.01 0.05 -0.12 -0.06 0.01 -0.11 -0.06 0.02 -0.04

33 6 0.01 0.05 -0.07 -0.04 0.03 -0.04 -0.06 0.02 0.03

34 6 -0.00 -0.01 0.00 -0.00 -0.02 0.03 -0.02 0.00 0.05

35 6 -0.01 -0.07 0.02 0.02 -0.09 0.01 0.02 -0.02 0.00

36 6 -0.02 -0.08 -0.03 -0.00 -0.11 -0.06 0.02 -0.02 -0.06

37 6 0.00 0.01 0.00 -0.00 -0.02 -0.03 -0.02 0.00 -0.05

38 6 0.01 0.07 0.02 0.02 -0.09 -0.01 0.02 -0.02 -0.00

39 6 0.02 0.08 -0.03 -0.00 -0.11 0.06 0.02 -0.02 0.06

40 6 0.01 0.01 -0.10 -0.04 -0.06 0.12 -0.02 0.00 0.08

41 6 -0.01 -0.05 -0.12 -0.06 0.01 0.11 -0.06 0.02 0.04

42 6 -0.01 -0.05 -0.07 -0.04 0.03 0.04 -0.06 0.02 -0.03

43 6 -0.00 0.00 0.00 0.00 0.02 0.00 0.02 -0.01 -0.04

44 6 -0.03 0.07 0.03 -0.02 0.08 0.02 0.01 -0.08 -0.03

45 6 -0.04 0.08 -0.01 -0.04 0.10 -0.01 0.03 -0.09 0.05

46 6 -0.02 0.01 -0.09 -0.04 0.05 -0.06 0.05 -0.03 0.12

47 6 0.01 -0.06 -0.12 -0.02 -0.02 -0.08 0.06 0.05 0.10

48 6 0.02 -0.06 -0.07 0.00 -0.03 -0.05 0.04 0.06 0.02

49 1 0.00 -0.04 -0.11 0.00 0.00 0.04 -0.01 -0.01 0.05

50 1 0.00 -0.04 -0.11 0.00 -0.00 -0.00 -0.01 -0.01 0.04

51 1 -0.03 -0.00 0.16 0.05 0.00 -0.19 -0.02 -0.02 -0.00

52 1 -0.03 -0.00 0.16 0.05 -0.00 -0.17 -0.02 -0.02 0.10

53 1 0.03 0.00 0.16 0.05 0.00 0.19 -0.02 -0.02 0.00

54 1 0.03 0.00 0.16 0.05 -0.00 0.17 -0.02 -0.02 -0.10

55 1 -0.00 0.04 -0.11 0.00 -0.00 0.00 -0.01 -0.01 -0.04

56 1 -0.00 0.04 -0.10 0.00 0.00 -0.04 -0.01 -0.01 -0.05

57 1 -0.04 0.12 -0.09 0.01 -0.08 0.06 0.05 0.12 -0.01

58 1 -0.03 0.11 -0.18 -0.02 -0.05 0.12 0.08 0.10 -0.15

59 1 0.02 -0.01 -0.12 -0.06 0.06 0.09 0.06 -0.04 -0.18

60 1 0.06 -0.13 0.01 -0.05 0.15 -0.00 0.02 -0.15 -0.06

61 1 0.05 -0.12 0.09 -0.01 0.12 -0.06 -0.01 -0.13 0.07

62 1 -0.01 -0.01 -0.13 -0.06 -0.08 -0.18 -0.02 0.00 -0.14

63 1 0.01 0.10 -0.17 -0.09 0.06 -0.15 -0.09 0.04 -0.06

64 1 0.02 0.10 -0.09 -0.05 0.09 -0.03 -0.09 0.04 0.06

65 1 -0.02 -0.12 0.07 0.05 -0.13 0.06 0.06 -0.03 0.02

66 1 -0.02 -0.13 -0.01 0.01 -0.17 -0.07 0.06 -0.03 -0.10

67 1 0.02 0.12 0.07 0.05 -0.13 -0.06 0.06 -0.03 -0.02

68 1 0.02 0.13 -0.01 0.01 -0.17 0.07 0.06 -0.03 0.10

69 1 0.01 0.02 -0.13 -0.06 -0.08 0.18 -0.02 0.00 0.14

70 1 -0.01 -0.10 -0.17 -0.09 0.06 0.15 -0.09 0.04 0.06

71 1 -0.02 -0.10 -0.09 -0.05 0.09 0.03 -0.09 0.04 -0.06

72 1 -0.05 0.12 0.09 -0.01 0.12 0.06 -0.01 -0.13 -0.07

73 1 -0.06 0.13 0.01 -0.05 0.15 0.00 0.02 -0.15 0.06

74 1 -0.02 0.01 -0.12 -0.06 0.06 -0.09 0.06 -0.04 0.18

75 1 0.03 -0.11 -0.18 -0.02 -0.05 -0.12 0.08 0.10 0.15

76 1 0.04 -0.12 -0.09 0.01 -0.08 -0.06 0.05 0.12 0.01

77 1 0.00 0.01 0.10 0.01 0.01 0.06 -0.00 0.05 0.27

78 1 -0.00 -0.01 0.10 0.01 0.01 -0.06 -0.00 0.05 -0.27

7 8 9

A A A

Frequencies -- 45.3658 53.4451 54.3047

Red. masses -- 5.2804 4.5815 5.1947

Frc consts -- 0.0064 0.0077 0.0090

IR Inten -- 0.6760 0.0085 0.9871

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.02 0.01 0.00 0.02 -0.00 -0.03 0.03 -0.02

2 6 0.00 0.01 -0.02 -0.03 0.03 -0.01 -0.02 0.03 -0.01

3 7 0.01 0.01 -0.04 -0.05 -0.00 -0.01 -0.02 0.03 -0.03

4 6 0.00 0.02 -0.03 -0.03 -0.03 -0.00 -0.02 0.03 -0.06

5 6 -0.00 0.03 0.00 0.00 -0.01 0.01 -0.03 0.03 -0.05

6 6 0.00 0.01 -0.03 -0.03 -0.05 0.00 -0.02 0.03 -0.07

7 6 -0.01 0.01 -0.02 -0.02 -0.04 0.00 -0.02 0.03 -0.06

8 7 -0.01 0.01 -0.04 0.00 -0.06 -0.00 -0.02 0.03 -0.06

9 6 -0.02 0.01 -0.02 0.02 -0.04 0.00 -0.02 0.03 -0.04

10 6 -0.03 0.00 0.01 0.01 -0.01 0.01 -0.02 0.03 -0.04

11 6 -0.02 0.00 0.01 -0.02 -0.01 0.01 -0.02 0.03 -0.04

12 6 0.01 -0.01 -0.03 -0.04 0.04 -0.01 -0.02 0.03 0.02

13 6 0.02 -0.01 -0.02 -0.02 0.04 -0.00 -0.02 0.03 0.04

14 6 0.03 -0.00 0.01 -0.01 0.01 0.01 -0.02 0.03 0.04

15 6 0.02 -0.00 0.01 0.02 0.01 0.01 -0.02 0.03 0.04

16 6 0.01 -0.01 -0.02 0.02 0.04 0.00 -0.02 0.03 0.06

17 7 0.01 -0.01 -0.04 -0.00 0.06 -0.00 -0.02 0.03 0.06

18 6 -0.00 -0.01 -0.03 0.03 0.05 0.00 -0.02 0.03 0.07

19 6 -0.00 -0.02 -0.03 0.03 0.03 -0.00 -0.02 0.03 0.06

20 6 0.00 -0.03 0.00 -0.00 0.01 0.01 -0.03 0.03 0.05

21 6 0.00 -0.02 0.01 -0.00 -0.02 -0.00 -0.03 0.03 0.02

22 6 -0.00 -0.01 -0.02 0.03 -0.03 -0.01 -0.02 0.03 0.01

23 7 -0.01 -0.01 -0.04 0.05 0.00 -0.01 -0.02 0.03 0.03

24 6 -0.01 0.01 -0.03 0.04 -0.04 -0.01 -0.02 0.03 -0.02

25 6 0.03 -0.01 -0.02 -0.03 -0.05 0.00 0.01 0.01 -0.05

26 6 0.04 0.00 -0.03 0.03 -0.10 0.06 0.00 0.02 -0.07

27 6 0.10 -0.05 0.01 0.04 -0.11 0.06 0.08 -0.05 0.01

28 6 0.15 -0.11 0.06 -0.02 -0.07 -0.01 0.16 -0.13 0.11

29 6 0.13 -0.12 0.06 -0.08 -0.01 -0.07 0.16 -0.13 0.11

30 6 0.07 -0.06 0.02 -0.09 -0.01 -0.07 0.08 -0.06 0.02

31 6 -0.11 -0.14 0.05 -0.08 0.00 0.02 -0.06 -0.01 -0.00

32 6 -0.10 -0.11 0.05 -0.02 0.08 -0.06 -0.05 0.01 -0.01

33 6 -0.05 -0.05 0.01 -0.00 0.09 -0.07 -0.04 0.03 -0.00

34 6 -0.01 -0.03 -0.02 -0.04 0.03 -0.01 -0.03 0.02 0.01

35 6 -0.01 -0.06 -0.01 -0.10 -0.03 0.06 -0.03 -0.00 0.01

36 6 -0.06 -0.11 0.02 -0.12 -0.05 0.08 -0.04 -0.02 0.01

37 6 0.01 0.03 -0.02 0.04 -0.03 -0.01 -0.03 0.02 -0.01

38 6 0.01 0.06 -0.01 0.10 0.03 0.06 -0.03 -0.00 -0.01

39 6 0.06 0.11 0.02 0.12 0.05 0.08 -0.04 -0.02 -0.01

40 6 0.11 0.14 0.05 0.08 -0.00 0.02 -0.06 -0.01 0.00

41 6 0.10 0.11 0.05 0.02 -0.08 -0.06 -0.05 0.01 0.01

42 6 0.05 0.05 0.01 0.00 -0.09 -0.07 -0.04 0.03 0.00

43 6 -0.03 0.01 -0.02 0.03 0.05 0.00 0.01 0.01 0.05

44 6 -0.07 0.06 0.02 0.09 0.01 -0.07 0.08 -0.06 -0.02

45 6 -0.13 0.12 0.06 0.08 0.02 -0.07 0.16 -0.13 -0.11

46 6 -0.15 0.11 0.06 0.02 0.07 -0.01 0.16 -0.13 -0.11

47 6 -0.10 0.05 0.01 -0.05 0.11 0.06 0.08 -0.05 -0.01

48 6 -0.04 -0.00 -0.03 -0.03 0.10 0.06 0.00 0.02 0.07

49 1 -0.01 0.02 0.03 0.02 0.04 -0.01 -0.03 0.03 -0.00

50 1 -0.01 0.04 0.02 0.03 -0.03 0.02 -0.03 0.03 -0.06

51 1 -0.03 -0.00 0.03 0.02 0.01 0.02 -0.03 0.03 -0.02

52 1 -0.02 -0.00 0.04 -0.03 0.00 0.02 -0.02 0.02 -0.03

53 1 0.03 0.00 0.03 -0.02 -0.01 0.02 -0.03 0.03 0.02

54 1 0.02 0.00 0.04 0.03 -0.00 0.02 -0.02 0.02 0.03

55 1 0.01 -0.04 0.02 -0.03 0.03 0.01 -0.03 0.03 0.06

56 1 0.01 -0.02 0.03 -0.02 -0.04 -0.01 -0.03 0.03 0.00

57 1 0.02 0.04 -0.06 0.08 -0.14 0.11 -0.05 0.07 -0.12

58 1 0.11 -0.05 0.01 0.10 -0.15 0.11 0.08 -0.05 0.01

59 1 0.19 -0.15 0.09 -0.01 -0.07 -0.01 0.23 -0.19 0.18

60 1 0.16 -0.16 0.09 -0.13 0.02 -0.13 0.22 -0.19 0.17

61 1 0.06 -0.07 0.02 -0.14 0.02 -0.11 0.08 -0.06 0.03

62 1 -0.15 -0.19 0.08 -0.09 -0.01 0.03 -0.07 -0.02 -0.00

63 1 -0.14 -0.13 0.07 0.02 0.12 -0.11 -0.06 0.02 -0.01

64 1 -0.05 -0.04 0.01 0.04 0.15 -0.13 -0.04 0.05 -0.00

65 1 0.02 -0.04 -0.03 -0.14 -0.07 0.11 -0.02 -0.01 0.02

66 1 -0.06 -0.13 0.03 -0.17 -0.11 0.14 -0.04 -0.04 0.01

67 1 -0.02 0.04 -0.03 0.14 0.07 0.11 -0.02 -0.01 -0.02

68 1 0.06 0.13 0.03 0.17 0.11 0.14 -0.04 -0.04 -0.01

69 1 0.15 0.19 0.08 0.09 0.01 0.03 -0.07 -0.02 0.00

70 1 0.14 0.13 0.07 -0.02 -0.12 -0.11 -0.06 0.02 0.01

71 1 0.05 0.04 0.01 -0.04 -0.15 -0.13 -0.04 0.05 0.00

72 1 -0.05 0.07 0.02 0.14 -0.02 -0.11 0.08 -0.06 -0.03

73 1 -0.16 0.16 0.09 0.13 -0.02 -0.13 0.22 -0.19 -0.17

74 1 -0.19 0.15 0.09 0.01 0.07 -0.01 0.23 -0.19 -0.18

75 1 -0.11 0.05 0.01 -0.10 0.15 0.11 0.08 -0.05 -0.01

76 1 -0.02 -0.04 -0.06 -0.08 0.13 0.11 -0.05 0.07 0.12

77 1 0.02 0.01 -0.06 -0.09 -0.01 -0.01 -0.01 0.03 -0.03

78 1 -0.02 -0.01 -0.06 0.09 0.01 -0.01 -0.01 0.03 0.03

10 11 12

A A A

Frequencies -- 56.8766 61.1056 81.3829

Red. masses -- 5.1135 4.2106 5.2067

Frc consts -- 0.0097 0.0093 0.0203

IR Inten -- 0.4516 0.5086 0.0002

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 -0.02 0.04 0.01 0.01 -0.02 0.03 0.03 -0.01

2 6 -0.03 -0.02 0.02 -0.00 0.01 -0.03 -0.02 0.04 -0.01

3 7 -0.03 -0.03 -0.01 -0.01 0.01 0.01 -0.04 -0.01 -0.00

4 6 -0.03 -0.02 -0.00 -0.00 0.01 0.04 -0.01 -0.05 0.01

5 6 -0.03 -0.01 0.03 0.01 0.01 0.03 0.03 -0.03 0.00

6 6 -0.03 -0.02 -0.03 -0.01 0.01 0.05 -0.02 -0.07 0.04

7 6 -0.03 -0.02 -0.04 -0.01 0.01 0.05 -0.01 -0.07 0.03

8 7 -0.03 -0.02 -0.03 -0.02 0.01 0.08 0.01 -0.08 0.00

9 6 -0.03 -0.02 -0.04 -0.01 0.01 0.05 0.02 -0.07 -0.03

10 6 -0.03 -0.02 -0.03 0.00 0.01 0.00 0.02 -0.06 -0.02

11 6 -0.03 -0.02 -0.04 0.00 0.01 0.01 -0.01 -0.06 0.03

12 6 -0.03 -0.02 0.04 -0.01 0.01 -0.04 -0.03 0.07 -0.03

13 6 -0.03 -0.02 0.04 -0.01 0.01 -0.05 -0.02 0.07 -0.03

14 6 -0.03 -0.02 0.03 0.00 0.01 -0.00 -0.02 0.06 -0.02

15 6 -0.03 -0.02 0.04 0.00 0.01 -0.01 0.01 0.06 0.03

16 6 -0.03 -0.02 0.04 -0.01 0.01 -0.05 0.01 0.07 0.03

17 7 -0.03 -0.02 0.03 -0.02 0.01 -0.08 -0.01 0.08 0.00

18 6 -0.03 -0.02 0.03 -0.01 0.01 -0.05 0.02 0.07 0.04

19 6 -0.03 -0.02 0.00 -0.00 0.01 -0.04 0.01 0.05 0.01

20 6 -0.03 -0.01 -0.03 0.01 0.01 -0.03 -0.03 0.03 0.00

21 6 -0.03 -0.02 -0.04 0.01 0.01 0.02 -0.03 -0.03 -0.01

22 6 -0.03 -0.02 -0.02 -0.00 0.01 0.03 0.02 -0.04 -0.01

23 7 -0.03 -0.03 0.01 -0.01 0.01 -0.01 0.04 0.01 -0.00

24 6 -0.03 -0.02 -0.04 -0.01 0.01 0.04 0.03 -0.07 -0.03

25 6 -0.02 -0.03 -0.02 0.01 -0.00 0.03 -0.02 -0.07 0.04

26 6 0.02 -0.07 0.03 0.08 -0.03 0.07 -0.08 -0.02 -0.03

27 6 0.04 -0.09 0.05 0.11 -0.06 0.06 -0.12 0.02 -0.08

28 6 0.02 -0.07 0.03 0.05 -0.05 -0.01 -0.10 -0.01 -0.05

29 6 -0.03 -0.03 -0.03 -0.03 -0.01 -0.06 -0.03 -0.07 0.03

30 6 -0.05 -0.01 -0.05 -0.05 0.01 -0.04 0.01 -0.10 0.07

31 6 0.14 0.17 -0.09 -0.03 -0.00 0.02 -0.09 0.00 0.04

32 6 0.11 0.11 -0.04 0.05 0.07 -0.08 -0.11 -0.03 0.08

33 6 0.03 0.02 0.02 0.05 0.08 -0.10 -0.08 0.01 0.03

34 6 -0.01 0.01 0.03 -0.01 0.01 -0.03 -0.03 0.07 -0.03

35 6 0.02 0.06 0.00 -0.09 -0.06 0.07 -0.00 0.10 -0.07

36 6 0.09 0.15 -0.06 -0.10 -0.07 0.09 -0.03 0.07 -0.03

37 6 -0.01 0.01 -0.03 -0.01 0.01 0.03 0.03 -0.07 -0.03

38 6 0.02 0.06 -0.00 -0.09 -0.06 -0.07 0.00 -0.10 -0.07

39 6 0.09 0.15 0.06 -0.10 -0.07 -0.09 0.03 -0.07 -0.03

40 6 0.14 0.17 0.09 -0.03 -0.00 -0.02 0.09 -0.00 0.04

41 6 0.11 0.11 0.04 0.05 0.07 0.08 0.11 0.03 0.08

42 6 0.03 0.02 -0.02 0.05 0.08 0.10 0.08 -0.01 0.03

43 6 -0.02 -0.03 0.02 0.01 -0.00 -0.03 0.02 0.07 0.04

44 6 -0.05 -0.01 0.05 -0.05 0.01 0.04 -0.01 0.10 0.07

45 6 -0.03 -0.03 0.03 -0.03 -0.01 0.06 0.03 0.07 0.03

46 6 0.02 -0.07 -0.03 0.05 -0.05 0.01 0.10 0.01 -0.05

47 6 0.04 -0.09 -0.05 0.11 -0.06 -0.06 0.12 -0.02 -0.08

48 6 0.02 -0.07 -0.03 0.08 -0.03 -0.07 0.08 0.02 -0.03

49 1 -0.03 -0.01 0.06 0.02 0.01 -0.05 0.05 0.05 -0.00

50 1 -0.04 -0.01 0.04 0.02 0.01 0.04 0.06 -0.05 0.00

51 1 -0.03 -0.01 -0.03 0.01 0.00 -0.03 0.03 -0.06 -0.04

52 1 -0.03 -0.02 -0.04 0.01 0.01 -0.02 -0.02 -0.06 0.05

53 1 -0.03 -0.01 0.03 0.01 0.00 0.03 -0.03 0.06 -0.04

54 1 -0.03 -0.02 0.04 0.01 0.01 0.02 0.02 0.06 0.05

55 1 -0.04 -0.01 -0.04 0.02 0.01 -0.04 -0.06 0.05 0.00

56 1 -0.03 -0.01 -0.06 0.02 0.01 0.05 -0.05 -0.05 -0.00

57 1 0.04 -0.09 0.05 0.12 -0.04 0.12 -0.10 0.00 -0.06

58 1 0.08 -0.12 0.09 0.17 -0.08 0.09 -0.17 0.06 -0.13

59 1 0.04 -0.09 0.05 0.08 -0.06 -0.02 -0.13 0.02 -0.08

60 1 -0.05 -0.01 -0.05 -0.07 -0.00 -0.11 -0.00 -0.09 0.06

61 1 -0.09 0.02 -0.08 -0.11 0.03 -0.07 0.05 -0.14 0.12

62 1 0.20 0.24 -0.15 -0.04 -0.01 0.04 -0.12 -0.03 0.08

63 1 0.14 0.12 -0.06 0.11 0.12 -0.14 -0.16 -0.08 0.14

64 1 0.02 -0.02 0.04 0.11 0.13 -0.17 -0.10 -0.02 0.06

65 1 -0.01 0.05 0.02 -0.14 -0.10 0.11 0.03 0.15 -0.12

66 1 0.11 0.20 -0.09 -0.16 -0.13 0.17 -0.01 0.10 -0.06

67 1 -0.01 0.05 -0.02 -0.14 -0.10 -0.11 -0.03 -0.15 -0.12

68 1 0.11 0.20 0.09 -0.16 -0.13 -0.17 0.01 -0.10 -0.06

69 1 0.20 0.24 0.15 -0.04 -0.01 -0.04 0.12 0.03 0.08

70 1 0.14 0.12 0.06 0.11 0.12 0.14 0.16 0.08 0.14

71 1 0.02 -0.02 -0.04 0.11 0.13 0.17 0.10 0.02 0.06

72 1 -0.09 0.02 0.08 -0.11 0.03 0.07 -0.05 0.14 0.12

73 1 -0.05 -0.01 0.05 -0.07 -0.00 0.11 0.00 0.09 0.06

74 1 0.04 -0.09 -0.05 0.08 -0.06 0.02 0.13 -0.02 -0.08

75 1 0.08 -0.12 -0.09 0.17 -0.08 -0.09 0.17 -0.06 -0.13

76 1 0.04 -0.09 -0.05 0.12 -0.04 -0.12 0.10 -0.00 -0.06

77 1 -0.02 -0.03 -0.03 -0.01 0.01 0.02 -0.11 -0.01 -0.01

78 1 -0.02 -0.03 0.03 -0.01 0.01 -0.02 0.11 0.01 -0.01

13 14 15

A A A

Frequencies -- 83.3987 92.2707 93.4827

Red. masses -- 5.3317 3.5020 4.8738

Frc consts -- 0.0218 0.0176 0.0251

IR Inten -- 0.0064 0.5960 0.0278

Atom AN X Y Z X Y Z X Y Z

1 6 0.09 0.00 -0.04 0.00 -0.03 -0.14 -0.00 0.04 0.13

2 6 0.08 0.01 -0.05 0.00 0.01 0.01 -0.00 0.02 0.05

3 7 0.07 0.01 -0.00 -0.00 0.03 0.10 -0.00 0.01 0.03

4 6 0.08 0.01 0.03 -0.00 0.01 0.01 -0.00 0.02 0.09

5 6 0.09 0.01 0.01 0.00 -0.03 -0.15 -0.00 0.04 0.15

6 6 0.07 -0.01 0.06 -0.00 0.01 0.02 0.01 0.01 0.03

7 6 0.04 -0.02 0.04 -0.01 0.01 0.01 0.01 0.01 -0.05

8 7 -0.00 0.01 0.00 -0.00 0.01 -0.00 0.01 0.00 -0.05

9 6 -0.04 -0.02 -0.03 0.00 0.01 -0.00 0.02 0.00 -0.08

10 6 -0.02 -0.07 -0.00 -0.00 0.02 0.01 0.03 0.00 -0.13

11 6 0.02 -0.07 0.03 -0.01 0.02 0.01 0.03 0.00 -0.10

12 6 0.07 0.02 -0.06 0.00 0.01 0.01 -0.01 0.01 -0.03

13 6 0.04 0.02 -0.03 0.00 0.01 0.00 -0.02 -0.00 -0.08

14 6 0.02 0.07 -0.00 -0.00 0.02 -0.01 -0.03 -0.00 -0.13

15 6 -0.02 0.07 0.03 -0.01 0.02 -0.01 -0.03 -0.00 -0.10

16 6 -0.04 0.02 0.04 -0.01 0.01 -0.01 -0.01 -0.01 -0.05

17 7 0.00 -0.01 0.00 -0.00 0.01 0.00 -0.01 -0.00 -0.05

18 6 -0.07 0.01 0.06 -0.00 0.01 -0.02 -0.01 -0.01 0.03

19 6 -0.08 -0.01 0.03 -0.00 0.01 -0.01 0.00 -0.02 0.09

20 6 -0.09 -0.01 0.01 0.00 -0.03 0.15 0.00 -0.04 0.15

21 6 -0.09 -0.00 -0.04 0.00 -0.03 0.14 0.00 -0.04 0.13

22 6 -0.08 -0.01 -0.05 0.00 0.01 -0.01 0.00 -0.02 0.05

23 7 -0.07 -0.01 -0.00 -0.00 0.03 -0.10 0.00 -0.01 0.03

24 6 -0.07 -0.02 -0.06 0.00 0.01 -0.01 0.01 -0.01 -0.03

25 6 0.07 -0.01 0.07 -0.00 0.01 0.00 0.01 0.01 0.02

26 6 0.07 -0.01 0.07 0.05 -0.03 0.05 -0.03 0.07 -0.04

27 6 0.01 0.05 -0.00 0.07 -0.05 0.06 -0.03 0.08 -0.07

28 6 -0.05 0.11 -0.07 0.03 -0.03 0.01 0.01 0.02 -0.02

29 6 -0.04 0.10 -0.06 -0.03 0.02 -0.05 0.06 -0.03 0.05

30 6 0.03 0.04 0.01 -0.05 0.03 -0.05 0.05 -0.03 0.07

31 6 -0.04 -0.12 0.08 -0.03 -0.02 0.02 -0.01 0.02 0.01

32 6 0.01 -0.06 0.02 -0.06 -0.05 0.06 0.05 0.07 -0.06

33 6 0.06 0.00 -0.06 -0.04 -0.03 0.05 0.04 0.06 -0.07

34 6 0.07 0.01 -0.07 0.00 0.01 0.00 -0.01 0.01 -0.02

35 6 0.04 -0.03 -0.02 0.04 0.04 -0.04 -0.07 -0.03 0.05

36 6 -0.02 -0.10 0.05 0.03 0.03 -0.04 -0.07 -0.03 0.07

37 6 -0.07 -0.01 -0.07 0.00 0.01 -0.00 0.01 -0.01 -0.02

38 6 -0.04 0.03 -0.02 0.04 0.04 0.04 0.07 0.03 0.05

39 6 0.02 0.10 0.05 0.03 0.03 0.04 0.07 0.03 0.07

40 6 0.04 0.12 0.08 -0.03 -0.02 -0.02 0.01 -0.02 0.01

41 6 -0.01 0.06 0.02 -0.06 -0.05 -0.06 -0.05 -0.07 -0.06

42 6 -0.06 -0.00 -0.06 -0.04 -0.03 -0.05 -0.04 -0.06 -0.07

43 6 -0.07 0.01 0.07 -0.00 0.01 -0.00 -0.01 -0.01 0.02

44 6 -0.03 -0.04 0.01 -0.05 0.03 0.05 -0.05 0.03 0.07

45 6 0.04 -0.10 -0.06 -0.03 0.02 0.05 -0.06 0.03 0.05

46 6 0.05 -0.11 -0.07 0.03 -0.03 -0.01 -0.01 -0.02 -0.02

47 6 -0.01 -0.05 -0.00 0.07 -0.05 -0.06 0.03 -0.08 -0.07

48 6 -0.07 0.01 0.07 0.05 -0.03 -0.05 0.03 -0.07 -0.04

49 1 0.10 0.00 -0.07 -0.00 -0.07 -0.25 0.00 0.05 0.15

50 1 0.10 0.01 0.03 0.02 -0.07 -0.25 -0.01 0.06 0.20

51 1 -0.04 -0.11 -0.01 -0.00 0.02 0.01 0.04 0.01 -0.15

52 1 0.04 -0.10 0.05 -0.01 0.02 0.02 0.03 -0.00 -0.11

53 1 0.04 0.11 -0.01 -0.00 0.02 -0.01 -0.04 -0.01 -0.15

54 1 -0.04 0.10 0.05 -0.01 0.02 -0.02 -0.03 0.00 -0.11

55 1 -0.10 -0.01 0.03 0.02 -0.07 0.25 0.01 -0.06 0.20

56 1 -0.10 -0.00 -0.07 -0.00 -0.06 0.25 -0.00 -0.05 0.15

57 1 0.11 -0.04 0.11 0.08 -0.05 0.08 -0.05 0.11 -0.07

58 1 0.00 0.06 -0.01 0.12 -0.09 0.11 -0.07 0.12 -0.12

59 1 -0.11 0.16 -0.14 0.05 -0.04 0.02 0.01 0.03 -0.04

60 1 -0.08 0.14 -0.11 -0.07 0.05 -0.09 0.09 -0.08 0.09

61 1 0.03 0.03 0.02 -0.09 0.06 -0.09 0.09 -0.07 0.11

62 1 -0.09 -0.18 0.14 -0.04 -0.04 0.03 -0.01 0.02 0.02

63 1 -0.01 -0.08 0.03 -0.10 -0.09 0.10 0.10 0.11 -0.11

64 1 0.09 0.04 -0.09 -0.06 -0.05 0.07 0.08 0.09 -0.12

65 1 0.05 -0.02 -0.03 0.07 0.07 -0.08 -0.12 -0.06 0.08

66 1 -0.05 -0.14 0.09 0.05 0.05 -0.07 -0.12 -0.07 0.12

67 1 -0.05 0.02 -0.03 0.07 0.07 0.08 0.12 0.06 0.08

68 1 0.05 0.14 0.09 0.05 0.05 0.07 0.12 0.07 0.12

69 1 0.09 0.18 0.14 -0.04 -0.04 -0.03 0.01 -0.02 0.02

70 1 0.01 0.08 0.03 -0.10 -0.09 -0.10 -0.10 -0.10 -0.11

71 1 -0.09 -0.04 -0.09 -0.06 -0.05 -0.07 -0.08 -0.09 -0.12

72 1 -0.03 -0.03 0.02 -0.09 0.06 0.09 -0.09 0.07 0.11

73 1 0.08 -0.14 -0.11 -0.07 0.05 0.09 -0.09 0.08 0.09

74 1 0.11 -0.16 -0.14 0.05 -0.04 -0.02 -0.01 -0.03 -0.04

75 1 -0.00 -0.06 -0.01 0.12 -0.09 -0.11 0.07 -0.12 -0.12

76 1 -0.11 0.04 0.11 0.08 -0.05 -0.08 0.05 -0.11 -0.07

77 1 0.08 0.01 0.00 -0.00 0.08 0.30 -0.00 -0.00 -0.03

78 1 -0.08 -0.01 0.00 -0.00 0.08 -0.30 0.00 0.00 -0.03

16 17 18

A A A

Frequencies -- 99.9633 114.2691 137.8536

Red. masses -- 5.3761 4.4878 4.7988

Frc consts -- 0.0317 0.0345 0.0537

IR Inten -- 0.0008 1.5413 1.4952

Atom AN X Y Z X Y Z X Y Z

1 6 -0.04 -0.03 -0.08 0.01 -0.09 -0.12 -0.01 -0.01 -0.06

2 6 -0.03 -0.03 -0.10 0.00 -0.04 0.05 -0.01 -0.02 -0.08

3 7 -0.03 -0.01 -0.01 -0.00 -0.01 0.16 -0.02 0.00 0.01

4 6 -0.04 0.02 0.08 0.00 -0.04 0.05 -0.02 0.01 0.09

5 6 -0.04 0.01 0.04 0.01 -0.09 -0.11 -0.01 0.01 0.05

6 6 -0.05 0.03 0.13 0.02 -0.01 0.03 -0.02 0.01 0.08

7 6 -0.03 0.03 0.09 0.05 0.00 0.02 -0.01 0.00 0.02

8 7 -0.01 0.03 0.01 0.03 0.00 0.10 -0.03 -0.00 0.14

9 6 0.02 0.04 -0.07 0.05 0.00 0.01 -0.01 -0.00 0.02

10 6 0.01 0.05 -0.03 0.08 0.01 -0.13 0.05 0.01 -0.20

11 6 -0.03 0.04 0.08 0.08 0.01 -0.13 0.05 0.00 -0.20

12 6 -0.03 -0.05 -0.12 -0.02 -0.01 0.03 -0.01 -0.01 -0.07

13 6 -0.02 -0.04 -0.07 -0.05 -0.00 0.01 -0.01 -0.00 -0.02

14 6 -0.01 -0.05 -0.03 -0.08 -0.01 -0.13 0.05 0.01 0.20

15 6 0.03 -0.04 0.08 -0.08 -0.01 -0.13 0.05 0.00 0.20

16 6 0.03 -0.03 0.09 -0.05 -0.00 0.02 -0.01 0.00 -0.02

17 7 0.01 -0.03 0.01 -0.03 -0.00 0.10 -0.03 -0.00 -0.14

18 6 0.05 -0.03 0.13 -0.02 0.01 0.03 -0.02 0.01 -0.08

19 6 0.04 -0.02 0.08 -0.00 0.04 0.05 -0.02 0.01 -0.09

20 6 0.04 -0.01 0.04 -0.01 0.09 -0.11 -0.01 0.01 -0.05

21 6 0.04 0.03 -0.08 -0.01 0.09 -0.12 -0.01 -0.01 0.06

22 6 0.03 0.03 -0.10 -0.00 0.04 0.05 -0.01 -0.02 0.08

23 7 0.03 0.01 -0.01 0.00 0.01 0.16 -0.02 0.00 -0.01

24 6 0.03 0.05 -0.12 0.02 0.01 0.03 -0.01 -0.01 0.07

25 6 -0.03 0.02 0.09 0.00 0.01 -0.01 -0.01 0.01 0.05

26 6 0.04 0.05 0.06 0.01 0.01 -0.01 -0.01 0.05 0.01

27 6 0.09 0.02 -0.01 0.02 -0.01 0.01 0.00 0.04 -0.02

28 6 0.05 -0.04 -0.05 0.04 -0.02 0.02 0.02 -0.01 -0.01

29 6 -0.03 -0.07 -0.03 0.02 -0.01 0.01 0.01 -0.05 0.03

30 6 -0.07 -0.04 0.04 0.00 0.00 -0.01 -0.01 -0.03 0.05

31 6 0.05 0.04 0.05 -0.04 -0.03 0.03 0.02 0.01 0.01

32 6 0.07 -0.04 0.03 -0.02 -0.01 0.01 0.01 -0.04 0.03

33 6 0.04 -0.08 -0.04 -0.00 0.01 -0.01 -0.00 -0.05 -0.00

34 6 -0.02 -0.03 -0.09 -0.00 0.01 -0.01 -0.01 -0.01 -0.05

35 6 -0.05 0.04 -0.07 -0.01 0.01 -0.01 -0.01 0.03 -0.05

36 6 -0.01 0.08 0.00 -0.02 -0.01 0.01 0.01 0.05 -0.03

37 6 0.02 0.03 -0.09 0.00 -0.01 -0.01 -0.01 -0.01 0.05

38 6 0.05 -0.04 -0.07 0.01 -0.01 -0.01 -0.01 0.03 0.05

39 6 0.01 -0.08 0.00 0.02 0.01 0.01 0.01 0.05 0.03

40 6 -0.05 -0.04 0.05 0.04 0.03 0.03 0.02 0.01 -0.01

41 6 -0.07 0.04 0.03 0.02 0.01 0.01 0.01 -0.04 -0.03

42 6 -0.04 0.08 -0.04 0.00 -0.01 -0.01 -0.00 -0.05 0.00

43 6 0.03 -0.02 0.09 -0.00 -0.01 -0.01 -0.01 0.01 -0.05

44 6 0.07 0.04 0.04 -0.00 -0.00 -0.01 -0.01 -0.03 -0.05

45 6 0.03 0.07 -0.03 -0.02 0.01 0.01 0.01 -0.05 -0.03

46 6 -0.05 0.04 -0.05 -0.04 0.02 0.02 0.02 -0.01 0.01

47 6 -0.09 -0.02 -0.01 -0.02 0.01 0.01 0.00 0.04 0.02

48 6 -0.04 -0.05 0.06 -0.01 -0.01 -0.01 -0.01 0.05 -0.01

49 1 -0.04 -0.04 -0.13 0.01 -0.12 -0.23 -0.00 -0.02 -0.11

50 1 -0.04 0.02 0.08 0.01 -0.12 -0.23 -0.01 0.01 0.08

51 1 0.02 0.05 -0.08 0.11 0.01 -0.23 0.09 0.02 -0.34

52 1 -0.04 0.04 0.14 0.11 0.00 -0.22 0.09 -0.00 -0.33

53 1 -0.02 -0.05 -0.08 -0.11 -0.01 -0.23 0.09 0.02 0.34

54 1 0.04 -0.04 0.14 -0.11 -0.00 -0.22 0.09 -0.00 0.33

55 1 0.04 -0.02 0.08 -0.01 0.12 -0.23 -0.01 0.01 -0.08

56 1 0.04 0.04 -0.13 -0.01 0.12 -0.23 -0.00 -0.02 0.11

57 1 0.07 0.10 0.10 -0.00 0.02 -0.01 -0.01 0.08 0.01

58 1 0.15 0.05 -0.02 0.03 -0.01 0.01 0.00 0.07 -0.06

59 1 0.08 -0.07 -0.10 0.05 -0.04 0.04 0.03 -0.02 -0.03

60 1 -0.06 -0.12 -0.07 0.02 -0.02 0.01 0.02 -0.09 0.03

61 1 -0.14 -0.06 0.05 -0.01 0.01 -0.01 -0.02 -0.05 0.07

62 1 0.07 0.07 0.10 -0.05 -0.05 0.05 0.03 0.02 0.03

63 1 0.12 -0.08 0.07 -0.03 -0.02 0.02 0.00 -0.07 0.07

64 1 0.06 -0.14 -0.06 0.00 0.02 -0.02 -0.00 -0.09 0.00

65 1 -0.10 0.07 -0.10 0.00 0.01 -0.02 -0.01 0.05 -0.07

66 1 -0.04 0.14 0.02 -0.03 -0.02 0.02 0.02 0.09 -0.04

67 1 0.10 -0.07 -0.10 -0.00 -0.01 -0.02 -0.01 0.05 0.07

68 1 0.04 -0.14 0.02 0.03 0.02 0.02 0.02 0.09 0.04

69 1 -0.07 -0.07 0.10 0.05 0.05 0.05 0.03 0.02 -0.03

70 1 -0.12 0.08 0.07 0.03 0.02 0.02 0.00 -0.07 -0.07

71 1 -0.06 0.14 -0.06 -0.00 -0.02 -0.02 -0.00 -0.09 -0.00

72 1 0.14 0.06 0.05 0.01 -0.01 -0.01 -0.02 -0.05 -0.07

73 1 0.06 0.12 -0.07 -0.02 0.02 0.01 0.02 -0.09 -0.03

74 1 -0.08 0.07 -0.10 -0.05 0.04 0.04 0.03 -0.02 0.03

75 1 -0.15 -0.05 -0.02 -0.03 0.01 0.01 0.00 0.07 0.06

76 1 -0.07 -0.10 0.10 0.00 -0.02 -0.01 -0.01 0.08 -0.01

77 1 -0.03 -0.01 -0.00 -0.00 0.01 0.26 -0.01 0.00 0.01

78 1 0.03 0.01 -0.00 0.00 -0.01 0.26 -0.01 0.00 -0.01

19 20 21

A A A

Frequencies -- 164.3566 179.0815 184.8099

Red. masses -- 7.3115 5.6621 6.4612

Frc consts -- 0.1164 0.1070 0.1300

IR Inten -- 0.4333 0.1270 12.4031

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 -0.12 0.10 0.00 0.02 -0.06 0.00 0.02 0.05

2 6 0.00 -0.15 -0.03 0.00 0.01 -0.09 0.01 -0.01 -0.06

3 7 0.01 -0.19 -0.13 0.00 -0.01 -0.18 0.00 -0.03 -0.15

4 6 0.02 -0.15 -0.03 -0.00 0.00 -0.11 -0.01 -0.01 -0.06

5 6 0.01 -0.12 0.10 0.00 0.02 -0.08 -0.00 0.02 0.05

6 6 0.06 -0.04 -0.02 -0.03 0.00 0.07 -0.03 -0.02 -0.00

7 6 0.14 0.00 0.02 -0.03 0.01 0.12 -0.05 -0.01 0.11

8 7 0.15 0.01 -0.01 -0.00 0.00 0.03 -0.09 -0.01 0.28

9 6 0.13 0.02 0.02 0.03 0.02 -0.09 -0.05 0.00 0.11

10 6 0.13 0.01 0.08 0.03 0.03 -0.09 -0.01 0.00 -0.09

11 6 0.13 0.01 0.08 -0.02 0.02 0.09 -0.01 -0.00 -0.09

12 6 -0.04 -0.05 -0.02 0.03 0.02 0.08 0.04 -0.02 -0.00

13 6 -0.13 -0.02 0.02 0.03 0.02 0.08 0.05 -0.00 0.11

14 6 -0.13 -0.01 0.08 0.03 0.03 0.09 0.01 -0.00 -0.09

15 6 -0.13 -0.01 0.08 -0.02 0.02 -0.09 0.01 0.00 -0.09

16 6 -0.14 -0.00 0.02 -0.03 0.01 -0.12 0.05 0.01 0.11

17 7 -0.15 -0.01 -0.01 -0.00 0.00 -0.03 0.09 0.01 0.28

18 6 -0.06 0.04 -0.02 -0.03 0.00 -0.07 0.03 0.02 -0.00

19 6 -0.02 0.15 -0.03 -0.00 0.00 0.11 0.01 0.01 -0.06

20 6 -0.01 0.12 0.10 0.00 0.02 0.08 0.00 -0.02 0.05

21 6 -0.01 0.12 0.10 0.00 0.02 0.06 -0.00 -0.02 0.05

22 6 -0.00 0.15 -0.03 0.00 0.01 0.09 -0.01 0.01 -0.06

23 7 -0.01 0.19 -0.13 0.00 -0.01 0.18 -0.00 0.03 -0.15

24 6 0.04 0.05 -0.02 0.03 0.02 -0.08 -0.04 0.02 -0.00

25 6 0.01 -0.00 -0.03 -0.02 -0.00 0.10 -0.04 -0.03 -0.03

26 6 0.00 -0.01 -0.02 0.01 0.02 0.07 -0.07 -0.03 -0.04

27 6 0.00 -0.01 -0.01 0.02 0.02 -0.00 -0.07 -0.04 -0.01

28 6 0.01 -0.00 0.00 -0.01 -0.02 -0.05 -0.04 -0.05 0.02

29 6 0.02 0.00 -0.00 -0.04 -0.06 -0.01 -0.02 -0.05 0.02

30 6 0.02 0.01 -0.02 -0.05 -0.05 0.06 -0.03 -0.04 -0.02

31 6 -0.01 -0.01 0.00 0.01 -0.01 -0.06 0.04 -0.05 0.02

32 6 0.00 -0.01 -0.01 -0.04 0.02 -0.00 0.07 -0.03 -0.01

33 6 0.00 -0.01 -0.02 -0.03 0.03 0.09 0.07 -0.03 -0.04

34 6 -0.00 -0.01 -0.03 0.02 0.00 0.12 0.04 -0.02 -0.03

35 6 -0.01 -0.00 -0.02 0.06 -0.05 0.09 0.04 -0.03 -0.02

36 6 -0.01 -0.00 -0.00 0.06 -0.05 -0.01 0.03 -0.05 0.02

37 6 0.00 0.01 -0.03 0.02 0.00 -0.12 -0.04 0.02 -0.03

38 6 0.01 0.00 -0.02 0.06 -0.05 -0.09 -0.04 0.03 -0.02

39 6 0.01 0.00 -0.00 0.06 -0.05 0.01 -0.03 0.05 0.02

40 6 0.01 0.01 0.00 0.01 -0.01 0.06 -0.04 0.05 0.02

41 6 -0.00 0.01 -0.01 -0.04 0.02 0.00 -0.07 0.03 -0.01

42 6 -0.00 0.01 -0.02 -0.03 0.03 -0.09 -0.07 0.03 -0.03

43 6 -0.01 0.00 -0.03 -0.02 -0.00 -0.10 0.04 0.03 -0.03

44 6 -0.02 -0.01 -0.02 -0.05 -0.05 -0.06 0.03 0.04 -0.02

45 6 -0.02 -0.00 -0.00 -0.04 -0.06 0.01 0.02 0.05 0.02

46 6 -0.01 0.00 0.00 -0.01 -0.02 0.05 0.04 0.05 0.02

47 6 -0.00 0.01 -0.01 0.02 0.02 0.00 0.07 0.04 -0.01

48 6 -0.00 0.01 -0.02 0.01 0.02 -0.07 0.07 0.03 -0.04

49 1 0.02 -0.09 0.19 -0.00 0.04 0.00 -0.00 0.04 0.13

50 1 -0.00 -0.09 0.19 0.01 0.03 -0.02 -0.01 0.04 0.13

51 1 0.12 -0.00 0.12 0.06 0.03 -0.19 0.04 0.01 -0.25

52 1 0.12 0.01 0.11 -0.04 0.02 0.16 0.04 0.00 -0.25

53 1 -0.12 0.00 0.12 0.06 0.03 0.19 -0.04 -0.01 -0.25

54 1 -0.12 -0.01 0.11 -0.04 0.02 -0.16 -0.04 -0.00 -0.25

55 1 0.00 0.09 0.19 0.01 0.03 0.02 0.01 -0.04 0.13

56 1 -0.02 0.09 0.19 -0.00 0.04 -0.00 0.00 -0.04 0.13

57 1 0.00 -0.02 -0.02 0.03 0.05 0.10 -0.08 -0.04 -0.06

58 1 -0.00 -0.02 -0.00 0.06 0.05 -0.03 -0.08 -0.04 -0.02

59 1 0.01 -0.01 0.02 -0.01 -0.02 -0.11 -0.02 -0.07 0.05

60 1 0.03 0.01 0.01 -0.07 -0.09 -0.04 0.00 -0.05 0.05

61 1 0.03 0.01 -0.02 -0.08 -0.08 0.09 -0.02 -0.03 -0.02

62 1 -0.01 -0.01 0.02 0.02 -0.00 -0.14 0.03 -0.06 0.05

63 1 0.01 -0.02 -0.00 -0.08 0.06 -0.04 0.09 -0.03 -0.02

64 1 0.01 -0.02 -0.02 -0.06 0.06 0.12 0.09 -0.03 -0.05

65 1 -0.02 -0.00 -0.02 0.10 -0.07 0.12 0.03 -0.03 -0.02

66 1 -0.02 -0.00 0.00 0.09 -0.09 -0.05 0.00 -0.05 0.05

67 1 0.02 0.00 -0.02 0.10 -0.07 -0.12 -0.03 0.03 -0.02

68 1 0.02 0.00 0.00 0.09 -0.09 0.05 -0.00 0.05 0.05

69 1 0.01 0.01 0.02 0.02 -0.00 0.14 -0.03 0.06 0.05

70 1 -0.01 0.02 -0.00 -0.08 0.06 0.04 -0.09 0.03 -0.02

71 1 -0.01 0.02 -0.02 -0.06 0.06 -0.12 -0.09 0.03 -0.05

72 1 -0.03 -0.01 -0.02 -0.08 -0.08 -0.09 0.02 0.03 -0.02

73 1 -0.03 -0.01 0.01 -0.07 -0.09 0.04 -0.00 0.05 0.05

74 1 -0.01 0.01 0.02 -0.01 -0.02 0.11 0.02 0.07 0.05

75 1 0.00 0.02 -0.00 0.06 0.05 0.03 0.08 0.04 -0.02

76 1 -0.00 0.02 -0.02 0.03 0.05 -0.10 0.08 0.04 -0.06

77 1 0.01 -0.20 -0.19 -0.00 -0.02 -0.23 0.00 -0.04 -0.18

78 1 -0.01 0.20 -0.19 -0.00 -0.02 0.23 -0.00 0.04 -0.18

22 23 24

A A A

Frequencies -- 186.9295 202.4249 217.8382

Red. masses -- 6.8119 7.2463 5.9491

Frc consts -- 0.1402 0.1749 0.1663

IR Inten -- 0.2344 2.2045 27.7731

Atom AN X Y Z X Y Z X Y Z

1 6 0.02 0.02 0.07 -0.01 0.06 -0.02 -0.01 0.07 0.03

2 6 0.01 0.03 0.09 -0.02 0.05 -0.06 0.02 0.06 0.03

3 7 0.00 0.00 0.03 -0.00 0.04 -0.11 -0.00 0.07 0.05

4 6 0.01 -0.03 -0.06 0.02 0.05 -0.06 -0.03 0.06 0.03

5 6 0.02 -0.02 -0.05 -0.00 0.06 -0.02 -0.01 0.07 0.03

6 6 0.01 -0.02 -0.06 0.03 0.04 -0.01 -0.07 0.01 -0.00

7 6 0.01 -0.00 0.13 0.01 0.02 0.09 -0.06 0.02 0.01

8 7 -0.02 -0.00 0.29 0.00 -0.00 0.16 -0.00 -0.01 0.00

9 6 0.00 -0.00 0.15 0.02 -0.02 0.08 0.04 0.02 -0.00

10 6 0.04 -0.00 0.01 0.03 0.00 0.01 0.02 0.09 -0.00

11 6 0.05 -0.00 -0.01 0.03 0.00 0.01 -0.04 0.08 0.01

12 6 0.00 0.02 0.04 -0.04 0.04 -0.01 0.06 0.01 0.00

13 6 0.00 -0.00 -0.15 -0.02 0.02 0.08 0.04 0.02 0.00

14 6 0.04 -0.00 -0.01 -0.03 -0.00 0.01 0.02 0.09 0.00

15 6 0.05 -0.00 0.01 -0.03 -0.00 0.01 -0.04 0.08 -0.01

16 6 0.01 -0.00 -0.13 -0.01 -0.02 0.09 -0.06 0.02 -0.01

17 7 -0.02 -0.00 -0.29 -0.00 0.00 0.16 -0.00 -0.01 -0.00

18 6 0.01 -0.02 0.06 -0.03 -0.04 -0.01 -0.07 0.01 0.00

19 6 0.01 -0.03 0.06 -0.02 -0.05 -0.06 -0.03 0.06 -0.03

20 6 0.02 -0.02 0.05 0.00 -0.06 -0.02 -0.01 0.07 -0.03

21 6 0.02 0.02 -0.07 0.01 -0.06 -0.02 -0.01 0.07 -0.03

22 6 0.01 0.03 -0.09 0.02 -0.05 -0.06 0.02 0.06 -0.03

23 7 0.00 0.00 -0.03 0.00 -0.04 -0.11 -0.00 0.07 -0.05

24 6 0.00 0.02 -0.04 0.04 -0.04 -0.01 0.06 0.01 -0.00

25 6 -0.00 -0.00 -0.13 0.06 0.07 -0.03 -0.10 -0.00 -0.04

26 6 -0.05 -0.04 -0.10 0.08 0.08 -0.02 -0.12 -0.00 -0.04

27 6 -0.05 -0.05 0.00 0.08 0.08 0.00 -0.08 -0.05 -0.00

28 6 -0.00 -0.02 0.07 0.09 0.11 0.02 -0.03 -0.11 0.04

29 6 0.03 0.04 0.01 0.08 0.12 0.01 -0.07 -0.08 0.00

30 6 0.02 0.04 -0.09 0.08 0.11 -0.02 -0.11 -0.03 -0.04

31 6 -0.01 0.02 -0.06 -0.11 0.09 0.02 0.06 -0.11 0.04

32 6 -0.05 0.04 -0.01 -0.09 0.07 0.00 0.09 -0.04 -0.00

33 6 -0.05 0.03 0.08 -0.09 0.07 -0.02 0.13 0.01 -0.04

34 6 -0.01 0.00 0.10 -0.07 0.06 -0.03 0.10 0.01 -0.03

35 6 0.01 -0.03 0.08 -0.09 0.10 -0.02 0.12 -0.03 -0.04

36 6 0.02 -0.02 -0.01 -0.10 0.11 0.00 0.08 -0.08 0.00

37 6 -0.01 0.00 -0.10 0.07 -0.06 -0.03 0.10 0.01 0.03

38 6 0.01 -0.03 -0.08 0.09 -0.10 -0.02 0.12 -0.03 0.04

39 6 0.02 -0.02 0.01 0.10 -0.11 0.00 0.08 -0.08 -0.00

40 6 -0.01 0.02 0.06 0.11 -0.09 0.02 0.06 -0.11 -0.04

41 6 -0.05 0.04 0.01 0.09 -0.07 0.00 0.09 -0.04 0.00

42 6 -0.05 0.03 -0.08 0.09 -0.07 -0.02 0.13 0.01 0.04

43 6 -0.00 -0.00 0.13 -0.06 -0.07 -0.03 -0.10 -0.00 0.04

44 6 0.02 0.04 0.09 -0.08 -0.11 -0.02 -0.11 -0.03 0.04

45 6 0.03 0.04 -0.01 -0.08 -0.12 0.01 -0.07 -0.08 -0.00

46 6 -0.00 -0.02 -0.07 -0.09 -0.11 0.02 -0.03 -0.11 -0.04

47 6 -0.05 -0.05 -0.00 -0.08 -0.08 0.00 -0.08 -0.05 0.00

48 6 -0.05 -0.04 0.10 -0.08 -0.08 -0.02 -0.12 -0.00 0.04

49 1 0.02 0.03 0.10 0.00 0.08 0.02 -0.01 0.05 0.01

50 1 0.02 -0.04 -0.10 -0.01 0.08 0.02 -0.01 0.06 0.01

51 1 0.07 -0.00 -0.10 0.06 0.01 -0.06 0.05 0.13 -0.01

52 1 0.08 0.00 -0.15 0.06 -0.00 -0.06 -0.08 0.12 0.01

53 1 0.07 -0.00 0.10 -0.06 -0.01 -0.06 0.05 0.13 0.01

54 1 0.08 0.00 0.15 -0.06 0.00 -0.06 -0.08 0.12 -0.01

55 1 0.02 -0.04 0.10 0.01 -0.08 0.02 -0.01 0.06 -0.01

56 1 0.02 0.03 -0.10 -0.00 -0.08 0.02 -0.01 0.05 -0.01

57 1 -0.09 -0.08 -0.14 0.08 0.08 -0.02 -0.14 0.01 -0.07

58 1 -0.09 -0.09 0.04 0.07 0.06 0.02 -0.05 -0.05 -0.00

59 1 0.02 -0.04 0.16 0.10 0.10 0.04 0.02 -0.16 0.09

60 1 0.06 0.07 0.06 0.08 0.12 0.01 -0.05 -0.10 0.02

61 1 0.06 0.07 -0.12 0.10 0.13 -0.03 -0.15 -0.03 -0.05

62 1 0.01 0.04 -0.13 -0.11 0.09 0.04 0.01 -0.17 0.09

63 1 -0.08 0.06 -0.03 -0.08 0.06 0.02 0.07 -0.04 -0.00

64 1 -0.08 0.05 0.11 -0.09 0.07 -0.02 0.15 0.02 -0.07

65 1 0.04 -0.04 0.10 -0.12 0.11 -0.03 0.16 -0.02 -0.05

66 1 0.05 -0.04 -0.04 -0.10 0.11 0.00 0.07 -0.10 0.03

67 1 0.04 -0.04 -0.10 0.12 -0.11 -0.03 0.16 -0.02 0.05

68 1 0.05 -0.04 0.04 0.10 -0.11 0.00 0.07 -0.10 -0.03

69 1 0.01 0.04 0.13 0.11 -0.09 0.04 0.01 -0.17 -0.09

70 1 -0.08 0.06 0.03 0.08 -0.06 0.02 0.07 -0.04 0.00

71 1 -0.08 0.05 -0.11 0.09 -0.07 -0.02 0.15 0.02 0.07

72 1 0.06 0.07 0.12 -0.10 -0.13 -0.03 -0.15 -0.03 0.05

73 1 0.06 0.07 -0.06 -0.08 -0.12 0.01 -0.05 -0.10 -0.02

74 1 0.02 -0.04 -0.16 -0.10 -0.10 0.04 0.02 -0.16 -0.09

75 1 -0.09 -0.09 -0.04 -0.07 -0.06 0.02 -0.05 -0.05 0.00

76 1 -0.09 -0.08 0.14 -0.08 -0.08 -0.02 -0.14 0.01 0.07

77 1 0.01 0.00 0.03 0.00 0.05 -0.09 0.00 0.07 0.09

78 1 0.01 0.00 -0.03 -0.00 -0.05 -0.09 0.00 0.07 -0.09

25 26 27

A A A

Frequencies -- 222.0124 222.1911 247.9083

Red. masses -- 6.2349 5.3501 5.2940

Frc consts -- 0.1811 0.1556 0.1917

IR Inten -- 0.1004 0.6525 0.0619

Atom AN X Y Z X Y Z X Y Z

1 6 -0.09 -0.05 -0.02 0.00 0.01 0.06 -0.01 0.11 -0.03

2 6 -0.01 -0.07 -0.02 0.00 0.01 0.07 -0.02 0.11 -0.01

3 7 0.02 -0.00 -0.01 -0.00 0.03 0.15 -0.01 0.14 0.03

4 6 -0.02 0.06 0.01 -0.00 0.01 0.07 0.00 0.11 -0.00

5 6 -0.09 0.03 0.01 -0.00 0.01 0.06 -0.00 0.11 -0.03

6 6 -0.01 0.06 -0.00 0.00 -0.00 -0.05 -0.01 -0.00 -0.03

7 6 -0.08 0.02 0.02 -0.01 -0.00 0.02 -0.03 -0.02 -0.03

8 7 -0.09 -0.00 0.03 -0.01 -0.00 0.02 0.01 -0.03 -0.00

9 6 -0.08 -0.03 0.01 -0.01 -0.00 0.02 0.04 -0.01 0.03

10 6 -0.09 -0.01 0.02 -0.02 -0.00 0.08 0.03 0.02 0.02

11 6 -0.09 -0.01 0.02 -0.02 -0.00 0.08 -0.01 0.02 -0.01

12 6 -0.01 -0.07 0.01 -0.00 -0.00 -0.05 0.01 -0.00 -0.04

13 6 -0.08 -0.03 -0.01 0.01 0.00 0.02 0.04 -0.01 -0.03

14 6 -0.09 -0.01 -0.02 0.02 0.00 0.08 0.03 0.02 -0.02

15 6 -0.09 -0.01 -0.02 0.02 0.00 0.08 -0.01 0.02 0.01

16 6 -0.08 0.02 -0.02 0.01 0.00 0.02 -0.03 -0.02 0.03

17 7 -0.09 -0.00 -0.03 0.01 0.00 0.02 0.01 -0.03 0.00

18 6 -0.01 0.06 0.00 -0.00 0.00 -0.05 -0.01 -0.00 0.03

19 6 -0.02 0.06 -0.01 0.00 -0.01 0.07 0.00 0.11 0.00

20 6 -0.09 0.03 -0.01 0.00 -0.01 0.06 -0.00 0.11 0.03

21 6 -0.09 -0.05 0.02 -0.00 -0.01 0.06 -0.01 0.11 0.03

22 6 -0.01 -0.07 0.02 -0.00 -0.01 0.07 -0.02 0.11 0.01

23 7 0.02 -0.00 0.01 0.00 -0.03 0.15 -0.01 0.14 -0.03

24 6 -0.01 -0.07 -0.01 0.00 0.00 -0.05 0.01 -0.00 0.04

25 6 0.01 0.09 -0.02 -0.01 0.01 -0.14 0.06 -0.07 0.01

26 6 0.04 0.11 -0.03 -0.06 -0.02 -0.11 0.04 -0.10 0.03

27 6 0.08 0.08 0.01 -0.05 -0.04 0.00 -0.03 -0.05 0.00

28 6 0.10 0.07 0.04 0.01 -0.02 0.07 -0.07 0.02 -0.04

29 6 0.05 0.10 0.00 0.02 0.05 -0.00 0.01 -0.01 0.01

30 6 0.01 0.12 -0.03 0.01 0.06 -0.11 0.08 -0.07 0.03

31 6 0.11 -0.05 -0.04 -0.01 -0.02 0.07 0.08 0.04 -0.05

32 6 0.08 -0.07 -0.01 0.05 -0.04 0.00 0.04 -0.05 0.01

33 6 0.04 -0.10 0.04 0.06 -0.01 -0.11 -0.04 -0.13 0.04

34 6 0.01 -0.09 0.03 0.01 0.01 -0.14 -0.06 -0.09 0.01

35 6 0.02 -0.11 0.03 -0.01 0.06 -0.12 -0.09 -0.09 0.04

36 6 0.06 -0.08 0.00 -0.03 0.05 -0.00 -0.02 -0.01 0.01

37 6 0.01 -0.09 -0.03 -0.01 -0.01 -0.14 -0.06 -0.09 -0.01

38 6 0.02 -0.11 -0.03 0.01 -0.06 -0.12 -0.09 -0.09 -0.04

39 6 0.06 -0.08 -0.00 0.03 -0.05 -0.00 -0.02 -0.01 -0.01

40 6 0.11 -0.05 0.04 0.01 0.02 0.07 0.08 0.04 0.05

41 6 0.08 -0.07 0.01 -0.05 0.03 0.00 0.04 -0.05 -0.01

42 6 0.04 -0.10 -0.03 -0.06 0.01 -0.11 -0.04 -0.13 -0.04

43 6 0.01 0.09 0.02 0.01 -0.01 -0.14 0.06 -0.07 -0.01

44 6 0.01 0.12 0.03 -0.01 -0.06 -0.11 0.08 -0.07 -0.03

45 6 0.05 0.10 -0.00 -0.02 -0.05 -0.00 0.01 -0.01 -0.01

46 6 0.11 0.07 -0.04 -0.01 0.02 0.07 -0.07 0.02 0.04

47 6 0.08 0.08 -0.01 0.05 0.04 0.00 -0.03 -0.05 -0.00

48 6 0.04 0.11 0.03 0.06 0.02 -0.11 0.04 -0.10 -0.03

49 1 -0.13 -0.10 -0.02 0.00 -0.00 0.02 -0.01 0.11 -0.06

50 1 -0.14 0.07 0.03 -0.01 -0.00 0.02 -0.00 0.11 -0.06

51 1 -0.09 -0.01 0.01 -0.04 -0.01 0.13 0.04 0.04 0.03

52 1 -0.08 -0.01 0.01 -0.04 0.01 0.12 -0.03 0.04 -0.02

53 1 -0.09 -0.01 -0.01 0.04 0.01 0.13 0.04 0.04 -0.03

54 1 -0.08 -0.01 -0.02 0.04 -0.01 0.12 -0.03 0.04 0.02

55 1 -0.14 0.07 -0.03 0.01 0.00 0.02 -0.00 0.11 0.06

56 1 -0.13 -0.10 0.02 -0.01 0.00 0.02 -0.01 0.11 0.06

57 1 0.04 0.14 -0.03 -0.09 -0.06 -0.15 0.05 -0.15 0.04

58 1 0.09 0.07 0.03 -0.07 -0.09 0.05 -0.06 -0.05 -0.00

59 1 0.15 0.04 0.08 0.04 -0.06 0.18 -0.15 0.09 -0.10

60 1 0.05 0.08 -0.00 0.05 0.09 0.04 0.01 0.02 0.01

61 1 0.01 0.14 -0.05 0.03 0.09 -0.15 0.12 -0.08 0.05

62 1 0.15 -0.00 -0.08 -0.04 -0.06 0.18 0.16 0.14 -0.12

63 1 0.09 -0.05 -0.03 0.08 -0.08 0.05 0.07 -0.04 -0.00

64 1 0.04 -0.13 0.04 0.10 -0.04 -0.15 -0.05 -0.18 0.06

65 1 0.02 -0.13 0.06 -0.04 0.08 -0.15 -0.14 -0.11 0.06

66 1 0.05 -0.07 0.00 -0.06 0.08 0.03 -0.02 0.03 0.01

67 1 0.02 -0.13 -0.06 0.04 -0.09 -0.15 -0.14 -0.11 -0.06

68 1 0.05 -0.07 -0.00 0.06 -0.08 0.03 -0.02 0.03 -0.01

69 1 0.15 -0.00 0.08 0.04 0.06 0.18 0.16 0.14 0.12

70 1 0.09 -0.05 0.03 -0.08 0.08 0.05 0.07 -0.04 0.00

71 1 0.04 -0.13 -0.04 -0.10 0.04 -0.15 -0.05 -0.18 -0.06

72 1 0.01 0.14 0.05 -0.03 -0.09 -0.15 0.12 -0.08 -0.05

73 1 0.05 0.08 0.00 -0.05 -0.09 0.04 0.01 0.02 -0.01

74 1 0.15 0.03 -0.08 -0.04 0.06 0.18 -0.15 0.09 0.10

75 1 0.09 0.07 -0.03 0.07 0.09 0.05 -0.06 -0.05 0.00

76 1 0.04 0.14 0.03 0.09 0.06 -0.15 0.05 -0.15 -0.04

77 1 0.09 0.00 -0.01 -0.00 0.02 0.11 -0.02 0.16 0.11

78 1 0.09 0.00 0.01 0.00 -0.02 0.11 -0.02 0.16 -0.11

28 29 30

A A A

Frequencies -- 249.1008 255.9836 282.0783

Red. masses -- 5.1887 4.4799 5.5173

Frc consts -- 0.1897 0.1730 0.2587

IR Inten -- 2.6949 0.5333 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.02 0.02 -0.01 0.00 0.00 0.00 0.00 -0.03 -0.16

2 6 -0.02 0.03 -0.02 0.01 -0.00 -0.01 -0.01 -0.03 -0.18

3 7 -0.04 -0.01 0.00 0.00 -0.01 -0.04 -0.02 -0.00 0.00

4 6 -0.01 -0.05 0.02 -0.01 -0.00 -0.01 -0.01 0.03 0.18

5 6 0.02 -0.03 0.01 -0.00 0.00 0.00 -0.00 0.03 0.15

6 6 -0.00 -0.00 0.04 -0.02 0.02 0.04 0.00 -0.00 0.01

7 6 0.10 0.02 -0.00 0.00 0.01 -0.01 0.02 -0.02 -0.13

8 7 0.12 0.01 -0.06 0.01 0.00 -0.04 0.00 -0.01 -0.00

9 6 0.09 -0.00 -0.01 0.01 -0.01 -0.01 -0.02 -0.03 0.13

10 6 0.10 0.00 0.04 -0.00 -0.00 0.00 -0.03 -0.03 0.14

11 6 0.10 0.01 0.04 -0.00 0.00 0.00 0.03 -0.02 -0.14

12 6 -0.00 0.00 -0.03 0.02 0.02 0.03 0.00 0.00 -0.01

13 6 0.09 -0.00 0.01 -0.01 0.01 -0.01 0.02 0.03 0.13

14 6 0.10 0.00 -0.04 0.00 0.00 0.00 0.03 0.03 0.14

15 6 0.10 0.01 -0.04 0.00 -0.00 0.00 -0.03 0.02 -0.14

16 6 0.10 0.02 0.00 -0.00 -0.01 -0.01 -0.02 0.02 -0.13

17 7 0.12 0.01 0.06 -0.01 -0.00 -0.04 -0.00 0.01 -0.00

18 6 -0.00 -0.00 -0.04 0.02 -0.02 0.04 -0.00 0.00 0.01

19 6 -0.01 -0.05 -0.02 0.01 0.00 -0.01 0.01 -0.03 0.18

20 6 0.02 -0.03 -0.01 0.00 -0.00 0.00 0.00 -0.03 0.15

21 6 0.02 0.02 0.01 -0.00 -0.00 0.00 -0.00 0.03 -0.16

22 6 -0.02 0.03 0.02 -0.01 0.00 -0.01 0.01 0.03 -0.18

23 7 -0.04 -0.01 -0.00 -0.00 0.01 -0.04 0.02 0.00 0.00

24 6 -0.00 0.00 0.03 -0.02 -0.02 0.03 -0.00 -0.00 -0.01

25 6 -0.09 0.07 -0.00 -0.09 0.08 0.03 -0.01 -0.01 -0.02

26 6 -0.08 0.11 -0.04 -0.07 0.13 -0.01 -0.02 -0.00 -0.02

27 6 0.01 0.04 -0.00 0.02 0.06 -0.00 -0.02 0.00 -0.01

28 6 0.06 -0.06 0.05 0.07 -0.05 0.04 0.00 -0.01 0.02

29 6 -0.04 -0.02 -0.01 -0.05 -0.02 -0.01 0.00 -0.01 0.01

30 6 -0.13 0.06 -0.04 -0.13 0.06 -0.02 -0.01 0.01 -0.02

31 6 0.04 0.06 -0.04 -0.06 -0.06 0.04 -0.00 0.01 -0.01

32 6 0.01 -0.03 0.00 -0.03 0.05 -0.00 -0.02 -0.00 0.01

33 6 -0.06 -0.10 0.03 0.05 0.14 -0.02 -0.02 0.00 0.02

34 6 -0.07 -0.07 0.00 0.08 0.09 0.03 -0.01 0.01 0.02

35 6 -0.10 -0.06 0.03 0.12 0.08 -0.02 -0.01 -0.01 0.02

36 6 -0.04 0.01 0.01 0.05 -0.01 -0.01 0.00 0.01 -0.01

37 6 -0.07 -0.07 -0.00 -0.08 -0.09 0.03 0.01 -0.01 0.02

38 6 -0.10 -0.06 -0.03 -0.12 -0.08 -0.02 0.01 0.01 0.02

39 6 -0.04 0.01 -0.01 -0.05 0.01 -0.01 -0.00 -0.01 -0.01

40 6 0.04 0.06 0.04 0.06 0.06 0.04 0.00 -0.01 -0.01

41 6 0.01 -0.03 -0.00 0.03 -0.05 -0.00 0.02 0.00 0.01

42 6 -0.06 -0.10 -0.03 -0.05 -0.14 -0.02 0.02 -0.00 0.02

43 6 -0.09 0.07 0.00 0.09 -0.08 0.03 0.01 0.01 -0.02

44 6 -0.13 0.06 0.04 0.13 -0.06 -0.02 0.01 -0.01 -0.02

45 6 -0.04 -0.02 0.01 0.05 0.02 -0.01 -0.00 0.01 0.01

46 6 0.06 -0.06 -0.05 -0.07 0.05 0.04 -0.00 0.01 0.02

47 6 0.01 0.04 0.00 -0.02 -0.06 -0.00 0.02 -0.00 -0.01

48 6 -0.08 0.11 0.04 0.07 -0.13 -0.01 0.02 0.00 -0.02

49 1 0.04 0.04 -0.01 0.00 0.00 0.01 0.01 -0.05 -0.25

50 1 0.05 -0.05 0.01 -0.00 0.00 0.01 -0.00 0.05 0.25

51 1 0.09 -0.00 0.07 0.00 -0.00 0.00 -0.06 -0.03 0.27

52 1 0.09 0.01 0.07 -0.00 0.00 0.01 0.06 -0.02 -0.27

53 1 0.09 -0.00 -0.07 -0.00 0.00 0.00 0.06 0.03 0.27

54 1 0.09 0.01 -0.07 0.00 -0.00 0.01 -0.06 0.02 -0.27

55 1 0.05 -0.05 -0.01 0.00 -0.00 0.01 0.00 -0.05 0.25

56 1 0.04 0.04 0.01 -0.00 -0.00 0.01 -0.01 0.05 -0.25

57 1 -0.10 0.17 -0.05 -0.08 0.20 -0.02 -0.02 -0.01 -0.02

58 1 0.05 0.04 -0.00 0.07 0.07 -0.01 -0.04 0.00 -0.02

59 1 0.16 -0.15 0.12 0.17 -0.14 0.09 0.01 -0.02 0.04

60 1 -0.04 -0.06 -0.01 -0.05 -0.07 -0.02 0.02 -0.01 0.02

61 1 -0.19 0.07 -0.06 -0.21 0.06 -0.03 -0.01 0.02 -0.04

62 1 0.12 0.15 -0.10 -0.15 -0.16 0.09 0.01 0.02 -0.03

63 1 0.05 -0.03 0.00 -0.08 0.06 -0.01 -0.04 -0.01 0.02

64 1 -0.07 -0.15 0.05 0.05 0.21 -0.03 -0.02 0.01 0.02

65 1 -0.15 -0.07 0.05 0.19 0.09 -0.03 -0.01 -0.02 0.04

66 1 -0.04 0.05 0.01 0.06 -0.07 -0.01 0.02 0.01 -0.02

67 1 -0.15 -0.07 -0.05 -0.19 -0.09 -0.03 0.01 0.02 0.04

68 1 -0.04 0.05 -0.01 -0.06 0.07 -0.01 -0.02 -0.01 -0.02

69 1 0.12 0.15 0.10 0.15 0.16 0.09 -0.01 -0.02 -0.03

70 1 0.05 -0.03 -0.00 0.08 -0.06 -0.01 0.04 0.01 0.02

71 1 -0.07 -0.15 -0.05 -0.05 -0.21 -0.03 0.02 -0.01 0.02

72 1 -0.19 0.07 0.06 0.21 -0.06 -0.03 0.01 -0.02 -0.04

73 1 -0.04 -0.06 0.01 0.05 0.07 -0.02 -0.02 0.01 0.02

74 1 0.16 -0.15 -0.12 -0.17 0.14 0.09 -0.01 0.02 0.04

75 1 0.05 0.04 0.00 -0.07 -0.07 -0.01 0.04 -0.00 -0.02

76 1 -0.10 0.17 0.05 0.08 -0.20 -0.02 0.02 0.01 -0.02

77 1 -0.10 -0.02 -0.01 -0.00 -0.01 -0.03 -0.03 -0.00 0.00

78 1 -0.10 -0.02 0.01 0.00 0.01 -0.03 0.03 0.00 0.00

31 32 33

A A A

Frequencies -- 289.4132 307.6043 310.9301

Red. masses -- 4.4759 5.4529 4.8261

Frc consts -- 0.2209 0.3040 0.2749

IR Inten -- 0.0005 0.3600 0.0703

Atom AN X Y Z X Y Z X Y Z

1 6 -0.09 -0.04 0.01 -0.02 0.04 0.17 -0.00 -0.01 -0.01

2 6 -0.03 -0.05 0.02 -0.01 0.04 0.19 0.01 -0.00 -0.00

3 7 0.00 0.00 -0.00 -0.01 -0.00 0.00 0.00 -0.01 -0.02

4 6 -0.03 0.05 -0.02 -0.01 -0.04 -0.19 -0.01 -0.01 -0.01

5 6 -0.10 0.03 -0.01 -0.01 -0.04 -0.17 -0.00 -0.01 -0.02

6 6 -0.03 0.03 -0.05 -0.01 0.00 -0.03 -0.01 0.01 -0.03

7 6 -0.04 0.02 -0.06 -0.00 0.01 0.02 0.03 0.01 -0.16

8 7 0.00 -0.00 0.00 -0.01 -0.00 0.04 -0.00 0.01 0.00

9 6 0.04 0.03 0.06 -0.00 -0.01 0.01 -0.03 0.00 0.16

10 6 0.02 0.08 0.04 0.01 0.00 -0.04 -0.04 0.00 0.17

11 6 -0.02 0.08 -0.04 0.01 -0.00 -0.03 0.04 0.01 -0.17

12 6 -0.03 -0.03 0.05 -0.01 -0.00 0.03 0.00 0.01 -0.03

13 6 -0.04 -0.03 0.06 -0.00 -0.01 -0.01 -0.03 0.00 -0.16

14 6 -0.02 -0.08 0.04 0.01 0.00 0.04 -0.04 0.00 -0.17

15 6 0.02 -0.08 -0.04 0.01 -0.00 0.03 0.04 0.01 0.17

16 6 0.04 -0.02 -0.06 -0.00 0.01 -0.02 0.03 0.01 0.16

17 7 -0.00 0.00 0.00 -0.01 -0.00 -0.04 -0.00 0.01 -0.00

18 6 0.03 -0.03 -0.05 -0.01 0.00 0.03 -0.01 0.01 0.03

19 6 0.03 -0.05 -0.02 -0.01 -0.04 0.19 -0.01 -0.01 0.01

20 6 0.10 -0.03 -0.01 -0.01 -0.04 0.17 -0.00 -0.01 0.02

21 6 0.09 0.04 0.01 -0.02 0.04 -0.17 -0.00 -0.01 0.01

22 6 0.03 0.05 0.02 -0.01 0.04 -0.19 0.01 -0.00 0.00

23 7 -0.00 -0.00 -0.00 -0.01 -0.00 -0.00 0.00 -0.01 0.02

24 6 0.03 0.03 0.05 -0.01 -0.00 -0.03 0.00 0.01 0.03

25 6 0.04 -0.04 0.02 -0.02 0.03 0.08 -0.04 0.02 0.08

26 6 0.07 -0.08 0.07 0.03 0.05 0.07 0.00 0.03 0.07

27 6 0.01 -0.03 0.01 0.05 0.04 0.01 0.02 0.03 0.00

28 6 -0.06 0.05 -0.07 0.02 0.02 -0.04 -0.01 -0.01 -0.03

29 6 0.02 -0.02 0.01 -0.02 -0.02 0.00 -0.03 -0.06 0.01

30 6 0.08 -0.07 0.07 -0.03 -0.00 0.07 -0.05 -0.03 0.07

31 6 -0.05 -0.05 0.07 0.02 -0.02 0.04 0.01 -0.01 -0.03

32 6 0.01 0.03 -0.01 0.06 -0.03 -0.01 -0.02 0.02 -0.00

33 6 0.06 0.09 -0.07 0.03 -0.05 -0.07 -0.00 0.03 0.07

34 6 0.03 0.04 -0.02 -0.02 -0.03 -0.08 0.03 0.02 0.07

35 6 0.07 0.08 -0.07 -0.03 0.00 -0.08 0.05 -0.02 0.06

36 6 0.02 0.02 -0.02 -0.02 0.02 -0.00 0.04 -0.05 0.01

37 6 -0.03 -0.04 -0.02 -0.02 -0.03 0.08 0.03 0.02 -0.07

38 6 -0.07 -0.08 -0.07 -0.03 0.00 0.08 0.05 -0.02 -0.06

39 6 -0.02 -0.02 -0.02 -0.02 0.02 0.00 0.04 -0.05 -0.01

40 6 0.05 0.05 0.07 0.02 -0.02 -0.04 0.01 -0.01 0.03

41 6 -0.01 -0.03 -0.01 0.06 -0.03 0.01 -0.02 0.02 0.00

42 6 -0.06 -0.09 -0.07 0.03 -0.05 0.07 -0.00 0.03 -0.07

43 6 -0.04 0.04 0.02 -0.02 0.03 -0.08 -0.04 0.02 -0.08

44 6 -0.08 0.07 0.07 -0.03 -0.00 -0.07 -0.05 -0.03 -0.07

45 6 -0.02 0.02 0.01 -0.02 -0.02 -0.00 -0.03 -0.06 -0.01

46 6 0.06 -0.05 -0.07 0.02 0.02 0.04 -0.01 -0.01 0.03

47 6 -0.01 0.03 0.01 0.05 0.04 -0.01 0.02 0.03 -0.00

48 6 -0.07 0.08 0.07 0.03 0.05 -0.07 0.00 0.03 -0.07

49 1 -0.13 -0.07 0.01 -0.02 0.07 0.27 -0.00 -0.02 -0.03

50 1 -0.14 0.06 -0.01 -0.01 -0.07 -0.27 0.00 -0.02 -0.03

51 1 0.04 0.12 0.07 0.03 0.01 -0.10 -0.08 -0.00 0.31

52 1 -0.05 0.11 -0.07 0.03 -0.01 -0.09 0.08 0.01 -0.31

53 1 -0.04 -0.12 0.07 0.03 0.01 0.10 -0.08 -0.00 -0.31

54 1 0.05 -0.11 -0.07 0.03 -0.01 0.09 0.08 0.01 0.31

55 1 0.14 -0.06 -0.01 -0.01 -0.07 0.27 0.00 -0.02 0.03

56 1 0.13 0.07 0.01 -0.02 0.07 -0.27 -0.00 -0.02 0.03

57 1 0.10 -0.11 0.10 0.04 0.10 0.09 0.02 0.07 0.10

58 1 0.00 -0.02 0.00 0.09 0.06 -0.01 0.05 0.06 -0.03

59 1 -0.15 0.13 -0.16 0.02 0.03 -0.10 -0.01 -0.01 -0.09

60 1 0.02 -0.01 0.01 -0.04 -0.06 -0.03 -0.04 -0.10 -0.01

61 1 0.12 -0.09 0.10 -0.06 -0.03 0.09 -0.10 -0.04 0.08

62 1 -0.13 -0.15 0.16 0.02 -0.02 0.10 0.01 -0.01 -0.09

63 1 -0.00 0.02 -0.00 0.10 -0.05 0.01 -0.05 0.05 -0.03

64 1 0.08 0.13 -0.10 0.05 -0.09 -0.09 -0.03 0.06 0.09

65 1 0.11 0.10 -0.10 -0.06 0.02 -0.10 0.10 -0.03 0.07

66 1 0.02 0.01 -0.01 -0.05 0.05 0.03 0.06 -0.09 -0.01

67 1 -0.11 -0.10 -0.10 -0.06 0.02 0.10 0.10 -0.03 -0.07

68 1 -0.02 -0.01 -0.01 -0.05 0.05 -0.03 0.06 -0.09 0.01

69 1 0.13 0.15 0.16 0.02 -0.02 -0.10 0.01 -0.01 0.09

70 1 0.00 -0.02 -0.00 0.10 -0.05 -0.01 -0.05 0.05 0.03

71 1 -0.08 -0.13 -0.10 0.05 -0.09 0.09 -0.03 0.06 -0.09

72 1 -0.12 0.09 0.10 -0.06 -0.03 -0.09 -0.10 -0.04 -0.08

73 1 -0.02 0.01 0.01 -0.04 -0.06 0.03 -0.04 -0.10 0.01

74 1 0.15 -0.13 -0.16 0.02 0.03 0.10 -0.01 -0.01 0.09

75 1 -0.00 0.02 0.00 0.09 0.06 0.01 0.05 0.06 0.03

76 1 -0.10 0.11 0.10 0.04 0.10 -0.09 0.02 0.07 -0.10

77 1 0.05 0.01 0.00 -0.01 -0.00 -0.01 -0.00 0.00 0.04

78 1 -0.05 -0.01 0.00 -0.01 -0.00 0.01 -0.00 0.00 -0.04

34 35 36

A A A

Frequencies -- 319.7050 332.9039 372.0131

Red. masses -- 4.8847 7.6169 6.3865

Frc consts -- 0.2942 0.4974 0.5207

IR Inten -- 0.0006 0.5235 0.0107

Atom AN X Y Z X Y Z X Y Z

1 6 0.03 0.04 0.08 0.02 -0.15 0.03 0.05 -0.06 0.01

2 6 -0.01 0.05 0.09 0.03 -0.13 0.03 0.11 -0.08 0.02

3 7 -0.02 0.00 -0.00 0.00 -0.18 0.02 0.17 0.00 -0.00

4 6 0.00 -0.05 -0.09 -0.02 -0.14 0.02 0.10 0.08 -0.02

5 6 0.03 -0.04 -0.08 0.00 -0.16 0.03 0.05 0.06 -0.00

6 6 0.01 -0.01 -0.03 -0.02 -0.01 -0.00 0.06 0.06 0.00

7 6 0.05 0.00 -0.11 -0.14 -0.03 -0.03 0.05 0.09 0.00

8 7 0.00 0.01 0.00 -0.19 -0.01 -0.02 -0.01 0.12 0.00

9 6 -0.05 -0.00 0.12 -0.14 0.01 -0.02 -0.07 0.09 -0.00

10 6 -0.04 -0.03 0.12 -0.17 -0.01 -0.03 -0.05 0.05 -0.00

11 6 0.05 -0.03 -0.12 -0.17 -0.02 -0.04 0.03 0.05 -0.00

12 6 0.01 0.01 0.03 0.02 -0.01 0.00 0.07 -0.05 -0.00

13 6 0.05 0.00 0.12 0.14 -0.01 -0.02 0.07 -0.09 -0.00

14 6 0.04 0.03 0.12 0.17 0.01 -0.03 0.05 -0.05 -0.00

15 6 -0.05 0.03 -0.12 0.17 0.02 -0.04 -0.03 -0.05 -0.00

16 6 -0.05 -0.00 -0.11 0.14 0.03 -0.03 -0.05 -0.09 0.00

17 7 -0.00 -0.01 0.00 0.19 0.01 -0.02 0.01 -0.12 0.00

18 6 -0.01 0.01 -0.03 0.02 0.01 -0.00 -0.06 -0.06 0.00

19 6 -0.00 0.05 -0.09 0.02 0.14 0.02 -0.10 -0.08 -0.02

20 6 -0.03 0.04 -0.08 -0.00 0.16 0.03 -0.05 -0.06 -0.00

21 6 -0.03 -0.04 0.08 -0.02 0.15 0.03 -0.05 0.06 0.01

22 6 0.01 -0.05 0.09 -0.03 0.13 0.03 -0.11 0.08 0.02

23 7 0.02 -0.00 -0.00 -0.00 0.18 0.02 -0.17 -0.00 -0.00

24 6 -0.01 -0.01 0.03 -0.02 0.01 0.00 -0.07 0.05 -0.00

25 6 -0.04 0.03 0.09 0.01 0.01 -0.00 0.01 0.01 0.01

26 6 -0.00 0.07 0.07 0.04 0.03 -0.00 -0.07 -0.03 0.02

27 6 0.03 0.05 0.00 0.04 0.04 -0.01 -0.07 -0.05 0.02

28 6 0.02 -0.01 -0.03 0.05 0.06 -0.00 -0.08 -0.10 -0.00

29 6 -0.03 -0.04 0.00 0.03 0.05 0.01 -0.05 -0.08 -0.02

30 6 -0.07 -0.00 0.07 0.03 0.04 0.01 -0.04 -0.07 -0.02

31 6 0.02 0.01 0.03 -0.05 0.04 0.00 -0.09 0.09 -0.00

32 6 0.04 -0.04 -0.00 -0.04 0.03 -0.01 -0.08 0.04 -0.02

33 6 0.01 -0.07 -0.07 -0.04 0.02 -0.01 -0.08 0.02 -0.02

34 6 -0.04 -0.04 -0.09 -0.01 0.01 -0.00 0.01 -0.01 -0.01

35 6 -0.07 -0.01 -0.07 -0.02 0.04 0.01 -0.05 0.06 0.02

36 6 -0.04 0.04 -0.01 -0.03 0.04 0.01 -0.06 0.07 0.02

37 6 0.04 0.04 -0.09 0.01 -0.01 -0.00 -0.01 0.01 -0.01

38 6 0.07 0.01 -0.07 0.02 -0.04 0.01 0.05 -0.06 0.02

39 6 0.04 -0.04 -0.01 0.03 -0.04 0.01 0.06 -0.07 0.02

40 6 -0.02 -0.01 0.03 0.05 -0.04 0.00 0.09 -0.09 -0.00

41 6 -0.04 0.04 -0.00 0.04 -0.03 -0.01 0.08 -0.04 -0.02

42 6 -0.01 0.07 -0.07 0.04 -0.02 -0.01 0.08 -0.02 -0.02

43 6 0.04 -0.03 0.09 -0.01 -0.01 -0.00 -0.01 -0.01 0.01

44 6 0.07 0.00 0.07 -0.03 -0.04 0.01 0.04 0.07 -0.02

45 6 0.03 0.04 0.00 -0.03 -0.05 0.01 0.05 0.08 -0.02

46 6 -0.02 0.01 -0.03 -0.05 -0.06 -0.00 0.08 0.10 -0.00

47 6 -0.03 -0.05 0.00 -0.04 -0.04 -0.01 0.07 0.05 0.02

48 6 0.00 -0.07 0.07 -0.04 -0.03 -0.00 0.07 0.03 0.02

49 1 0.05 0.08 0.13 0.00 -0.16 0.05 -0.01 -0.12 0.01

50 1 0.06 -0.07 -0.13 0.02 -0.17 0.04 -0.02 0.10 -0.01

51 1 -0.08 -0.06 0.22 -0.18 -0.02 -0.04 -0.08 -0.00 -0.01

52 1 0.09 -0.04 -0.22 -0.18 -0.00 -0.05 0.07 0.01 0.00

53 1 0.08 0.06 0.22 0.18 0.02 -0.04 0.08 0.00 -0.01

54 1 -0.09 0.04 -0.22 0.18 0.00 -0.05 -0.07 -0.01 0.00

55 1 -0.06 0.07 -0.13 -0.02 0.17 0.04 0.02 -0.10 -0.01

56 1 -0.05 -0.08 0.13 -0.00 0.16 0.05 0.01 0.12 0.01

57 1 0.01 0.12 0.09 0.05 0.04 0.01 -0.09 -0.06 -0.01

58 1 0.08 0.08 -0.03 0.03 0.03 -0.00 -0.03 -0.03 -0.00

59 1 0.04 -0.02 -0.07 0.04 0.06 -0.00 -0.07 -0.11 0.00

60 1 -0.06 -0.09 -0.03 0.03 0.03 0.01 -0.05 -0.05 -0.02

61 1 -0.12 -0.02 0.08 0.05 0.05 0.00 -0.10 -0.09 -0.00

62 1 0.03 0.03 0.07 -0.05 0.04 0.00 -0.09 0.10 -0.01

63 1 0.09 -0.07 0.03 -0.03 0.03 -0.00 -0.04 0.03 -0.00

64 1 0.03 -0.12 -0.09 -0.04 0.04 0.00 -0.10 0.05 0.01

65 1 -0.12 0.00 -0.08 -0.04 0.04 -0.00 -0.11 0.07 0.00

66 1 -0.07 0.08 0.02 -0.03 0.02 0.00 -0.06 0.04 0.02

67 1 0.12 -0.00 -0.08 0.04 -0.04 -0.00 0.11 -0.07 0.00

68 1 0.07 -0.08 0.02 0.03 -0.02 0.00 0.06 -0.04 0.02

69 1 -0.03 -0.03 0.07 0.05 -0.04 0.00 0.09 -0.10 -0.01

70 1 -0.09 0.07 0.03 0.03 -0.03 -0.00 0.04 -0.03 -0.00

71 1 -0.03 0.12 -0.09 0.04 -0.04 0.00 0.10 -0.05 0.01

72 1 0.12 0.02 0.08 -0.05 -0.05 0.00 0.10 0.09 -0.00

73 1 0.06 0.09 -0.03 -0.03 -0.03 0.01 0.05 0.05 -0.02

74 1 -0.04 0.02 -0.07 -0.04 -0.06 -0.00 0.07 0.11 0.00

75 1 -0.08 -0.08 -0.03 -0.03 -0.03 -0.00 0.03 0.03 -0.00

76 1 -0.01 -0.12 0.09 -0.05 -0.04 0.01 0.09 0.06 -0.01

77 1 -0.04 -0.00 -0.00 -0.02 -0.21 -0.07 0.34 0.02 0.01

78 1 0.04 0.00 -0.00 0.02 0.21 -0.07 -0.34 -0.02 0.01

37 38 39

A A A

Frequencies -- 379.3269 384.0557 400.2613

Red. masses -- 5.2016 5.7169 4.3404

Frc consts -- 0.4410 0.4968 0.4097

IR Inten -- 46.1499 6.0759 3.2948

Atom AN X Y Z X Y Z X Y Z

1 6 0.02 -0.10 0.03 0.19 0.03 0.02 -0.07 -0.10 0.02

2 6 0.03 -0.08 0.02 0.11 0.02 0.01 0.08 -0.12 0.03

3 7 0.01 -0.12 0.04 0.11 0.01 -0.00 0.16 0.01 -0.00

4 6 -0.02 -0.08 0.02 0.11 -0.01 -0.01 0.06 0.13 -0.04

5 6 -0.00 -0.10 0.02 0.19 -0.00 -0.02 -0.09 0.09 -0.02

6 6 -0.03 0.03 -0.03 0.04 -0.01 0.03 0.03 0.04 -0.01

7 6 -0.04 0.08 -0.00 -0.08 -0.03 -0.02 0.02 0.02 0.01

8 7 -0.00 0.05 -0.00 -0.13 -0.01 -0.03 0.03 0.00 0.02

9 6 0.03 0.08 0.00 -0.09 0.02 -0.01 0.02 -0.02 0.01

10 6 0.02 0.20 -0.01 -0.11 -0.00 -0.03 0.02 -0.00 0.00

11 6 -0.05 0.19 0.01 -0.11 -0.01 -0.03 0.02 0.00 0.00

12 6 0.02 0.04 -0.04 0.04 0.02 -0.03 0.04 -0.04 0.01

13 6 0.03 0.08 -0.00 -0.09 0.02 0.01 0.02 -0.02 -0.01

14 6 0.02 0.20 0.01 -0.11 -0.00 0.03 0.02 -0.00 -0.00

15 6 -0.05 0.19 -0.01 -0.11 -0.01 0.03 0.02 0.00 -0.00

16 6 -0.04 0.08 0.00 -0.08 -0.03 0.02 0.02 0.02 -0.01

17 7 -0.00 0.05 0.00 -0.13 -0.01 0.03 0.03 0.00 -0.02

18 6 -0.03 0.03 0.03 0.04 -0.01 -0.03 0.03 0.04 0.01

19 6 -0.02 -0.08 -0.02 0.11 -0.01 0.01 0.06 0.13 0.04

20 6 -0.00 -0.10 -0.02 0.19 -0.00 0.02 -0.09 0.09 0.02

21 6 0.02 -0.10 -0.03 0.19 0.03 -0.02 -0.07 -0.10 -0.02

22 6 0.03 -0.08 -0.02 0.11 0.02 -0.01 0.08 -0.12 -0.03

23 7 0.01 -0.12 -0.04 0.11 0.01 0.00 0.16 0.01 0.00

24 6 0.02 0.04 0.04 0.04 0.02 0.03 0.04 -0.04 -0.01

25 6 -0.01 0.01 -0.03 0.02 -0.01 0.04 0.01 0.01 0.03

26 6 0.03 -0.05 0.03 -0.04 0.03 -0.01 -0.05 0.01 0.00

27 6 -0.00 -0.02 0.01 -0.04 0.03 -0.02 -0.02 -0.03 0.02

28 6 -0.04 0.02 -0.04 0.02 -0.05 0.04 -0.03 -0.06 0.01

29 6 0.03 -0.03 0.02 -0.03 -0.01 -0.01 -0.05 -0.03 -0.03

30 6 0.04 -0.03 0.01 -0.06 0.02 -0.03 -0.02 -0.04 0.01

31 6 0.04 0.03 -0.04 0.01 0.06 -0.04 -0.04 0.06 -0.01

32 6 0.00 -0.02 0.01 -0.03 -0.03 0.02 -0.03 0.02 -0.02

33 6 -0.03 -0.06 0.03 -0.04 -0.04 0.01 -0.05 -0.02 -0.00

34 6 0.01 0.01 -0.03 0.01 0.01 -0.04 0.01 -0.00 -0.03

35 6 -0.03 -0.03 0.01 -0.05 -0.02 0.03 -0.02 0.04 -0.01

36 6 -0.03 -0.03 0.03 -0.03 0.01 0.01 -0.05 0.02 0.03

37 6 0.01 0.01 0.03 0.01 0.01 0.04 0.01 -0.00 0.03

38 6 -0.03 -0.03 -0.01 -0.05 -0.02 -0.03 -0.02 0.04 0.01

39 6 -0.03 -0.03 -0.03 -0.03 0.01 -0.01 -0.05 0.02 -0.03

40 6 0.04 0.03 0.04 0.01 0.06 0.04 -0.04 0.06 0.01

41 6 0.00 -0.02 -0.01 -0.03 -0.03 -0.02 -0.03 0.02 0.02

42 6 -0.03 -0.06 -0.03 -0.04 -0.04 -0.01 -0.05 -0.02 0.00

43 6 -0.01 0.01 0.03 0.02 -0.01 -0.04 0.01 0.01 -0.03

44 6 0.04 -0.03 -0.01 -0.06 0.02 0.03 -0.02 -0.04 -0.01

45 6 0.03 -0.03 -0.02 -0.03 -0.01 0.01 -0.05 -0.03 0.03

46 6 -0.04 0.02 0.04 0.02 -0.05 -0.04 -0.03 -0.06 -0.01

47 6 -0.00 -0.02 -0.01 -0.04 0.03 0.02 -0.02 -0.03 -0.02

48 6 0.03 -0.05 -0.03 -0.04 0.03 0.01 -0.05 0.01 -0.00

49 1 -0.00 -0.11 0.03 0.22 0.07 0.04 -0.19 -0.21 0.03

50 1 0.02 -0.11 0.03 0.22 -0.03 -0.04 -0.22 0.18 -0.03

51 1 0.07 0.26 -0.02 -0.12 -0.02 -0.04 0.04 0.01 -0.01

52 1 -0.11 0.25 0.02 -0.12 0.00 -0.05 0.04 -0.01 -0.00

53 1 0.07 0.26 0.02 -0.12 -0.02 0.04 0.04 0.01 0.01

54 1 -0.11 0.25 -0.02 -0.12 0.00 0.05 0.04 -0.01 0.00

55 1 0.02 -0.11 -0.03 0.22 -0.03 0.04 -0.22 0.18 0.03

56 1 -0.00 -0.11 -0.03 0.22 0.07 -0.04 -0.19 -0.21 -0.03

57 1 0.06 -0.09 0.06 -0.06 0.06 -0.04 -0.09 0.02 -0.03

58 1 0.00 -0.03 0.02 -0.05 0.06 -0.06 0.02 -0.02 0.02

59 1 -0.10 0.07 -0.09 0.08 -0.11 0.09 -0.02 -0.07 0.01

60 1 0.06 -0.04 0.06 -0.04 -0.01 -0.03 -0.07 0.01 -0.06

61 1 0.06 -0.05 0.04 -0.12 0.04 -0.06 -0.05 -0.06 0.03

62 1 0.09 0.09 -0.09 0.06 0.11 -0.09 -0.03 0.07 -0.01

63 1 0.00 -0.03 0.02 -0.04 -0.06 0.06 0.01 0.02 -0.02

64 1 -0.05 -0.11 0.07 -0.06 -0.06 0.04 -0.08 -0.03 0.03

65 1 -0.06 -0.05 0.04 -0.11 -0.05 0.06 -0.06 0.05 -0.02

66 1 -0.06 -0.05 0.06 -0.05 -0.00 0.03 -0.07 -0.01 0.05

67 1 -0.06 -0.05 -0.04 -0.11 -0.05 -0.06 -0.06 0.05 0.02

68 1 -0.06 -0.05 -0.06 -0.05 -0.00 -0.03 -0.07 -0.01 -0.05

69 1 0.09 0.09 0.09 0.06 0.11 0.09 -0.03 0.07 0.01

70 1 0.00 -0.03 -0.02 -0.04 -0.06 -0.06 0.01 0.02 0.02

71 1 -0.05 -0.11 -0.07 -0.06 -0.06 -0.04 -0.08 -0.03 -0.03

72 1 0.06 -0.05 -0.04 -0.12 0.04 0.06 -0.05 -0.06 -0.03

73 1 0.06 -0.04 -0.06 -0.04 -0.01 0.03 -0.07 0.01 0.06

74 1 -0.10 0.07 0.09 0.08 -0.11 -0.09 -0.02 -0.07 -0.01

75 1 0.00 -0.03 -0.02 -0.05 0.06 0.06 0.02 -0.02 -0.02

76 1 0.06 -0.09 -0.06 -0.06 0.06 0.04 -0.09 0.02 0.03

77 1 0.01 -0.13 -0.03 0.14 0.01 0.01 0.36 0.03 0.02

78 1 0.01 -0.13 0.03 0.14 0.01 -0.01 0.36 0.03 -0.02

40 41 42

A A A

Frequencies -- 414.2791 415.6752 419.2342

Red. masses -- 3.2309 3.5140 2.9698

Frc consts -- 0.3267 0.3577 0.3075

IR Inten -- 0.0069 8.6429 0.0386

Atom AN X Y Z X Y Z X Y Z

1 6 0.07 0.03 -0.00 0.01 0.00 0.00 0.02 0.01 0.00

2 6 0.01 0.03 -0.00 -0.00 0.00 -0.00 0.00 0.01 -0.00

3 7 -0.01 0.00 0.00 -0.00 -0.00 0.01 -0.00 -0.00 -0.00

4 6 0.01 -0.03 0.00 0.00 -0.01 0.00 0.00 -0.01 0.00

5 6 0.07 -0.02 0.00 0.01 -0.01 0.00 0.02 -0.01 0.01

6 6 0.00 -0.00 0.00 0.02 0.03 -0.01 0.00 0.00 0.00

7 6 -0.01 0.03 0.00 0.05 0.05 0.01 -0.00 0.01 0.00

8 7 0.00 -0.00 -0.00 -0.01 0.10 -0.00 -0.00 0.00 0.00

9 6 0.01 0.03 -0.00 -0.06 0.05 -0.01 -0.00 0.01 -0.00

10 6 0.01 0.08 0.00 -0.05 -0.02 -0.01 0.00 0.02 -0.01

11 6 -0.02 0.08 -0.00 0.04 -0.02 0.01 -0.00 0.02 -0.01

12 6 0.00 0.00 -0.00 -0.02 0.03 -0.01 -0.00 0.00 0.00

13 6 -0.01 -0.03 -0.00 -0.06 0.05 0.01 0.00 -0.01 -0.00

14 6 -0.01 -0.08 0.00 -0.05 -0.02 0.01 -0.00 -0.02 -0.01

15 6 0.02 -0.08 -0.00 0.04 -0.02 -0.01 0.00 -0.02 -0.01

16 6 0.01 -0.03 0.00 0.05 0.05 -0.01 0.00 -0.01 0.00

17 7 -0.00 -0.00 -0.00 -0.01 0.10 0.00 0.00 -0.00 0.00

18 6 -0.00 0.00 0.00 0.02 0.03 0.01 -0.00 -0.00 0.00

19 6 -0.01 0.03 0.00 0.00 -0.01 -0.00 -0.00 0.01 0.00

20 6 -0.07 0.02 0.00 0.01 -0.01 -0.00 -0.02 0.01 0.01

21 6 -0.07 -0.03 -0.00 0.01 0.00 -0.00 -0.02 -0.01 0.00

22 6 -0.01 -0.03 -0.00 -0.00 0.00 0.00 -0.00 -0.01 -0.00

23 7 0.01 -0.00 0.00 -0.00 -0.00 -0.01 0.00 0.00 -0.00

24 6 -0.00 -0.00 -0.00 -0.02 0.03 0.01 0.00 -0.00 0.00

25 6 0.00 0.00 -0.00 -0.01 0.02 -0.02 -0.00 0.00 -0.00

26 6 0.06 -0.06 0.07 -0.07 0.04 -0.06 -0.05 0.05 -0.06

27 6 -0.06 0.05 -0.07 0.05 -0.08 0.08 0.05 -0.05 0.06

28 6 -0.00 0.00 -0.00 -0.04 -0.02 -0.01 -0.00 0.00 -0.00

29 6 0.07 -0.05 0.07 -0.06 0.03 -0.07 -0.05 0.04 -0.06

30 6 -0.06 0.05 -0.07 0.07 -0.08 0.07 0.06 -0.05 0.06

31 6 -0.00 -0.00 0.00 0.04 -0.01 -0.02 -0.00 -0.00 0.00

32 6 -0.04 -0.04 0.05 -0.02 -0.06 0.06 -0.06 -0.06 0.07

33 6 0.04 0.05 -0.05 0.05 0.02 -0.03 0.06 0.07 -0.08

34 6 0.00 -0.00 0.01 0.00 0.02 -0.02 0.00 -0.00 0.00

35 6 -0.03 -0.04 0.05 -0.04 -0.07 0.04 -0.06 -0.07 0.08

36 6 0.04 0.04 -0.05 0.04 0.01 -0.04 0.06 0.06 -0.07

37 6 -0.00 0.00 0.01 0.00 0.02 0.02 -0.00 0.00 0.00

38 6 0.03 0.04 0.05 -0.04 -0.07 -0.04 0.06 0.07 0.08

39 6 -0.04 -0.04 -0.05 0.04 0.01 0.04 -0.06 -0.06 -0.07

40 6 0.00 0.00 0.00 0.04 -0.01 0.02 0.00 0.00 0.00

41 6 0.04 0.04 0.05 -0.02 -0.06 -0.06 0.06 0.07 0.07

42 6 -0.04 -0.05 -0.05 0.05 0.02 0.03 -0.06 -0.07 -0.08

43 6 -0.00 -0.00 -0.00 -0.01 0.02 0.02 0.00 -0.00 -0.00

44 6 0.06 -0.05 -0.07 0.07 -0.08 -0.07 -0.06 0.05 0.06

45 6 -0.07 0.05 0.07 -0.06 0.03 0.07 0.05 -0.04 -0.06

46 6 0.00 -0.00 -0.00 -0.04 -0.02 0.01 0.00 -0.00 -0.00

47 6 0.06 -0.05 -0.07 0.05 -0.08 -0.08 -0.05 0.05 0.06

48 6 -0.06 0.06 0.07 -0.07 0.04 0.06 0.05 -0.05 -0.06

49 1 0.11 0.07 -0.01 0.02 0.01 0.01 0.03 0.02 -0.00

50 1 0.12 -0.05 0.01 0.01 -0.01 0.01 0.03 -0.01 0.00

51 1 0.03 0.11 0.01 -0.09 -0.09 -0.02 0.00 0.03 0.00

52 1 -0.05 0.11 -0.00 0.09 -0.08 0.02 -0.01 0.02 -0.00

53 1 -0.03 -0.11 0.01 -0.09 -0.09 0.02 -0.00 -0.03 0.00

54 1 0.05 -0.11 -0.00 0.09 -0.08 -0.02 0.01 -0.02 -0.00

55 1 -0.12 0.05 0.01 0.01 -0.01 -0.01 -0.03 0.01 0.00

56 1 -0.11 -0.07 -0.01 0.02 0.01 -0.01 -0.03 -0.02 -0.00

57 1 0.14 -0.13 0.15 -0.14 0.08 -0.14 -0.11 0.11 -0.13

58 1 -0.13 0.12 -0.15 0.14 -0.15 0.17 0.11 -0.11 0.13

59 1 -0.01 0.00 -0.00 -0.05 -0.00 -0.03 -0.01 0.00 -0.01

60 1 0.15 -0.12 0.16 -0.13 0.10 -0.14 -0.11 0.10 -0.12

61 1 -0.13 0.12 -0.15 0.15 -0.16 0.17 0.12 -0.11 0.13

62 1 -0.01 -0.01 0.00 0.06 0.00 -0.03 -0.00 -0.00 -0.00

63 1 -0.08 -0.09 0.10 -0.08 -0.11 0.12 -0.12 -0.14 0.15

64 1 0.08 0.11 -0.11 0.08 0.04 -0.08 0.13 0.15 -0.16

65 1 -0.08 -0.09 0.10 -0.07 -0.13 0.11 -0.13 -0.14 0.16

66 1 0.09 0.10 -0.11 0.07 0.06 -0.08 0.13 0.14 -0.16

67 1 0.08 0.09 0.10 -0.07 -0.13 -0.11 0.13 0.14 0.16

68 1 -0.09 -0.10 -0.11 0.07 0.06 0.08 -0.13 -0.14 -0.16

69 1 0.01 0.01 0.00 0.06 0.00 0.03 0.00 0.00 -0.00

70 1 0.08 0.09 0.10 -0.08 -0.11 -0.12 0.12 0.14 0.15

71 1 -0.08 -0.11 -0.11 0.08 0.04 0.08 -0.13 -0.15 -0.16

72 1 0.13 -0.12 -0.15 0.15 -0.16 -0.17 -0.12 0.11 0.13

73 1 -0.15 0.12 0.16 -0.13 0.10 0.14 0.11 -0.10 -0.12

74 1 0.01 -0.00 -0.00 -0.05 -0.00 0.03 0.01 -0.00 -0.01

75 1 0.13 -0.12 -0.15 0.14 -0.15 -0.17 -0.11 0.11 0.13

76 1 -0.14 0.13 0.15 -0.14 0.08 0.14 0.11 -0.11 -0.13

77 1 -0.05 -0.00 0.00 -0.01 -0.03 -0.10 -0.02 -0.01 -0.01

78 1 0.05 0.00 -0.00 -0.01 -0.03 0.10 0.02 0.01 -0.01

43 44 45

A A A

Frequencies -- 419.6567 424.8994 429.3593

Red. masses -- 3.0387 4.2073 3.9735

Frc consts -- 0.3153 0.4475 0.4316

IR Inten -- 8.9786 26.8817 0.0135

Atom AN X Y Z X Y Z X Y Z

1 6 0.02 0.02 -0.00 -0.00 0.00 -0.01 0.12 0.07 -0.02

2 6 -0.01 0.02 -0.01 -0.01 0.01 -0.00 -0.01 0.08 -0.03

3 7 -0.02 -0.00 -0.00 -0.00 0.01 0.01 -0.06 -0.00 -0.00

4 6 -0.01 -0.02 0.01 0.01 0.01 -0.00 -0.00 -0.07 0.03

5 6 0.02 -0.01 0.00 0.00 0.00 -0.01 0.13 -0.05 0.02

6 6 -0.01 -0.02 0.01 0.03 0.04 0.01 -0.00 0.00 0.00

7 6 -0.02 -0.02 -0.01 0.09 0.08 0.04 0.01 0.07 -0.00

8 7 -0.01 -0.03 -0.00 -0.01 0.15 0.00 -0.00 0.04 -0.00

9 6 0.01 -0.01 0.00 -0.10 0.06 -0.03 -0.01 0.06 0.01

10 6 0.00 0.01 -0.01 -0.07 -0.06 -0.02 -0.00 0.12 0.01

11 6 -0.02 0.00 -0.01 0.08 -0.05 0.02 -0.01 0.12 -0.01

12 6 0.00 -0.00 -0.01 -0.04 0.04 0.00 0.00 -0.00 -0.00

13 6 0.01 -0.01 -0.00 -0.10 0.06 0.03 0.01 -0.06 0.01

14 6 0.00 0.01 0.01 -0.07 -0.06 0.02 0.00 -0.12 0.01

15 6 -0.02 0.00 0.01 0.08 -0.05 -0.02 0.01 -0.12 -0.01

16 6 -0.02 -0.02 0.01 0.09 0.08 -0.04 -0.01 -0.07 -0.00

17 7 -0.01 -0.03 0.00 -0.01 0.15 -0.00 0.00 -0.04 -0.00

18 6 -0.01 -0.02 -0.01 0.03 0.04 -0.01 0.00 -0.00 0.00

19 6 -0.01 -0.02 -0.01 0.01 0.01 0.00 0.00 0.07 0.03

20 6 0.02 -0.01 -0.00 0.00 0.00 0.01 -0.13 0.05 0.02

21 6 0.02 0.02 0.00 -0.00 0.00 0.01 -0.12 -0.07 -0.02

22 6 -0.01 0.02 0.01 -0.01 0.01 0.00 0.01 -0.08 -0.03

23 7 -0.02 -0.00 0.00 -0.00 0.01 -0.01 0.06 0.00 -0.00

24 6 0.00 -0.00 0.01 -0.04 0.04 -0.00 -0.00 0.00 -0.00

25 6 0.00 -0.01 0.00 0.00 0.02 -0.03 -0.01 0.01 -0.03

26 6 -0.05 0.05 -0.07 0.02 -0.06 0.05 -0.02 0.01 -0.04

27 6 0.06 -0.04 0.05 -0.06 0.00 -0.02 0.03 -0.04 0.04

28 6 0.02 0.01 0.01 -0.05 -0.03 -0.01 -0.02 0.01 -0.02

29 6 -0.05 0.06 -0.05 0.03 -0.06 0.03 -0.01 0.02 -0.02

30 6 0.05 -0.04 0.06 -0.03 0.00 -0.06 0.05 -0.04 0.04

31 6 -0.00 -0.00 0.00 0.05 -0.02 -0.01 -0.02 -0.01 0.02

32 6 0.05 0.07 -0.07 0.07 0.02 -0.03 0.03 0.05 -0.05

33 6 -0.06 -0.06 0.08 -0.02 -0.07 0.07 -0.03 -0.03 0.05

34 6 -0.00 0.00 0.01 -0.01 0.02 -0.03 -0.01 -0.01 0.02

35 6 0.06 0.07 -0.07 0.04 0.02 -0.07 0.05 0.05 -0.05

36 6 -0.05 -0.06 0.07 -0.03 -0.08 0.04 -0.02 -0.03 0.03

37 6 -0.00 0.00 -0.01 -0.01 0.02 0.03 0.01 0.01 0.02

38 6 0.06 0.07 0.07 0.04 0.02 0.07 -0.05 -0.05 -0.05

39 6 -0.05 -0.06 -0.07 -0.03 -0.08 -0.05 0.02 0.03 0.03

40 6 -0.00 -0.00 -0.00 0.05 -0.02 0.01 0.02 0.01 0.02

41 6 0.05 0.07 0.07 0.07 0.02 0.03 -0.03 -0.05 -0.05

42 6 -0.06 -0.06 -0.08 -0.02 -0.07 -0.07 0.03 0.03 0.05

43 6 0.00 -0.01 -0.00 0.00 0.02 0.03 0.01 -0.01 -0.03

44 6 0.05 -0.04 -0.06 -0.03 0.00 0.06 -0.05 0.04 0.04

45 6 -0.05 0.06 0.05 0.03 -0.06 -0.03 0.01 -0.02 -0.02

46 6 0.02 0.01 -0.01 -0.05 -0.03 0.01 0.02 -0.01 -0.02

47 6 0.06 -0.04 -0.05 -0.06 0.00 0.02 -0.03 0.04 0.04

48 6 -0.05 0.05 0.07 0.02 -0.06 -0.05 0.02 -0.01 -0.04

49 1 0.04 0.04 0.00 0.00 0.01 0.01 0.21 0.15 -0.03

50 1 0.05 -0.03 -0.00 -0.00 0.01 0.01 0.23 -0.12 0.03

51 1 0.01 0.03 0.01 -0.15 -0.17 -0.03 0.01 0.15 0.02

52 1 -0.04 0.02 -0.01 0.17 -0.15 0.03 -0.03 0.14 -0.02

53 1 0.01 0.03 -0.01 -0.15 -0.17 0.03 -0.01 -0.15 0.02

54 1 -0.04 0.02 0.01 0.17 -0.15 -0.03 0.03 -0.14 -0.02

55 1 0.05 -0.03 0.00 -0.00 0.01 -0.01 -0.23 0.12 0.03

56 1 0.04 0.04 -0.00 0.00 0.01 -0.01 -0.21 -0.15 -0.03

57 1 -0.11 0.12 -0.13 0.07 -0.15 0.10 -0.05 0.03 -0.07

58 1 0.10 -0.09 0.11 -0.08 0.03 -0.06 0.07 -0.09 0.09

59 1 0.02 0.01 0.01 -0.06 -0.02 -0.02 -0.04 0.03 -0.03

60 1 -0.11 0.11 -0.12 0.10 -0.09 0.11 -0.03 0.04 -0.04

61 1 0.12 -0.08 0.12 -0.08 0.02 -0.09 0.11 -0.08 0.09

62 1 -0.01 -0.01 0.00 0.07 -0.01 -0.02 -0.03 -0.04 0.03

63 1 0.12 0.15 -0.16 0.09 0.06 -0.08 0.07 0.11 -0.11

64 1 -0.12 -0.14 0.16 -0.07 -0.18 0.13 -0.06 -0.05 0.08

65 1 0.14 0.15 -0.16 0.10 0.05 -0.11 0.11 0.11 -0.11

66 1 -0.12 -0.14 0.15 -0.10 -0.12 0.13 -0.04 -0.06 0.06

67 1 0.14 0.15 0.16 0.10 0.05 0.11 -0.11 -0.11 -0.11

68 1 -0.12 -0.14 -0.15 -0.10 -0.12 -0.13 0.04 0.06 0.06

69 1 -0.01 -0.01 -0.00 0.07 -0.01 0.02 0.03 0.04 0.03

70 1 0.12 0.15 0.16 0.09 0.06 0.08 -0.07 -0.11 -0.11

71 1 -0.12 -0.14 -0.16 -0.07 -0.18 -0.13 0.06 0.05 0.08

72 1 0.12 -0.08 -0.12 -0.08 0.02 0.09 -0.11 0.08 0.09

73 1 -0.11 0.11 0.12 0.10 -0.09 -0.11 0.03 -0.04 -0.04

74 1 0.02 0.01 -0.01 -0.06 -0.02 0.02 0.04 -0.03 -0.03

75 1 0.10 -0.09 -0.11 -0.08 0.03 0.06 -0.07 0.09 0.09

76 1 -0.11 0.12 0.13 0.07 -0.15 -0.10 0.05 -0.03 -0.07

77 1 -0.05 0.00 0.02 -0.00 -0.02 -0.13 -0.18 -0.01 -0.00

78 1 -0.05 0.00 -0.02 -0.00 -0.02 0.13 0.18 0.01 -0.00

46 47 48

A A A

Frequencies -- 444.4840 495.1005 502.0035

Red. masses -- 4.7334 4.1944 1.4150

Frc consts -- 0.5510 0.6058 0.2101

IR Inten -- 0.0065 1.9920 36.4563

Atom AN X Y Z X Y Z X Y Z

1 6 -0.05 0.03 -0.01 -0.00 -0.00 -0.01 -0.00 -0.00 -0.03

2 6 -0.07 0.04 -0.01 -0.02 0.01 0.01 0.00 0.00 -0.01

3 7 -0.10 -0.00 0.00 0.00 0.00 -0.06 -0.00 0.02 0.11

4 6 -0.06 -0.05 0.01 0.02 0.01 0.01 -0.00 0.00 -0.01

5 6 -0.05 -0.04 0.01 0.01 -0.00 -0.01 0.00 -0.00 -0.03

6 6 -0.00 0.03 -0.00 0.02 -0.02 0.10 -0.00 -0.01 -0.02

7 6 0.10 0.07 0.04 -0.01 -0.02 0.01 -0.01 -0.01 -0.00

8 7 -0.01 0.15 0.00 -0.01 0.00 -0.06 0.00 -0.02 -0.00

9 6 -0.11 0.06 -0.04 -0.01 0.02 0.01 0.01 -0.01 0.00

10 6 -0.08 -0.11 -0.03 -0.00 0.00 -0.01 0.01 -0.01 -0.01

11 6 0.10 -0.09 0.03 -0.00 -0.00 -0.01 -0.01 -0.01 0.01

12 6 0.00 -0.03 0.00 -0.02 -0.02 0.11 0.01 -0.01 -0.02

13 6 0.11 -0.06 -0.04 0.01 -0.02 0.01 0.01 -0.01 -0.00

14 6 0.08 0.11 -0.03 0.00 -0.00 -0.01 0.01 -0.01 0.01

15 6 -0.10 0.09 0.03 0.00 0.00 -0.01 -0.01 -0.01 -0.01

16 6 -0.10 -0.07 0.04 0.01 0.02 0.01 -0.01 -0.01 0.00

17 7 0.01 -0.15 0.00 0.01 -0.00 -0.06 0.00 -0.02 0.00

18 6 0.00 -0.03 -0.00 -0.02 0.02 0.10 -0.00 -0.01 0.02

19 6 0.06 0.05 0.01 -0.02 -0.01 0.01 -0.00 0.00 0.01

20 6 0.05 0.04 0.01 -0.01 0.00 -0.01 0.00 -0.00 0.03

21 6 0.05 -0.03 -0.01 0.00 0.00 -0.01 -0.00 -0.00 0.03

22 6 0.07 -0.04 -0.01 0.02 -0.01 0.01 0.00 0.00 0.01

23 7 0.10 0.00 0.00 -0.00 -0.00 -0.06 -0.00 0.02 -0.11

24 6 -0.00 0.03 0.00 0.02 0.02 0.11 0.01 -0.01 0.02

25 6 -0.03 0.04 -0.06 0.11 -0.10 0.08 -0.01 0.00 0.01

26 6 0.02 -0.04 0.02 0.00 -0.02 -0.03 0.00 0.01 0.01

27 6 -0.00 -0.02 0.01 -0.05 0.02 -0.05 0.01 0.01 -0.00

28 6 -0.05 0.02 -0.04 0.05 -0.05 0.08 0.01 0.00 -0.00

29 6 0.03 -0.03 0.03 -0.03 0.05 -0.05 -0.00 -0.00 0.00

30 6 0.01 -0.01 -0.02 0.02 -0.00 -0.03 -0.01 0.00 0.01

31 6 -0.05 -0.02 0.04 -0.05 -0.06 0.08 -0.01 0.01 -0.00

32 6 -0.01 0.02 -0.02 0.05 0.03 -0.05 -0.01 0.00 -0.00

33 6 0.02 0.04 -0.02 -0.00 -0.02 -0.03 -0.00 0.01 0.01

34 6 -0.03 -0.04 0.06 -0.10 -0.11 0.08 0.01 0.00 0.00

35 6 0.01 0.01 0.02 -0.02 -0.00 -0.03 0.01 0.01 0.01

36 6 0.03 0.03 -0.03 0.02 0.05 -0.05 0.00 -0.00 0.00

37 6 0.03 0.04 0.06 0.10 0.11 0.08 0.01 0.00 -0.00

38 6 -0.01 -0.01 0.02 0.02 0.00 -0.03 0.01 0.01 -0.01

39 6 -0.03 -0.03 -0.03 -0.02 -0.05 -0.05 0.00 -0.00 -0.00

40 6 0.05 0.02 0.04 0.05 0.06 0.08 -0.01 0.01 0.00

41 6 0.01 -0.02 -0.02 -0.05 -0.03 -0.05 -0.01 0.00 0.00

42 6 -0.02 -0.04 -0.02 0.00 0.02 -0.03 -0.00 0.01 -0.01

43 6 0.03 -0.04 -0.06 -0.11 0.10 0.08 -0.01 0.00 -0.01

44 6 -0.01 0.01 -0.02 -0.02 0.00 -0.03 -0.01 0.00 -0.01

45 6 -0.03 0.03 0.03 0.03 -0.05 -0.05 -0.00 -0.00 -0.00

46 6 0.05 -0.02 -0.04 -0.05 0.05 0.08 0.01 0.00 0.00

47 6 0.00 0.02 0.01 0.05 -0.02 -0.05 0.01 0.01 0.00

48 6 -0.02 0.04 0.02 -0.00 0.02 -0.03 0.00 0.01 -0.01

49 1 -0.02 0.06 -0.02 0.00 0.01 -0.01 -0.00 0.02 0.06

50 1 -0.01 -0.06 0.02 -0.00 0.01 -0.01 -0.00 0.02 0.06

51 1 -0.17 -0.24 -0.05 -0.01 -0.01 -0.02 0.01 0.00 -0.01

52 1 0.21 -0.21 0.04 -0.01 0.00 -0.02 -0.02 -0.00 0.01

53 1 0.17 0.24 -0.04 0.01 0.01 -0.02 0.01 0.00 0.01

54 1 -0.21 0.21 0.04 0.01 -0.00 -0.02 -0.02 -0.00 -0.01

55 1 0.01 0.06 0.02 0.00 -0.01 -0.01 -0.00 0.02 -0.06

56 1 0.02 -0.06 -0.02 -0.00 -0.01 -0.01 -0.00 0.02 -0.06

57 1 0.07 -0.11 0.07 -0.07 0.02 -0.12 0.00 0.02 0.01

58 1 0.02 -0.05 0.04 -0.15 0.08 -0.13 0.01 0.01 -0.00

59 1 -0.09 0.05 -0.07 0.09 -0.09 0.15 0.01 0.00 -0.01

60 1 0.09 -0.06 0.09 -0.11 0.15 -0.13 -0.01 -0.01 -0.00

61 1 0.03 -0.03 0.01 -0.03 0.07 -0.11 -0.01 0.01 0.01

62 1 -0.08 -0.06 0.07 -0.08 -0.10 0.15 -0.01 0.01 -0.01

63 1 0.01 0.05 -0.04 0.15 0.11 -0.14 -0.01 0.00 0.00

64 1 0.05 0.11 -0.07 0.07 0.03 -0.12 -0.01 0.01 0.01

65 1 0.03 0.04 -0.01 0.02 0.07 -0.12 0.01 0.00 0.01

66 1 0.08 0.07 -0.09 0.08 0.16 -0.13 0.00 -0.01 0.00

67 1 -0.03 -0.04 -0.01 -0.02 -0.07 -0.12 0.01 0.00 -0.01

68 1 -0.08 -0.07 -0.09 -0.08 -0.16 -0.13 0.00 -0.01 -0.00

69 1 0.08 0.06 0.07 0.08 0.10 0.15 -0.01 0.01 0.01

70 1 -0.01 -0.05 -0.04 -0.15 -0.11 -0.14 -0.01 0.00 -0.00

71 1 -0.05 -0.11 -0.07 -0.07 -0.03 -0.12 -0.01 0.01 -0.01

72 1 -0.03 0.03 0.01 0.03 -0.07 -0.11 -0.01 0.01 -0.01

73 1 -0.09 0.06 0.09 0.11 -0.15 -0.13 -0.01 -0.01 0.00

74 1 0.09 -0.05 -0.07 -0.09 0.09 0.15 0.01 0.00 0.01

75 1 -0.02 0.05 0.04 0.15 -0.08 -0.13 0.01 0.01 0.00

76 1 -0.07 0.11 0.07 0.07 -0.02 -0.12 0.00 0.02 -0.01

77 1 -0.16 -0.01 -0.00 -0.00 0.02 0.03 0.01 -0.15 -0.67

78 1 0.16 0.01 -0.00 0.00 -0.02 0.03 0.01 -0.15 0.67

49 50 51

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Frequencies -- 516.8965 517.5315 530.9467

Red. masses -- 4.1177 3.7784 4.4786

Frc consts -- 0.6482 0.5963 0.7439

IR Inten -- 2.1993 3.1003 0.0022

Atom AN X Y Z X Y Z X Y Z

1 6 -0.07 0.01 0.05 -0.00 -0.02 -0.02 -0.06 0.03 0.07

2 6 -0.03 0.00 0.01 -0.01 0.00 0.02 -0.04 0.01 0.00

3 7 -0.04 -0.00 -0.00 0.00 -0.01 -0.03 -0.06 -0.00 -0.00

4 6 -0.03 -0.01 -0.01 0.01 0.00 0.02 -0.04 -0.02 -0.00

5 6 -0.07 -0.02 -0.05 0.00 -0.02 -0.03 -0.05 -0.04 -0.07

6 6 -0.01 -0.02 0.08 0.02 0.02 0.10 0.00 0.01 0.11

7 6 0.00 -0.01 0.02 0.01 0.03 0.00 0.03 0.05 0.02

8 7 0.02 0.00 -0.05 -0.00 0.05 -0.00 -0.00 0.05 0.00

9 6 -0.00 0.01 0.02 -0.01 0.03 -0.00 -0.04 0.05 -0.02

10 6 0.02 0.00 -0.01 -0.02 0.07 0.06 -0.05 0.03 0.07

11 6 0.02 -0.00 -0.00 0.01 0.07 -0.06 0.04 0.04 -0.06

12 6 -0.01 0.02 -0.09 -0.02 0.01 0.09 0.00 -0.01 -0.11

13 6 -0.00 0.01 -0.02 -0.01 0.03 0.00 0.04 -0.05 -0.02

14 6 0.02 0.00 0.01 -0.02 0.07 -0.06 0.05 -0.03 0.07

15 6 0.02 -0.00 0.00 0.01 0.07 0.06 -0.04 -0.04 -0.06

16 6 0.00 -0.01 -0.02 0.01 0.03 -0.00 -0.03 -0.05 0.02

17 7 0.02 0.00 0.05 -0.00 0.05 0.00 0.00 -0.05 0.00

18 6 -0.01 -0.02 -0.08 0.02 0.02 -0.10 -0.00 -0.01 0.11

19 6 -0.03 -0.01 0.01 0.01 0.00 -0.02 0.04 0.02 -0.00

20 6 -0.07 -0.02 0.05 0.00 -0.02 0.03 0.05 0.04 -0.07

21 6 -0.07 0.01 -0.05 -0.00 -0.02 0.02 0.06 -0.03 0.07

22 6 -0.03 0.00 -0.01 -0.01 0.00 -0.02 0.04 -0.01 0.00

23 7 -0.04 -0.00 0.00 0.00 -0.01 0.03 0.06 0.00 -0.00

24 6 -0.01 0.02 0.09 -0.02 0.01 -0.09 -0.00 0.01 -0.11

25 6 0.09 -0.10 0.08 0.11 -0.08 0.07 0.10 -0.08 0.07

26 6 0.02 -0.03 -0.02 0.00 -0.03 -0.02 0.02 -0.04 -0.02

27 6 -0.04 0.02 -0.05 -0.05 0.01 -0.04 -0.05 0.01 -0.04

28 6 0.06 -0.03 0.07 0.03 -0.06 0.07 0.04 -0.05 0.06

29 6 -0.02 0.05 -0.04 -0.03 0.04 -0.05 -0.02 0.04 -0.04

30 6 0.03 0.00 -0.02 0.04 -0.02 -0.03 0.04 -0.02 -0.02

31 6 0.06 0.04 -0.07 -0.02 -0.06 0.06 0.03 0.05 -0.06

32 6 -0.04 -0.03 0.06 0.05 0.02 -0.03 -0.05 -0.02 0.04

33 6 0.02 0.04 0.03 0.00 -0.03 -0.02 0.01 0.04 0.02

34 6 0.09 0.12 -0.09 -0.09 -0.08 0.07 0.09 0.09 -0.07

35 6 0.03 0.00 0.02 -0.03 -0.02 -0.02 0.04 0.02 0.02

36 6 -0.02 -0.06 0.04 0.02 0.03 -0.05 -0.01 -0.04 0.04

37 6 0.09 0.12 0.09 -0.09 -0.08 -0.07 -0.09 -0.09 -0.07

38 6 0.03 0.00 -0.02 -0.03 -0.02 0.02 -0.04 -0.02 0.02

39 6 -0.02 -0.06 -0.04 0.02 0.03 0.05 0.01 0.04 0.04

40 6 0.06 0.04 0.07 -0.02 -0.06 -0.06 -0.03 -0.05 -0.06

41 6 -0.04 -0.03 -0.06 0.05 0.02 0.03 0.05 0.02 0.04

42 6 0.02 0.04 -0.03 0.00 -0.03 0.02 -0.01 -0.04 0.02

43 6 0.09 -0.10 -0.08 0.11 -0.08 -0.07 -0.10 0.08 0.07

44 6 0.03 0.00 0.02 0.04 -0.02 0.03 -0.04 0.02 -0.02

45 6 -0.02 0.05 0.04 -0.03 0.04 0.05 0.02 -0.04 -0.04

46 6 0.06 -0.03 -0.07 0.03 -0.06 -0.07 -0.04 0.05 0.06

47 6 -0.04 0.02 0.05 -0.05 0.01 0.04 0.05 -0.01 -0.04

48 6 0.02 -0.03 0.02 0.00 -0.03 0.02 -0.02 0.04 -0.02

49 1 -0.09 0.00 0.07 -0.00 -0.00 0.02 -0.05 0.05 0.10

50 1 -0.08 -0.02 -0.08 -0.01 -0.00 0.01 -0.04 -0.05 -0.10

51 1 0.02 -0.00 -0.03 -0.03 0.07 0.10 -0.08 -0.01 0.12

52 1 0.02 -0.00 -0.02 0.02 0.08 -0.11 0.08 0.01 -0.12

53 1 0.02 -0.00 0.03 -0.03 0.07 -0.10 0.08 0.01 0.12

54 1 0.02 -0.00 0.02 0.02 0.08 0.11 -0.08 -0.01 -0.12

55 1 -0.08 -0.02 0.08 -0.01 -0.00 -0.01 0.04 0.05 -0.10

56 1 -0.09 0.00 -0.07 -0.00 -0.00 -0.02 0.05 -0.05 0.10

57 1 -0.05 0.02 -0.10 -0.07 0.00 -0.11 -0.05 -0.00 -0.10

58 1 -0.15 0.09 -0.14 -0.15 0.08 -0.12 -0.15 0.08 -0.13

59 1 0.09 -0.06 0.12 0.06 -0.08 0.12 0.05 -0.06 0.11

60 1 -0.10 0.14 -0.13 -0.10 0.15 -0.13 -0.09 0.15 -0.12

61 1 -0.02 0.07 -0.10 -0.02 0.04 -0.09 -0.01 0.05 -0.10

62 1 0.08 0.07 -0.13 -0.04 -0.08 0.11 0.04 0.06 -0.11

63 1 -0.15 -0.11 0.15 0.12 0.09 -0.11 -0.14 -0.09 0.12

64 1 -0.05 -0.03 0.11 0.07 0.01 -0.10 -0.05 0.00 0.10

65 1 -0.01 -0.08 0.11 0.02 0.03 -0.09 -0.00 -0.05 0.10

66 1 -0.09 -0.16 0.14 0.07 0.14 -0.12 -0.07 -0.15 0.12

67 1 -0.01 -0.08 -0.11 0.02 0.03 0.09 0.00 0.05 0.10

68 1 -0.09 -0.16 -0.14 0.07 0.14 0.12 0.07 0.15 0.12

69 1 0.08 0.07 0.13 -0.04 -0.08 -0.11 -0.04 -0.06 -0.11

70 1 -0.15 -0.11 -0.15 0.12 0.09 0.11 0.14 0.09 0.12

71 1 -0.05 -0.03 -0.11 0.07 0.01 0.10 0.05 -0.00 0.10

72 1 -0.02 0.07 0.10 -0.02 0.04 0.09 0.01 -0.05 -0.10

73 1 -0.10 0.14 0.13 -0.10 0.15 0.13 0.09 -0.15 -0.12

74 1 0.09 -0.06 -0.12 0.06 -0.08 -0.12 -0.05 0.06 0.11

75 1 -0.15 0.09 0.14 -0.15 0.08 0.12 0.15 -0.08 -0.13

76 1 -0.05 0.02 0.10 -0.07 0.00 0.11 0.05 0.00 -0.10

77 1 -0.08 0.00 0.03 0.00 -0.07 -0.28 -0.10 -0.01 -0.01

78 1 -0.08 0.00 -0.03 0.00 -0.07 0.28 0.10 0.01 -0.01

52 53 54

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Frequencies -- 570.2525 570.4781 579.3434

Red. masses -- 4.3904 4.8203 4.4386

Frc consts -- 0.8412 0.9243 0.8777

IR Inten -- 16.2654 55.4236 0.0001

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.00 -0.04 -0.00 0.00 -0.01 -0.01 -0.00 -0.11

2 6 0.01 0.02 0.06 0.00 0.02 0.07 -0.02 0.03 0.03

3 7 0.00 -0.01 -0.08 0.00 -0.03 -0.16 -0.05 -0.00 -0.00

4 6 -0.01 0.02 0.06 -0.01 0.02 0.08 -0.02 -0.03 -0.03

5 6 -0.00 0.01 -0.04 -0.00 -0.00 -0.02 -0.01 0.00 0.11

6 6 -0.04 -0.00 0.17 -0.03 0.02 0.18 0.02 -0.01 -0.16

7 6 -0.03 -0.02 0.05 -0.01 0.00 0.04 0.04 0.03 -0.04

8 7 0.00 -0.03 0.00 0.02 0.00 -0.10 -0.00 0.04 -0.00

9 6 0.03 -0.01 -0.05 -0.01 -0.01 0.04 -0.04 0.02 0.05

10 6 -0.01 -0.01 0.11 -0.01 -0.00 -0.02 -0.00 0.01 -0.10

11 6 0.01 -0.01 -0.11 -0.01 -0.00 -0.02 0.00 0.01 0.10

12 6 0.04 0.01 0.17 0.02 0.03 0.18 0.02 0.01 0.16

13 6 0.03 -0.01 0.05 0.01 0.01 0.04 0.04 -0.02 0.05

14 6 -0.01 -0.01 -0.11 0.01 0.00 -0.02 0.00 -0.01 -0.10

15 6 0.01 -0.01 0.11 0.01 0.00 -0.02 -0.00 -0.01 0.10

16 6 -0.03 -0.02 -0.05 0.01 -0.00 0.04 -0.04 -0.03 -0.04

17 7 0.00 -0.03 -0.00 -0.02 -0.00 -0.10 0.00 -0.04 -0.00

18 6 -0.04 -0.00 -0.17 0.03 -0.02 0.18 -0.02 0.01 -0.16

19 6 -0.01 0.02 -0.06 0.01 -0.02 0.08 0.02 0.03 -0.03

20 6 -0.00 0.01 0.04 0.00 0.00 -0.02 0.01 -0.00 0.11

21 6 -0.00 0.00 0.04 0.00 -0.00 -0.02 0.01 0.00 -0.11

22 6 0.01 0.02 -0.06 -0.00 -0.02 0.08 0.02 -0.03 0.03

23 7 0.00 -0.01 0.08 -0.00 0.03 -0.16 0.05 0.00 -0.00

24 6 0.04 0.01 -0.17 -0.02 -0.03 0.18 -0.02 -0.01 0.16

25 6 -0.04 0.02 -0.08 -0.03 0.03 -0.08 0.04 -0.03 0.07

26 6 0.02 -0.00 -0.05 0.01 -0.00 -0.05 -0.01 -0.01 0.04

27 6 0.03 -0.02 0.03 0.01 -0.02 0.04 -0.02 0.01 -0.04

28 6 -0.03 0.05 -0.02 -0.05 0.04 -0.02 0.04 -0.04 0.03

29 6 0.02 -0.01 0.04 0.02 -0.01 0.04 -0.01 0.02 -0.04

30 6 -0.00 -0.01 -0.04 0.01 -0.01 -0.05 0.01 0.01 0.04

31 6 0.03 0.06 -0.03 0.04 0.04 -0.02 0.04 0.05 -0.03

32 6 -0.03 -0.02 0.03 -0.01 -0.02 0.04 -0.02 -0.01 0.04

33 6 -0.01 -0.00 -0.05 -0.01 -0.01 -0.05 -0.01 0.01 -0.04

34 6 0.04 0.03 -0.08 0.03 0.03 -0.08 0.03 0.04 -0.07

35 6 0.00 -0.01 -0.04 -0.01 -0.01 -0.05 0.01 -0.01 -0.04

36 6 -0.02 -0.01 0.05 -0.02 -0.02 0.04 -0.01 -0.02 0.04

37 6 0.04 0.03 0.08 -0.03 -0.03 -0.08 -0.03 -0.04 -0.07

38 6 0.00 -0.01 0.04 0.01 0.01 -0.05 -0.01 0.01 -0.04

39 6 -0.02 -0.01 -0.05 0.02 0.02 0.04 0.01 0.02 0.04

40 6 0.03 0.06 0.03 -0.04 -0.04 -0.02 -0.04 -0.05 -0.03

41 6 -0.02 -0.02 -0.03 0.01 0.02 0.04 0.02 0.01 0.04

42 6 -0.01 -0.00 0.05 0.01 0.01 -0.05 0.01 -0.01 -0.04

43 6 -0.04 0.02 0.07 0.03 -0.03 -0.08 -0.04 0.03 0.07

44 6 -0.00 -0.01 0.03 -0.01 0.01 -0.05 -0.01 -0.01 0.04

45 6 0.02 -0.01 -0.04 -0.02 0.01 0.04 0.01 -0.02 -0.04

46 6 -0.03 0.05 0.02 0.05 -0.04 -0.02 -0.04 0.04 0.03

47 6 0.03 -0.02 -0.03 -0.01 0.02 0.04 0.02 -0.01 -0.04

48 6 0.01 -0.00 0.05 -0.01 0.00 -0.05 0.01 0.01 0.04

49 1 -0.00 0.01 -0.03 -0.00 -0.03 -0.11 0.02 -0.00 -0.20

50 1 0.00 0.01 -0.02 0.00 -0.03 -0.12 0.02 0.01 0.20

51 1 -0.03 0.00 0.20 0.00 0.00 -0.04 -0.00 -0.02 -0.19

52 1 0.03 0.01 -0.20 0.00 -0.00 -0.04 0.01 -0.03 0.19

53 1 -0.03 0.00 -0.20 -0.00 -0.00 -0.04 0.00 0.02 -0.19

54 1 0.03 0.01 0.20 -0.00 0.00 -0.05 -0.01 0.03 0.19

55 1 0.00 0.01 0.02 -0.00 0.03 -0.12 -0.02 -0.01 0.20

56 1 -0.00 0.01 0.02 0.00 0.03 -0.11 -0.02 0.00 -0.20

57 1 0.07 -0.07 0.01 0.07 -0.09 0.01 -0.06 0.07 -0.02

58 1 0.07 -0.11 0.13 0.06 -0.10 0.13 -0.08 0.09 -0.14

59 1 -0.03 0.05 -0.03 -0.04 0.03 -0.02 0.04 -0.04 0.04

60 1 0.10 -0.06 0.13 0.11 -0.05 0.14 -0.10 0.07 -0.14

61 1 0.09 -0.04 0.02 0.10 -0.05 0.00 -0.07 0.05 -0.02

62 1 0.03 0.06 -0.03 0.04 0.04 -0.02 0.03 0.04 -0.04

63 1 -0.06 -0.12 0.14 -0.05 -0.11 0.14 -0.07 -0.11 0.14

64 1 -0.06 -0.08 0.01 -0.05 -0.10 0.01 -0.05 -0.07 0.02

65 1 -0.09 -0.06 0.02 -0.09 -0.07 0.00 -0.07 -0.06 0.02

66 1 -0.09 -0.07 0.14 -0.10 -0.06 0.13 -0.09 -0.08 0.14

67 1 -0.09 -0.06 -0.02 0.09 0.07 0.00 0.07 0.06 0.02

68 1 -0.09 -0.07 -0.14 0.10 0.06 0.13 0.09 0.08 0.14

69 1 0.02 0.05 0.03 -0.04 -0.04 -0.02 -0.03 -0.04 -0.04

70 1 -0.05 -0.12 -0.14 0.05 0.11 0.14 0.07 0.11 0.14

71 1 -0.06 -0.08 -0.01 0.05 0.10 0.01 0.05 0.07 0.02

72 1 0.09 -0.04 -0.02 -0.10 0.05 0.00 0.07 -0.05 -0.02

73 1 0.10 -0.06 -0.13 -0.11 0.05 0.14 0.10 -0.07 -0.14

74 1 -0.03 0.05 0.03 0.04 -0.04 -0.02 -0.04 0.04 0.04

75 1 0.06 -0.10 -0.13 -0.06 0.11 0.14 0.08 -0.09 -0.14

76 1 0.07 -0.07 -0.01 -0.07 0.09 0.01 0.06 -0.06 -0.02

77 1 0.00 -0.05 -0.28 -0.00 0.08 0.33 -0.10 -0.01 -0.01

78 1 0.00 -0.05 0.28 0.00 -0.08 0.32 0.10 0.01 -0.01

55 56 57

A A A

Frequencies -- 580.0490 614.6769 635.0454

Red. masses -- 5.3170 1.4380 6.2316

Frc consts -- 1.0540 0.3201 1.4807

IR Inten -- 17.2650 64.7625 0.0025

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.02 -0.13 0.00 0.00 0.03 -0.01 0.00 0.03

2 6 -0.01 0.02 0.04 -0.00 0.00 0.02 0.00 -0.01 -0.02

3 7 -0.02 -0.00 0.00 0.00 -0.01 -0.07 0.01 -0.00 0.00

4 6 -0.01 -0.03 -0.04 -0.00 0.00 0.02 0.00 0.01 0.01

5 6 -0.00 0.02 0.13 -0.00 0.00 0.03 -0.01 -0.00 -0.02

6 6 0.02 -0.03 -0.20 0.00 -0.01 -0.05 0.00 -0.01 0.01

7 6 0.02 -0.01 -0.06 0.00 -0.00 -0.03 -0.00 -0.00 0.01

8 7 -0.02 -0.00 0.13 -0.01 -0.00 0.04 -0.00 -0.02 0.02

9 6 0.01 0.01 -0.06 0.00 0.00 -0.03 0.01 0.00 -0.04

10 6 0.01 0.00 0.02 -0.00 0.00 0.01 -0.00 0.00 0.02

11 6 0.01 0.00 0.03 -0.00 -0.00 0.01 0.01 0.00 -0.02

12 6 0.01 0.04 0.20 -0.00 -0.01 -0.04 0.01 0.01 -0.05

13 6 0.01 0.01 0.06 -0.00 -0.00 -0.03 -0.01 -0.00 -0.04

14 6 0.01 0.00 -0.02 0.00 -0.00 0.01 0.00 -0.00 0.02

15 6 0.01 0.00 -0.03 0.00 0.00 0.01 -0.01 -0.00 -0.02

16 6 0.02 -0.01 0.06 -0.00 0.00 -0.03 0.00 0.00 0.01

17 7 -0.02 -0.00 -0.13 0.01 0.00 0.04 0.00 0.02 0.02

18 6 0.02 -0.03 0.20 -0.00 0.01 -0.05 -0.00 0.01 0.01

19 6 -0.01 -0.03 0.04 0.00 -0.00 0.02 -0.00 -0.01 0.01

20 6 -0.00 0.02 -0.13 0.00 -0.00 0.03 0.01 0.00 -0.02

21 6 0.00 -0.02 0.13 -0.00 -0.00 0.03 0.01 -0.00 0.03

22 6 -0.01 0.02 -0.04 0.00 -0.00 0.02 -0.00 0.01 -0.02

23 7 -0.02 -0.00 -0.00 -0.00 0.01 -0.07 -0.01 0.00 0.00

24 6 0.01 0.04 -0.20 0.00 0.01 -0.04 -0.01 -0.01 -0.05

25 6 0.02 -0.04 0.08 -0.00 -0.00 0.01 -0.02 0.02 0.03

26 6 -0.02 -0.00 0.04 -0.01 -0.00 0.01 -0.08 -0.03 0.04

27 6 -0.01 0.01 -0.05 -0.00 -0.01 -0.01 -0.01 -0.09 -0.05

28 6 0.06 -0.03 0.02 0.01 -0.01 -0.00 0.02 -0.01 -0.04

29 6 -0.02 0.02 -0.03 0.01 0.01 -0.01 0.09 0.03 -0.05

30 6 -0.01 0.02 0.07 -0.00 0.01 0.02 0.01 0.08 0.05

31 6 0.05 0.03 -0.02 -0.01 -0.01 -0.00 0.03 0.03 0.08

32 6 -0.01 -0.01 0.05 0.00 -0.01 -0.01 -0.05 0.18 0.11

33 6 -0.01 -0.00 -0.04 0.01 -0.00 0.01 -0.17 0.03 -0.08

34 6 0.01 0.04 -0.07 0.00 -0.00 0.01 -0.04 -0.05 -0.06

35 6 -0.01 -0.02 -0.06 -0.00 0.01 0.02 0.05 -0.17 -0.09

36 6 -0.02 -0.02 0.03 -0.01 0.00 -0.01 0.19 -0.02 0.10

37 6 0.01 0.04 0.08 -0.00 0.00 0.01 0.04 0.05 -0.06

38 6 -0.01 -0.02 0.06 0.00 -0.01 0.02 -0.05 0.17 -0.09

39 6 -0.02 -0.02 -0.03 0.01 -0.00 -0.01 -0.19 0.02 0.10

40 6 0.05 0.03 0.02 0.01 0.01 -0.00 -0.03 -0.03 0.08

41 6 -0.01 -0.01 -0.05 -0.00 0.01 -0.01 0.05 -0.18 0.10

42 6 -0.01 -0.00 0.04 -0.01 0.00 0.01 0.17 -0.03 -0.08

43 6 0.02 -0.04 -0.08 0.00 0.00 0.01 0.02 -0.02 0.03

44 6 -0.01 0.02 -0.07 0.00 -0.01 0.02 -0.01 -0.08 0.05

45 6 -0.02 0.02 0.03 -0.01 -0.01 -0.01 -0.09 -0.03 -0.05

46 6 0.06 -0.03 -0.02 -0.01 0.01 -0.00 -0.02 0.01 -0.04

47 6 -0.01 0.01 0.05 0.00 0.01 -0.01 0.01 0.09 -0.05

48 6 -0.02 -0.00 -0.04 0.01 0.00 0.01 0.08 0.03 0.04

49 1 0.02 -0.04 -0.23 0.00 -0.05 -0.15 -0.02 -0.01 0.03

50 1 0.01 0.04 0.23 0.01 -0.05 -0.15 -0.01 -0.01 -0.06

51 1 -0.01 -0.00 0.08 -0.02 -0.00 0.05 -0.01 0.01 0.07

52 1 -0.01 0.00 0.09 -0.02 0.00 0.06 0.00 0.01 -0.02

53 1 -0.01 -0.00 -0.08 0.02 0.00 0.05 0.01 -0.01 0.07

54 1 -0.01 0.00 -0.09 0.02 -0.00 0.06 -0.00 -0.01 -0.02

55 1 0.01 0.04 -0.23 -0.01 0.05 -0.15 0.01 0.01 -0.06

56 1 0.02 -0.04 0.23 -0.00 0.05 -0.15 0.02 0.01 0.03

57 1 -0.06 0.10 -0.00 -0.02 0.02 0.01 -0.06 0.01 0.07

58 1 -0.06 0.09 -0.14 -0.01 0.01 -0.03 0.04 -0.08 -0.06

59 1 0.05 -0.02 0.02 0.00 0.00 0.01 -0.04 0.04 0.06

60 1 -0.12 0.04 -0.14 -0.01 0.00 -0.03 0.08 -0.03 -0.05

61 1 -0.08 0.06 0.01 -0.02 0.02 0.01 -0.02 0.06 0.07

62 1 0.04 0.03 -0.02 0.00 0.00 0.00 -0.08 -0.09 -0.13

63 1 -0.05 -0.09 0.14 0.00 0.01 -0.03 0.07 0.18 0.11

64 1 -0.05 -0.11 0.01 0.01 0.02 0.01 -0.12 -0.04 -0.14

65 1 -0.07 -0.07 -0.01 0.02 0.02 0.01 -0.03 -0.12 -0.14

66 1 -0.10 -0.05 0.14 0.01 0.00 -0.03 0.18 0.09 0.11

67 1 -0.07 -0.07 0.01 -0.02 -0.02 0.01 0.03 0.12 -0.14

68 1 -0.10 -0.05 -0.14 -0.01 -0.00 -0.03 -0.18 -0.09 0.11

69 1 0.04 0.03 0.03 -0.00 -0.00 0.00 0.08 0.09 -0.13

70 1 -0.05 -0.09 -0.14 -0.00 -0.01 -0.03 -0.07 -0.18 0.11

71 1 -0.05 -0.11 -0.01 -0.01 -0.02 0.01 0.12 0.04 -0.14

72 1 -0.09 0.06 -0.01 0.02 -0.02 0.01 0.02 -0.06 0.07

73 1 -0.12 0.04 0.14 0.01 -0.00 -0.03 -0.08 0.03 -0.05

74 1 0.05 -0.02 -0.03 -0.00 -0.00 0.01 0.04 -0.04 0.06

75 1 -0.06 0.09 0.14 0.01 -0.01 -0.03 -0.04 0.08 -0.06

76 1 -0.06 0.10 0.00 0.02 -0.02 0.01 0.06 -0.01 0.07

77 1 -0.05 0.00 0.02 -0.01 0.14 0.63 0.01 0.02 0.07

78 1 -0.05 0.00 -0.02 0.01 -0.14 0.63 -0.01 -0.02 0.07

58 59 60

A A A

Frequencies -- 635.1488 636.2712 636.7873

Red. masses -- 6.3187 6.3076 5.8664

Frc consts -- 1.5019 1.5045 1.4016

IR Inten -- 0.8544 1.2925 0.0294

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.00 0.03 -0.01 0.01 0.02 -0.00 0.00 -0.01

2 6 0.00 -0.01 -0.03 -0.00 -0.00 -0.01 -0.00 0.00 0.01

3 7 0.00 -0.00 0.02 0.00 0.00 -0.01 0.00 0.00 -0.00

4 6 -0.00 -0.00 0.00 -0.00 0.01 0.04 0.00 0.01 0.02

5 6 -0.00 -0.01 -0.02 -0.00 -0.01 -0.03 -0.00 -0.00 -0.02

6 6 0.00 0.01 -0.00 0.00 0.00 0.05 0.00 0.00 0.06

7 6 0.00 0.00 -0.01 -0.01 -0.00 0.03 -0.01 -0.00 0.04

8 7 -0.00 0.00 -0.02 -0.00 -0.00 -0.02 0.00 -0.01 -0.04

9 6 -0.01 -0.00 0.03 -0.00 -0.00 -0.00 -0.01 -0.00 0.02

10 6 0.00 -0.00 -0.02 -0.01 0.00 0.01 -0.00 0.00 0.00

11 6 -0.01 -0.00 0.02 0.00 0.00 -0.02 -0.00 0.00 -0.01

12 6 0.00 0.00 -0.05 0.01 -0.01 -0.01 -0.00 0.01 0.04

13 6 -0.01 -0.00 -0.03 -0.00 -0.00 0.00 0.01 0.00 0.02

14 6 0.00 -0.00 0.02 -0.01 0.00 -0.01 0.00 -0.00 0.00

15 6 -0.01 -0.00 -0.02 0.00 0.00 0.02 0.00 -0.00 -0.01

16 6 0.00 0.00 0.01 -0.01 -0.00 -0.03 0.01 0.00 0.04

17 7 -0.00 0.00 0.02 -0.00 -0.00 0.02 -0.00 0.01 -0.04

18 6 0.00 0.01 0.00 0.00 0.00 -0.05 -0.00 -0.00 0.06

19 6 -0.00 -0.00 -0.00 -0.00 0.01 -0.04 -0.00 -0.01 0.02

20 6 -0.00 -0.01 0.02 -0.00 -0.01 0.03 0.00 0.00 -0.02

21 6 -0.00 0.00 -0.03 -0.01 0.01 -0.02 0.00 -0.00 -0.01

22 6 0.00 -0.01 0.03 -0.00 -0.00 0.01 0.00 -0.00 0.01

23 7 0.00 -0.00 -0.02 0.00 0.00 0.01 -0.00 -0.00 -0.00

24 6 0.00 0.00 0.05 0.01 -0.01 0.01 0.00 -0.01 0.04

25 6 0.01 0.00 -0.01 -0.05 0.04 0.07 -0.04 0.04 0.06

26 6 0.02 0.01 -0.01 -0.19 -0.06 0.09 -0.16 -0.05 0.08

27 6 -0.00 0.03 0.02 -0.03 -0.21 -0.12 -0.02 -0.18 -0.10

28 6 -0.01 -0.00 0.01 0.03 -0.03 -0.09 0.03 -0.03 -0.08

29 6 -0.02 -0.01 0.01 0.21 0.06 -0.12 0.18 0.05 -0.10

30 6 0.00 -0.02 -0.02 0.03 0.19 0.10 0.03 0.16 0.08

31 6 0.03 0.04 0.09 -0.00 0.01 0.01 -0.01 -0.02 -0.04

32 6 -0.06 0.20 0.12 -0.01 0.02 0.01 0.02 -0.08 -0.05

33 6 -0.19 0.03 -0.10 -0.02 0.00 -0.01 0.08 -0.01 0.04

34 6 -0.04 -0.05 -0.07 0.00 -0.01 -0.01 0.01 0.02 0.03

35 6 0.06 -0.18 -0.10 0.01 -0.02 -0.00 -0.03 0.07 0.03

36 6 0.21 -0.03 0.12 0.03 -0.00 0.02 -0.09 0.01 -0.05

37 6 -0.04 -0.05 0.07 0.00 -0.01 0.01 -0.01 -0.02 0.03

38 6 0.06 -0.18 0.10 0.01 -0.02 0.00 0.03 -0.07 0.03

39 6 0.21 -0.03 -0.12 0.03 -0.00 -0.02 0.09 -0.01 -0.05

40 6 0.03 0.04 -0.09 -0.00 0.01 -0.01 0.01 0.02 -0.04

41 6 -0.06 0.20 -0.12 -0.01 0.02 -0.01 -0.02 0.08 -0.05

42 6 -0.19 0.03 0.10 -0.02 0.00 0.01 -0.08 0.01 0.04

43 6 0.01 0.00 0.01 -0.05 0.04 -0.07 0.04 -0.04 0.06

44 6 0.00 -0.02 0.02 0.03 0.19 -0.10 -0.03 -0.16 0.08

45 6 -0.02 -0.01 -0.01 0.21 0.06 0.12 -0.18 -0.05 -0.10

46 6 -0.01 -0.00 -0.01 0.03 -0.03 0.09 -0.03 0.03 -0.08

47 6 -0.00 0.03 -0.02 -0.03 -0.21 0.12 0.02 0.18 -0.10

48 6 0.02 0.01 0.01 -0.19 -0.06 -0.09 0.16 0.05 0.08

49 1 -0.01 0.01 0.06 -0.01 0.02 0.05 -0.00 0.02 0.05

50 1 -0.00 -0.01 -0.03 -0.01 -0.01 -0.07 -0.01 0.02 0.02

51 1 0.01 -0.01 -0.06 -0.01 0.00 0.01 0.01 0.00 -0.05

52 1 -0.01 -0.00 0.02 0.01 0.01 -0.06 0.01 0.01 -0.08

53 1 0.01 -0.01 0.06 -0.01 0.00 -0.01 -0.01 -0.00 -0.05

54 1 -0.01 -0.00 -0.02 0.01 0.01 0.06 -0.01 -0.01 -0.08

55 1 -0.00 -0.01 0.03 -0.01 -0.01 0.07 0.01 -0.02 0.02

56 1 -0.01 0.01 -0.06 -0.01 0.02 -0.05 0.00 -0.02 0.05

57 1 0.01 -0.01 -0.02 -0.14 0.02 0.15 -0.12 0.01 0.13

58 1 -0.01 0.03 0.02 0.10 -0.18 -0.13 0.09 -0.16 -0.10

59 1 0.01 -0.01 -0.02 -0.10 0.08 0.15 -0.09 0.07 0.13

60 1 -0.02 0.01 0.01 0.20 -0.06 -0.13 0.19 -0.06 -0.10

61 1 0.00 -0.02 -0.02 -0.05 0.12 0.15 -0.03 0.10 0.14

62 1 -0.09 -0.10 -0.15 -0.02 -0.01 -0.02 0.04 0.04 0.06

63 1 0.07 0.19 0.13 0.01 0.02 0.01 -0.03 -0.08 -0.04

64 1 -0.13 -0.04 -0.15 -0.02 0.00 -0.02 0.05 0.01 0.06

65 1 -0.03 -0.13 -0.15 -0.01 -0.01 -0.01 0.01 0.05 0.06

66 1 0.19 0.09 0.13 0.03 0.00 0.01 -0.09 -0.04 -0.05

67 1 -0.03 -0.14 0.15 -0.01 -0.01 0.01 -0.01 -0.05 0.06

68 1 0.19 0.09 -0.13 0.03 0.00 -0.01 0.09 0.04 -0.05

69 1 -0.09 -0.10 0.15 -0.02 -0.01 0.02 -0.04 -0.04 0.06

70 1 0.07 0.19 -0.13 0.01 0.02 -0.01 0.03 0.08 -0.04

71 1 -0.13 -0.04 0.15 -0.02 0.00 0.02 -0.05 -0.01 0.06

72 1 0.00 -0.02 0.02 -0.05 0.12 -0.15 0.03 -0.10 0.14

73 1 -0.02 0.01 -0.01 0.20 -0.06 0.13 -0.19 0.06 -0.10

74 1 0.01 -0.01 0.02 -0.10 0.08 -0.15 0.09 -0.07 0.13

75 1 -0.01 0.03 -0.02 0.10 -0.18 0.13 -0.09 0.16 -0.10

76 1 0.01 -0.01 0.02 -0.14 0.02 -0.15 0.12 -0.01 0.13

77 1 -0.00 0.00 0.03 -0.00 -0.00 -0.03 0.01 -0.04 -0.19

78 1 -0.00 0.00 -0.03 -0.00 -0.00 0.03 -0.01 0.04 -0.19

61 62 63

A A A

Frequencies -- 649.5961 658.9246 661.6662

Red. masses -- 6.8004 4.0947 4.3768

Frc consts -- 1.6907 1.0475 1.1290

IR Inten -- 1.1555 14.5459 0.0569

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.03 -0.01 0.02 -0.05 -0.09 -0.01 0.05 0.12

2 6 -0.03 0.01 0.04 0.01 0.01 0.12 -0.00 -0.02 -0.16

3 7 0.00 -0.03 -0.04 0.03 0.00 0.01 -0.02 -0.00 -0.00

4 6 0.03 0.01 0.05 0.02 -0.01 -0.13 -0.01 0.03 0.16

5 6 0.00 -0.03 -0.01 0.01 0.05 0.09 -0.00 -0.05 -0.12

6 6 0.09 0.10 -0.01 -0.03 -0.04 0.03 0.01 0.04 -0.03

7 6 0.00 0.04 -0.05 -0.02 -0.02 0.12 -0.00 -0.02 -0.12

8 7 -0.03 -0.00 0.06 0.03 0.00 -0.13 -0.00 0.02 0.00

9 6 0.01 -0.04 -0.04 -0.02 0.01 0.10 0.01 -0.02 0.11

10 6 -0.03 -0.00 -0.01 0.01 0.00 -0.00 0.05 -0.02 -0.08

11 6 -0.04 -0.00 -0.00 0.01 0.00 -0.01 -0.04 -0.03 0.08

12 6 -0.10 0.08 -0.01 -0.03 0.03 -0.03 0.02 -0.04 0.03

13 6 -0.01 0.04 -0.04 -0.02 0.01 -0.10 -0.01 0.02 0.11

14 6 0.03 0.00 -0.01 0.01 0.00 0.00 -0.05 0.02 -0.08

15 6 0.04 0.00 -0.00 0.01 0.00 0.01 0.04 0.03 0.08

16 6 -0.00 -0.04 -0.05 -0.02 -0.02 -0.12 0.00 0.02 -0.12

17 7 0.03 0.00 0.06 0.03 0.00 0.13 0.00 -0.02 0.00

18 6 -0.09 -0.10 -0.01 -0.03 -0.04 -0.03 -0.01 -0.04 -0.03

19 6 -0.03 -0.01 0.05 0.02 -0.01 0.13 0.01 -0.03 0.16

20 6 -0.00 0.03 -0.01 0.01 0.05 -0.09 0.00 0.05 -0.12

21 6 -0.00 0.03 -0.01 0.02 -0.05 0.09 0.01 -0.05 0.12

22 6 0.03 -0.01 0.04 0.01 0.01 -0.12 0.00 0.02 -0.16

23 7 -0.00 0.03 -0.04 0.03 0.00 -0.01 0.02 0.00 -0.00

24 6 0.10 -0.08 -0.01 -0.03 0.03 0.03 -0.02 0.04 0.03

25 6 0.10 0.12 0.01 -0.04 -0.04 -0.00 0.02 0.03 0.00

26 6 -0.04 0.06 0.09 0.00 -0.03 -0.05 -0.01 0.01 0.03

27 6 -0.05 0.05 0.09 0.02 -0.03 -0.03 -0.02 0.02 0.02

28 6 -0.10 -0.12 -0.00 0.03 0.06 -0.01 -0.02 -0.04 0.00

29 6 0.05 -0.04 -0.08 -0.01 0.02 0.04 0.01 -0.01 -0.03

30 6 0.07 -0.03 -0.08 -0.03 0.02 0.03 0.02 -0.01 -0.02

31 6 0.12 -0.11 -0.00 0.04 -0.05 0.01 -0.03 0.04 -0.00

32 6 0.04 0.06 0.09 0.02 0.04 0.03 -0.02 -0.02 -0.02

33 6 0.03 0.07 0.08 -0.00 0.02 0.04 -0.01 -0.02 -0.04

34 6 -0.12 0.10 0.00 -0.05 0.03 0.00 0.03 -0.03 -0.00

35 6 -0.06 -0.04 -0.08 -0.03 -0.02 -0.03 0.02 0.01 0.02

36 6 -0.04 -0.05 -0.08 -0.01 -0.02 -0.03 0.01 0.01 0.03

37 6 0.12 -0.10 0.00 -0.05 0.03 -0.00 -0.03 0.03 -0.00

38 6 0.06 0.04 -0.08 -0.03 -0.02 0.03 -0.02 -0.01 0.02

39 6 0.04 0.05 -0.08 -0.01 -0.02 0.03 -0.01 -0.01 0.03

40 6 -0.12 0.11 -0.00 0.04 -0.05 -0.01 0.03 -0.04 -0.00

41 6 -0.04 -0.06 0.09 0.02 0.04 -0.03 0.02 0.02 -0.02

42 6 -0.03 -0.07 0.08 -0.00 0.02 -0.04 0.01 0.02 -0.04

43 6 -0.10 -0.12 0.01 -0.04 -0.04 0.00 -0.02 -0.03 0.00

44 6 -0.07 0.03 -0.08 -0.03 0.02 -0.03 -0.02 0.01 -0.02

45 6 -0.05 0.04 -0.08 -0.01 0.02 -0.04 -0.01 0.01 -0.03

46 6 0.10 0.12 -0.00 0.03 0.06 0.01 0.02 0.04 0.00

47 6 0.05 -0.05 0.09 0.02 -0.03 0.03 0.02 -0.02 0.02

48 6 0.04 -0.06 0.09 0.00 -0.03 0.05 0.01 -0.01 0.03

49 1 0.02 -0.02 -0.03 -0.00 -0.11 -0.23 0.01 0.12 0.32

50 1 -0.01 -0.03 -0.05 -0.02 0.12 0.27 0.03 -0.12 -0.33

51 1 -0.05 0.01 0.09 0.07 0.01 -0.27 0.09 0.01 -0.17

52 1 -0.05 -0.02 0.10 0.08 0.01 -0.29 -0.10 -0.01 0.19

53 1 0.05 -0.01 0.09 0.07 0.01 0.27 -0.09 -0.01 -0.17

54 1 0.05 0.02 0.10 0.08 0.01 0.29 0.10 0.01 0.19

55 1 0.01 0.03 -0.05 -0.02 0.12 -0.27 -0.03 0.12 -0.33

56 1 -0.02 0.02 -0.03 -0.00 -0.11 0.23 -0.01 -0.12 0.32

57 1 -0.08 -0.05 0.03 0.03 0.01 -0.01 -0.02 -0.01 0.02

58 1 0.07 0.13 0.02 -0.01 -0.09 0.02 0.01 0.05 -0.01

59 1 -0.10 -0.12 -0.01 0.04 0.05 0.02 -0.02 -0.03 -0.00

60 1 0.10 0.10 -0.02 -0.01 -0.07 0.04 0.01 0.04 -0.03

61 1 -0.04 -0.09 -0.04 0.03 0.03 0.03 -0.02 -0.01 -0.02

62 1 0.12 -0.11 -0.01 0.04 -0.04 -0.01 -0.04 0.03 0.00

63 1 -0.09 0.12 0.02 -0.02 0.08 -0.02 0.02 -0.06 0.01

64 1 0.09 -0.04 0.03 0.03 -0.00 0.01 -0.02 0.01 -0.02

65 1 0.06 -0.08 -0.04 0.03 -0.02 -0.03 -0.02 0.01 0.02

66 1 -0.11 0.08 -0.02 -0.01 0.06 -0.04 0.02 -0.04 0.03

67 1 -0.06 0.08 -0.04 0.03 -0.02 0.03 0.02 -0.01 0.02

68 1 0.11 -0.08 -0.02 -0.01 0.06 0.04 -0.02 0.04 0.03

69 1 -0.12 0.11 -0.01 0.04 -0.04 0.01 0.04 -0.03 0.00

70 1 0.09 -0.12 0.02 -0.02 0.08 0.02 -0.02 0.06 0.01

71 1 -0.09 0.04 0.03 0.03 -0.00 -0.01 0.02 -0.01 -0.02

72 1 0.04 0.09 -0.04 0.03 0.03 -0.03 0.02 0.01 -0.02

73 1 -0.10 -0.10 -0.02 -0.01 -0.07 -0.04 -0.01 -0.04 -0.03

74 1 0.10 0.12 -0.01 0.04 0.05 -0.02 0.02 0.03 -0.00

75 1 -0.07 -0.13 0.02 -0.01 -0.09 -0.02 -0.01 -0.05 -0.01

76 1 0.08 0.05 0.03 0.03 0.01 0.01 0.02 0.01 0.02

77 1 0.00 -0.06 -0.16 0.06 0.01 0.01 -0.04 -0.01 -0.03

78 1 -0.00 0.06 -0.16 0.06 0.01 -0.01 0.04 0.01 -0.03

64 65 66

A A A

Frequencies -- 669.8496 674.8035 677.1494

Red. masses -- 5.3029 5.0129 2.6010

Frc consts -- 1.4019 1.3449 0.7027

IR Inten -- 28.6729 9.9914 8.5717

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.02 0.03 0.02 -0.02 0.08 0.00 0.00 0.04

2 6 0.02 -0.03 -0.13 0.02 -0.06 -0.08 -0.01 -0.03 -0.10

3 7 -0.01 0.03 0.10 0.06 0.00 0.00 -0.00 0.01 0.06

4 6 -0.02 -0.03 -0.12 0.01 0.06 0.07 0.01 -0.03 -0.09

5 6 -0.00 0.01 0.02 0.02 0.02 -0.07 -0.00 -0.00 0.03

6 6 -0.06 -0.04 -0.01 -0.04 -0.06 0.00 0.01 0.01 -0.02

7 6 0.02 0.03 0.10 0.02 -0.03 -0.07 -0.02 0.00 0.10

8 7 -0.01 0.06 0.01 -0.01 -0.00 0.07 0.01 0.00 -0.11

9 6 -0.02 0.03 -0.11 0.01 0.03 -0.08 -0.02 -0.01 0.11

10 6 -0.07 0.02 0.06 0.02 0.00 0.01 -0.01 -0.00 -0.00

11 6 0.07 0.03 -0.06 0.02 0.00 0.00 -0.01 -0.00 0.00

12 6 0.07 -0.04 -0.01 -0.04 0.05 -0.00 -0.01 0.00 -0.02

13 6 -0.02 0.03 0.11 0.01 0.03 0.08 0.02 0.01 0.11

14 6 -0.07 0.02 -0.06 0.02 0.00 -0.01 0.01 0.00 -0.00

15 6 0.07 0.03 0.06 0.02 0.00 -0.00 0.01 0.00 0.00

16 6 0.02 0.03 -0.10 0.02 -0.03 0.07 0.02 -0.00 0.10

17 7 -0.01 0.06 -0.01 -0.01 -0.00 -0.07 -0.01 -0.00 -0.11

18 6 -0.06 -0.04 0.01 -0.04 -0.06 -0.00 -0.01 -0.01 -0.02

19 6 -0.02 -0.03 0.12 0.01 0.06 -0.07 -0.01 0.03 -0.09

20 6 -0.00 0.01 -0.02 0.02 0.02 0.07 0.00 0.00 0.03

21 6 -0.00 0.02 -0.03 0.02 -0.02 -0.08 -0.00 -0.00 0.04

22 6 0.02 -0.03 0.13 0.02 -0.06 0.08 0.01 0.03 -0.10

23 7 -0.01 0.03 -0.10 0.06 0.00 -0.00 0.00 -0.01 0.06

24 6 0.07 -0.04 0.01 -0.04 0.05 0.00 0.01 -0.00 -0.02

25 6 -0.06 -0.07 -0.00 -0.07 -0.09 -0.00 0.02 0.02 0.00

26 6 0.04 -0.05 -0.05 0.02 -0.05 -0.07 -0.00 0.01 0.01

27 6 0.02 -0.03 -0.06 0.04 -0.05 -0.06 -0.01 0.01 0.02

28 6 0.07 0.06 0.02 0.07 0.10 -0.01 -0.02 -0.02 0.00

29 6 -0.05 0.03 0.05 -0.05 0.02 0.08 0.01 -0.01 -0.01

30 6 -0.04 0.00 0.06 -0.07 0.02 0.06 0.01 -0.01 -0.01

31 6 -0.09 0.06 0.01 0.08 -0.08 0.01 0.02 -0.02 0.00

32 6 -0.02 -0.04 -0.07 0.03 0.05 0.06 0.00 0.02 0.02

33 6 -0.03 -0.07 -0.06 0.01 0.05 0.07 0.00 0.01 0.01

34 6 0.08 -0.07 -0.00 -0.09 0.07 -0.00 -0.02 0.02 0.00

35 6 0.04 0.01 0.07 -0.06 -0.03 -0.06 -0.01 -0.01 -0.02

36 6 0.05 0.04 0.05 -0.04 -0.03 -0.07 -0.01 -0.01 -0.01

37 6 0.08 -0.07 0.00 -0.09 0.07 0.00 0.02 -0.02 0.00

38 6 0.04 0.01 -0.07 -0.06 -0.03 0.06 0.01 0.01 -0.02

39 6 0.05 0.04 -0.05 -0.04 -0.03 0.07 0.01 0.01 -0.01

40 6 -0.09 0.06 -0.01 0.08 -0.08 -0.01 -0.02 0.02 0.00

41 6 -0.02 -0.04 0.07 0.03 0.05 -0.06 -0.00 -0.02 0.02

42 6 -0.03 -0.06 0.06 0.01 0.05 -0.07 -0.00 -0.01 0.01

43 6 -0.06 -0.07 0.00 -0.07 -0.09 0.00 -0.02 -0.02 0.00

44 6 -0.04 0.00 -0.06 -0.07 0.02 -0.06 -0.01 0.01 -0.01

45 6 -0.05 0.03 -0.05 -0.05 0.02 -0.08 -0.01 0.01 -0.01

46 6 0.07 0.06 -0.02 0.07 0.10 0.01 0.02 0.02 0.00

47 6 0.02 -0.03 0.06 0.04 -0.05 0.06 0.01 -0.01 0.02

48 6 0.04 -0.05 0.05 0.02 -0.05 0.07 0.00 -0.01 0.01

49 1 -0.01 0.06 0.19 -0.02 -0.02 0.20 0.01 0.02 0.10

50 1 0.00 0.05 0.17 -0.02 0.02 -0.19 -0.01 0.01 0.08

51 1 -0.13 -0.04 0.15 -0.05 -0.03 0.21 0.08 0.02 -0.32

52 1 0.13 -0.02 -0.13 -0.05 0.02 0.21 0.08 -0.00 -0.31

53 1 -0.13 -0.04 -0.15 -0.05 -0.03 -0.21 -0.08 -0.02 -0.32

54 1 0.13 -0.02 0.13 -0.05 0.02 -0.21 -0.08 0.00 -0.31

55 1 0.00 0.05 -0.17 -0.02 0.02 0.19 0.01 -0.01 0.08

56 1 -0.01 0.06 -0.19 -0.02 -0.02 -0.20 -0.01 -0.02 0.10

57 1 0.04 0.03 -0.04 0.06 0.03 -0.02 -0.02 -0.00 -0.01

58 1 -0.09 -0.05 -0.06 -0.05 -0.12 -0.00 0.01 0.03 0.00

59 1 0.06 0.07 0.01 0.07 0.10 -0.01 -0.02 -0.02 -0.01

60 1 -0.11 -0.04 -0.02 -0.08 -0.10 0.03 0.01 0.02 -0.00

61 1 0.02 0.05 0.02 0.01 0.08 0.02 -0.00 -0.02 -0.00

62 1 -0.08 0.07 0.01 0.08 -0.08 0.01 0.02 -0.02 -0.01

63 1 0.11 -0.05 -0.05 -0.06 0.11 -0.00 -0.02 0.03 0.00

64 1 -0.05 0.02 -0.04 0.07 -0.02 0.01 0.02 0.00 -0.01

65 1 -0.03 0.05 0.03 0.02 -0.07 -0.02 0.01 -0.02 -0.00

66 1 0.12 -0.03 -0.02 -0.09 0.09 -0.04 -0.02 0.02 -0.00

67 1 -0.03 0.05 -0.03 0.02 -0.07 0.02 -0.01 0.02 -0.00

68 1 0.12 -0.03 0.02 -0.09 0.09 0.04 0.02 -0.02 -0.00

69 1 -0.08 0.07 -0.01 0.08 -0.08 -0.01 -0.02 0.02 -0.01

70 1 0.11 -0.05 0.05 -0.06 0.11 0.00 0.02 -0.03 0.00

71 1 -0.05 0.02 0.04 0.07 -0.02 -0.01 -0.02 -0.00 -0.01

72 1 0.02 0.05 -0.02 0.01 0.08 -0.02 0.00 0.02 -0.00

73 1 -0.11 -0.04 0.02 -0.08 -0.10 -0.03 -0.01 -0.02 -0.00

74 1 0.06 0.07 -0.01 0.07 0.10 0.01 0.02 0.02 -0.01

75 1 -0.09 -0.05 0.06 -0.05 -0.12 0.00 -0.01 -0.03 0.00

76 1 0.04 0.03 0.04 0.06 0.03 0.02 0.02 0.00 -0.01

77 1 -0.01 0.06 0.24 0.17 0.01 0.00 -0.00 0.10 0.44

78 1 -0.01 0.06 -0.24 0.17 0.01 -0.00 0.00 -0.10 0.43

67 68 69

A A A

Frequencies -- 685.2225 690.5320 712.1623

Red. masses -- 4.4089 5.7726 1.6876

Frc consts -- 1.2197 1.6218 0.5043

IR Inten -- 3.8905 0.0993 47.7423

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.01 0.02 0.03 -0.02 0.06 0.01 -0.00 0.00

2 6 -0.02 -0.04 -0.14 0.01 -0.05 -0.07 0.00 0.00 0.00

3 7 -0.00 0.03 0.10 0.05 0.00 -0.00 0.00 -0.00 0.00

4 6 0.03 -0.04 -0.14 0.00 0.05 0.08 -0.00 -0.00 -0.00

5 6 0.00 -0.01 0.02 0.03 0.02 -0.06 0.00 0.00 -0.00

6 6 0.04 0.01 0.02 -0.05 -0.03 -0.02 -0.01 0.01 -0.00

7 6 -0.04 -0.02 0.08 0.04 0.02 -0.03 -0.01 -0.00 0.01

8 7 0.00 -0.05 0.00 -0.01 0.08 0.00 0.00 0.01 -0.00

9 6 0.04 -0.01 -0.09 -0.04 0.02 0.03 0.01 -0.01 -0.00

10 6 0.01 0.00 0.08 -0.04 0.02 -0.04 0.00 -0.00 0.01

11 6 -0.01 0.00 -0.08 0.04 0.02 0.04 -0.00 -0.00 -0.01

12 6 -0.04 0.00 0.02 -0.05 0.02 0.02 -0.00 -0.00 0.00

13 6 0.04 -0.01 0.09 0.04 -0.02 0.03 -0.01 0.01 -0.00

14 6 0.01 0.00 -0.08 0.04 -0.02 -0.04 -0.00 0.00 0.01

15 6 -0.01 0.00 0.08 -0.04 -0.02 0.04 0.00 0.00 -0.01

16 6 -0.04 -0.02 -0.08 -0.04 -0.02 -0.03 0.01 0.00 0.01

17 7 0.00 -0.05 -0.00 0.01 -0.08 0.00 -0.00 -0.01 -0.00

18 6 0.04 0.01 -0.02 0.05 0.03 -0.02 0.01 -0.01 -0.00

19 6 0.03 -0.04 0.14 -0.00 -0.05 0.08 0.00 0.00 -0.00

20 6 0.00 -0.01 -0.02 -0.03 -0.02 -0.06 -0.00 -0.00 -0.00

21 6 -0.00 -0.01 -0.02 -0.03 0.02 0.06 -0.01 0.00 0.00

22 6 -0.02 -0.04 0.14 -0.01 0.05 -0.07 -0.00 -0.00 0.00

23 7 -0.00 0.03 -0.10 -0.05 -0.00 -0.00 -0.00 0.00 0.00

24 6 -0.04 0.00 -0.02 0.05 -0.02 0.02 0.00 0.00 0.00

25 6 0.05 0.06 0.01 -0.08 -0.10 -0.01 -0.04 0.03 -0.04

26 6 -0.03 0.05 0.04 0.04 -0.07 -0.07 0.02 -0.02 0.04

27 6 -0.02 0.03 0.06 0.03 -0.06 -0.09 -0.05 0.05 -0.06

28 6 -0.06 -0.05 -0.01 0.09 0.10 0.01 0.02 -0.02 0.02

29 6 0.04 -0.02 -0.04 -0.07 0.03 0.08 -0.05 0.05 -0.06

30 6 0.03 -0.00 -0.05 -0.07 0.01 0.08 0.03 -0.02 0.04

31 6 0.07 -0.04 -0.01 0.11 -0.08 -0.01 0.00 0.00 -0.00

32 6 0.01 0.03 0.06 0.02 0.06 0.09 -0.01 -0.01 0.01

33 6 0.02 0.05 0.04 0.03 0.08 0.07 0.00 0.00 -0.01

34 6 -0.06 0.05 0.00 -0.10 0.08 0.00 -0.01 -0.01 0.01

35 6 -0.03 -0.01 -0.05 -0.06 -0.02 -0.09 0.00 0.00 -0.01

36 6 -0.04 -0.03 -0.04 -0.07 -0.04 -0.07 -0.01 -0.01 0.01

37 6 -0.06 0.05 -0.00 0.10 -0.08 0.00 0.01 0.01 0.01

38 6 -0.03 -0.01 0.05 0.06 0.02 -0.09 -0.00 -0.00 -0.01

39 6 -0.04 -0.03 0.04 0.07 0.04 -0.07 0.01 0.01 0.01

40 6 0.07 -0.04 0.01 -0.11 0.08 -0.01 -0.00 -0.00 -0.00

41 6 0.01 0.03 -0.06 -0.02 -0.06 0.09 0.01 0.01 0.01

42 6 0.02 0.05 -0.04 -0.03 -0.08 0.07 -0.00 -0.00 -0.01

43 6 0.05 0.06 -0.01 0.08 0.10 -0.01 0.04 -0.03 -0.04

44 6 0.03 -0.00 0.05 0.07 -0.01 0.08 -0.03 0.02 0.04

45 6 0.04 -0.02 0.04 0.07 -0.03 0.08 0.05 -0.05 -0.06

46 6 -0.06 -0.05 0.01 -0.09 -0.10 0.01 -0.02 0.02 0.02

47 6 -0.02 0.03 -0.06 -0.03 0.06 -0.09 0.05 -0.05 -0.06

48 6 -0.03 0.05 -0.04 -0.04 0.07 -0.07 -0.02 0.02 0.04

49 1 0.01 0.08 0.28 0.02 -0.00 0.17 0.00 -0.00 -0.00

50 1 -0.03 0.08 0.28 0.02 0.00 -0.17 0.01 0.00 -0.00

51 1 0.01 0.04 0.17 -0.07 -0.03 -0.07 0.00 0.00 0.02

52 1 -0.02 0.04 -0.15 0.06 -0.02 0.09 -0.01 -0.00 -0.01

53 1 0.01 0.04 -0.17 0.07 0.03 -0.07 -0.00 -0.00 0.02

54 1 -0.02 0.04 0.15 -0.06 0.02 0.09 0.01 0.00 -0.01

55 1 -0.03 0.08 -0.28 -0.02 -0.00 -0.17 -0.01 -0.00 -0.00

56 1 0.01 0.08 -0.28 -0.02 0.00 0.17 -0.00 0.00 -0.00

57 1 -0.05 -0.01 0.01 0.07 0.02 -0.03 0.19 -0.18 0.22

58 1 0.08 0.06 0.04 -0.10 -0.12 -0.05 0.09 -0.08 0.09

59 1 -0.06 -0.06 -0.01 0.09 0.10 0.00 0.24 -0.22 0.27

60 1 0.09 0.04 0.02 -0.14 -0.09 -0.01 0.08 -0.08 0.09

61 1 -0.01 -0.05 -0.01 0.01 0.08 0.02 0.20 -0.17 0.22

62 1 0.06 -0.05 -0.01 0.10 -0.08 -0.01 0.03 0.04 -0.04

63 1 -0.08 0.04 0.04 -0.12 0.10 0.05 0.01 0.01 -0.01

64 1 0.05 0.00 0.00 0.08 -0.01 0.02 0.02 0.03 -0.03

65 1 0.02 -0.04 -0.01 0.02 -0.07 -0.03 0.03 0.03 -0.03

66 1 -0.09 0.02 0.02 -0.15 0.07 0.00 0.01 0.01 -0.01

67 1 0.02 -0.04 0.01 -0.02 0.07 -0.03 -0.03 -0.03 -0.03

68 1 -0.09 0.02 -0.02 0.15 -0.07 0.00 -0.01 -0.01 -0.01

69 1 0.06 -0.05 0.01 -0.10 0.08 -0.01 -0.03 -0.04 -0.04

70 1 -0.08 0.04 -0.04 0.12 -0.10 0.05 -0.01 -0.01 -0.01

71 1 0.05 0.00 -0.00 -0.08 0.01 0.02 -0.02 -0.03 -0.04

72 1 -0.01 -0.05 0.01 -0.01 -0.08 0.02 -0.20 0.17 0.22

73 1 0.09 0.04 -0.02 0.14 0.09 -0.01 -0.08 0.08 0.09

74 1 -0.06 -0.06 0.01 -0.09 -0.10 0.00 -0.24 0.22 0.27

75 1 0.08 0.06 -0.04 0.10 0.12 -0.05 -0.09 0.08 0.09

76 1 -0.05 -0.01 -0.01 -0.07 -0.02 -0.03 -0.19 0.18 0.22

77 1 -0.01 0.06 0.22 0.18 0.01 -0.03 0.01 -0.00 0.00

78 1 -0.01 0.06 -0.22 -0.18 -0.01 -0.03 -0.01 0.00 0.00

70 71 72

A A A

Frequencies -- 712.6600 713.9410 714.4206

Red. masses -- 1.6148 1.7238 1.6397

Frc consts -- 0.4832 0.5177 0.4931

IR Inten -- 81.5579 85.0490 75.4287

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 0.01 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 -0.01 -0.00 0.01 0.00 0.00 -0.00

10 6 -0.00 0.00 0.00 -0.00 0.00 -0.01 0.00 -0.00 0.01

11 6 0.00 0.00 0.01 0.00 0.00 0.00 -0.00 -0.00 -0.00

12 6 0.00 -0.00 0.00 0.01 0.01 -0.00 0.00 0.00 0.00

13 6 -0.00 0.00 -0.00 0.01 0.00 0.01 0.00 0.00 0.00

14 6 -0.00 0.00 -0.00 0.00 -0.00 -0.01 0.00 -0.00 -0.01

15 6 0.00 0.00 -0.01 -0.00 -0.00 0.00 -0.00 -0.00 0.00

16 6 0.00 -0.00 -0.00 -0.01 -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 0.00 -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 -0.01 -0.01 -0.00 0.00 0.00 -0.00

25 6 0.04 -0.03 0.04 -0.01 0.00 -0.01 0.00 0.00 -0.00

26 6 -0.02 0.02 -0.03 0.01 -0.01 0.00 -0.00 0.00 0.00

27 6 0.05 -0.05 0.06 -0.01 0.01 -0.01 -0.00 0.00 0.00

28 6 -0.02 0.02 -0.02 0.01 -0.00 0.00 -0.00 -0.00 0.00

29 6 0.05 -0.05 0.06 -0.01 0.01 -0.01 0.00 0.00 -0.00

30 6 -0.03 0.02 -0.03 0.00 -0.00 0.01 0.00 -0.00 -0.00

31 6 -0.00 0.00 0.00 -0.02 -0.03 0.03 -0.02 -0.03 0.02

32 6 0.00 -0.00 -0.00 0.05 0.06 -0.06 0.05 0.06 -0.06

33 6 -0.00 -0.00 -0.00 -0.02 -0.03 0.04 -0.02 -0.02 0.04

34 6 0.00 -0.00 -0.00 0.03 0.04 -0.04 0.03 0.04 -0.04

35 6 0.00 0.00 0.00 -0.03 -0.03 0.04 -0.02 -0.03 0.03

36 6 0.00 0.00 0.00 0.05 0.05 -0.06 0.05 0.05 -0.06

37 6 0.00 -0.00 0.00 -0.03 -0.04 -0.04 0.03 0.04 0.04

38 6 0.00 0.00 -0.00 0.03 0.03 0.04 -0.02 -0.03 -0.03

39 6 0.00 0.00 -0.00 -0.05 -0.06 -0.07 0.05 0.05 0.06

40 6 -0.00 0.00 -0.00 0.02 0.03 0.03 -0.02 -0.03 -0.02

41 6 0.00 -0.00 0.00 -0.05 -0.06 -0.06 0.05 0.06 0.06

42 6 -0.00 -0.00 0.00 0.02 0.03 0.04 -0.02 -0.02 -0.04

43 6 0.04 -0.03 -0.04 0.01 -0.00 -0.01 0.00 0.00 0.00

44 6 -0.03 0.02 0.03 -0.00 0.00 0.01 0.00 -0.00 0.00

45 6 0.05 -0.05 -0.06 0.01 -0.01 -0.01 0.00 0.00 0.00

46 6 -0.02 0.02 0.02 -0.01 0.00 0.00 -0.00 -0.00 -0.00

47 6 0.05 -0.05 -0.06 0.01 -0.01 -0.01 -0.00 0.00 -0.00

48 6 -0.02 0.02 0.03 -0.01 0.01 0.00 -0.00 0.00 -0.00

49 1 -0.00 0.00 -0.00 -0.01 -0.00 -0.00 -0.00 0.00 0.01

50 1 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.01

51 1 0.00 0.00 -0.02 -0.00 0.00 -0.01 0.01 -0.00 -0.01

52 1 0.01 0.00 -0.02 0.01 -0.00 0.01 -0.00 0.00 -0.01

53 1 0.00 0.00 0.02 0.00 -0.00 -0.01 0.01 -0.00 0.01

54 1 0.01 0.00 0.02 -0.01 0.00 0.01 -0.00 0.00 0.01

55 1 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.01

56 1 -0.00 0.00 0.00 0.01 0.00 -0.00 -0.00 0.00 -0.01

57 1 -0.19 0.18 -0.22 0.03 -0.03 0.04 0.00 -0.01 0.01

58 1 -0.10 0.08 -0.10 0.01 -0.01 0.01 0.01 0.00 0.01

59 1 -0.24 0.22 -0.27 0.04 -0.03 0.04 0.01 -0.01 0.01

60 1 -0.09 0.09 -0.10 0.01 -0.01 0.01 0.01 0.00 0.00

61 1 -0.20 0.17 -0.22 0.03 -0.03 0.04 0.01 -0.01 0.01

62 1 -0.01 -0.01 0.01 -0.21 -0.25 0.27 -0.21 -0.25 0.27

63 1 0.00 -0.01 0.00 -0.08 -0.08 0.09 -0.09 -0.09 0.10

64 1 -0.01 -0.01 0.01 -0.17 -0.20 0.22 -0.17 -0.20 0.23

65 1 -0.01 -0.00 0.01 -0.18 -0.20 0.22 -0.18 -0.20 0.22

66 1 0.00 -0.01 0.00 -0.07 -0.08 0.08 -0.08 -0.09 0.09

67 1 -0.01 -0.00 -0.01 0.18 0.20 0.22 -0.18 -0.20 -0.22

68 1 0.00 -0.01 -0.00 0.07 0.08 0.08 -0.08 -0.09 -0.09

69 1 -0.01 -0.01 -0.01 0.21 0.25 0.27 -0.21 -0.25 -0.27

70 1 0.00 -0.01 -0.00 0.08 0.08 0.09 -0.09 -0.09 -0.10

71 1 -0.01 -0.01 -0.01 0.17 0.20 0.23 -0.17 -0.20 -0.23

72 1 -0.20 0.17 0.22 -0.03 0.03 0.04 0.01 -0.01 -0.01

73 1 -0.09 0.09 0.10 -0.01 0.01 0.01 0.01 0.00 -0.00

74 1 -0.24 0.22 0.27 -0.04 0.03 0.04 0.01 -0.01 -0.01

75 1 -0.10 0.08 0.10 -0.01 0.01 0.01 0.01 0.00 -0.01

76 1 -0.19 0.18 0.22 -0.03 0.03 0.04 0.00 -0.01 -0.01

77 1 -0.01 -0.00 -0.00 -0.00 -0.00 0.00 -0.01 -0.00 0.00

78 1 -0.01 -0.00 0.00 0.00 0.00 0.00 -0.01 -0.00 -0.00

73 74 75

A A A

Frequencies -- 718.7073 724.3248 731.6276

Red. masses -- 2.7562 2.1934 3.1056

Frc consts -- 0.8388 0.6780 0.9794

IR Inten -- 26.7229 243.1301 59.7637

Atom AN X Y Z X Y Z X Y Z

1 6 -0.01 -0.01 -0.04 0.00 0.00 -0.00 -0.00 -0.01 -0.02

2 6 0.00 0.03 0.10 0.01 0.02 0.09 -0.01 -0.02 -0.07

3 7 -0.00 -0.00 -0.00 0.00 -0.03 -0.05 -0.00 0.02 0.04

4 6 0.01 -0.03 -0.10 -0.02 0.03 0.10 0.01 -0.01 -0.06

5 6 -0.01 0.01 0.04 -0.00 0.00 -0.00 0.00 -0.01 -0.02

6 6 0.00 -0.00 0.11 -0.01 0.01 -0.08 0.01 -0.00 0.10

7 6 0.02 -0.01 -0.09 -0.01 0.01 0.07 0.04 0.00 -0.13

8 7 -0.03 -0.00 0.08 0.03 0.00 -0.05 -0.00 0.01 -0.00

9 6 0.01 0.01 -0.08 -0.01 -0.01 0.06 -0.04 -0.01 0.14

10 6 0.01 0.00 -0.03 -0.00 -0.00 0.02 0.01 0.02 -0.06

11 6 0.01 -0.00 -0.02 -0.00 0.00 0.02 -0.01 0.02 0.07

12 6 0.00 0.00 -0.10 0.01 0.01 -0.07 -0.01 -0.00 0.11

13 6 0.01 0.01 0.08 0.01 0.01 0.06 -0.04 -0.01 -0.14

14 6 0.01 0.00 0.03 0.00 0.00 0.02 0.01 0.02 0.06

15 6 0.01 -0.00 0.02 0.00 -0.00 0.02 -0.01 0.02 -0.07

16 6 0.02 -0.01 0.09 0.01 -0.01 0.07 0.04 0.00 0.13

17 7 -0.03 -0.00 -0.08 -0.03 -0.00 -0.05 -0.00 0.01 0.00

18 6 0.00 -0.00 -0.11 0.01 -0.01 -0.08 0.01 -0.00 -0.10

19 6 0.01 -0.03 0.10 0.02 -0.03 0.10 0.01 -0.01 0.06

20 6 -0.01 0.01 -0.04 0.00 -0.00 -0.00 0.00 -0.01 0.02

21 6 -0.01 -0.01 0.04 -0.00 -0.00 -0.00 -0.00 -0.01 0.02

22 6 0.00 0.03 -0.10 -0.01 -0.02 0.09 -0.01 -0.02 0.07

23 7 -0.00 -0.00 0.00 -0.00 0.03 -0.05 -0.00 0.02 -0.04

24 6 0.00 0.00 0.10 -0.01 -0.01 -0.07 -0.01 -0.00 -0.11

25 6 0.01 -0.01 0.01 -0.01 0.01 -0.01 0.01 -0.02 0.02

26 6 -0.02 0.01 -0.02 0.01 -0.01 0.02 -0.01 -0.00 -0.04

27 6 0.00 -0.01 0.01 -0.00 0.01 -0.00 0.00 -0.02 -0.01

28 6 -0.02 0.01 -0.02 0.02 -0.01 0.02 -0.01 0.03 -0.02

29 6 0.02 -0.00 0.00 -0.01 0.00 0.00 0.00 0.00 0.01

30 6 -0.00 0.01 -0.03 0.01 -0.01 0.02 -0.02 0.02 -0.02

31 6 -0.02 -0.01 0.01 -0.01 -0.01 0.01 0.01 0.03 -0.02

32 6 -0.00 0.01 -0.01 -0.00 0.01 -0.00 -0.00 -0.02 -0.01

33 6 -0.01 -0.01 0.02 -0.01 -0.01 0.01 0.01 0.00 -0.04

34 6 0.01 0.01 -0.01 0.01 0.01 -0.01 -0.01 -0.02 0.02

35 6 -0.00 -0.01 0.03 -0.01 -0.01 0.02 0.02 0.02 -0.02

36 6 0.02 0.00 0.00 0.01 0.00 0.00 -0.01 0.00 0.01

37 6 0.01 0.01 0.01 -0.01 -0.01 -0.01 -0.01 -0.02 -0.02

38 6 -0.00 -0.01 -0.03 0.01 0.01 0.02 0.02 0.02 0.02

39 6 0.02 0.00 -0.00 -0.01 -0.00 0.00 -0.01 0.00 -0.01

40 6 -0.02 -0.01 -0.01 0.01 0.01 0.01 0.01 0.03 0.02

41 6 -0.00 0.01 0.01 0.00 -0.01 -0.00 -0.00 -0.02 0.01

42 6 -0.01 -0.01 -0.02 0.01 0.01 0.01 0.01 0.00 0.04

43 6 0.01 -0.01 -0.01 0.01 -0.01 -0.01 0.01 -0.02 -0.02

44 6 -0.00 0.01 0.03 -0.01 0.01 0.02 -0.02 0.01 0.02

45 6 0.02 -0.00 -0.00 0.01 -0.00 0.00 0.00 0.00 -0.01

46 6 -0.02 0.01 0.02 -0.02 0.01 0.02 -0.01 0.03 0.02

47 6 0.00 -0.01 -0.01 0.00 -0.01 -0.00 0.00 -0.02 0.01

48 6 -0.02 0.01 0.02 -0.01 0.01 0.02 -0.01 -0.00 0.04

49 1 -0.02 -0.06 -0.18 -0.01 -0.08 -0.25 0.01 0.10 0.33

50 1 -0.03 0.06 0.19 0.02 -0.08 -0.26 -0.02 0.10 0.32

51 1 -0.11 -0.02 0.36 0.08 0.02 -0.26 0.05 0.03 -0.18

52 1 -0.11 0.00 0.37 0.09 -0.01 -0.27 -0.04 0.02 0.16

53 1 -0.11 -0.02 -0.36 -0.08 -0.02 -0.26 0.05 0.03 0.18

54 1 -0.11 0.00 -0.37 -0.09 0.01 -0.27 -0.04 0.02 -0.16

55 1 -0.03 0.06 -0.19 -0.02 0.08 -0.26 -0.02 0.10 -0.32

56 1 -0.02 -0.06 0.18 0.01 0.08 -0.25 0.01 0.10 -0.33

57 1 0.00 -0.02 0.00 -0.01 0.02 -0.01 0.03 -0.03 0.01

58 1 0.05 -0.06 0.06 -0.06 0.06 -0.07 0.06 -0.11 0.09

59 1 0.01 -0.01 0.04 -0.03 0.03 -0.05 0.05 -0.03 0.07

60 1 0.08 -0.03 0.06 -0.08 0.05 -0.07 0.08 -0.07 0.09

61 1 0.02 -0.01 -0.00 -0.03 0.02 -0.02 0.03 -0.01 0.02

62 1 0.01 0.02 -0.04 0.03 0.04 -0.05 -0.04 -0.03 0.07

63 1 0.04 0.06 -0.06 0.05 0.07 -0.07 -0.04 -0.11 0.09

64 1 0.01 0.02 -0.01 0.02 0.03 -0.02 -0.02 -0.03 0.01

65 1 0.02 0.02 -0.01 0.03 0.03 -0.02 -0.03 -0.01 0.01

66 1 0.07 0.04 -0.06 0.07 0.06 -0.07 -0.07 -0.08 0.09

67 1 0.02 0.02 0.01 -0.03 -0.03 -0.02 -0.03 -0.01 -0.01

68 1 0.07 0.04 0.06 -0.07 -0.06 -0.07 -0.07 -0.08 -0.09

69 1 0.01 0.02 0.04 -0.03 -0.04 -0.05 -0.04 -0.03 -0.07

70 1 0.05 0.06 0.06 -0.05 -0.07 -0.07 -0.04 -0.11 -0.09

71 1 0.01 0.02 0.01 -0.02 -0.03 -0.02 -0.02 -0.03 -0.01

72 1 0.02 -0.01 0.00 0.03 -0.02 -0.02 0.03 -0.01 -0.02

73 1 0.08 -0.03 -0.06 0.08 -0.05 -0.07 0.08 -0.07 -0.09

74 1 0.01 -0.01 -0.04 0.03 -0.03 -0.05 0.05 -0.03 -0.07

75 1 0.05 -0.06 -0.06 0.06 -0.06 -0.07 0.06 -0.11 -0.09

76 1 0.00 -0.02 -0.00 0.01 -0.02 -0.01 0.03 -0.03 -0.01

77 1 -0.02 0.00 0.01 0.00 -0.08 -0.26 -0.00 0.04 0.10

78 1 -0.02 0.00 -0.01 -0.00 0.08 -0.26 -0.00 0.04 -0.10

76 77 78

A A A

Frequencies -- 732.8223 763.0575 765.1055

Red. masses -- 3.8347 2.0310 3.3198

Frc consts -- 1.2133 0.6967 1.1450

IR Inten -- 0.0777 5.5352 0.0032

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 -0.00 -0.02 -0.01 -0.00 0.01 0.05 -0.02 -0.01

2 6 0.00 0.02 0.08 -0.03 0.00 0.01 -0.01 0.01 0.07

3 7 -0.00 -0.00 -0.00 -0.00 0.02 -0.01 0.00 0.00 -0.00

4 6 0.00 -0.02 -0.07 0.03 0.01 0.02 0.00 -0.00 -0.06

5 6 -0.03 -0.00 0.02 -0.00 -0.00 0.01 0.05 0.02 0.02

6 6 0.02 -0.02 0.12 0.05 -0.04 -0.04 -0.06 0.06 0.07

7 6 0.06 0.01 -0.15 0.00 -0.03 0.01 -0.04 -0.02 -0.07

8 7 0.00 -0.02 -0.00 -0.03 -0.01 -0.01 -0.01 0.08 -0.00

9 6 -0.06 -0.00 0.16 -0.01 0.03 -0.01 0.05 -0.01 0.07

10 6 0.00 0.03 -0.08 -0.00 0.01 0.02 0.05 -0.05 -0.00

11 6 -0.01 0.02 0.08 0.01 0.00 0.02 -0.05 -0.06 0.01

12 6 0.02 0.02 -0.13 -0.03 -0.03 -0.02 -0.06 -0.08 -0.08

13 6 0.06 0.00 0.16 0.01 -0.03 -0.01 -0.05 0.01 0.07

14 6 -0.00 -0.03 -0.08 0.00 -0.01 0.02 -0.05 0.05 -0.00

15 6 0.01 -0.02 0.08 -0.01 -0.00 0.02 0.05 0.06 0.01

16 6 -0.06 -0.01 -0.15 -0.00 0.03 0.01 0.04 0.02 -0.07

17 7 -0.00 0.02 -0.00 0.03 0.01 -0.01 0.01 -0.08 -0.00

18 6 -0.02 0.02 0.12 -0.05 0.04 -0.04 0.06 -0.06 0.07

19 6 -0.00 0.02 -0.07 -0.03 -0.01 0.02 -0.00 0.00 -0.06

20 6 0.03 0.00 0.02 0.00 0.00 0.01 -0.05 -0.02 0.02

21 6 0.03 0.00 -0.02 0.01 0.00 0.01 -0.05 0.02 -0.01

22 6 -0.00 -0.02 0.07 0.03 -0.00 0.01 0.01 -0.01 0.07

23 7 0.00 0.00 -0.00 0.00 -0.02 -0.01 -0.00 -0.00 -0.00

24 6 -0.02 -0.02 -0.13 0.03 0.03 -0.02 0.06 0.08 -0.08

25 6 0.02 -0.02 0.02 0.05 -0.05 0.06 -0.04 0.03 -0.04

26 6 -0.02 0.01 -0.04 -0.03 0.03 -0.03 0.02 -0.03 0.01

27 6 0.00 -0.02 -0.01 0.01 0.00 0.01 -0.01 -0.01 -0.01

28 6 -0.02 0.03 -0.02 -0.04 0.03 -0.04 0.02 -0.02 0.03

29 6 0.01 0.00 0.01 -0.01 -0.01 0.01 0.01 0.01 -0.01

30 6 -0.02 0.02 -0.03 -0.03 0.02 -0.03 0.02 -0.01 0.02

31 6 -0.02 -0.03 0.02 0.03 0.03 -0.03 0.03 0.03 -0.04

32 6 -0.00 0.02 0.01 -0.01 0.00 0.01 -0.01 0.02 0.01

33 6 -0.01 -0.01 0.04 0.02 0.03 -0.03 0.02 0.04 -0.02

34 6 0.01 0.03 -0.02 -0.04 -0.04 0.05 -0.05 -0.05 0.06

35 6 -0.01 -0.02 0.03 0.03 0.02 -0.02 0.03 0.02 -0.03

36 6 0.01 -0.00 -0.01 0.00 -0.01 0.01 0.01 -0.01 0.01

37 6 -0.01 -0.03 -0.02 0.04 0.04 0.05 0.05 0.05 0.06

38 6 0.01 0.02 0.03 -0.03 -0.02 -0.02 -0.03 -0.02 -0.03

39 6 -0.01 0.00 -0.01 -0.00 0.01 0.01 -0.01 0.01 0.01

40 6 0.02 0.03 0.02 -0.03 -0.03 -0.03 -0.03 -0.03 -0.04

41 6 0.00 -0.02 0.01 0.01 -0.00 0.01 0.01 -0.02 0.01

42 6 0.01 0.01 0.04 -0.02 -0.03 -0.03 -0.02 -0.04 -0.02

43 6 -0.02 0.02 0.02 -0.05 0.05 0.06 0.04 -0.03 -0.04

44 6 0.02 -0.02 -0.03 0.03 -0.02 -0.03 -0.02 0.01 0.02

45 6 -0.01 -0.00 0.01 0.01 0.01 0.01 -0.01 -0.01 -0.01

46 6 0.02 -0.03 -0.02 0.04 -0.03 -0.04 -0.02 0.02 0.03

47 6 -0.00 0.02 -0.01 -0.01 -0.00 0.01 0.01 0.01 -0.01

48 6 0.02 -0.01 -0.04 0.03 -0.03 -0.03 -0.02 0.03 0.01

49 1 -0.04 -0.05 -0.15 0.01 -0.03 -0.14 0.07 -0.04 -0.14

50 1 -0.05 0.04 0.14 -0.02 -0.04 -0.16 0.06 0.03 0.07

51 1 0.04 0.03 -0.21 0.02 -0.02 -0.13 0.09 -0.02 -0.05

52 1 -0.04 0.02 0.19 0.03 0.03 -0.14 -0.08 -0.02 0.00

53 1 -0.04 -0.03 -0.21 -0.02 0.02 -0.13 -0.09 0.02 -0.05

54 1 0.04 -0.02 0.19 -0.03 -0.03 -0.14 0.08 0.02 0.00

55 1 0.05 -0.04 0.14 0.02 0.04 -0.16 -0.06 -0.03 0.07

56 1 0.04 0.05 -0.15 -0.01 0.03 -0.14 -0.07 0.04 -0.14

57 1 0.05 -0.05 0.03 0.02 -0.01 0.03 -0.02 0.00 -0.03

58 1 0.10 -0.13 0.13 0.16 -0.13 0.18 -0.12 0.08 -0.13

59 1 0.08 -0.06 0.10 0.14 -0.12 0.13 -0.11 0.10 -0.08

60 1 0.12 -0.10 0.13 0.15 -0.16 0.18 -0.10 0.11 -0.13

61 1 0.05 -0.03 0.03 0.02 -0.02 0.03 -0.01 0.03 -0.03

62 1 0.07 0.07 -0.11 -0.10 -0.11 0.11 -0.13 -0.15 0.13

63 1 0.08 0.15 -0.14 -0.12 -0.13 0.15 -0.16 -0.15 0.19

64 1 0.04 0.06 -0.04 -0.02 -0.02 0.02 -0.03 -0.01 0.04

65 1 0.05 0.04 -0.03 -0.01 -0.02 0.02 -0.01 -0.03 0.04

66 1 0.11 0.11 -0.13 -0.10 -0.14 0.15 -0.13 -0.17 0.19

67 1 -0.05 -0.04 -0.03 0.01 0.02 0.02 0.01 0.03 0.04

68 1 -0.11 -0.11 -0.13 0.10 0.14 0.15 0.13 0.17 0.19

69 1 -0.07 -0.07 -0.11 0.10 0.11 0.11 0.13 0.15 0.13

70 1 -0.08 -0.15 -0.13 0.12 0.13 0.15 0.16 0.15 0.19

71 1 -0.04 -0.06 -0.04 0.02 0.02 0.02 0.03 0.01 0.04

72 1 -0.05 0.03 0.03 -0.02 0.02 0.03 0.01 -0.03 -0.03

73 1 -0.12 0.10 0.13 -0.15 0.16 0.18 0.10 -0.11 -0.13

74 1 -0.08 0.06 0.10 -0.14 0.12 0.13 0.11 -0.10 -0.08

75 1 -0.10 0.13 0.13 -0.16 0.13 0.18 0.12 -0.08 -0.13

76 1 -0.05 0.05 0.03 -0.02 0.01 0.03 0.02 -0.00 -0.03

77 1 -0.01 -0.00 -0.01 -0.00 -0.00 -0.11 0.04 0.00 -0.03

78 1 0.01 0.00 -0.01 0.00 0.00 -0.11 -0.04 -0.00 -0.03

79 80 81

A A A

Frequencies -- 769.2494 770.1234 788.4449

Red. masses -- 2.1376 2.0403 1.4510

Frc consts -- 0.7453 0.7129 0.5314

IR Inten -- 135.0092 136.7752 55.4973

Atom AN X Y Z X Y Z X Y Z

1 6 0.03 -0.01 -0.02 -0.01 0.00 -0.03 0.00 -0.02 -0.06

2 6 0.01 -0.01 0.02 0.02 0.01 -0.01 -0.00 0.01 0.05

3 7 0.01 -0.01 0.00 -0.00 -0.02 0.00 0.00 -0.00 -0.03

4 6 -0.02 0.01 -0.02 -0.02 -0.00 0.01 0.00 0.01 0.05

5 6 0.03 0.01 -0.01 -0.02 -0.01 -0.03 0.00 -0.02 -0.06

6 6 -0.05 0.04 0.05 -0.02 0.01 0.01 0.01 0.00 -0.02

7 6 -0.01 0.02 -0.01 -0.02 -0.01 -0.03 0.01 -0.00 -0.03

8 7 0.02 0.00 0.00 -0.01 -0.00 -0.00 -0.00 -0.00 0.01

9 6 0.01 -0.02 0.02 0.01 0.02 0.02 0.01 0.00 -0.03

10 6 0.01 -0.02 -0.02 0.02 -0.03 0.01 -0.01 -0.00 0.04

11 6 -0.01 -0.01 -0.02 -0.01 -0.04 0.02 -0.01 -0.00 0.04

12 6 -0.01 -0.02 -0.01 0.04 0.04 0.04 -0.01 0.00 -0.02

13 6 0.01 -0.02 -0.02 0.01 0.02 -0.02 -0.01 -0.00 -0.03

14 6 0.01 -0.02 0.02 0.02 -0.03 -0.01 0.01 0.00 0.04

15 6 -0.01 -0.01 0.02 -0.01 -0.04 -0.02 0.01 0.00 0.04

16 6 -0.01 0.02 0.01 -0.02 -0.01 0.03 -0.01 0.00 -0.03

17 7 0.02 0.00 -0.00 -0.01 -0.00 0.00 0.00 0.00 0.01

18 6 -0.05 0.04 -0.05 -0.02 0.01 -0.01 -0.01 -0.00 -0.02

19 6 -0.02 0.01 0.02 -0.02 -0.00 -0.01 -0.00 -0.01 0.05

20 6 0.03 0.01 0.01 -0.02 -0.01 0.03 -0.00 0.02 -0.06

21 6 0.03 -0.01 0.02 -0.01 0.00 0.03 -0.00 0.02 -0.06

22 6 0.01 -0.01 -0.02 0.02 0.01 0.01 0.00 -0.01 0.05

23 7 0.01 -0.01 -0.00 -0.00 -0.02 -0.00 -0.00 0.00 -0.03

24 6 -0.01 -0.02 0.01 0.04 0.04 -0.04 0.01 -0.00 -0.02

25 6 -0.08 0.07 -0.08 -0.02 0.02 -0.02 0.00 -0.00 0.00

26 6 0.03 -0.04 0.04 0.01 -0.00 0.02 -0.00 0.00 -0.00

27 6 -0.01 -0.00 -0.01 -0.00 0.00 0.00 0.00 -0.00 -0.00

28 6 0.05 -0.04 0.05 0.01 -0.02 0.01 0.00 0.00 -0.00

29 6 0.00 0.01 -0.01 0.01 0.00 -0.01 -0.01 -0.00 0.00

30 6 0.04 -0.03 0.04 0.02 -0.01 0.01 -0.00 -0.00 0.01

31 6 0.02 0.01 -0.02 -0.04 -0.05 0.05 -0.00 0.00 -0.00

32 6 -0.00 0.01 0.01 0.01 -0.00 -0.01 -0.00 -0.00 -0.00

33 6 0.01 0.02 -0.01 -0.03 -0.04 0.04 0.00 0.00 -0.01

34 6 -0.02 -0.02 0.03 0.06 0.07 -0.08 -0.00 -0.00 0.00

35 6 0.01 0.01 -0.02 -0.04 -0.03 0.03 0.00 0.00 0.00

36 6 -0.00 -0.00 -0.00 -0.01 0.01 -0.01 0.01 -0.00 0.00

37 6 -0.02 -0.02 -0.03 0.06 0.07 0.08 0.00 0.00 0.00

38 6 0.01 0.01 0.02 -0.04 -0.03 -0.03 -0.00 -0.00 0.00

39 6 -0.00 -0.00 0.00 -0.01 0.01 0.01 -0.01 0.00 0.00

40 6 0.02 0.01 0.02 -0.04 -0.05 -0.05 0.00 -0.00 -0.00

41 6 -0.00 0.01 -0.01 0.01 -0.00 0.01 0.00 0.00 -0.00

42 6 0.01 0.02 0.01 -0.03 -0.04 -0.04 -0.00 -0.00 -0.01

43 6 -0.08 0.07 0.08 -0.02 0.02 0.02 -0.00 0.00 0.00

44 6 0.04 -0.03 -0.04 0.02 -0.01 -0.01 0.00 0.00 0.01

45 6 0.00 0.01 0.01 0.01 0.00 0.01 0.01 0.00 0.00

46 6 0.05 -0.04 -0.05 0.01 -0.02 -0.01 -0.00 -0.00 -0.00

47 6 -0.01 -0.00 0.01 -0.00 0.00 -0.00 -0.00 0.00 -0.00

48 6 0.03 -0.04 -0.04 0.01 -0.00 -0.02 0.00 -0.00 -0.00

49 1 0.03 0.01 0.08 -0.03 0.07 0.24 0.00 0.11 0.39

50 1 0.03 0.05 0.15 -0.01 0.05 0.21 -0.02 0.12 0.40

51 1 -0.02 -0.01 0.13 0.04 -0.03 -0.10 0.06 0.01 -0.24

52 1 -0.04 -0.04 0.16 -0.00 -0.02 -0.05 0.06 0.00 -0.24

53 1 -0.02 -0.01 -0.13 0.04 -0.03 0.10 -0.06 -0.01 -0.24

54 1 -0.04 -0.04 -0.16 -0.00 -0.02 0.05 -0.06 -0.00 -0.24

55 1 0.03 0.05 -0.15 -0.01 0.05 -0.21 0.02 -0.12 0.40

56 1 0.03 0.01 -0.08 -0.03 0.07 -0.24 -0.00 -0.11 0.39

57 1 -0.02 0.01 -0.02 -0.01 0.00 0.00 0.00 -0.00 0.00

58 1 -0.20 0.17 -0.23 -0.04 0.05 -0.05 0.01 -0.01 0.01

59 1 -0.17 0.15 -0.17 -0.05 0.03 -0.04 0.01 -0.00 0.00

60 1 -0.19 0.19 -0.23 -0.04 0.06 -0.06 -0.01 -0.01 0.00

61 1 -0.01 0.02 -0.02 -0.00 0.00 -0.01 -0.01 0.00 -0.00

62 1 -0.05 -0.06 0.06 0.15 0.16 -0.16 -0.01 -0.01 0.01

63 1 -0.07 -0.06 0.08 0.17 0.19 -0.22 -0.01 -0.02 0.01

64 1 -0.01 -0.00 0.01 0.02 0.01 -0.02 -0.00 -0.00 0.00

65 1 -0.00 -0.01 0.00 0.01 0.02 -0.02 0.01 0.01 -0.00

66 1 -0.07 -0.06 0.08 0.15 0.20 -0.22 0.01 -0.01 0.01

67 1 -0.00 -0.01 -0.00 0.01 0.02 0.02 -0.01 -0.01 -0.00

68 1 -0.07 -0.06 -0.08 0.15 0.20 0.22 -0.01 0.01 0.01

69 1 -0.05 -0.06 -0.06 0.15 0.16 0.16 0.01 0.01 0.01

70 1 -0.07 -0.06 -0.08 0.17 0.19 0.22 0.01 0.02 0.01

71 1 -0.01 -0.00 -0.01 0.02 0.01 0.02 0.00 0.00 0.00

72 1 -0.01 0.02 0.02 -0.00 0.00 0.01 0.01 -0.00 -0.00

73 1 -0.19 0.19 0.23 -0.04 0.06 0.06 0.01 0.01 0.00

74 1 -0.17 0.15 0.17 -0.05 0.03 0.04 -0.01 0.00 0.00

75 1 -0.20 0.17 0.23 -0.04 0.05 0.05 -0.01 0.01 0.01

76 1 -0.02 0.01 0.02 -0.01 0.00 -0.00 -0.00 0.00 0.00

77 1 0.05 0.00 0.03 -0.02 -0.01 0.06 -0.00 0.03 0.14

78 1 0.05 0.00 -0.03 -0.02 -0.01 -0.06 0.00 -0.03 0.14

82 83 84

A A A

Frequencies -- 792.3677 801.1600 804.9485

Red. masses -- 1.9169 2.0281 2.2157

Frc consts -- 0.7091 0.7670 0.8459

IR Inten -- 0.1122 1.5397 290.1345

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.03 -0.07 0.00 -0.00 0.00 0.00 -0.01 -0.03

2 6 -0.01 0.02 0.08 -0.00 0.00 0.02 -0.01 0.01 0.05

3 7 0.00 -0.00 -0.04 -0.00 0.00 -0.00 -0.00 -0.00 -0.02

4 6 0.00 0.02 0.08 -0.00 -0.00 -0.02 0.00 0.01 0.05

5 6 0.00 -0.03 -0.07 0.00 0.00 -0.00 0.00 -0.01 -0.04

6 6 0.02 -0.01 -0.06 -0.01 0.01 0.05 0.01 -0.01 -0.07

7 6 -0.00 0.00 0.04 0.02 0.01 -0.10 -0.02 -0.01 0.10

8 7 0.00 -0.00 0.00 -0.01 -0.00 0.05 0.00 0.00 -0.05

9 6 0.00 0.00 -0.04 0.02 -0.00 -0.10 -0.02 0.00 0.10

10 6 -0.01 0.01 0.01 -0.03 -0.00 0.08 0.02 -0.00 -0.07

11 6 0.01 0.01 -0.01 -0.02 -0.00 0.08 0.02 0.00 -0.07

12 6 -0.02 -0.01 -0.06 -0.01 -0.01 -0.05 -0.01 -0.02 -0.06

13 6 0.00 0.00 0.04 0.02 -0.00 0.10 0.02 -0.00 0.10

14 6 -0.01 0.01 -0.01 -0.03 -0.00 -0.08 -0.02 0.00 -0.07

15 6 0.01 0.01 0.01 -0.02 -0.00 -0.08 -0.02 -0.00 -0.07

16 6 -0.00 0.00 -0.04 0.02 0.01 0.10 0.02 0.01 0.10

17 7 0.00 -0.00 -0.00 -0.01 -0.00 -0.05 -0.00 -0.00 -0.05

18 6 0.02 -0.01 0.06 -0.01 0.01 -0.05 -0.01 0.01 -0.07

19 6 0.00 0.02 -0.08 -0.00 -0.00 0.02 -0.00 -0.01 0.05

20 6 0.00 -0.03 0.07 0.00 0.00 0.00 -0.00 0.01 -0.04

21 6 0.00 -0.03 0.07 0.00 -0.00 -0.00 -0.00 0.01 -0.03

22 6 -0.01 0.02 -0.08 -0.00 0.00 -0.02 0.01 -0.01 0.05

23 7 0.00 -0.00 0.04 -0.00 0.00 0.00 0.00 0.00 -0.02

24 6 -0.02 -0.01 0.06 -0.01 -0.01 0.05 0.01 0.02 -0.06

25 6 0.02 -0.02 0.02 -0.01 0.01 -0.01 0.01 -0.01 0.01

26 6 -0.01 0.01 -0.01 0.00 -0.01 -0.00 -0.01 0.01 0.00

27 6 0.00 0.00 -0.00 -0.00 -0.01 -0.01 0.00 0.00 0.00

28 6 -0.01 0.01 -0.01 0.01 -0.00 0.01 -0.01 0.00 -0.01

29 6 -0.01 -0.00 0.01 0.00 0.00 -0.00 -0.00 -0.00 0.00

30 6 -0.01 0.00 0.00 0.01 -0.01 0.01 -0.01 0.01 -0.00

31 6 0.00 0.01 -0.01 0.01 0.00 -0.01 0.00 0.00 -0.01

32 6 -0.00 0.00 -0.00 -0.00 0.01 0.01 -0.00 0.01 0.00

33 6 0.01 0.01 -0.01 0.00 0.01 0.00 0.00 0.01 0.00

34 6 -0.02 -0.02 0.02 -0.01 -0.01 0.01 -0.01 -0.01 0.01

35 6 0.01 0.01 0.00 0.01 0.01 -0.00 0.01 0.01 -0.00

36 6 0.01 -0.00 0.01 0.00 -0.00 -0.00 0.00 -0.00 0.00

37 6 -0.02 -0.02 -0.02 -0.01 -0.01 -0.01 0.01 0.01 0.01

38 6 0.01 0.01 -0.00 0.01 0.01 0.00 -0.01 -0.01 -0.00

39 6 0.01 -0.00 -0.01 0.00 -0.00 0.00 -0.00 0.00 0.00

40 6 0.00 0.01 0.01 0.01 0.00 0.01 -0.00 -0.00 -0.01

41 6 -0.00 0.00 0.00 -0.00 0.01 -0.01 0.00 -0.01 0.00

42 6 0.01 0.01 0.01 0.00 0.01 -0.00 -0.00 -0.01 0.00

43 6 0.02 -0.02 -0.02 -0.01 0.01 0.01 -0.01 0.01 0.01

44 6 -0.01 0.00 -0.00 0.01 -0.01 -0.01 0.01 -0.01 -0.00

45 6 -0.01 -0.00 -0.01 0.00 0.00 0.00 0.00 0.00 0.00

46 6 -0.01 0.01 0.01 0.01 -0.00 -0.01 0.01 -0.00 -0.01

47 6 0.00 0.00 0.00 -0.00 -0.01 0.01 -0.00 -0.00 0.00

48 6 -0.01 0.01 0.01 0.00 -0.01 0.00 0.01 -0.01 0.00

49 1 0.00 0.13 0.44 0.01 -0.01 -0.05 0.00 0.06 0.21

50 1 -0.03 0.13 0.44 0.00 0.01 0.05 -0.01 0.06 0.22

51 1 -0.02 0.00 0.04 0.12 0.02 -0.45 -0.10 -0.02 0.39

52 1 0.02 0.00 -0.03 0.12 0.01 -0.46 -0.11 -0.01 0.39

53 1 -0.02 0.00 -0.04 0.12 0.02 0.45 0.10 0.02 0.39

54 1 0.02 0.00 0.03 0.12 0.01 0.46 0.11 0.01 0.39

55 1 -0.03 0.13 -0.44 0.00 0.01 -0.05 0.01 -0.06 0.22

56 1 0.00 0.13 -0.44 0.01 -0.01 0.05 -0.00 -0.06 0.21

57 1 -0.00 0.01 -0.00 0.02 -0.02 0.01 -0.01 0.02 -0.01

58 1 0.04 -0.03 0.04 -0.02 -0.00 -0.02 0.02 -0.01 0.02

59 1 0.04 -0.03 0.03 -0.02 0.02 -0.01 0.03 -0.03 0.01

60 1 0.02 -0.04 0.04 -0.03 0.03 -0.03 0.02 -0.03 0.03

61 1 -0.01 0.01 0.00 0.01 0.00 -0.01 -0.01 -0.00 0.01

62 1 -0.04 -0.04 0.03 -0.02 -0.02 0.01 -0.02 -0.02 0.01

63 1 -0.04 -0.04 0.05 -0.02 -0.00 0.02 -0.02 -0.00 0.01

64 1 -0.00 0.01 0.00 0.01 0.02 -0.01 0.01 0.02 -0.00

65 1 0.01 0.01 0.00 0.00 -0.00 0.01 0.01 0.00 0.01

66 1 -0.01 -0.05 0.04 -0.02 -0.03 0.03 -0.01 -0.03 0.02

67 1 0.01 0.01 -0.00 0.00 -0.00 -0.01 -0.01 -0.00 0.01

68 1 -0.01 -0.05 -0.04 -0.02 -0.03 -0.03 0.01 0.03 0.02

69 1 -0.04 -0.04 -0.03 -0.02 -0.02 -0.01 0.02 0.02 0.01

70 1 -0.04 -0.04 -0.05 -0.02 -0.00 -0.02 0.02 0.00 0.01

71 1 -0.00 0.01 -0.00 0.01 0.02 0.01 -0.01 -0.02 -0.00

72 1 -0.01 0.01 -0.00 0.01 0.00 0.01 0.01 0.00 0.01

73 1 0.02 -0.04 -0.04 -0.03 0.03 0.03 -0.02 0.03 0.03

74 1 0.04 -0.03 -0.03 -0.02 0.02 0.01 -0.03 0.03 0.01

75 1 0.04 -0.03 -0.04 -0.02 -0.00 0.02 -0.02 0.01 0.02

76 1 -0.00 0.01 0.00 0.02 -0.02 -0.01 0.01 -0.02 -0.01

77 1 -0.00 0.02 0.09 0.01 0.00 0.00 -0.00 0.02 0.08

78 1 -0.00 0.02 -0.09 0.01 0.00 -0.00 0.00 -0.02 0.08

85 86 87

A A A

Frequencies -- 810.2492 846.0698 854.7620

Red. masses -- 3.9468 5.2184 4.5359

Frc consts -- 1.5266 2.2009 1.9526

IR Inten -- 0.6265 30.1556 0.2814

Atom AN X Y Z X Y Z X Y Z

1 6 -0.05 0.01 0.01 -0.01 -0.03 0.00 -0.01 -0.03 0.01

2 6 0.01 0.00 -0.01 -0.09 -0.01 0.02 -0.09 -0.01 0.01

3 7 0.03 0.00 -0.00 -0.01 0.11 -0.04 -0.01 0.11 -0.03

4 6 0.01 -0.00 0.02 0.09 0.00 0.02 0.09 0.00 0.01

5 6 -0.05 -0.01 -0.01 0.01 -0.03 0.00 0.02 -0.03 0.01

6 6 0.06 -0.08 0.04 0.11 -0.11 0.02 0.11 -0.10 0.02

7 6 0.08 0.01 -0.00 0.10 -0.06 0.01 0.01 -0.11 0.00

8 7 0.01 -0.15 -0.00 0.00 -0.09 -0.00 -0.15 -0.01 -0.04

9 6 -0.08 0.00 0.01 -0.10 -0.07 -0.01 -0.01 0.10 0.00

10 6 -0.06 0.06 -0.03 -0.09 0.12 -0.02 0.05 0.01 0.01

11 6 0.06 0.07 0.02 0.08 0.13 0.02 0.06 -0.01 0.01

12 6 0.05 0.09 -0.04 -0.09 -0.12 0.02 -0.09 -0.11 0.02

13 6 0.08 -0.00 0.01 -0.10 -0.07 0.01 0.01 -0.10 0.00

14 6 0.06 -0.06 -0.03 -0.09 0.12 0.02 -0.05 -0.01 0.01

15 6 -0.06 -0.07 0.02 0.08 0.13 -0.02 -0.06 0.01 0.01

16 6 -0.08 -0.01 -0.00 0.10 -0.06 -0.01 -0.01 0.11 0.00

17 7 -0.01 0.15 -0.00 0.00 -0.09 0.00 0.15 0.01 -0.04

18 6 -0.06 0.08 0.04 0.11 -0.11 -0.02 -0.11 0.10 0.02

19 6 -0.01 0.00 0.02 0.09 0.00 -0.02 -0.09 -0.00 0.01

20 6 0.05 0.01 -0.01 0.01 -0.03 -0.00 -0.02 0.03 0.01

21 6 0.05 -0.01 0.01 -0.01 -0.03 -0.00 0.01 0.03 0.01

22 6 -0.01 -0.00 -0.01 -0.09 -0.01 -0.02 0.09 0.01 0.01

23 7 -0.03 -0.00 -0.00 -0.01 0.11 0.04 0.01 -0.11 -0.03

24 6 -0.05 -0.09 -0.04 -0.09 -0.12 -0.02 0.09 0.11 0.02

25 6 -0.07 0.06 -0.08 -0.05 0.04 -0.06 -0.05 0.04 -0.06

26 6 0.01 -0.01 0.03 -0.00 0.00 0.02 -0.01 0.01 0.01

27 6 -0.00 0.02 0.00 0.01 0.01 0.01 0.00 0.01 0.00

28 6 0.04 -0.04 0.04 0.03 -0.03 0.02 0.03 -0.03 0.02

29 6 -0.00 0.00 -0.01 -0.01 -0.01 0.00 -0.00 -0.01 0.01

30 6 0.02 -0.02 0.02 -0.00 0.00 0.02 -0.00 -0.00 0.02

31 6 0.03 0.04 -0.04 -0.02 -0.03 0.02 -0.03 -0.03 0.02

32 6 0.00 -0.01 -0.00 -0.01 0.01 0.01 -0.01 0.01 0.01

33 6 0.02 0.01 -0.03 -0.00 0.00 0.02 0.00 0.01 0.02

34 6 -0.06 -0.07 0.08 0.04 0.05 -0.06 0.04 0.05 -0.06

35 6 0.02 0.02 -0.03 0.00 0.00 0.01 0.01 0.01 0.01

36 6 -0.00 -0.00 0.01 0.01 -0.00 0.00 0.01 -0.00 0.00

37 6 0.06 0.07 0.08 0.04 0.05 0.06 -0.04 -0.05 -0.06

38 6 -0.02 -0.02 -0.03 0.00 0.00 -0.01 -0.01 -0.01 0.01

39 6 0.00 0.00 0.01 0.01 -0.00 -0.00 -0.01 0.00 0.00

40 6 -0.03 -0.04 -0.04 -0.02 -0.03 -0.02 0.03 0.03 0.02

41 6 -0.00 0.01 -0.00 -0.01 0.01 -0.01 0.01 -0.01 0.01

42 6 -0.02 -0.01 -0.03 -0.00 0.00 -0.02 -0.00 -0.01 0.02

43 6 0.07 -0.06 -0.08 -0.05 0.04 0.06 0.05 -0.04 -0.06

44 6 -0.02 0.02 0.02 -0.00 0.00 -0.02 0.00 0.00 0.02

45 6 0.00 -0.00 -0.01 -0.01 -0.01 -0.00 0.00 0.01 0.01

46 6 -0.04 0.04 0.04 0.03 -0.03 -0.02 -0.03 0.03 0.02

47 6 0.00 -0.02 0.00 0.01 0.01 -0.01 -0.00 -0.01 0.00

48 6 -0.01 0.01 0.03 -0.00 0.00 -0.02 0.01 -0.01 0.01

49 1 -0.08 -0.03 0.00 0.09 0.06 -0.02 0.09 0.05 -0.03

50 1 -0.09 0.02 0.01 -0.10 0.05 -0.01 -0.10 0.03 -0.03

51 1 -0.09 0.02 -0.05 -0.09 0.12 -0.03 -0.03 -0.13 -0.03

52 1 0.07 0.03 0.11 0.07 0.14 0.05 -0.05 0.13 -0.04

53 1 0.09 -0.02 -0.05 -0.09 0.12 0.03 0.03 0.13 -0.03

54 1 -0.07 -0.03 0.11 0.07 0.14 -0.05 0.05 -0.13 -0.04

55 1 0.09 -0.02 0.01 -0.10 0.05 0.01 0.10 -0.03 -0.03

56 1 0.08 0.03 0.00 0.09 0.06 0.02 -0.09 -0.05 -0.03

57 1 0.03 -0.02 0.05 0.05 -0.04 0.07 0.10 -0.08 0.14

58 1 -0.10 0.13 -0.14 -0.06 0.10 -0.09 -0.02 0.06 -0.05

59 1 -0.13 0.11 -0.16 -0.11 0.10 -0.16 -0.12 0.11 -0.17

60 1 -0.12 0.11 -0.14 -0.09 0.05 -0.09 -0.13 0.08 -0.13

61 1 0.03 -0.03 0.04 0.06 -0.06 0.09 0.02 -0.03 0.05

62 1 -0.12 -0.13 0.16 0.09 0.11 -0.16 0.10 0.12 -0.17

63 1 -0.10 -0.16 0.15 0.06 0.12 -0.11 0.06 0.12 -0.11

64 1 0.03 0.02 -0.05 -0.03 -0.03 0.05 -0.04 -0.03 0.07

65 1 0.03 0.04 -0.05 -0.06 -0.08 0.10 -0.07 -0.09 0.11

66 1 -0.11 -0.12 0.14 0.07 0.04 -0.07 0.07 0.04 -0.07

67 1 -0.03 -0.04 -0.05 -0.06 -0.07 -0.10 0.07 0.09 0.11

68 1 0.11 0.12 0.14 0.07 0.04 0.07 -0.07 -0.04 -0.07

69 1 0.12 0.13 0.16 0.09 0.11 0.16 -0.10 -0.12 -0.17

70 1 0.10 0.16 0.15 0.06 0.12 0.11 -0.06 -0.12 -0.11

71 1 -0.03 -0.02 -0.05 -0.03 -0.03 -0.05 0.04 0.03 0.07

72 1 -0.03 0.03 0.04 0.06 -0.06 -0.09 -0.02 0.03 0.05

73 1 0.12 -0.11 -0.14 -0.09 0.05 0.09 0.13 -0.08 -0.13

74 1 0.13 -0.11 -0.16 -0.11 0.10 0.16 0.12 -0.11 -0.17

75 1 0.10 -0.13 -0.14 -0.06 0.10 0.09 0.02 -0.06 -0.05

76 1 -0.03 0.02 0.05 0.05 -0.04 -0.07 -0.10 0.08 0.14

77 1 0.03 0.00 0.00 -0.01 0.11 -0.06 -0.00 0.11 -0.08

78 1 -0.03 -0.00 0.00 -0.01 0.11 0.06 0.00 -0.11 -0.08

88 89 90

A A A

Frequencies -- 857.0060 857.3532 858.3865

Red. masses -- 1.5391 1.2568 2.8485

Frc consts -- 0.6660 0.5443 1.2366

IR Inten -- 37.4130 0.1016 82.4859

Atom AN X Y Z X Y Z X Y Z

1 6 -0.04 0.02 -0.00 -0.00 0.00 0.00 0.08 -0.04 0.01

2 6 0.02 0.02 -0.01 0.00 0.00 -0.00 -0.05 -0.04 0.01

3 7 0.01 0.00 0.00 0.00 -0.00 0.00 -0.03 0.00 -0.00

4 6 0.02 -0.02 0.00 -0.00 -0.00 -0.00 -0.05 0.03 -0.01

5 6 -0.03 -0.02 0.00 -0.00 -0.00 -0.00 0.07 0.04 -0.01

6 6 0.04 -0.02 0.00 0.00 0.01 -0.00 -0.07 0.06 -0.01

7 6 -0.00 -0.03 0.01 -0.00 0.01 0.01 -0.00 0.07 0.00

8 7 -0.04 -0.00 -0.01 0.01 0.00 0.00 0.11 0.01 0.02

9 6 -0.00 0.03 0.00 0.00 -0.01 0.00 0.01 -0.07 -0.00

10 6 0.02 0.00 0.00 -0.00 -0.00 -0.00 -0.04 -0.01 -0.01

11 6 0.01 -0.00 0.00 -0.01 -0.00 -0.00 -0.04 0.01 -0.01

12 6 0.03 0.03 -0.00 0.00 0.01 -0.00 -0.07 -0.07 0.01

13 6 -0.00 0.03 -0.00 -0.00 0.01 0.00 0.01 -0.07 0.00

14 6 0.02 0.00 -0.00 0.00 0.00 -0.00 -0.04 -0.01 0.01

15 6 0.01 -0.00 -0.00 0.01 0.00 -0.00 -0.04 0.01 0.01

16 6 -0.00 -0.03 -0.01 0.00 -0.01 0.01 -0.00 0.07 -0.00

17 7 -0.04 -0.00 0.01 -0.01 -0.00 0.00 0.11 0.01 -0.02

18 6 0.04 -0.02 -0.00 -0.00 -0.01 -0.00 -0.07 0.06 0.01

19 6 0.02 -0.02 -0.00 0.00 0.00 -0.00 -0.05 0.03 0.01

20 6 -0.03 -0.02 -0.00 0.00 0.00 -0.00 0.07 0.04 0.01

21 6 -0.04 0.02 0.00 0.00 -0.00 0.00 0.08 -0.04 -0.01

22 6 0.02 0.02 0.01 -0.00 -0.00 -0.00 -0.05 -0.04 -0.01

23 7 0.01 0.00 -0.00 -0.00 0.00 0.00 -0.03 0.00 0.00

24 6 0.03 0.03 0.00 -0.00 -0.01 -0.00 -0.07 -0.07 -0.01

25 6 -0.01 0.01 -0.01 0.00 -0.00 0.00 0.03 -0.03 0.04

26 6 -0.03 0.03 -0.03 -0.03 0.03 -0.03 -0.02 0.02 -0.03

27 6 -0.03 0.03 -0.03 -0.03 0.02 -0.03 -0.03 0.02 -0.03

28 6 0.01 -0.00 0.01 0.00 0.00 -0.00 -0.02 0.02 -0.01

29 6 0.02 -0.03 0.04 0.03 -0.03 0.03 0.03 -0.02 0.02

30 6 0.02 -0.02 0.03 0.03 -0.03 0.03 0.03 -0.02 0.02

31 6 0.01 0.01 -0.01 0.00 0.00 -0.00 -0.02 -0.02 0.02

32 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.01 0.00

33 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.01 0.01 0.01

34 6 -0.01 -0.01 0.01 -0.00 -0.00 0.00 0.03 0.03 -0.04

35 6 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 0.01

36 6 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.01 -0.01 0.01

37 6 -0.01 -0.01 -0.01 0.00 0.00 0.00 0.03 0.03 0.04

38 6 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.01

39 6 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.01 -0.01 -0.01

40 6 0.01 0.01 0.01 -0.00 -0.00 -0.00 -0.02 -0.02 -0.02

41 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.01 -0.00

42 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.01 0.01 -0.01

43 6 -0.01 0.01 0.01 -0.00 0.00 0.00 0.03 -0.03 -0.04

44 6 0.02 -0.02 -0.03 -0.03 0.03 0.03 0.03 -0.02 -0.02

45 6 0.02 -0.03 -0.04 -0.03 0.03 0.03 0.03 -0.02 -0.02

46 6 0.01 -0.00 -0.01 -0.00 -0.00 -0.00 -0.02 0.02 0.01

47 6 -0.03 0.03 0.03 0.03 -0.02 -0.03 -0.03 0.02 0.03

48 6 -0.03 0.03 0.03 0.03 -0.03 -0.03 -0.02 0.02 0.03

49 1 -0.04 0.01 -0.02 -0.00 -0.00 -0.01 0.11 -0.01 -0.00

50 1 -0.05 -0.01 0.01 -0.00 -0.00 0.01 0.10 0.03 -0.00

51 1 -0.01 -0.03 0.01 0.00 0.01 0.02 0.02 0.09 0.03

52 1 -0.02 0.04 -0.01 -0.01 -0.00 0.00 0.03 -0.08 0.02

53 1 -0.01 -0.03 -0.01 -0.00 -0.01 0.02 0.02 0.09 -0.03

54 1 -0.02 0.04 0.01 0.01 0.00 0.00 0.03 -0.08 -0.02

55 1 -0.05 -0.01 -0.01 0.00 0.00 0.01 0.10 0.03 0.00

56 1 -0.04 0.01 0.02 0.00 0.00 -0.01 0.11 -0.01 0.00

57 1 0.21 -0.19 0.24 0.20 -0.18 0.22 0.11 -0.11 0.11

58 1 0.17 -0.16 0.19 0.20 -0.19 0.23 0.18 -0.19 0.22

59 1 -0.03 0.03 -0.05 0.01 -0.00 0.01 0.07 -0.06 0.10

60 1 -0.22 0.18 -0.23 -0.20 0.17 -0.21 -0.10 0.11 -0.12

61 1 -0.18 0.16 -0.18 -0.21 0.18 -0.22 -0.19 0.17 -0.22

62 1 -0.02 -0.03 0.04 -0.01 -0.01 0.01 0.06 0.07 -0.11

63 1 -0.01 -0.02 0.02 0.00 -0.00 0.00 0.02 0.04 -0.04

64 1 0.01 0.01 -0.02 0.00 0.00 -0.01 -0.05 -0.06 0.08

65 1 0.01 0.02 -0.02 0.00 0.00 -0.00 -0.02 -0.02 0.04

66 1 -0.02 -0.01 0.02 -0.01 -0.01 0.01 0.07 0.05 -0.07

67 1 0.01 0.02 0.02 -0.00 -0.00 -0.00 -0.02 -0.02 -0.04

68 1 -0.02 -0.01 -0.02 0.01 0.01 0.01 0.07 0.05 0.07

69 1 -0.02 -0.03 -0.04 0.01 0.01 0.01 0.06 0.07 0.11

70 1 -0.01 -0.02 -0.02 -0.00 0.00 0.00 0.02 0.04 0.04

71 1 0.01 0.01 0.02 -0.00 -0.00 -0.01 -0.05 -0.06 -0.08

72 1 -0.18 0.16 0.18 0.21 -0.18 -0.22 -0.19 0.17 0.22

73 1 -0.22 0.18 0.23 0.20 -0.17 -0.22 -0.10 0.11 0.12

74 1 -0.03 0.03 0.05 -0.01 0.00 0.01 0.07 -0.06 -0.10

75 1 0.17 -0.16 -0.19 -0.20 0.19 0.23 0.18 -0.19 -0.22

76 1 0.21 -0.19 -0.24 -0.20 0.18 0.22 0.11 -0.11 -0.11

77 1 -0.04 -0.00 -0.00 -0.01 -0.01 0.01 0.07 0.01 -0.00

78 1 -0.04 -0.00 0.00 0.01 0.01 0.01 0.07 0.01 0.00

91 92 93

A A A

Frequencies -- 859.3650 859.3867 875.5448

Red. masses -- 1.2493 1.2497 1.3804

Frc consts -- 0.5436 0.5438 0.6235

IR Inten -- 0.0034 2.6717 0.0366

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 -0.03 -0.08

2 6 0.01 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.02

3 7 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00

4 6 -0.00 -0.00 0.00 0.01 0.00 -0.00 -0.00 -0.00 -0.02

5 6 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.03 0.08

6 6 -0.00 0.00 -0.00 0.01 -0.01 0.00 -0.01 -0.00 0.01

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 -0.01 -0.00 0.00 -0.00 -0.00 -0.00

9 6 0.00 -0.00 -0.01 -0.00 0.00 -0.01 -0.00 -0.00 0.00

10 6 0.00 -0.00 0.00 0.01 0.00 0.00 -0.00 0.00 -0.00

11 6 -0.00 -0.00 0.00 0.00 0.00 0.00 0.01 0.00 0.00

12 6 0.01 -0.00 -0.00 -0.01 0.01 -0.00 -0.01 0.00 -0.01

13 6 -0.00 0.00 -0.01 -0.00 0.00 0.01 0.00 0.00 0.00

14 6 -0.00 0.00 0.00 0.01 0.00 -0.00 0.00 -0.00 0.00

15 6 0.00 0.00 0.00 0.00 0.00 -0.00 -0.01 -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 -0.01 -0.00 -0.00 0.00 0.00 -0.00

18 6 0.00 -0.00 -0.00 0.01 -0.01 -0.00 0.01 0.00 0.01

19 6 0.00 0.00 0.00 0.01 0.00 0.00 0.00 0.00 -0.02

20 6 0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.03 0.08

21 6 0.00 -0.01 0.00 -0.00 -0.00 0.00 -0.00 0.03 -0.08

22 6 -0.01 -0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.02

23 7 -0.00 0.00 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00

24 6 -0.01 0.00 -0.00 -0.01 0.01 0.00 0.01 -0.00 -0.02

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 0.01 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 -0.03 -0.03 0.04 0.03 0.03 -0.03 -0.00 -0.00 -0.00

33 6 -0.03 -0.03 0.03 0.02 0.03 -0.03 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 0.02 0.03 -0.03 -0.02 -0.03 0.03 0.00 0.00 0.00

36 6 0.02 0.03 -0.04 -0.02 -0.03 0.03 0.01 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 -0.02 -0.03 -0.03 -0.03 -0.03 -0.03 -0.00 -0.00 0.00

39 6 -0.02 -0.03 -0.03 -0.02 -0.03 -0.04 -0.01 -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 0.03 0.03 0.03 0.03 0.03 0.04 0.00 0.00 -0.00

42 6 0.02 0.03 0.03 0.03 0.03 0.03 -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 -0.01 -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 -0.00 -0.01 0.00 0.00 0.01 -0.01 0.13 0.47

50 1 0.00 0.00 0.02 -0.01 -0.00 -0.02 0.02 -0.13 -0.46

51 1 0.01 0.01 0.00 0.01 0.00 -0.00 -0.01 -0.00 -0.01

52 1 0.00 0.00 -0.02 -0.00 0.01 -0.02 0.01 -0.00 0.01

53 1 -0.01 -0.01 0.00 0.01 0.00 0.00 0.01 0.00 -0.01

54 1 -0.00 -0.00 -0.02 -0.00 0.01 0.02 -0.01 0.00 0.01

55 1 -0.00 -0.00 0.02 -0.01 -0.00 0.02 -0.02 0.13 -0.47

56 1 0.01 0.00 -0.01 0.00 0.00 -0.01 0.01 -0.13 0.48

57 1 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.01 -0.01 0.01

58 1 -0.00 0.00 -0.00 -0.01 0.01 -0.01 0.01 -0.00 0.01

59 1 0.00 -0.00 0.00 -0.01 0.01 -0.01 -0.00 0.00 0.00

60 1 0.01 -0.00 0.00 0.00 -0.00 0.00 0.00 0.01 -0.01

61 1 0.00 -0.00 0.00 0.01 -0.01 0.01 -0.00 0.00 -0.01

62 1 -0.01 -0.01 0.01 0.00 0.01 -0.01 -0.00 -0.00 -0.00

63 1 0.17 0.21 -0.22 -0.17 -0.20 0.22 0.01 0.01 -0.01

64 1 0.18 0.21 -0.22 -0.17 -0.20 0.21 0.01 0.01 -0.01

65 1 -0.19 -0.21 0.22 0.18 0.20 -0.22 -0.00 -0.01 0.01

66 1 -0.19 -0.20 0.23 0.18 0.20 -0.22 -0.00 -0.01 0.01

67 1 0.18 0.20 0.22 0.19 0.21 0.23 0.00 0.01 0.01

68 1 0.18 0.20 0.22 0.18 0.20 0.23 0.00 0.02 0.01

69 1 0.01 0.01 0.01 0.00 0.01 0.01 0.00 0.00 -0.00

70 1 -0.16 -0.20 -0.22 -0.17 -0.21 -0.23 -0.01 -0.01 -0.01

71 1 -0.17 -0.20 -0.22 -0.17 -0.20 -0.22 -0.01 -0.01 -0.01

72 1 -0.00 0.00 0.00 0.01 -0.01 -0.01 -0.00 -0.00 -0.01

73 1 -0.01 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.01 -0.01

74 1 -0.00 0.00 0.00 -0.01 0.01 0.01 0.00 -0.00 0.00

75 1 0.00 -0.00 -0.00 -0.01 0.01 0.01 -0.01 0.00 0.01

76 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.01 0.01 0.01

77 1 -0.01 -0.00 0.00 0.00 0.00 -0.00 0.01 0.00 0.00

78 1 0.01 0.00 0.00 0.00 0.00 0.00 -0.01 -0.00 0.00

94 95 96

A A A

Frequencies -- 875.6072 886.6466 897.1891

Red. masses -- 1.3805 4.9142 4.7952

Frc consts -- 0.6236 2.2762 2.2742

IR Inten -- 0.4052 0.0033 6.0950

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.03 -0.08 0.13 -0.10 0.05 0.01 0.06 -0.02

2 6 -0.00 0.00 0.02 -0.08 -0.09 0.01 0.09 -0.00 0.01

3 7 0.00 0.00 -0.00 -0.06 -0.00 -0.00 0.00 -0.06 0.01

4 6 -0.00 -0.00 -0.02 -0.09 0.08 -0.01 -0.10 -0.01 0.01

5 6 -0.00 0.03 0.08 0.11 0.12 -0.04 -0.01 0.07 -0.03

6 6 -0.01 -0.00 0.01 -0.12 -0.04 -0.01 -0.14 -0.09 -0.00

7 6 0.00 -0.00 -0.01 0.01 0.04 -0.01 0.04 -0.02 -0.01

8 7 -0.00 -0.00 0.00 0.01 -0.08 -0.00 -0.01 -0.06 -0.00

9 6 0.00 0.00 -0.01 -0.02 0.03 0.02 -0.04 -0.01 0.01

10 6 0.00 0.00 0.00 -0.09 0.01 -0.03 -0.12 0.05 -0.04

11 6 0.00 0.00 0.00 0.08 0.02 0.03 0.14 0.07 0.04

12 6 -0.01 0.00 -0.02 -0.13 0.03 0.01 0.13 -0.05 -0.00

13 6 0.00 0.00 0.01 0.02 -0.03 0.02 -0.04 -0.01 -0.01

14 6 0.00 0.00 -0.00 0.09 -0.01 -0.03 -0.12 0.05 0.04

15 6 0.00 0.00 -0.00 -0.08 -0.02 0.03 0.14 0.07 -0.04

16 6 0.00 -0.00 0.01 -0.01 -0.04 -0.01 0.04 -0.02 0.01

17 7 -0.00 -0.00 -0.00 -0.01 0.08 -0.00 -0.01 -0.06 0.00

18 6 -0.01 -0.00 -0.01 0.12 0.04 -0.01 -0.14 -0.09 0.00

19 6 -0.00 -0.00 0.02 0.09 -0.08 -0.01 -0.10 -0.01 -0.01

20 6 -0.00 0.03 -0.08 -0.11 -0.12 -0.04 -0.01 0.07 0.03

21 6 0.00 -0.03 0.08 -0.13 0.10 0.05 0.01 0.06 0.02

22 6 -0.00 0.00 -0.02 0.08 0.09 0.01 0.09 -0.00 -0.01

23 7 0.00 0.00 0.00 0.06 0.00 -0.00 0.00 -0.06 -0.01

24 6 -0.01 0.00 0.02 0.13 -0.03 0.01 0.13 -0.05 0.00

25 6 -0.00 -0.00 -0.00 -0.01 -0.03 0.01 -0.02 -0.04 0.01

26 6 -0.00 0.00 0.00 -0.00 0.02 0.02 -0.01 0.03 0.03

27 6 -0.00 0.00 0.00 -0.01 0.05 0.03 -0.01 0.07 0.05

28 6 -0.00 -0.00 0.00 -0.02 -0.01 -0.01 -0.03 -0.01 -0.01

29 6 0.01 0.00 -0.00 0.06 0.01 -0.04 0.08 0.01 -0.05

30 6 0.00 -0.00 -0.00 0.04 -0.01 -0.02 0.05 -0.01 -0.03

31 6 -0.00 0.00 -0.00 -0.03 0.01 0.01 0.03 -0.01 -0.01

32 6 -0.00 -0.00 -0.00 -0.00 -0.05 -0.03 -0.00 0.06 0.04

33 6 0.00 -0.00 0.00 -0.00 -0.02 -0.02 0.00 0.02 0.03

34 6 -0.00 -0.00 0.00 -0.01 0.03 -0.01 0.02 -0.04 0.01

35 6 0.00 0.00 0.00 0.03 0.02 0.02 -0.04 -0.02 -0.03

36 6 0.01 0.00 0.00 0.06 -0.00 0.04 -0.07 -0.00 -0.05

37 6 -0.00 -0.00 -0.00 0.01 -0.03 -0.01 0.02 -0.04 -0.01

38 6 0.00 0.00 -0.00 -0.03 -0.02 0.02 -0.04 -0.02 0.03

39 6 0.01 0.00 -0.00 -0.06 0.00 0.04 -0.07 -0.00 0.05

40 6 -0.00 0.00 0.00 0.03 -0.01 0.01 0.03 -0.01 0.01

41 6 -0.00 -0.00 0.00 0.00 0.05 -0.03 -0.00 0.06 -0.04

42 6 0.00 -0.00 -0.00 0.00 0.02 -0.02 0.00 0.02 -0.03

43 6 -0.00 -0.00 0.00 0.01 0.03 0.01 -0.02 -0.04 -0.01

44 6 0.00 -0.00 0.00 -0.04 0.01 -0.02 0.05 -0.01 0.03

45 6 0.01 0.00 0.00 -0.06 -0.01 -0.04 0.08 0.01 0.05

46 6 -0.00 -0.00 -0.00 0.02 0.01 -0.01 -0.03 -0.01 0.01

47 6 -0.00 0.00 -0.00 0.01 -0.05 0.03 -0.01 0.07 -0.05

48 6 -0.00 0.00 -0.00 0.00 -0.02 0.02 -0.01 0.03 -0.03

49 1 -0.01 0.13 0.48 0.09 -0.16 -0.02 -0.09 -0.02 0.03

50 1 0.02 -0.13 -0.47 0.07 0.17 0.02 0.09 0.03 0.04

51 1 -0.00 -0.00 -0.00 -0.19 -0.16 -0.08 -0.25 -0.14 -0.07

52 1 0.00 0.00 -0.00 0.21 -0.14 0.08 0.27 -0.08 0.07

53 1 -0.00 -0.00 0.00 0.19 0.16 -0.08 -0.25 -0.14 0.07

54 1 0.00 0.00 0.00 -0.21 0.14 0.08 0.27 -0.08 -0.07

55 1 0.02 -0.13 0.46 -0.07 -0.17 0.02 0.09 0.03 -0.04

56 1 -0.01 0.13 -0.47 -0.09 0.16 -0.02 -0.09 -0.02 -0.03

57 1 0.01 -0.01 0.01 -0.03 0.04 -0.00 -0.04 0.06 0.00

58 1 0.01 -0.00 0.01 0.08 0.03 0.07 0.11 0.06 0.08

59 1 -0.01 0.00 -0.00 0.03 -0.06 0.07 0.03 -0.07 0.07

60 1 -0.00 0.01 -0.01 0.08 0.08 -0.01 0.10 0.11 -0.03

61 1 0.00 0.00 -0.01 -0.03 0.04 -0.09 -0.02 0.04 -0.11

62 1 -0.01 -0.00 0.00 0.02 0.05 -0.06 -0.02 -0.06 0.07

63 1 0.01 0.00 -0.01 0.09 -0.02 -0.07 -0.10 0.03 0.07

64 1 0.01 0.01 -0.01 -0.02 -0.04 -0.00 0.03 0.06 -0.01

65 1 -0.00 -0.00 0.01 -0.02 -0.04 0.09 0.01 0.04 -0.10

66 1 -0.00 -0.02 0.01 0.09 -0.07 0.02 -0.10 0.08 -0.02

67 1 -0.00 -0.00 -0.01 0.02 0.04 0.09 0.01 0.04 0.10

68 1 -0.00 -0.02 -0.01 -0.09 0.07 0.02 -0.10 0.08 0.02

69 1 -0.01 -0.00 -0.00 -0.02 -0.05 -0.06 -0.02 -0.06 -0.07

70 1 0.01 0.00 0.01 -0.09 0.02 -0.07 -0.10 0.03 -0.07

71 1 0.01 0.01 0.01 0.02 0.04 -0.00 0.03 0.06 0.01

72 1 0.00 0.00 0.01 0.03 -0.04 -0.09 -0.02 0.04 0.11

73 1 -0.00 0.01 0.01 -0.08 -0.08 -0.01 0.10 0.11 0.03

74 1 -0.01 0.00 0.00 -0.03 0.06 0.07 0.03 -0.07 -0.07

75 1 0.01 -0.00 -0.01 -0.08 -0.03 0.07 0.11 0.06 -0.08

76 1 0.01 -0.01 -0.01 0.03 -0.04 -0.00 -0.04 0.06 -0.00

77 1 0.01 0.00 0.00 0.16 0.01 -0.00 0.01 -0.06 0.03

78 1 0.01 0.00 -0.00 -0.16 -0.01 -0.00 0.01 -0.06 -0.03

97 98 99

A A A

Frequencies -- 897.6877 901.3060 928.4836

Red. masses -- 6.3827 6.5904 1.3204

Frc consts -- 3.0304 3.1543 0.6706

IR Inten -- 15.1113 0.3731 0.0004

Atom AN X Y Z X Y Z X Y Z

1 6 0.10 -0.12 0.05 0.00 -0.07 0.02 -0.00 -0.00 -0.00

2 6 -0.06 -0.07 0.00 -0.10 -0.00 -0.02 0.00 0.00 0.00

3 7 -0.04 0.00 -0.00 -0.00 0.05 -0.01 0.00 0.00 -0.00

4 6 -0.05 0.07 -0.00 0.10 0.01 -0.02 0.00 -0.00 -0.00

5 6 0.09 0.12 -0.04 0.01 -0.07 0.03 -0.00 0.00 0.00

6 6 -0.09 -0.11 -0.01 0.15 0.13 0.01 -0.00 -0.00 0.01

7 6 -0.03 -0.09 -0.01 0.03 0.08 0.02 0.00 -0.01 -0.01

8 7 -0.11 -0.00 -0.03 0.08 0.01 0.02 -0.00 0.00 -0.00

9 6 -0.04 0.09 -0.02 0.04 -0.08 0.02 -0.00 -0.01 0.01

10 6 0.15 0.01 0.04 -0.12 -0.01 -0.03 0.02 0.01 -0.08

11 6 0.12 -0.00 0.03 -0.12 -0.01 -0.03 -0.02 0.00 0.08

12 6 -0.14 0.11 0.00 -0.17 0.10 0.00 -0.00 0.00 -0.01

13 6 -0.04 0.09 0.02 -0.04 0.08 0.02 0.00 0.01 0.01

14 6 0.15 0.01 -0.04 0.12 0.01 -0.03 -0.02 -0.01 -0.08

15 6 0.12 -0.00 -0.03 0.12 0.01 -0.03 0.02 -0.00 0.08

16 6 -0.03 -0.09 0.01 -0.03 -0.08 0.02 -0.00 0.01 -0.01

17 7 -0.11 -0.00 0.03 -0.08 -0.01 0.02 0.00 -0.00 -0.00

18 6 -0.09 -0.11 0.01 -0.15 -0.13 0.01 0.00 0.00 0.01

19 6 -0.05 0.07 0.00 -0.10 -0.01 -0.02 -0.00 0.00 -0.00

20 6 0.09 0.12 0.04 -0.01 0.07 0.03 0.00 -0.00 0.00

21 6 0.10 -0.12 -0.05 -0.00 0.07 0.02 0.00 0.00 -0.00

22 6 -0.06 -0.07 -0.00 0.10 0.00 -0.02 -0.00 -0.00 0.00

23 7 -0.04 0.00 0.00 0.00 -0.05 -0.01 -0.00 -0.00 -0.00

24 6 -0.14 0.11 -0.00 0.17 -0.10 0.00 0.00 -0.00 -0.01

25 6 -0.04 -0.03 -0.01 0.04 0.06 -0.00 -0.00 0.00 -0.00

26 6 -0.02 0.04 0.03 0.01 -0.04 -0.04 0.00 -0.00 0.00

27 6 -0.01 0.07 0.05 0.01 -0.09 -0.07 0.00 -0.00 0.00

28 6 -0.01 -0.03 0.00 0.03 0.02 0.01 -0.00 0.00 -0.00

29 6 0.07 0.01 -0.05 -0.10 -0.01 0.07 0.00 0.00 -0.00

30 6 0.03 -0.00 -0.03 -0.05 0.01 0.04 0.00 -0.00 0.00

31 6 -0.03 0.03 -0.00 -0.03 0.02 0.00 -0.00 0.00 -0.00

32 6 0.00 -0.09 -0.06 0.00 -0.10 -0.07 0.00 -0.00 -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 0.04 0.00 -0.05 0.05 -0.01 -0.00 -0.00 0.00

35 6 0.04 0.01 0.04 0.05 0.02 0.04 0.00 0.00 -0.00

36 6 0.09 0.00 0.06 0.10 0.00 0.07 0.00 -0.00 0.00

37 6 -0.05 0.04 -0.00 0.05 -0.05 -0.01 0.00 0.00 0.00

38 6 0.04 0.01 -0.04 -0.05 -0.02 0.04 -0.00 -0.00 -0.00

39 6 0.09 0.00 -0.06 -0.10 -0.00 0.07 -0.00 0.00 0.00

40 6 -0.03 0.03 0.00 0.03 -0.02 0.00 0.00 -0.00 -0.00

41 6 0.00 -0.09 0.06 -0.00 0.10 -0.07 -0.00 0.00 -0.00

42 6 -0.01 -0.04 0.04 0.01 0.04 -0.04 -0.00 -0.00 -0.00

43 6 -0.04 -0.03 0.01 -0.04 -0.06 -0.00 0.00 -0.00 -0.00

44 6 0.03 -0.00 0.03 0.05 -0.01 0.04 -0.00 0.00 0.00

45 6 0.07 0.01 0.05 0.10 0.01 0.07 -0.00 -0.00 -0.00

46 6 -0.01 -0.03 -0.00 -0.03 -0.02 0.01 0.00 -0.00 -0.00

47 6 -0.01 0.07 -0.05 -0.01 0.09 -0.07 -0.00 0.00 0.00

48 6 -0.02 0.04 -0.03 -0.01 0.04 -0.04 -0.00 0.00 0.00

49 1 0.02 -0.21 -0.01 0.12 0.02 -0.03 -0.00 -0.00 0.01

50 1 -0.02 0.21 -0.00 -0.12 -0.01 -0.05 -0.00 -0.00 -0.01

51 1 0.09 -0.10 -0.00 -0.06 0.10 0.01 -0.13 -0.01 0.48

52 1 0.02 0.14 -0.03 -0.05 -0.11 0.02 0.13 0.02 -0.47

53 1 0.09 -0.10 0.00 0.06 -0.10 0.01 0.13 0.01 0.48

54 1 0.02 0.14 0.03 0.05 0.11 0.02 -0.13 -0.02 -0.47

55 1 -0.02 0.21 0.00 0.12 0.01 -0.05 0.00 0.00 -0.01

56 1 0.02 -0.21 0.01 -0.12 -0.02 -0.03 0.00 0.00 0.01

57 1 0.01 0.01 0.07 0.03 -0.06 -0.04 -0.01 0.01 -0.01

58 1 0.09 0.09 0.05 -0.13 -0.10 -0.09 -0.00 0.00 -0.00

59 1 -0.04 -0.00 -0.03 -0.00 0.05 -0.04 0.00 -0.01 0.01

60 1 0.06 0.11 -0.06 -0.11 -0.14 0.06 0.01 -0.00 0.00

61 1 0.04 -0.01 -0.02 -0.01 -0.02 0.09 -0.00 0.00 -0.01

62 1 -0.04 0.01 0.01 -0.01 0.05 -0.04 -0.00 0.00 -0.00

63 1 0.13 -0.09 -0.06 0.15 -0.09 -0.08 -0.00 -0.00 0.00

64 1 0.01 -0.03 -0.07 -0.02 -0.06 -0.04 -0.00 -0.00 0.00

65 1 0.04 0.01 0.05 0.02 -0.02 0.10 0.00 0.00 0.00

66 1 0.10 -0.12 0.07 0.13 -0.13 0.06 0.01 0.00 -0.00

67 1 0.04 0.01 -0.05 -0.02 0.02 0.10 -0.00 -0.00 0.00

68 1 0.10 -0.12 -0.07 -0.13 0.13 0.06 -0.01 -0.00 -0.00

69 1 -0.04 0.01 -0.01 0.01 -0.05 -0.04 0.00 -0.00 -0.00

70 1 0.13 -0.09 0.06 -0.15 0.09 -0.08 0.00 0.00 0.00

71 1 0.01 -0.03 0.07 0.02 0.06 -0.04 0.00 0.00 0.00

72 1 0.04 -0.01 0.02 0.01 0.02 0.09 0.00 -0.00 -0.01

73 1 0.06 0.11 0.06 0.11 0.14 0.06 -0.01 0.00 0.00

74 1 -0.04 -0.00 0.03 0.00 -0.05 -0.04 -0.00 0.01 0.01

75 1 0.09 0.09 -0.05 0.13 0.10 -0.09 0.00 -0.00 -0.00

76 1 0.01 0.01 -0.07 -0.03 0.06 -0.04 0.01 -0.01 -0.01

77 1 0.12 0.01 -0.01 0.00 0.05 -0.02 -0.00 0.00 0.00

78 1 0.12 0.01 0.01 -0.00 -0.05 -0.02 0.00 -0.00 0.00

100 101 102

A A A

Frequencies -- 928.7844 940.6065 940.8880

Red. masses -- 1.3175 1.4767 1.4968

Frc consts -- 0.6696 0.7698 0.7807

IR Inten -- 0.0399 2.3618 3.3669

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 0.01 -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 0.01 -0.00 -0.01 -0.01 0.00

4 6 0.00 -0.00 -0.00 0.01 -0.01 -0.00 -0.01 0.01 0.00

5 6 0.00 -0.00 0.00 -0.01 -0.02 0.01 0.01 0.01 -0.01

6 6 0.00 0.00 0.01 0.01 0.01 0.01 -0.01 -0.00 -0.01

7 6 0.00 -0.00 -0.01 0.00 0.00 -0.00 -0.00 0.01 0.00

8 7 0.00 -0.00 -0.00 -0.02 -0.02 -0.00 0.03 0.01 0.01

9 6 -0.00 -0.00 0.01 -0.00 0.01 0.00 0.01 -0.00 0.00

10 6 0.02 0.00 -0.08 0.01 0.00 0.00 -0.02 -0.00 -0.01

11 6 -0.02 0.00 0.08 0.01 -0.00 -0.00 -0.02 -0.00 -0.00

12 6 -0.00 0.00 0.01 0.00 -0.00 -0.00 0.00 0.00 0.00

13 6 -0.00 -0.00 -0.01 0.00 -0.01 0.00 0.01 -0.00 -0.00

14 6 0.02 0.00 0.08 -0.01 -0.00 0.00 -0.02 -0.00 0.01

15 6 -0.02 0.00 -0.08 -0.01 0.00 -0.00 -0.02 -0.00 0.00

16 6 0.00 -0.00 0.01 -0.00 -0.00 -0.00 -0.00 0.01 -0.00

17 7 0.00 -0.00 0.00 0.02 0.02 -0.00 0.03 0.01 -0.01

18 6 0.00 0.00 -0.01 -0.01 -0.01 0.01 -0.01 -0.00 0.01

19 6 0.00 -0.00 0.00 -0.01 0.01 -0.00 -0.01 0.01 -0.00

20 6 0.00 -0.00 -0.00 0.01 0.02 0.01 0.01 0.01 0.01

21 6 -0.00 -0.00 -0.00 0.01 -0.00 -0.00 0.01 -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 -0.01 -0.00 -0.01 -0.01 -0.00

24 6 -0.00 0.00 -0.01 -0.00 0.00 -0.00 0.00 0.00 -0.00

25 6 -0.00 0.00 -0.00 -0.03 0.03 -0.04 0.03 -0.03 0.04

26 6 0.00 -0.00 0.00 0.04 -0.04 0.04 -0.04 0.04 -0.04

27 6 0.00 -0.00 -0.00 -0.00 -0.01 -0.01 0.00 0.00 0.01

28 6 -0.00 0.00 -0.00 -0.04 0.04 -0.04 0.04 -0.04 0.04

29 6 -0.00 0.00 -0.00 -0.01 0.00 0.00 0.01 -0.00 -0.00

30 6 0.00 -0.00 0.00 0.04 -0.04 0.05 -0.04 0.03 -0.05

31 6 0.00 0.00 0.00 -0.01 -0.01 0.01 0.01 0.01 -0.01

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 0.01 0.01 -0.01 -0.01 -0.01 0.01

34 6 0.00 0.00 -0.00 -0.00 -0.01 0.01 0.01 0.01 -0.01

35 6 -0.00 -0.00 0.00 0.01 0.01 -0.01 -0.01 -0.01 0.01

36 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00

37 6 0.00 0.00 0.00 0.00 0.01 0.01 0.01 0.01 0.01

38 6 -0.00 -0.00 -0.00 -0.01 -0.01 -0.01 -0.01 -0.01 -0.01

39 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.00 0.00 0.00

40 6 0.00 0.00 -0.00 0.01 0.01 0.01 0.01 0.01 0.01

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 -0.01 -0.01 -0.01 -0.01 -0.01 -0.01

43 6 -0.00 0.00 0.00 0.03 -0.03 -0.04 0.03 -0.03 -0.04

44 6 0.00 -0.00 -0.00 -0.04 0.04 0.05 -0.04 0.03 0.05

45 6 -0.00 0.00 0.00 0.01 -0.00 0.00 0.01 -0.00 0.00

46 6 -0.00 0.00 0.00 0.04 -0.04 -0.04 0.04 -0.04 -0.04

47 6 0.00 -0.00 0.00 0.00 0.01 -0.01 0.00 0.00 -0.01

48 6 0.00 -0.00 -0.00 -0.04 0.04 0.04 -0.04 0.04 0.04

49 1 0.00 0.00 -0.00 0.01 0.02 -0.00 -0.01 -0.01 0.00

50 1 -0.00 -0.00 -0.00 -0.01 -0.02 -0.00 0.02 0.01 0.00

51 1 -0.13 -0.01 0.48 0.01 -0.01 -0.02 -0.02 0.01 0.02

52 1 0.12 0.02 -0.47 -0.01 0.01 0.02 0.01 -0.03 -0.02

53 1 -0.13 -0.01 -0.48 -0.01 0.01 -0.02 -0.02 0.01 -0.02

54 1 0.12 0.02 0.47 0.01 -0.01 0.02 0.01 -0.03 0.02

55 1 -0.00 -0.00 0.00 0.01 0.02 -0.00 0.02 0.01 -0.00

56 1 0.00 0.00 0.00 -0.01 -0.02 -0.00 -0.01 -0.01 -0.00

57 1 -0.01 0.01 -0.01 -0.21 0.19 -0.24 0.21 -0.19 0.23

58 1 -0.01 0.00 -0.00 -0.00 -0.01 -0.00 -0.00 0.01 -0.00

59 1 0.01 -0.01 0.01 0.23 -0.20 0.26 -0.22 0.20 -0.25

60 1 0.00 -0.01 0.01 -0.00 -0.01 0.01 0.00 0.01 -0.00

61 1 -0.01 0.01 -0.01 -0.23 0.20 -0.24 0.22 -0.20 0.24

62 1 -0.00 -0.00 0.00 0.05 0.05 -0.06 -0.06 -0.07 0.08

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 -0.01 -0.04 -0.05 0.06 0.06 0.07 -0.07

65 1 0.00 0.00 -0.00 -0.05 -0.05 0.06 0.06 0.07 -0.07

66 1 -0.00 -0.00 0.01 0.00 0.00 -0.00 -0.00 -0.00 0.00

67 1 0.00 0.00 0.00 0.05 0.05 0.06 0.06 0.07 0.07

68 1 -0.00 -0.00 -0.01 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

69 1 -0.00 -0.00 -0.00 -0.05 -0.05 -0.06 -0.06 -0.07 -0.08

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 0.01 0.04 0.05 0.06 0.06 0.07 0.07

72 1 -0.01 0.01 0.01 0.23 -0.20 -0.24 0.23 -0.20 -0.24

73 1 0.00 -0.01 -0.01 0.00 0.01 0.01 0.00 0.01 0.00

74 1 0.01 -0.01 -0.01 -0.23 0.20 0.26 -0.23 0.20 0.25

75 1 -0.01 0.00 0.00 0.00 0.01 -0.00 -0.00 0.01 0.00

76 1 -0.01 0.01 0.01 0.21 -0.19 -0.24 0.21 -0.19 -0.23

77 1 0.00 0.00 0.00 0.01 0.01 -0.01 -0.01 -0.01 0.01

78 1 0.00 0.00 -0.00 -0.01 -0.01 -0.01 -0.01 -0.01 -0.01

103 104 105

A A A

Frequencies -- 942.6962 943.0863 968.1522

Red. masses -- 1.4892 1.4788 6.6497

Frc consts -- 0.7797 0.7749 3.6723

IR Inten -- 6.3333 2.4823 0.0690

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 -0.01 0.01 0.00 -0.01 0.00 0.04 -0.01 -0.00

2 6 -0.01 -0.00 -0.00 -0.02 -0.01 -0.00 -0.04 -0.05 0.01

3 7 -0.01 0.01 -0.00 -0.01 0.02 -0.01 -0.07 -0.01 0.00

4 6 0.01 0.00 -0.00 0.01 0.00 -0.00 -0.04 0.05 -0.02

5 6 0.01 -0.00 0.00 0.00 -0.01 0.00 0.04 0.03 0.00

6 6 0.01 0.00 0.00 0.01 -0.00 0.00 0.06 0.10 -0.00

7 6 -0.00 -0.01 0.00 0.01 -0.00 0.00 -0.03 0.18 -0.01

8 7 -0.03 0.01 -0.01 0.02 -0.01 0.00 0.01 -0.24 -0.00

9 6 0.00 0.00 -0.00 -0.00 -0.01 -0.00 0.01 0.18 0.01

10 6 0.01 0.00 0.00 -0.01 0.00 -0.00 0.08 -0.08 0.00

11 6 0.01 0.00 0.00 -0.01 0.00 -0.00 -0.05 -0.09 -0.00

12 6 -0.02 0.00 0.01 -0.01 -0.00 0.01 0.07 -0.09 0.00

13 6 -0.00 -0.00 -0.00 -0.00 -0.01 0.00 -0.01 -0.18 0.01

14 6 -0.01 -0.00 0.00 -0.01 0.00 0.00 -0.08 0.08 0.00

15 6 -0.01 -0.00 0.00 -0.01 0.00 0.00 0.05 0.09 -0.00

16 6 0.00 0.01 0.00 0.01 -0.00 -0.00 0.03 -0.18 -0.01

17 7 0.03 -0.01 -0.01 0.02 -0.01 -0.00 -0.01 0.24 -0.00

18 6 -0.01 -0.00 0.00 0.01 -0.00 -0.00 -0.06 -0.10 -0.00

19 6 -0.01 -0.00 -0.00 0.01 0.00 0.00 0.04 -0.05 -0.02

20 6 -0.01 0.00 0.00 0.00 -0.01 -0.00 -0.04 -0.03 0.00

21 6 -0.01 0.01 0.01 0.00 -0.01 -0.00 -0.04 0.01 -0.00

22 6 0.01 0.00 -0.00 -0.02 -0.01 0.00 0.04 0.05 0.01

23 7 0.01 -0.01 -0.00 -0.01 0.02 0.01 0.07 0.01 0.00

24 6 0.02 -0.00 0.01 -0.01 -0.00 -0.01 -0.07 0.09 0.00

25 6 -0.01 0.01 -0.01 -0.01 0.01 -0.01 0.07 0.07 0.01

26 6 0.01 -0.01 0.01 0.01 -0.01 0.01 0.01 -0.01 -0.04

27 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.07 -0.06

28 6 -0.01 0.01 -0.01 -0.01 0.01 -0.01 0.02 0.00 0.01

29 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.08 0.01 0.04

30 6 0.01 -0.01 0.01 0.01 -0.01 0.02 -0.01 -0.00 0.02

31 6 0.03 0.04 -0.04 0.03 0.04 -0.04 0.02 0.00 -0.01

32 6 0.00 -0.01 -0.01 0.00 -0.00 -0.00 -0.01 0.07 0.05

33 6 -0.03 -0.04 0.04 -0.03 -0.04 0.04 0.00 0.01 0.04

34 6 0.02 0.04 -0.04 0.02 0.03 -0.04 0.07 -0.06 -0.01

35 6 -0.03 -0.04 0.05 -0.03 -0.04 0.05 -0.01 -0.00 -0.02

36 6 0.01 0.00 0.00 0.01 0.00 0.00 -0.07 -0.02 -0.04

37 6 -0.02 -0.04 -0.04 0.02 0.03 0.04 -0.07 0.06 -0.01

38 6 0.03 0.04 0.05 -0.03 -0.04 -0.05 0.01 0.00 -0.02

39 6 -0.01 -0.00 0.00 0.01 0.00 -0.00 0.07 0.02 -0.04

40 6 -0.03 -0.04 -0.04 0.03 0.04 0.04 -0.02 -0.00 -0.01

41 6 -0.00 0.01 -0.01 0.00 -0.00 0.00 0.01 -0.07 0.05

42 6 0.03 0.04 0.04 -0.03 -0.04 -0.04 -0.00 -0.01 0.04

43 6 0.01 -0.01 -0.01 -0.01 0.01 0.01 -0.07 -0.07 0.01

44 6 -0.01 0.01 0.01 0.01 -0.01 -0.02 0.01 0.00 0.02

45 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.08 -0.01 0.04

46 6 0.01 -0.01 -0.01 -0.01 0.01 0.01 -0.02 -0.00 0.01

47 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.07 -0.06

48 6 -0.01 0.01 0.01 0.01 -0.01 -0.01 -0.01 0.01 -0.04

49 1 0.02 -0.01 -0.00 0.02 0.00 -0.00 0.07 0.02 0.04

50 1 -0.02 0.01 -0.01 -0.02 0.01 -0.01 0.07 -0.00 -0.04

51 1 0.00 -0.02 0.00 0.01 0.03 -0.01 -0.01 -0.18 0.04

52 1 0.00 0.02 -0.00 -0.02 0.00 0.01 0.04 -0.17 -0.04

53 1 -0.00 0.02 0.00 0.01 0.03 0.01 0.01 0.18 0.04

54 1 -0.00 -0.02 -0.00 -0.02 0.00 -0.01 -0.04 0.17 -0.04

55 1 0.02 -0.01 -0.01 -0.02 0.01 0.01 -0.07 0.00 -0.04

56 1 -0.02 0.01 -0.00 0.02 0.00 0.00 -0.07 -0.02 0.04

57 1 -0.05 0.04 -0.05 -0.07 0.06 -0.07 0.08 -0.08 0.03

58 1 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.08 -0.09 -0.06

59 1 0.05 -0.04 0.06 0.07 -0.06 0.08 -0.05 0.06 -0.05

60 1 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.01 -0.11 0.12

61 1 -0.05 0.04 -0.05 -0.07 0.06 -0.07 -0.07 0.01 0.01

62 1 -0.20 -0.23 0.26 -0.20 -0.23 0.25 -0.04 -0.06 0.04

63 1 0.01 -0.00 -0.01 0.01 0.00 -0.01 -0.08 0.08 0.05

64 1 0.19 0.21 -0.24 0.18 0.21 -0.23 0.06 0.08 -0.02

65 1 0.21 0.23 -0.24 0.20 0.22 -0.24 -0.06 -0.02 -0.01

66 1 0.00 -0.02 0.01 0.00 -0.01 0.01 -0.03 0.10 -0.11

67 1 -0.21 -0.23 -0.24 0.20 0.22 0.24 0.06 0.02 -0.01

68 1 -0.00 0.02 0.01 0.00 -0.01 -0.01 0.03 -0.10 -0.11

69 1 0.20 0.23 0.26 -0.20 -0.23 -0.25 0.04 0.06 0.04

70 1 -0.01 0.00 -0.01 0.01 0.00 0.01 0.08 -0.08 0.05

71 1 -0.19 -0.21 -0.24 0.18 0.21 0.23 -0.06 -0.08 -0.02

72 1 0.05 -0.04 -0.05 -0.07 0.06 0.07 0.07 -0.01 0.01

73 1 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.01 0.11 0.12

74 1 -0.05 0.04 0.06 0.07 -0.06 -0.08 0.05 -0.06 -0.05

75 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.08 0.09 -0.06

76 1 0.05 -0.04 -0.05 -0.07 0.06 0.07 -0.08 0.08 0.03

77 1 -0.01 0.02 -0.01 -0.01 0.02 -0.01 -0.20 -0.02 0.01

78 1 0.01 -0.02 -0.01 -0.01 0.02 0.01 0.20 0.02 0.01

106 107 108

A A A

Frequencies -- 980.9581 980.9721 981.1491

Red. masses -- 2.9150 1.3657 1.9149

Frc consts -- 1.6527 0.7743 1.0861

IR Inten -- 2.2461 9.2434 1.4500

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.02 0.00 -0.00 0.00 0.00 -0.00 -0.01 0.00

2 6 -0.03 -0.01 0.01 0.00 0.00 -0.00 -0.01 -0.00 0.00

3 7 -0.01 0.07 -0.02 0.00 -0.00 -0.00 -0.00 0.04 -0.01

4 6 0.02 -0.01 0.01 0.00 -0.00 0.00 0.01 -0.01 0.00

5 6 0.00 -0.03 0.01 -0.00 -0.00 0.00 0.00 -0.02 0.00

6 6 -0.01 -0.06 0.00 -0.00 -0.00 0.00 -0.01 -0.04 0.00

7 6 0.02 -0.01 0.00 0.00 -0.00 -0.00 0.02 -0.02 0.00

8 7 0.13 -0.01 0.03 0.00 0.00 0.00 0.08 0.01 0.02

9 6 0.03 0.03 0.01 0.00 0.00 -0.00 0.01 0.01 0.00

10 6 -0.10 -0.01 -0.02 -0.00 -0.00 -0.00 -0.06 -0.00 -0.01

11 6 -0.10 -0.01 -0.02 -0.00 -0.00 0.00 -0.06 -0.00 -0.01

12 6 0.02 -0.07 0.00 -0.00 0.01 -0.00 0.01 -0.04 0.00

13 6 -0.03 -0.03 0.01 0.00 0.00 -0.00 -0.01 -0.01 0.00

14 6 0.10 0.01 -0.02 -0.01 -0.00 0.00 0.06 0.00 -0.01

15 6 0.10 0.01 -0.02 -0.01 -0.00 0.00 0.06 0.00 -0.01

16 6 -0.02 0.01 0.00 0.00 -0.00 0.00 -0.02 0.02 0.00

17 7 -0.13 0.01 0.03 0.01 0.00 -0.00 -0.08 -0.01 0.02

18 6 0.01 0.06 0.00 -0.00 -0.01 -0.00 0.01 0.04 0.00

19 6 -0.02 0.01 0.01 0.00 -0.00 -0.00 -0.01 0.01 0.00

20 6 -0.00 0.03 0.01 -0.00 -0.00 -0.00 -0.00 0.02 0.00

21 6 -0.00 0.02 0.00 -0.00 0.00 -0.00 0.00 0.01 0.00

22 6 0.03 0.01 0.01 0.00 0.00 0.00 0.01 0.00 0.00

23 7 0.01 -0.07 -0.02 0.00 0.00 0.00 0.00 -0.04 -0.01

24 6 -0.02 0.07 0.00 -0.00 0.00 0.00 -0.01 0.04 0.00

25 6 -0.03 -0.02 -0.01 0.00 0.00 -0.00 -0.02 -0.02 -0.01

26 6 0.03 -0.03 0.05 0.04 -0.03 0.04 -0.04 0.03 -0.02

27 6 -0.03 0.05 -0.01 -0.03 0.03 -0.04 0.03 -0.01 0.06

28 6 -0.00 0.01 -0.01 -0.00 0.00 -0.00 0.00 0.00 -0.00

29 6 0.06 -0.03 0.02 0.04 -0.03 0.04 -0.01 0.03 -0.05

30 6 -0.02 0.02 -0.04 -0.04 0.03 -0.04 0.04 -0.04 0.03

31 6 0.00 0.01 -0.01 -0.00 -0.00 0.00 -0.00 0.00 -0.00

32 6 -0.01 0.03 0.03 0.00 -0.00 -0.00 -0.00 0.02 0.02

33 6 0.01 0.01 0.02 -0.00 -0.00 -0.00 0.00 0.00 0.01

34 6 0.04 -0.02 -0.01 -0.00 0.00 0.00 0.02 -0.01 -0.01

35 6 -0.01 -0.01 -0.01 0.00 0.00 0.00 -0.01 -0.01 -0.00

36 6 -0.03 -0.00 -0.02 0.00 -0.00 0.00 -0.01 -0.00 -0.01

37 6 -0.04 0.02 -0.01 -0.00 0.00 -0.00 -0.02 0.01 -0.01

38 6 0.01 0.01 -0.01 0.00 0.00 0.00 0.01 0.01 -0.00

39 6 0.03 0.00 -0.02 0.00 -0.00 -0.00 0.01 0.00 -0.01

40 6 -0.00 -0.01 -0.01 0.00 -0.00 -0.00 0.00 -0.00 -0.00

41 6 0.01 -0.03 0.03 0.00 -0.00 0.00 0.00 -0.02 0.02

42 6 -0.01 -0.01 0.02 -0.00 -0.00 0.00 -0.00 -0.00 0.01

43 6 0.03 0.02 -0.01 -0.00 0.00 0.00 0.02 0.02 -0.01

44 6 0.02 -0.02 -0.04 -0.04 0.03 0.04 -0.04 0.04 0.03

45 6 -0.05 0.03 0.02 0.04 -0.03 -0.04 0.01 -0.03 -0.05

46 6 0.00 -0.01 -0.01 -0.00 0.00 0.00 -0.00 -0.00 -0.00

47 6 0.03 -0.05 -0.01 -0.04 0.03 0.04 -0.03 0.01 0.06

48 6 -0.02 0.02 0.05 0.04 -0.03 -0.04 0.04 -0.03 -0.02

49 1 0.07 0.03 -0.00 -0.01 -0.00 -0.00 0.03 0.01 -0.00

50 1 -0.05 0.00 -0.00 -0.00 -0.00 0.00 -0.04 0.00 0.00

51 1 -0.10 -0.01 -0.02 -0.00 0.00 0.00 -0.06 0.01 -0.02

52 1 -0.09 -0.03 -0.03 -0.00 0.00 -0.01 -0.06 -0.00 -0.01

53 1 0.10 0.01 -0.02 -0.01 0.00 -0.00 0.06 -0.01 -0.02

54 1 0.09 0.03 -0.03 -0.01 -0.00 0.01 0.06 0.00 -0.01

55 1 0.05 -0.00 -0.00 -0.00 -0.00 -0.00 0.04 -0.00 0.00

56 1 -0.07 -0.03 -0.00 -0.00 -0.00 0.00 -0.03 -0.01 -0.00

57 1 -0.21 0.19 -0.20 -0.20 0.18 -0.22 0.17 -0.15 0.22

58 1 0.19 -0.12 0.20 0.19 -0.18 0.21 -0.18 0.21 -0.20

59 1 0.04 -0.03 0.02 0.01 -0.01 0.01 0.02 -0.01 0.01

60 1 -0.17 0.19 -0.22 -0.20 0.18 -0.22 0.21 -0.15 0.19

61 1 0.18 -0.15 0.17 0.20 -0.18 0.22 -0.19 0.18 -0.23

62 1 -0.04 -0.03 0.03 0.00 0.00 -0.00 -0.02 -0.02 0.01

63 1 -0.02 0.06 0.00 -0.00 -0.01 0.00 -0.01 0.03 -0.00

64 1 0.02 0.03 0.00 0.00 0.00 -0.00 0.01 0.01 0.01

65 1 -0.00 0.01 -0.04 -0.00 -0.00 0.01 0.00 0.01 -0.02

66 1 -0.02 0.03 -0.04 0.00 0.00 -0.00 -0.02 0.01 -0.01

67 1 0.00 -0.01 -0.04 -0.00 -0.00 -0.00 -0.00 -0.01 -0.02

68 1 0.03 -0.03 -0.04 0.00 0.00 0.00 0.02 -0.01 -0.01

69 1 0.04 0.04 0.03 0.00 0.00 0.00 0.02 0.02 0.01

70 1 0.02 -0.06 0.00 -0.00 -0.01 -0.00 0.01 -0.03 -0.00

71 1 -0.02 -0.03 0.00 0.00 0.00 0.00 -0.01 -0.01 0.01

72 1 -0.16 0.13 0.15 0.21 -0.18 -0.22 0.19 -0.18 -0.23

73 1 0.15 -0.17 -0.20 -0.21 0.18 0.23 -0.21 0.15 0.19

74 1 -0.04 0.03 0.02 0.01 -0.01 -0.01 -0.02 0.01 0.01

75 1 -0.17 0.10 0.18 0.20 -0.18 -0.22 0.18 -0.21 -0.21

76 1 0.19 -0.17 -0.18 -0.20 0.18 0.23 -0.17 0.15 0.22

77 1 0.00 0.07 -0.04 0.00 -0.00 0.00 0.01 0.04 -0.02

78 1 -0.00 -0.07 -0.04 0.00 0.00 0.00 -0.01 -0.04 -0.02

109 110 111

A A A

Frequencies -- 982.7983 982.8708 983.5313

Red. masses -- 1.3612 1.3682 6.7019

Frc consts -- 0.7746 0.7787 3.8197

IR Inten -- 5.4065 0.0080 168.8285

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 -0.05 0.02 -0.00

2 6 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.04 0.04 -0.02

3 7 0.00 -0.00 0.00 -0.00 -0.00 0.00 0.08 0.01 0.00

4 6 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.04 -0.03 0.02

5 6 -0.00 0.00 -0.00 0.00 0.00 -0.00 -0.05 -0.03 0.00

6 6 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.03 -0.15 0.01

7 6 -0.00 0.00 -0.00 -0.00 0.01 -0.00 0.05 -0.06 0.01

8 7 -0.00 -0.00 -0.00 -0.00 -0.01 -0.00 0.23 0.02 0.05

9 6 -0.00 -0.00 -0.00 0.00 0.01 0.00 0.04 0.06 0.01

10 6 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.17 -0.02 -0.04

11 6 0.00 0.00 0.00 0.00 -0.00 0.00 -0.17 -0.01 -0.04

12 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.05 0.14 -0.01

13 6 -0.00 -0.00 0.00 -0.00 -0.01 0.00 0.04 0.06 -0.01

14 6 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.17 -0.02 0.04

15 6 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.17 -0.01 0.04

16 6 -0.00 0.00 0.00 0.00 -0.01 -0.00 0.05 -0.06 -0.01

17 7 -0.00 -0.00 0.00 0.00 0.01 -0.00 0.23 0.02 -0.05

18 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.03 -0.15 -0.01

19 6 -0.00 -0.00 0.00 0.00 -0.00 -0.00 0.04 -0.03 -0.02

20 6 -0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.05 -0.03 -0.00

21 6 -0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.05 0.02 0.00

22 6 0.00 0.00 0.00 -0.00 0.00 -0.00 0.04 0.04 0.02

23 7 0.00 -0.00 -0.00 0.00 0.00 0.00 0.08 0.01 -0.00

24 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.05 0.14 0.01

25 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.07 -0.06 -0.03

26 6 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.03 0.01 0.04

27 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.01 0.06 0.07

28 6 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.02 -0.02

29 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.06 0.01 -0.05

30 6 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.03 -0.02 -0.01

31 6 -0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.01 0.02

32 6 -0.03 -0.04 0.05 -0.03 -0.03 0.05 0.01 -0.07 -0.06

33 6 0.03 0.04 -0.04 0.03 0.04 -0.04 -0.01 -0.01 -0.04

34 6 0.00 -0.00 0.00 0.00 -0.01 0.00 -0.08 0.05 0.02

35 6 -0.03 -0.04 0.04 -0.03 -0.04 0.03 0.01 0.02 0.02

36 6 0.03 0.04 -0.04 0.02 0.03 -0.04 0.07 0.01 0.04

37 6 0.00 -0.00 -0.00 -0.00 0.01 0.00 -0.08 0.05 -0.02

38 6 -0.03 -0.04 -0.04 0.03 0.04 0.04 0.01 0.02 -0.02

39 6 0.03 0.03 0.04 -0.03 -0.03 -0.04 0.07 0.01 -0.04

40 6 -0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.01 -0.02

41 6 -0.03 -0.04 -0.05 0.03 0.03 0.05 0.01 -0.07 0.06

42 6 0.03 0.04 0.04 -0.04 -0.04 -0.04 -0.01 -0.01 0.04

43 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.07 -0.06 0.03

44 6 -0.00 0.00 0.00 0.00 -0.00 0.00 0.03 -0.02 0.01

45 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.06 0.01 0.05

46 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.02 0.02

47 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.01 0.06 -0.07

48 6 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.03 0.01 -0.04

49 1 0.00 0.00 -0.00 0.00 0.00 0.00 -0.09 -0.02 -0.02

50 1 0.00 -0.00 0.00 0.01 -0.00 0.00 -0.09 0.01 0.02

51 1 0.00 0.00 -0.00 -0.00 -0.01 0.01 -0.20 -0.05 -0.06

52 1 0.01 -0.00 0.00 0.00 -0.01 -0.00 -0.20 0.02 -0.06

53 1 0.00 0.00 0.00 0.00 0.01 0.01 -0.20 -0.05 0.06

54 1 0.01 -0.00 -0.00 -0.00 0.01 -0.00 -0.20 0.02 0.06

55 1 0.00 -0.00 -0.00 -0.01 0.00 0.00 -0.09 0.01 -0.02

56 1 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.09 -0.02 0.02

57 1 -0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.03 0.03 0.05

58 1 0.00 -0.01 0.00 0.00 -0.01 0.00 -0.01 0.16 -0.03

59 1 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.08 -0.06 0.05

60 1 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.07 0.04 -0.04

61 1 0.00 -0.00 0.01 -0.00 -0.00 0.00 -0.02 0.05 -0.10

62 1 -0.01 -0.01 0.01 -0.01 -0.01 0.01 0.08 0.07 -0.05

63 1 0.18 0.22 -0.23 0.18 0.22 -0.23 0.05 -0.11 -0.02

64 1 -0.19 -0.22 0.24 -0.18 -0.21 0.24 -0.06 -0.08 0.01

65 1 0.17 0.19 -0.21 0.17 0.19 -0.21 0.02 -0.01 0.05

66 1 -0.17 -0.19 0.21 -0.17 -0.18 0.20 0.04 -0.08 0.10

67 1 0.17 0.19 0.21 -0.17 -0.19 -0.21 0.02 -0.01 -0.05

68 1 -0.17 -0.18 -0.21 0.17 0.19 0.21 0.04 -0.08 -0.10

69 1 -0.01 -0.01 -0.01 0.01 0.01 0.01 0.08 0.07 0.05

70 1 0.18 0.21 0.23 -0.18 -0.22 -0.23 0.05 -0.11 0.02

71 1 -0.18 -0.21 -0.24 0.19 0.22 0.24 -0.06 -0.08 -0.01

72 1 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.02 0.05 0.10

73 1 -0.00 0.00 0.00 0.00 0.00 0.00 0.07 0.04 0.04

74 1 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.08 -0.06 -0.05

75 1 0.00 -0.01 -0.00 -0.00 0.01 0.00 -0.01 0.16 0.03

76 1 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.03 0.03 -0.05

77 1 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.13 0.01 0.00

78 1 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.13 0.01 -0.00

112 113 114

A A A

Frequencies -- 1002.6752 1002.8229 1004.3058

Red. masses -- 1.3116 1.2966 1.3073

Frc consts -- 0.7769 0.7683 0.7769

IR Inten -- 0.3513 0.0960 0.5284

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 -0.01 0.00 -0.00 0.00 -0.00 -0.01 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 -0.02 -0.01 0.00 0.01 0.00 -0.00 0.02 -0.01 0.00

4 6 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00

5 6 0.01 0.02 -0.00 -0.00 -0.01 0.00 -0.00 -0.01 0.00

6 6 0.01 0.00 -0.00 -0.00 -0.00 0.00 -0.01 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 0.01 0.00 0.00

12 6 0.01 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 -0.00 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 -0.01 -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 -0.00 -0.00 0.00 0.00 -0.00

18 6 -0.01 -0.00 -0.00 -0.00 -0.00 -0.00 0.01 -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 -0.01 -0.02 -0.00 -0.00 -0.01 -0.00 0.00 0.01 0.00

21 6 -0.01 0.01 0.00 -0.00 0.00 0.00 0.01 -0.01 -0.00

22 6 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

23 7 0.02 0.01 0.00 0.01 0.00 0.00 -0.02 0.01 0.00

24 6 -0.01 -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 -0.00 -0.00 0.00

26 6 -0.01 0.01 -0.02 0.01 -0.02 0.02 -0.00 0.00 -0.00

27 6 0.04 -0.03 0.03 -0.03 0.03 -0.03 0.00 -0.00 0.01

28 6 -0.04 0.03 -0.04 0.04 -0.03 0.04 -0.00 0.00 -0.00

29 6 0.03 -0.03 0.04 -0.03 0.03 -0.04 0.01 -0.00 0.00

30 6 -0.02 0.02 -0.01 0.02 -0.02 0.01 -0.00 0.00 -0.00

31 6 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.04 0.03 -0.04

32 6 0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.03 -0.03 0.03

33 6 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.01 0.01 -0.02

34 6 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.01 0.00 0.00

35 6 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.02 0.02 -0.01

36 6 -0.00 0.00 -0.01 0.00 0.00 0.00 -0.03 -0.04 0.04

37 6 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.01 -0.00 0.00

38 6 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.02 -0.02 -0.01

39 6 0.00 -0.00 -0.01 0.00 0.00 -0.00 0.03 0.04 0.04

40 6 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.04 -0.03 -0.04

41 6 -0.00 -0.00 -0.00 0.00 -0.00 0.00 0.03 0.03 0.03

42 6 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.01 -0.01 -0.02

43 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

44 6 0.02 -0.02 -0.01 0.02 -0.02 -0.01 0.00 -0.00 -0.00

45 6 -0.03 0.03 0.04 -0.03 0.03 0.04 -0.01 0.00 0.00

46 6 0.04 -0.03 -0.04 0.04 -0.03 -0.04 0.00 -0.00 -0.00

47 6 -0.03 0.03 0.03 -0.04 0.03 0.04 -0.00 0.00 0.01

48 6 0.01 -0.01 -0.02 0.01 -0.02 -0.02 0.00 -0.00 -0.00

49 1 -0.02 -0.03 0.01 0.01 0.01 -0.00 0.01 0.03 -0.01

50 1 -0.02 0.03 -0.01 0.00 -0.01 0.00 0.03 -0.03 0.01

51 1 0.01 0.01 0.00 -0.01 -0.01 -0.00 -0.00 -0.01 -0.00

52 1 -0.01 0.01 -0.00 -0.00 0.00 0.00 0.01 -0.01 0.00

53 1 -0.01 -0.01 0.00 -0.01 -0.01 0.00 0.00 0.01 -0.00

54 1 0.01 -0.01 -0.00 -0.00 -0.00 -0.00 -0.01 0.01 0.00

55 1 0.02 -0.03 -0.01 0.00 -0.01 -0.00 -0.03 0.03 0.01

56 1 0.02 0.03 0.01 0.01 0.01 0.00 -0.01 -0.03 -0.01

57 1 0.12 -0.10 0.12 -0.12 0.11 -0.13 0.02 -0.01 0.02

58 1 -0.20 0.19 -0.24 0.20 -0.19 0.23 -0.02 0.02 -0.02

59 1 0.22 -0.21 0.25 -0.22 0.20 -0.25 0.02 -0.02 0.03

60 1 -0.21 0.18 -0.22 0.20 -0.18 0.22 -0.02 0.02 -0.02

61 1 0.12 -0.09 0.13 -0.12 0.10 -0.12 0.01 -0.01 0.01

62 1 0.02 0.02 -0.02 0.01 0.00 -0.01 -0.19 -0.23 0.25

63 1 -0.01 -0.01 0.02 -0.00 -0.01 0.00 0.16 0.19 -0.21

64 1 0.01 0.01 -0.01 0.00 0.00 -0.00 -0.09 -0.11 0.11

65 1 0.01 0.01 -0.01 0.00 0.00 -0.00 -0.11 -0.12 0.14

66 1 -0.02 -0.02 0.02 -0.00 -0.01 0.01 0.20 0.21 -0.24

67 1 -0.01 -0.01 -0.01 0.00 0.00 0.00 0.11 0.12 0.14

68 1 0.02 0.02 0.02 -0.00 -0.01 -0.01 -0.20 -0.21 -0.24

69 1 -0.02 -0.02 -0.02 0.01 0.00 0.01 0.19 0.23 0.25

70 1 0.01 0.01 0.02 -0.00 -0.01 -0.00 -0.16 -0.19 -0.21

71 1 -0.01 -0.01 -0.01 0.00 0.00 0.00 0.09 0.11 0.11

72 1 -0.11 0.09 0.12 -0.12 0.10 0.13 -0.01 0.01 0.01

73 1 0.20 -0.17 -0.21 0.21 -0.18 -0.22 0.02 -0.02 -0.02

74 1 -0.22 0.20 0.25 -0.22 0.21 0.25 -0.02 0.02 0.03

75 1 0.19 -0.18 -0.23 0.20 -0.19 -0.24 0.02 -0.02 -0.02

76 1 -0.11 0.10 0.12 -0.12 0.11 0.13 -0.02 0.01 0.02

77 1 -0.06 -0.01 0.00 0.02 0.01 -0.00 0.05 -0.00 0.00

78 1 0.06 0.01 0.00 0.02 0.01 0.00 -0.05 0.00 0.00

115 116 117

A A A

Frequencies -- 1004.3684 1011.0084 1011.4763

Red. masses -- 1.2970 5.3828 2.1618

Frc consts -- 0.7709 3.2417 1.3031

IR Inten -- 0.0021 56.3014 0.0027

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.01 0.00 0.00 -0.05 0.01 -0.04 0.08 -0.02

2 6 -0.00 -0.00 0.00 -0.01 -0.02 0.01 -0.03 0.01 0.00

3 7 -0.01 0.00 -0.00 -0.01 0.11 -0.03 0.11 0.01 -0.00

4 6 0.00 0.00 -0.00 0.01 -0.01 0.01 -0.03 -0.01 -0.00

5 6 0.00 0.00 -0.00 0.00 -0.04 0.01 -0.03 -0.09 0.02

6 6 0.00 0.00 -0.00 -0.04 -0.09 -0.01 -0.05 0.03 -0.00

7 6 -0.00 0.00 -0.00 0.03 -0.03 0.01 -0.04 0.03 -0.01

8 7 -0.00 -0.01 -0.00 -0.01 0.21 0.00 -0.00 -0.05 -0.00

9 6 0.00 -0.00 0.00 -0.03 -0.03 -0.01 0.03 0.03 0.01

10 6 -0.00 0.00 -0.00 0.08 -0.02 0.02 -0.02 -0.01 -0.01

11 6 0.00 0.00 0.00 -0.08 -0.03 -0.02 0.03 -0.00 0.01

12 6 0.00 -0.00 0.00 0.06 -0.09 -0.01 -0.04 -0.03 0.00

13 6 0.00 -0.00 -0.00 -0.03 -0.03 0.01 -0.03 -0.03 0.01

14 6 -0.00 0.00 0.00 0.08 -0.02 -0.02 0.02 0.01 -0.01

15 6 0.00 0.00 -0.00 -0.08 -0.03 0.02 -0.03 0.00 0.01

16 6 -0.00 0.00 0.00 0.03 -0.03 -0.01 0.04 -0.03 -0.01

17 7 -0.00 -0.01 0.00 -0.01 0.21 -0.00 0.00 0.05 -0.00

18 6 0.00 0.00 0.00 -0.04 -0.09 0.01 0.05 -0.03 -0.00

19 6 0.00 0.00 0.00 0.01 -0.01 -0.01 0.03 0.01 -0.00

20 6 0.00 0.00 0.00 0.00 -0.04 -0.01 0.03 0.09 0.02

21 6 0.00 -0.01 -0.00 0.00 -0.05 -0.01 0.04 -0.08 -0.02

22 6 -0.00 -0.00 -0.00 -0.01 -0.02 -0.01 0.03 -0.01 0.00

23 7 -0.01 0.00 0.00 -0.01 0.11 0.03 -0.11 -0.01 -0.00

24 6 0.00 -0.00 -0.00 0.06 -0.09 0.01 0.04 0.03 0.00

25 6 0.00 0.00 0.00 -0.06 -0.07 -0.00 -0.00 -0.01 0.01

26 6 0.00 -0.00 -0.00 -0.06 0.00 0.06 -0.01 0.01 -0.01

27 6 0.00 -0.00 -0.00 -0.01 0.06 0.05 0.00 -0.00 0.01

28 6 -0.00 -0.00 -0.00 0.05 0.06 0.00 -0.00 0.01 -0.00

29 6 -0.00 -0.00 0.00 0.06 0.00 -0.05 0.02 -0.00 -0.00

30 6 -0.00 0.00 0.00 0.01 -0.06 -0.06 -0.00 -0.00 -0.02

31 6 -0.04 -0.04 0.04 -0.06 0.05 0.00 0.00 -0.02 0.00

32 6 0.03 0.03 -0.03 -0.00 0.07 0.05 0.00 0.00 -0.01

33 6 -0.01 -0.01 0.02 0.06 0.01 0.06 -0.01 -0.01 0.00

34 6 0.00 0.00 -0.00 0.07 -0.07 -0.00 -0.01 0.01 -0.01

35 6 -0.02 -0.02 0.02 -0.00 -0.06 -0.06 -0.00 0.01 0.02

36 6 0.03 0.04 -0.04 -0.06 -0.00 -0.05 0.02 0.01 0.00

37 6 0.00 0.00 0.00 0.07 -0.07 0.00 0.01 -0.01 -0.01

38 6 -0.02 -0.02 -0.02 -0.00 -0.06 0.06 0.00 -0.01 0.02

39 6 0.03 0.04 0.04 -0.06 -0.00 0.05 -0.02 -0.01 0.00

40 6 -0.04 -0.04 -0.04 -0.06 0.05 -0.00 -0.00 0.02 0.00

41 6 0.03 0.03 0.03 -0.00 0.07 -0.05 -0.00 -0.00 -0.01

42 6 -0.01 -0.01 -0.02 0.06 0.01 -0.06 0.01 0.01 0.00

43 6 0.00 0.00 -0.00 -0.06 -0.07 0.00 0.00 0.01 0.01

44 6 -0.00 0.00 -0.00 0.01 -0.06 0.06 0.00 0.00 -0.02

45 6 -0.00 -0.00 -0.00 0.06 0.00 0.05 -0.02 0.00 -0.00

46 6 -0.00 -0.00 0.00 0.05 0.06 -0.00 0.00 -0.01 -0.00

47 6 0.00 -0.00 0.00 -0.01 0.06 -0.05 -0.00 0.00 0.01

48 6 0.00 -0.00 0.00 -0.06 0.00 -0.06 0.01 -0.01 -0.01

49 1 -0.00 -0.01 0.00 0.05 -0.01 0.01 0.15 0.24 -0.07

50 1 -0.01 0.01 -0.01 -0.06 -0.00 0.01 0.19 -0.23 0.08

51 1 -0.00 -0.00 -0.00 0.23 0.20 0.08 -0.10 -0.13 -0.03

52 1 0.01 -0.01 0.00 -0.26 0.17 -0.08 0.14 -0.12 0.03

53 1 -0.00 -0.00 0.00 0.23 0.20 -0.08 0.10 0.13 -0.03

54 1 0.01 -0.01 -0.00 -0.26 0.17 0.08 -0.14 0.12 0.03

55 1 -0.01 0.01 0.01 -0.06 -0.00 -0.01 -0.19 0.23 0.08

56 1 -0.00 -0.01 -0.00 0.05 -0.01 -0.01 -0.15 -0.24 -0.07

57 1 0.00 -0.00 -0.00 -0.07 0.02 0.06 0.04 -0.03 0.05

58 1 -0.00 -0.00 -0.01 0.01 0.07 0.06 -0.05 0.04 -0.04

59 1 0.00 -0.01 0.00 0.06 0.06 -0.01 0.03 -0.02 0.06

60 1 -0.01 0.00 -0.00 0.07 0.01 -0.05 -0.02 0.05 -0.05

61 1 0.00 0.00 0.00 0.03 -0.05 -0.07 0.03 -0.05 0.04

62 1 0.19 0.23 -0.25 -0.06 0.06 -0.02 0.04 0.02 -0.06

63 1 -0.16 -0.19 0.21 -0.03 0.07 0.06 -0.04 -0.04 0.04

64 1 0.09 0.11 -0.12 0.07 0.03 0.06 0.03 0.03 -0.05

65 1 0.11 0.12 -0.14 -0.02 -0.06 -0.07 0.03 0.05 -0.03

66 1 -0.20 -0.21 0.24 -0.08 -0.00 -0.05 -0.02 -0.05 0.05

67 1 0.11 0.12 0.14 -0.02 -0.06 0.07 -0.03 -0.05 -0.03

68 1 -0.20 -0.21 -0.24 -0.08 -0.00 0.05 0.02 0.05 0.05

69 1 0.19 0.23 0.25 -0.06 0.06 0.02 -0.04 -0.02 -0.06

70 1 -0.16 -0.19 -0.22 -0.03 0.07 -0.06 0.04 0.04 0.04

71 1 0.09 0.11 0.12 0.07 0.03 -0.06 -0.03 -0.03 -0.05

72 1 0.00 0.00 -0.00 0.03 -0.05 0.07 -0.03 0.05 0.04

73 1 -0.01 0.00 0.00 0.07 0.01 0.05 0.02 -0.05 -0.05

74 1 0.00 -0.01 -0.00 0.06 0.06 0.01 -0.03 0.02 0.06

75 1 -0.00 -0.00 0.01 0.01 0.07 -0.06 0.05 -0.04 -0.04

76 1 0.00 -0.00 0.00 -0.07 0.02 -0.06 -0.04 0.03 0.05

77 1 -0.02 0.00 -0.00 -0.02 0.12 -0.03 0.39 0.03 -0.00

78 1 -0.02 0.00 0.00 -0.02 0.12 0.03 -0.39 -0.03 -0.00

118 119 120

A A A

Frequencies -- 1018.5956 1018.6242 1019.3231

Red. masses -- 6.1590 5.0159 6.2162

Frc consts -- 3.7650 3.0664 3.8054

IR Inten -- 0.0075 61.1306 0.0329

Atom AN X Y Z X Y Z X Y Z

1 6 -0.01 0.01 -0.00 -0.02 0.05 -0.01 0.00 0.00 0.00

2 6 -0.01 0.00 0.00 -0.02 0.00 0.00 -0.00 0.00 -0.00

3 7 0.01 0.00 -0.00 0.06 0.00 0.00 0.01 -0.00 0.00

4 6 -0.01 -0.00 0.00 -0.02 -0.00 -0.00 -0.00 0.00 -0.00

5 6 -0.00 -0.01 0.00 -0.01 -0.05 0.01 -0.00 -0.01 0.00

6 6 -0.01 0.00 -0.00 -0.03 0.02 -0.00 0.00 0.02 -0.00

7 6 -0.01 -0.01 -0.00 -0.02 0.02 -0.00 -0.01 0.01 -0.00

8 7 0.00 -0.01 0.00 -0.03 -0.00 -0.01 -0.02 -0.00 -0.01

9 6 0.01 -0.01 0.00 -0.02 -0.02 -0.00 -0.00 -0.01 0.00

10 6 -0.02 0.00 -0.00 0.03 0.00 0.01 0.01 0.00 0.00

11 6 0.01 0.01 0.00 0.03 0.00 0.01 0.02 0.00 0.00

12 6 -0.01 -0.01 0.00 -0.02 -0.03 0.00 -0.01 0.02 -0.00

13 6 -0.01 0.01 0.00 -0.02 -0.02 0.00 0.00 0.01 0.00

14 6 0.02 -0.00 -0.00 0.03 0.00 -0.01 -0.01 -0.00 0.00

15 6 -0.01 -0.01 0.00 0.03 0.00 -0.01 -0.02 -0.00 0.00

16 6 0.01 0.01 -0.00 -0.02 0.02 0.00 0.01 -0.01 -0.00

17 7 -0.00 0.01 0.00 -0.03 -0.00 0.01 0.02 0.00 -0.01

18 6 0.01 -0.00 -0.00 -0.03 0.02 0.00 -0.00 -0.02 -0.00

19 6 0.01 0.00 0.00 -0.02 -0.00 0.00 0.00 -0.00 -0.00

20 6 0.00 0.01 0.00 -0.01 -0.05 -0.01 0.00 0.01 0.00

21 6 0.00 -0.01 -0.00 -0.02 0.05 0.01 -0.00 -0.00 0.00

22 6 0.00 -0.00 0.00 -0.02 0.00 -0.00 0.00 -0.00 -0.00

23 7 -0.01 -0.00 -0.00 0.06 0.00 -0.00 -0.01 0.00 0.00

24 6 0.01 0.01 0.00 -0.02 -0.03 -0.00 0.01 -0.02 -0.00

25 6 -0.00 -0.00 0.00 0.00 -0.01 0.01 0.01 0.00 0.00

26 6 0.17 0.00 -0.15 -0.13 0.00 0.10 -0.13 -0.00 0.11

27 6 -0.00 0.02 0.02 0.00 -0.01 -0.01 0.00 -0.02 -0.02

28 6 -0.14 -0.17 -0.00 0.10 0.13 0.00 0.11 0.13 0.00

29 6 0.02 0.00 -0.02 -0.00 -0.00 0.01 -0.02 -0.00 0.02

30 6 -0.03 0.16 0.15 0.02 -0.12 -0.12 0.02 -0.12 -0.12

31 6 -0.12 0.11 -0.00 0.12 -0.11 -0.00 -0.16 0.15 0.00

32 6 -0.00 -0.01 -0.01 0.00 0.01 0.01 -0.00 -0.03 -0.02

33 6 0.12 0.02 0.11 -0.12 -0.02 -0.10 0.16 0.02 0.15

34 6 -0.00 0.00 -0.00 -0.00 0.01 -0.01 -0.01 0.01 0.00

35 6 -0.00 -0.12 -0.11 -0.00 0.12 0.12 -0.00 -0.16 -0.15

36 6 0.01 0.00 0.02 -0.00 -0.00 -0.01 0.02 0.00 0.03

37 6 0.00 -0.00 -0.00 -0.00 0.01 0.01 0.01 -0.01 0.00

38 6 0.00 0.12 -0.11 -0.00 0.12 -0.12 0.00 0.16 -0.15

39 6 -0.01 -0.00 0.02 -0.00 -0.00 0.01 -0.02 -0.00 0.03

40 6 0.12 -0.11 -0.00 0.12 -0.11 0.00 0.16 -0.15 0.00

41 6 0.00 0.01 -0.01 0.00 0.01 -0.01 0.00 0.03 -0.02

42 6 -0.12 -0.02 0.11 -0.12 -0.02 0.10 -0.16 -0.02 0.15

43 6 0.00 0.00 0.00 0.00 -0.01 -0.01 -0.01 -0.00 0.00

44 6 0.03 -0.16 0.15 0.02 -0.12 0.12 -0.02 0.12 -0.12

45 6 -0.02 -0.00 -0.02 -0.00 -0.00 -0.01 0.02 0.00 0.02

46 6 0.14 0.17 -0.00 0.10 0.13 -0.00 -0.11 -0.13 0.00

47 6 0.00 -0.02 0.02 0.00 -0.01 0.01 -0.00 0.02 -0.02

48 6 -0.17 -0.00 -0.15 -0.12 0.00 -0.10 0.13 0.00 0.11

49 1 0.02 0.03 -0.01 0.10 0.15 -0.05 0.02 0.02 -0.00

50 1 0.03 -0.03 0.01 0.11 -0.13 0.05 0.00 -0.01 0.01

51 1 -0.03 -0.02 -0.02 0.07 0.06 0.02 0.02 0.02 0.00

52 1 0.03 -0.02 0.02 0.07 -0.04 0.02 0.04 -0.03 0.01

53 1 0.03 0.02 -0.02 0.07 0.06 -0.02 -0.02 -0.02 0.00

54 1 -0.03 0.02 0.02 0.08 -0.04 -0.02 -0.05 0.03 0.01

55 1 -0.03 0.03 0.01 0.11 -0.13 -0.05 -0.00 0.01 0.01

56 1 -0.02 -0.03 -0.01 0.10 0.15 0.05 -0.02 -0.02 -0.00

57 1 0.17 -0.02 -0.16 -0.11 0.00 0.14 -0.12 0.01 0.13

58 1 0.00 0.01 0.02 -0.03 0.00 -0.02 -0.01 -0.01 -0.02

59 1 -0.16 -0.17 -0.01 0.12 0.13 0.03 0.12 0.13 0.02

60 1 0.02 -0.01 -0.00 -0.01 0.02 -0.01 -0.02 0.01 0.01

61 1 -0.06 0.17 0.15 0.06 -0.15 -0.10 0.05 -0.13 -0.11

62 1 -0.14 0.10 0.00 0.13 -0.11 -0.03 -0.18 0.14 0.01

63 1 0.00 -0.01 -0.01 -0.02 -0.01 0.02 0.01 -0.01 -0.03

64 1 0.13 0.04 0.11 -0.10 -0.02 -0.14 0.16 0.05 0.16

65 1 -0.03 -0.13 -0.11 0.04 0.15 0.09 -0.04 -0.18 -0.15

66 1 0.01 0.01 0.00 -0.01 -0.03 0.01 0.02 0.01 0.01

67 1 0.03 0.13 -0.12 0.04 0.15 -0.09 0.04 0.18 -0.15

68 1 -0.02 -0.01 0.00 -0.01 -0.03 -0.01 -0.02 -0.01 0.01

69 1 0.14 -0.11 0.00 0.13 -0.10 0.03 0.18 -0.14 0.01

70 1 -0.00 0.01 -0.01 -0.02 -0.01 -0.02 -0.01 0.01 -0.03

71 1 -0.13 -0.04 0.11 -0.10 -0.02 0.14 -0.16 -0.05 0.16

72 1 0.06 -0.17 0.15 0.06 -0.15 0.10 -0.05 0.13 -0.11

73 1 -0.02 0.01 -0.00 -0.01 0.02 0.01 0.02 -0.01 0.01

74 1 0.16 0.17 -0.01 0.12 0.13 -0.03 -0.12 -0.13 0.02

75 1 -0.01 -0.01 0.02 -0.03 0.00 0.02 0.01 0.01 -0.02

76 1 -0.17 0.02 -0.16 -0.10 0.00 -0.14 0.12 -0.01 0.13

77 1 0.05 0.01 -0.00 0.21 0.01 0.00 0.03 -0.00 0.00

78 1 -0.05 -0.01 -0.00 0.21 0.01 -0.00 -0.03 0.00 0.00

121 122 123

A A A

Frequencies -- 1020.1441 1022.4201 1040.6291

Red. masses -- 6.0382 2.6728 4.3980

Frc consts -- 3.7024 1.6462 2.8061

IR Inten -- 63.0697 85.1556 62.0641

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 0.00 0.00 -0.04 0.09 -0.02 0.03 -0.16 0.04

2 6 0.00 0.01 -0.01 -0.03 0.00 0.00 -0.02 0.02 -0.01

3 7 -0.01 -0.04 0.01 0.12 0.01 0.00 -0.01 0.19 -0.05

4 6 0.00 0.01 -0.01 -0.02 -0.01 -0.00 0.01 0.02 -0.01

5 6 -0.00 0.02 -0.00 -0.03 -0.09 0.02 -0.00 -0.17 0.05

6 6 0.03 0.05 0.00 -0.06 0.01 -0.01 -0.07 0.05 -0.01

7 6 -0.02 0.01 -0.00 -0.03 0.02 -0.01 -0.08 0.05 -0.02

8 7 0.01 -0.09 0.00 -0.02 -0.00 -0.01 0.00 -0.06 -0.00

9 6 0.02 0.02 0.00 -0.02 -0.02 -0.01 0.08 0.06 0.02

10 6 -0.04 0.01 -0.01 0.04 0.00 0.01 -0.04 -0.01 -0.01

11 6 0.03 0.02 0.01 0.04 0.00 0.01 0.05 -0.00 0.01

12 6 -0.02 0.05 0.00 -0.07 -0.02 0.01 0.06 0.05 -0.01

13 6 0.02 0.02 -0.00 -0.02 -0.02 0.01 0.08 0.06 -0.02

14 6 -0.04 0.01 0.01 0.04 0.00 -0.01 -0.04 -0.01 0.01

15 6 0.03 0.02 -0.01 0.04 0.00 -0.01 0.05 -0.00 -0.01

16 6 -0.02 0.01 0.00 -0.03 0.02 0.01 -0.08 0.05 0.02

17 7 0.01 -0.09 -0.00 -0.02 -0.00 0.01 0.00 -0.06 0.00

18 6 0.03 0.05 -0.00 -0.06 0.01 0.01 -0.07 0.05 0.01

19 6 0.00 0.01 0.01 -0.02 -0.01 0.00 0.01 0.02 0.01

20 6 -0.00 0.02 0.00 -0.03 -0.09 -0.02 -0.00 -0.17 -0.05

21 6 0.01 0.00 -0.00 -0.04 0.09 0.02 0.03 -0.16 -0.04

22 6 0.00 0.01 0.01 -0.03 0.00 -0.00 -0.02 0.02 0.01

23 7 -0.01 -0.04 -0.01 0.12 0.01 -0.00 -0.01 0.19 0.05

24 6 -0.02 0.05 -0.00 -0.07 -0.02 -0.01 0.06 0.05 0.01

25 6 0.03 0.04 0.00 -0.01 -0.03 0.01 -0.00 -0.01 0.02

26 6 -0.13 -0.00 0.12 0.03 0.00 -0.04 0.01 -0.00 -0.02

27 6 0.01 -0.05 -0.05 -0.00 0.02 0.02 -0.01 0.01 0.02

28 6 0.11 0.13 0.00 -0.03 -0.02 0.00 -0.00 0.01 0.01

29 6 -0.05 -0.00 0.05 0.03 0.00 -0.02 0.03 -0.00 -0.02

30 6 0.02 -0.13 -0.12 -0.01 0.03 0.02 -0.01 -0.00 -0.00

31 6 -0.13 0.11 0.00 -0.04 0.03 -0.00 0.00 0.01 0.01

32 6 -0.00 -0.05 -0.04 -0.00 -0.02 -0.03 0.01 0.01 0.02

33 6 0.13 0.02 0.11 0.04 0.00 0.05 -0.01 -0.00 -0.02

34 6 -0.03 0.03 0.00 -0.02 0.03 -0.01 0.00 -0.01 0.02

35 6 -0.00 -0.13 -0.12 -0.01 -0.04 -0.03 0.01 0.00 -0.00

36 6 0.04 0.01 0.04 0.04 0.01 0.03 -0.02 -0.01 -0.02

37 6 -0.03 0.03 -0.00 -0.02 0.03 0.01 0.00 -0.01 -0.02

38 6 -0.00 -0.13 0.12 -0.01 -0.04 0.03 0.01 0.00 0.00

39 6 0.04 0.01 -0.04 0.04 0.01 -0.03 -0.02 -0.01 0.02

40 6 -0.13 0.11 -0.00 -0.04 0.03 0.00 0.00 0.01 -0.01

41 6 -0.00 -0.05 0.04 -0.00 -0.02 0.03 0.01 0.01 -0.02

42 6 0.13 0.02 -0.11 0.04 0.00 -0.05 -0.01 -0.00 0.02

43 6 0.03 0.04 -0.00 -0.01 -0.03 -0.01 -0.00 -0.01 -0.02

44 6 0.02 -0.13 0.12 -0.01 0.03 -0.02 -0.01 -0.00 0.00

45 6 -0.05 -0.00 -0.05 0.03 0.00 0.02 0.03 -0.00 0.02

46 6 0.11 0.13 -0.00 -0.03 -0.02 -0.00 -0.00 0.01 -0.01

47 6 0.01 -0.05 0.05 -0.00 0.02 -0.02 -0.01 0.01 -0.02

48 6 -0.13 -0.00 -0.12 0.03 0.00 0.04 0.01 -0.00 0.02

49 1 -0.01 -0.01 0.00 0.16 0.26 -0.08 0.13 -0.09 0.01

50 1 -0.03 0.03 -0.01 0.20 -0.24 0.09 -0.11 -0.12 0.02

51 1 -0.13 -0.11 -0.04 0.08 0.05 0.02 -0.20 -0.25 -0.07

52 1 0.12 -0.08 0.03 0.08 -0.04 0.02 0.24 -0.22 0.06

53 1 -0.13 -0.11 0.04 0.08 0.05 -0.02 -0.21 -0.25 0.07

54 1 0.12 -0.08 -0.03 0.08 -0.04 -0.02 0.24 -0.22 -0.06

55 1 -0.03 0.03 0.01 0.20 -0.24 -0.09 -0.11 -0.12 -0.02

56 1 -0.01 -0.01 -0.00 0.16 0.26 0.08 0.13 -0.09 -0.01

57 1 -0.13 0.02 0.13 0.06 -0.02 -0.01 0.04 -0.03 0.01

58 1 0.00 -0.04 -0.05 -0.03 0.02 0.02 -0.06 -0.01 0.02

59 1 0.12 0.13 0.02 -0.03 -0.02 0.02 -0.01 0.02 0.04

60 1 -0.05 0.01 0.04 0.02 0.02 -0.03 0.02 0.00 -0.04

61 1 0.05 -0.13 -0.12 0.00 -0.00 0.05 -0.02 -0.05 0.04

62 1 -0.14 0.11 0.02 -0.04 0.03 -0.03 0.01 0.02 0.04

63 1 0.01 -0.04 -0.05 -0.03 -0.03 -0.02 0.06 0.00 0.02

64 1 0.12 0.04 0.13 0.07 0.04 0.01 -0.03 -0.04 0.01

65 1 -0.03 -0.14 -0.12 0.00 -0.01 -0.06 0.03 -0.04 0.04

66 1 0.05 0.02 0.03 0.03 -0.02 0.04 -0.02 -0.00 -0.04

67 1 -0.03 -0.14 0.12 0.00 -0.01 0.06 0.03 -0.04 -0.04

68 1 0.05 0.02 -0.03 0.03 -0.02 -0.04 -0.02 -0.00 0.04

69 1 -0.14 0.11 -0.02 -0.04 0.03 0.03 0.01 0.02 -0.04

70 1 0.01 -0.04 0.05 -0.03 -0.03 0.02 0.06 0.00 -0.02

71 1 0.12 0.04 -0.13 0.07 0.04 -0.01 -0.03 -0.04 -0.01

72 1 0.05 -0.13 0.12 0.00 -0.00 -0.05 -0.02 -0.05 -0.04

73 1 -0.05 0.01 -0.04 0.02 0.02 0.04 0.02 0.00 0.04

74 1 0.12 0.13 -0.02 -0.03 -0.02 -0.02 -0.01 0.02 -0.04

75 1 0.00 -0.04 0.05 -0.03 0.02 -0.02 -0.06 -0.01 -0.02

76 1 -0.13 0.02 -0.13 0.06 -0.02 0.01 0.04 -0.03 -0.01

77 1 -0.03 -0.05 0.01 0.42 0.03 -0.00 -0.01 0.20 -0.08

78 1 -0.03 -0.05 -0.01 0.42 0.03 0.00 -0.01 0.20 0.08

124 125 126

A A A

Frequencies -- 1047.8613 1050.6987 1053.8769

Red. masses -- 3.6656 2.5100 2.0490

Frc consts -- 2.3714 1.6326 1.3408

IR Inten -- 2.4581 0.0111 40.9607

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 0.13 -0.04 -0.00 0.01 -0.00 -0.00 0.02 -0.00

2 6 0.01 -0.02 0.00 0.01 0.00 0.00 -0.01 0.00 -0.00

3 7 0.02 -0.15 0.04 -0.00 -0.01 0.00 0.02 -0.01 0.00

4 6 0.00 -0.01 0.00 0.01 -0.00 -0.00 -0.01 -0.00 -0.00

5 6 0.01 0.13 -0.03 0.00 0.01 -0.00 -0.01 -0.00 0.00

6 6 0.06 -0.04 0.01 -0.01 0.02 0.00 -0.01 -0.01 0.00

7 6 0.03 -0.06 0.01 -0.02 -0.05 -0.00 -0.00 -0.01 0.00

8 7 0.04 -0.00 0.01 -0.00 0.01 -0.00 0.02 -0.01 0.00

9 6 0.04 0.06 0.01 0.03 -0.04 0.01 -0.00 0.01 0.00

10 6 -0.06 -0.01 -0.01 -0.05 0.02 -0.01 -0.00 -0.00 -0.00

11 6 -0.04 0.01 -0.01 0.05 0.03 0.01 -0.00 0.00 -0.00

12 6 -0.06 -0.06 0.01 -0.01 -0.02 0.00 -0.03 0.02 0.00

13 6 -0.04 -0.06 0.01 -0.03 0.04 0.01 -0.00 0.01 -0.00

14 6 0.06 0.01 -0.01 0.05 -0.02 -0.01 -0.00 -0.00 0.00

15 6 0.04 -0.01 -0.01 -0.05 -0.03 0.01 -0.00 0.00 0.00

16 6 -0.03 0.06 0.01 0.02 0.05 -0.00 -0.00 -0.01 -0.00

17 7 -0.04 0.00 0.01 0.00 -0.01 -0.00 0.02 -0.01 -0.00

18 6 -0.06 0.04 0.01 0.01 -0.02 0.00 -0.01 -0.01 -0.00

19 6 -0.00 0.01 0.00 -0.01 0.00 -0.00 -0.01 -0.00 0.00

20 6 -0.01 -0.13 -0.03 -0.00 -0.01 -0.00 -0.01 -0.00 -0.00

21 6 0.03 -0.13 -0.04 0.00 -0.01 -0.00 -0.00 0.02 0.00

22 6 -0.01 0.02 0.00 -0.01 -0.00 0.00 -0.01 0.00 0.00

23 7 -0.02 0.15 0.04 0.00 0.01 0.00 0.02 -0.01 -0.00

24 6 0.06 0.06 0.01 0.01 0.02 0.00 -0.03 0.02 -0.00

25 6 0.01 0.02 -0.02 0.01 0.02 0.00 -0.00 0.00 -0.00

26 6 -0.01 0.01 0.03 -0.01 0.03 0.03 -0.00 0.02 0.02

27 6 0.02 -0.02 -0.04 0.03 -0.05 -0.07 0.02 -0.03 -0.04

28 6 -0.01 -0.03 -0.01 -0.03 -0.04 0.00 -0.03 -0.03 -0.00

29 6 -0.04 0.01 0.05 -0.05 0.02 0.06 -0.03 0.02 0.04

30 6 0.02 0.00 -0.00 0.03 0.00 -0.03 0.02 0.00 -0.02

31 6 0.02 -0.03 -0.01 -0.05 0.04 -0.00 -0.07 0.06 -0.00

32 6 -0.02 -0.03 -0.04 0.03 0.06 0.08 0.04 0.05 0.08

33 6 0.01 0.01 0.03 0.00 -0.04 -0.03 0.00 -0.04 -0.03

34 6 -0.01 0.02 -0.02 0.01 -0.01 -0.00 -0.01 0.01 -0.00

35 6 -0.02 0.00 -0.01 0.04 0.01 0.03 0.04 0.00 0.03

36 6 0.05 0.02 0.05 -0.06 -0.04 -0.08 -0.05 -0.05 -0.08

37 6 0.01 -0.02 -0.02 -0.01 0.01 -0.00 -0.01 0.01 0.00

38 6 0.02 -0.00 -0.01 -0.04 -0.01 0.03 0.04 0.00 -0.03

39 6 -0.05 -0.02 0.05 0.06 0.04 -0.08 -0.05 -0.05 0.08

40 6 -0.02 0.03 -0.01 0.05 -0.04 -0.00 -0.07 0.06 0.00

41 6 0.02 0.03 -0.04 -0.03 -0.06 0.08 0.04 0.05 -0.08

42 6 -0.01 -0.01 0.03 -0.00 0.04 -0.03 0.00 -0.04 0.03

43 6 -0.01 -0.02 -0.02 -0.01 -0.02 0.00 -0.00 0.00 0.00

44 6 -0.02 -0.00 -0.00 -0.03 -0.00 -0.03 0.02 0.00 0.02

45 6 0.04 -0.01 0.05 0.05 -0.02 0.06 -0.03 0.02 -0.04

46 6 0.01 0.03 -0.01 0.03 0.04 0.00 -0.03 -0.03 0.00

47 6 -0.02 0.02 -0.04 -0.03 0.05 -0.07 0.02 -0.03 0.04

48 6 0.01 -0.01 0.03 0.01 -0.03 0.03 -0.00 0.02 -0.02

49 1 -0.09 0.10 -0.02 0.00 0.01 -0.01 0.03 0.05 -0.01

50 1 0.10 0.09 -0.01 0.01 0.00 0.00 0.02 -0.02 0.01

51 1 -0.21 -0.24 -0.07 -0.11 -0.06 -0.04 -0.03 -0.04 -0.01

52 1 -0.19 0.18 -0.05 0.10 -0.03 0.03 -0.03 0.03 -0.01

53 1 0.21 0.24 -0.07 0.11 0.06 -0.04 -0.03 -0.04 0.01

54 1 0.19 -0.18 -0.05 -0.10 0.03 0.03 -0.03 0.03 0.01

55 1 -0.10 -0.09 -0.01 -0.01 -0.00 0.00 0.02 -0.02 -0.01

56 1 0.09 -0.10 -0.02 -0.00 -0.01 -0.01 0.03 0.05 0.01

57 1 -0.02 0.08 0.02 0.04 0.14 0.08 0.03 0.11 0.06

58 1 0.12 0.02 -0.07 0.18 0.02 -0.13 0.13 0.03 -0.09

59 1 -0.00 -0.04 -0.04 -0.05 -0.04 -0.00 -0.03 -0.03 -0.00

60 1 -0.02 0.06 0.09 0.00 0.16 0.14 0.01 0.13 0.10

61 1 0.07 0.08 -0.07 0.13 0.07 -0.08 0.10 0.05 -0.06

62 1 0.01 -0.05 -0.04 -0.07 0.04 -0.00 -0.08 0.06 -0.00

63 1 -0.15 0.01 -0.09 0.22 -0.00 0.16 0.26 -0.03 0.18

64 1 0.00 0.10 0.03 0.08 -0.17 -0.11 0.10 -0.21 -0.12

65 1 -0.10 0.07 -0.08 0.17 -0.06 0.10 0.21 -0.07 0.12

66 1 0.01 0.08 0.10 0.04 -0.21 -0.18 0.06 -0.26 -0.19

67 1 0.10 -0.07 -0.08 -0.17 0.06 0.10 0.21 -0.07 -0.12

68 1 -0.01 -0.08 0.10 -0.04 0.21 -0.18 0.06 -0.26 0.19

69 1 -0.01 0.05 -0.04 0.07 -0.04 -0.00 -0.08 0.06 0.00

70 1 0.15 -0.01 -0.09 -0.22 0.00 0.16 0.26 -0.03 -0.18

71 1 -0.00 -0.10 0.03 -0.08 0.17 -0.11 0.10 -0.21 0.12

72 1 -0.07 -0.08 -0.07 -0.13 -0.07 -0.08 0.10 0.05 0.06

73 1 0.02 -0.06 0.09 -0.00 -0.16 0.14 0.01 0.13 -0.10

74 1 0.00 0.04 -0.04 0.05 0.04 -0.00 -0.03 -0.03 0.00

75 1 -0.12 -0.02 -0.07 -0.18 -0.02 -0.13 0.13 0.03 0.09

76 1 0.02 -0.08 0.02 -0.04 -0.14 0.08 0.03 0.11 -0.06

77 1 -0.00 -0.16 0.07 -0.03 -0.01 0.00 0.09 -0.01 0.00

78 1 0.00 0.16 0.07 0.03 0.01 0.00 0.09 -0.01 -0.00

127 128 129

A A A

Frequencies -- 1054.9166 1055.5739 1066.9669

Red. masses -- 2.2999 2.0626 2.5641

Frc consts -- 1.5080 1.3540 1.7198

IR Inten -- 0.9900 8.3833 0.0166

Atom AN X Y Z X Y Z X Y Z

1 6 -0.01 0.05 -0.01 -0.00 -0.02 0.00 0.00 -0.01 0.00

2 6 -0.01 -0.00 0.00 0.00 -0.00 0.00 0.05 0.01 0.00

3 7 0.01 -0.07 0.02 0.00 0.04 -0.01 -0.03 0.01 -0.00

4 6 0.01 -0.00 0.00 -0.01 -0.00 0.00 0.05 -0.00 -0.00

5 6 -0.00 0.05 -0.01 0.00 -0.02 0.01 -0.00 -0.01 0.00

6 6 0.04 0.00 0.01 -0.03 -0.02 -0.00 -0.00 0.07 -0.00

7 6 0.02 -0.01 0.00 -0.00 -0.01 -0.00 -0.08 -0.07 -0.02

8 7 -0.00 -0.00 -0.00 0.00 0.03 0.00 -0.00 -0.02 -0.00

9 6 0.01 0.02 0.00 -0.00 -0.00 0.00 0.08 -0.06 0.01

10 6 -0.01 -0.00 -0.00 0.00 -0.00 0.00 -0.10 0.04 -0.02

11 6 -0.02 -0.00 -0.00 -0.00 -0.00 -0.00 0.09 0.05 0.02

12 6 -0.04 -0.00 0.00 0.02 -0.01 -0.00 0.01 -0.07 -0.00

13 6 -0.01 -0.02 0.00 -0.00 -0.00 -0.00 -0.08 0.06 0.01

14 6 0.01 0.00 -0.00 0.00 -0.00 -0.00 0.10 -0.04 -0.02

15 6 0.02 0.00 -0.00 -0.00 -0.00 0.00 -0.09 -0.05 0.02

16 6 -0.02 0.01 0.00 -0.00 -0.01 0.00 0.08 0.07 -0.02

17 7 0.00 0.00 -0.00 0.00 0.03 -0.00 0.00 0.02 -0.00

18 6 -0.04 -0.00 0.01 -0.03 -0.02 0.00 0.00 -0.07 -0.00

19 6 -0.01 0.00 0.00 -0.01 -0.00 -0.00 -0.05 0.00 -0.00

20 6 0.00 -0.05 -0.01 0.00 -0.02 -0.01 0.00 0.01 0.00

21 6 0.01 -0.05 -0.01 -0.00 -0.02 -0.00 -0.00 0.01 0.00

22 6 0.01 0.00 0.00 0.00 -0.00 -0.00 -0.05 -0.01 0.00

23 7 -0.01 0.07 0.02 0.00 0.04 0.01 0.03 -0.01 -0.00

24 6 0.04 0.00 0.00 0.02 -0.01 0.00 -0.01 0.07 -0.00

25 6 0.00 0.00 -0.01 -0.01 -0.01 0.00 0.03 0.03 0.00

26 6 0.00 -0.04 -0.03 -0.00 0.04 0.03 0.00 -0.01 -0.01

27 6 -0.04 0.04 0.07 0.05 -0.04 -0.08 -0.02 -0.00 0.01

28 6 0.05 0.05 -0.00 -0.06 -0.07 -0.00 0.02 0.03 0.00

29 6 0.05 -0.03 -0.07 -0.05 0.04 0.08 0.00 -0.02 -0.02

30 6 -0.03 0.00 0.03 0.04 0.00 -0.04 -0.02 -0.00 0.01

31 6 -0.05 0.04 -0.00 0.03 -0.03 0.00 0.03 -0.03 -0.00

32 6 0.03 0.04 0.05 -0.02 -0.02 -0.04 -0.02 0.00 -0.01

33 6 0.01 -0.03 -0.02 -0.00 0.02 0.02 -0.00 0.02 0.01

34 6 -0.01 0.01 -0.01 0.01 -0.01 0.00 0.03 -0.03 -0.00

35 6 0.03 0.00 0.03 -0.02 -0.00 -0.02 -0.02 -0.00 -0.01

36 6 -0.03 -0.03 -0.05 0.02 0.02 0.04 -0.00 0.02 0.02

37 6 0.01 -0.01 -0.01 0.01 -0.01 -0.00 -0.03 0.03 -0.00

38 6 -0.03 -0.00 0.03 -0.02 -0.00 0.02 0.02 0.00 -0.01

39 6 0.03 0.03 -0.05 0.02 0.02 -0.04 0.00 -0.02 0.02

40 6 0.05 -0.04 -0.00 0.03 -0.03 -0.00 -0.03 0.03 -0.00

41 6 -0.03 -0.04 0.05 -0.02 -0.02 0.04 0.02 -0.00 -0.01

42 6 -0.01 0.03 -0.02 -0.00 0.02 -0.02 0.00 -0.02 0.01

43 6 -0.00 -0.00 -0.01 -0.01 -0.01 -0.00 -0.03 -0.03 0.00

44 6 0.03 -0.00 0.03 0.04 0.00 0.04 0.02 0.00 0.01

45 6 -0.05 0.03 -0.07 -0.05 0.04 -0.08 -0.00 0.02 -0.02

46 6 -0.05 -0.05 -0.00 -0.06 -0.07 0.00 -0.02 -0.03 0.00

47 6 0.04 -0.04 0.07 0.05 -0.04 0.08 0.02 0.00 0.01

48 6 -0.00 0.04 -0.03 -0.00 0.04 -0.03 -0.00 0.01 -0.01

49 1 0.00 0.07 -0.02 -0.02 -0.03 0.01 -0.03 -0.04 0.01

50 1 -0.01 0.06 -0.02 0.04 -0.05 0.02 -0.05 0.02 -0.01

51 1 -0.05 -0.05 -0.01 0.00 -0.00 0.00 -0.22 -0.15 -0.07

52 1 -0.05 0.04 -0.01 -0.03 0.02 -0.01 0.27 -0.15 0.08

53 1 0.05 0.05 -0.01 0.00 -0.00 -0.00 0.22 0.15 -0.07

54 1 0.05 -0.04 -0.01 -0.03 0.02 0.01 -0.27 0.15 0.08

55 1 0.01 -0.06 -0.02 0.04 -0.05 -0.02 0.05 -0.02 -0.01

56 1 -0.00 -0.07 -0.02 -0.02 -0.03 -0.01 0.03 0.04 0.01

57 1 -0.07 -0.19 -0.12 0.07 0.22 0.13 -0.03 -0.10 -0.05

58 1 -0.22 -0.05 0.15 0.26 0.07 -0.17 -0.11 -0.06 0.05

59 1 0.07 0.05 -0.01 -0.07 -0.07 0.00 0.01 0.04 0.01

60 1 -0.03 -0.23 -0.17 0.03 0.26 0.19 -0.03 -0.12 -0.06

61 1 -0.17 -0.08 0.09 0.21 0.10 -0.11 -0.10 -0.05 0.05

62 1 -0.06 0.03 -0.02 0.04 -0.03 0.01 0.03 -0.03 0.00

63 1 0.17 -0.02 0.12 -0.13 0.02 -0.09 -0.12 0.04 -0.06

64 1 0.08 -0.14 -0.09 -0.06 0.11 0.06 -0.05 0.10 0.06

65 1 0.14 -0.03 0.07 -0.11 0.03 -0.06 -0.10 0.03 -0.05

66 1 0.05 -0.18 -0.12 -0.04 0.13 0.09 -0.05 0.13 0.06

67 1 -0.14 0.03 0.07 -0.11 0.03 0.06 0.10 -0.03 -0.05

68 1 -0.05 0.18 -0.12 -0.04 0.13 -0.09 0.05 -0.13 0.06

69 1 0.06 -0.03 -0.02 0.04 -0.03 -0.01 -0.03 0.03 0.00

70 1 -0.17 0.02 0.12 -0.13 0.02 0.09 0.12 -0.04 -0.06

71 1 -0.08 0.14 -0.09 -0.06 0.11 -0.06 0.05 -0.10 0.06

72 1 0.17 0.08 0.09 0.21 0.10 0.11 0.10 0.05 0.05

73 1 0.03 0.23 -0.17 0.03 0.26 -0.19 0.03 0.12 -0.06

74 1 -0.07 -0.05 -0.01 -0.07 -0.07 -0.00 -0.01 -0.04 0.01

75 1 0.22 0.05 0.15 0.26 0.07 0.17 0.11 0.06 0.05

76 1 0.07 0.19 -0.12 0.07 0.22 -0.13 0.03 0.10 -0.05

77 1 -0.00 -0.08 0.03 0.03 0.04 -0.01 -0.33 -0.01 -0.00

78 1 0.00 0.08 0.03 0.03 0.04 0.01 0.33 0.01 -0.00

130 131 132

A A A

Frequencies -- 1076.4175 1082.1488 1099.7239

Red. masses -- 1.2158 1.2066 1.1470

Frc consts -- 0.8300 0.8325 0.8173

IR Inten -- 371.4714 7.2872 50.9361

Atom AN X Y Z X Y Z X Y Z

1 6 -0.06 -0.01 0.00 0.06 0.00 -0.00 -0.00 -0.00 0.00

2 6 0.01 0.01 -0.00 -0.01 -0.00 0.00 0.01 0.01 -0.00

3 7 -0.00 0.03 -0.01 0.00 -0.03 0.01 0.00 0.00 -0.00

4 6 -0.01 0.00 -0.00 0.01 0.00 0.00 0.01 -0.01 0.00

5 6 0.06 0.00 0.00 -0.06 -0.00 0.00 -0.00 0.00 -0.00

6 6 0.01 0.00 0.00 -0.01 0.00 -0.00 0.00 -0.02 0.00

7 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.01 -0.00

8 7 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.02 -0.00 -0.00

9 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.01 -0.00

10 6 0.00 0.00 0.00 0.01 -0.00 0.00 -0.02 0.03 -0.00

11 6 -0.00 0.00 -0.00 0.01 0.00 0.00 -0.01 -0.03 -0.00

12 6 -0.01 -0.00 0.00 0.01 0.00 -0.00 0.00 0.02 -0.00

13 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.01 0.00

14 6 0.00 0.00 -0.00 -0.01 0.00 0.00 -0.02 0.03 0.00

15 6 -0.00 0.00 0.00 -0.01 -0.00 0.00 -0.01 -0.03 0.00

16 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.01 0.00

17 7 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.02 -0.00 0.00

18 6 0.01 0.00 -0.00 0.01 -0.00 -0.00 0.00 -0.02 -0.00

19 6 -0.01 0.00 0.00 -0.01 -0.00 0.00 0.01 -0.01 -0.00

20 6 0.06 0.00 -0.00 0.06 0.00 0.00 -0.00 0.00 0.00

21 6 -0.06 -0.01 -0.00 -0.06 -0.00 -0.00 -0.00 -0.00 -0.00

22 6 0.01 0.01 0.00 0.01 0.00 0.00 0.01 0.01 0.00

23 7 -0.00 0.03 0.01 -0.00 0.03 0.01 0.00 0.00 0.00

24 6 -0.01 -0.00 -0.00 -0.01 -0.00 -0.00 0.00 0.02 0.00

25 6 0.00 0.01 -0.00 -0.00 -0.01 0.00 -0.01 -0.01 -0.01

26 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.01 -0.00 0.01

27 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.01 0.00

28 6 0.01 0.01 -0.00 -0.01 -0.00 0.00 -0.00 -0.01 -0.01

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 0.01 0.00

31 6 -0.01 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.01 0.01

32 6 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.01 -0.01 -0.00

33 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.01 0.00 -0.01

34 6 -0.00 0.01 -0.00 0.00 -0.00 0.00 -0.01 0.01 0.01

35 6 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.01 -0.01 -0.00

36 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00

37 6 -0.00 0.01 0.00 -0.00 0.00 0.00 -0.01 0.01 -0.01

38 6 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.01 -0.01 0.00

39 6 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00

40 6 -0.01 0.00 0.00 -0.00 0.00 0.00 -0.00 0.01 -0.01

41 6 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.01 -0.01 0.00

42 6 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.01 0.00 0.01

43 6 0.00 0.01 0.00 0.00 0.01 0.00 -0.01 -0.01 0.01

44 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.01 -0.00

45 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00

46 6 0.01 0.01 0.00 0.01 0.00 0.00 -0.00 -0.01 0.01

47 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.01 -0.00

48 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.01 -0.00 -0.01

49 1 -0.40 -0.28 0.08 0.40 0.28 -0.08 -0.04 -0.04 0.01

50 1 0.43 -0.22 0.09 -0.43 0.22 -0.09 -0.04 0.03 -0.01

51 1 0.01 0.01 0.00 0.01 0.01 0.01 0.23 0.42 0.08

52 1 -0.01 0.01 -0.00 0.02 -0.01 0.01 0.28 -0.38 0.07

53 1 0.01 0.01 -0.00 -0.01 -0.01 0.01 0.23 0.42 -0.08

54 1 -0.01 0.01 0.00 -0.02 0.01 0.01 0.28 -0.38 -0.07

55 1 0.43 -0.22 -0.09 0.43 -0.22 -0.09 -0.04 0.03 0.01

56 1 -0.40 -0.28 -0.08 -0.40 -0.28 -0.08 -0.04 -0.04 -0.01

57 1 -0.01 -0.01 -0.01 0.01 0.01 0.01 -0.02 -0.01 -0.00

58 1 -0.02 -0.01 0.01 0.02 0.01 -0.01 0.05 0.03 -0.01

59 1 0.01 0.01 0.00 -0.01 -0.00 0.00 0.02 -0.03 -0.04

60 1 -0.01 -0.02 -0.01 0.01 0.02 0.01 -0.00 0.01 0.01

61 1 -0.02 -0.01 0.00 0.02 0.00 -0.00 0.04 0.04 -0.02

62 1 -0.01 0.00 -0.00 0.01 -0.00 0.00 0.02 0.03 0.04

63 1 0.02 -0.01 0.01 -0.02 0.00 -0.01 0.05 -0.03 0.01

64 1 0.01 -0.01 -0.01 -0.01 0.01 0.01 -0.02 0.01 0.00

65 1 0.02 -0.00 0.01 -0.01 0.00 -0.00 0.05 -0.04 0.02

66 1 0.01 -0.02 -0.01 -0.01 0.02 0.01 -0.00 -0.00 -0.01

67 1 0.02 -0.00 -0.01 0.01 -0.00 -0.00 0.05 -0.04 -0.02

68 1 0.01 -0.02 0.01 0.01 -0.02 0.01 -0.00 -0.00 0.01

69 1 -0.01 0.00 0.00 -0.01 0.00 0.00 0.02 0.03 -0.04

70 1 0.02 -0.01 -0.01 0.02 -0.00 -0.01 0.05 -0.03 -0.01

71 1 0.01 -0.01 0.01 0.01 -0.01 0.01 -0.02 0.01 -0.00

72 1 -0.02 -0.01 -0.00 -0.02 -0.00 -0.00 0.04 0.04 0.02

73 1 -0.01 -0.02 0.01 -0.01 -0.02 0.01 -0.00 0.01 -0.01

74 1 0.01 0.01 -0.00 0.01 0.00 0.00 0.02 -0.03 0.04

75 1 -0.02 -0.01 -0.01 -0.02 -0.01 -0.01 0.05 0.03 0.01

76 1 -0.01 -0.01 0.01 -0.01 -0.01 0.01 -0.02 -0.01 0.00

77 1 -0.00 0.03 -0.01 0.00 -0.04 0.01 -0.05 -0.00 -0.00

78 1 -0.00 0.03 0.01 -0.00 0.04 0.01 -0.05 -0.00 0.00

133 134 135

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Frequencies -- 1102.3379 1104.1028 1104.1041

Red. masses -- 1.3647 1.5892 1.5884

Frc consts -- 0.9770 1.1414 1.1409

IR Inten -- 9.4159 10.2968 5.9224

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.01 0.00 -0.00 0.01 -0.00 -0.00 0.00 -0.00

2 6 0.00 0.00 -0.00 -0.01 -0.01 0.00 -0.00 0.00 -0.00

3 7 -0.00 0.01 -0.00 0.00 -0.01 0.00 -0.00 -0.00 0.00

4 6 -0.00 0.00 -0.00 -0.01 0.00 -0.00 -0.00 0.00 -0.00

5 6 -0.00 -0.01 0.00 0.00 0.00 -0.00 0.00 0.00 0.00

6 6 -0.01 0.01 -0.01 0.00 0.00 0.01 -0.00 -0.00 0.01

7 6 -0.00 -0.01 0.00 0.00 0.00 0.00 -0.01 0.00 -0.00

8 7 0.02 0.00 0.00 0.00 -0.00 -0.00 -0.01 0.00 -0.00

9 6 -0.00 0.01 0.00 -0.01 -0.00 -0.00 0.01 0.01 0.01

10 6 0.01 -0.02 0.00 0.00 -0.00 0.00 -0.01 0.01 -0.00

11 6 0.01 0.03 0.00 -0.00 0.00 0.00 -0.00 -0.01 0.00

12 6 0.00 0.02 -0.01 -0.01 -0.01 -0.02 0.00 0.00 0.00

13 6 0.00 -0.01 0.00 -0.01 -0.01 0.01 0.00 0.00 -0.00

14 6 -0.01 0.02 0.00 0.01 -0.01 -0.00 -0.00 -0.00 0.00

15 6 -0.01 -0.03 0.00 0.00 0.01 0.00 0.00 0.00 0.00

16 6 0.00 0.01 0.00 0.01 -0.00 -0.00 -0.00 -0.00 -0.00

17 7 -0.02 -0.00 0.00 0.01 -0.00 -0.00 0.00 0.00 -0.00

18 6 0.01 -0.01 -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 -0.00 0.01 -0.00 -0.00

20 6 0.00 0.01 0.00 0.00 0.00 0.00 -0.00 -0.00 0.00

21 6 -0.00 0.01 0.00 -0.00 0.00 0.00 0.00 -0.01 -0.00

22 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.01 0.01 0.00

23 7 0.00 -0.01 -0.00 0.00 -0.00 -0.00 -0.00 0.01 0.00

24 6 -0.00 -0.02 -0.01 -0.00 -0.00 0.01 0.01 0.01 -0.01

25 6 -0.00 0.01 0.02 0.01 -0.00 -0.01 0.01 -0.02 -0.02

26 6 0.02 0.01 -0.01 -0.02 -0.02 0.01 -0.04 -0.03 0.02

27 6 -0.00 -0.02 -0.01 0.00 0.02 0.01 0.00 0.03 0.02

28 6 -0.01 0.01 0.02 0.01 -0.01 -0.02 0.02 -0.02 -0.03

29 6 0.02 0.00 -0.01 -0.02 -0.01 0.01 -0.03 -0.01 0.02

30 6 -0.01 -0.03 -0.01 0.01 0.03 0.01 0.02 0.05 0.02

31 6 0.01 0.02 0.03 0.03 0.04 0.06 -0.00 -0.00 -0.00

32 6 0.01 -0.03 -0.02 0.01 -0.05 -0.04 -0.00 0.00 0.00

33 6 -0.04 0.02 -0.02 -0.08 0.04 -0.03 0.01 -0.00 0.00

34 6 0.01 0.02 0.02 0.03 0.03 0.04 -0.00 -0.00 -0.00

35 6 0.02 -0.04 -0.02 0.05 -0.08 -0.03 -0.00 0.01 0.00

36 6 -0.03 0.00 -0.02 -0.06 0.01 -0.04 0.00 -0.00 0.00

37 6 -0.01 -0.02 0.02 0.01 0.01 -0.01 -0.03 -0.02 0.03

38 6 -0.02 0.04 -0.02 0.02 -0.03 0.01 -0.05 0.07 -0.03

39 6 0.03 -0.00 -0.02 -0.02 0.00 0.01 0.05 -0.01 -0.04

40 6 -0.01 -0.02 0.03 0.01 0.01 -0.02 -0.03 -0.03 0.05

41 6 -0.01 0.03 -0.02 0.00 -0.02 0.01 -0.01 0.05 -0.03

42 6 0.04 -0.02 -0.02 -0.03 0.01 0.01 0.08 -0.04 -0.02

43 6 0.00 -0.01 0.02 -0.01 0.01 -0.02 -0.02 0.01 -0.02

44 6 0.01 0.03 -0.01 -0.02 -0.04 0.01 -0.02 -0.04 0.01

45 6 -0.02 -0.00 -0.01 0.02 0.01 0.02 0.03 0.01 0.02

46 6 0.01 -0.01 0.02 -0.02 0.02 -0.03 -0.02 0.01 -0.03

47 6 0.00 0.02 -0.01 -0.00 -0.03 0.02 -0.00 -0.02 0.02

48 6 -0.02 -0.01 -0.01 0.04 0.02 0.01 0.04 0.02 0.01

49 1 0.01 -0.00 0.00 0.03 0.04 -0.01 -0.00 -0.00 0.00

50 1 -0.01 -0.01 0.00 0.04 -0.02 0.01 0.00 -0.00 -0.00

51 1 -0.17 -0.32 -0.06 0.00 -0.00 0.00 0.03 0.07 0.01

52 1 -0.21 0.29 -0.05 -0.01 0.02 -0.00 0.09 -0.12 0.02

53 1 0.17 0.32 -0.06 -0.03 -0.07 0.01 -0.01 -0.02 0.00

54 1 0.21 -0.29 -0.05 -0.09 0.12 0.02 -0.01 0.02 0.00

55 1 0.01 0.01 0.00 0.01 -0.00 -0.00 -0.04 0.02 0.00

56 1 -0.01 0.00 0.00 0.01 0.01 0.00 -0.03 -0.03 -0.01

57 1 0.06 0.09 0.03 -0.06 -0.11 -0.04 -0.11 -0.18 -0.06

58 1 -0.07 -0.06 0.01 0.05 0.04 -0.01 0.10 0.09 -0.02

59 1 -0.07 0.06 0.12 0.08 -0.06 -0.12 0.14 -0.11 -0.21

60 1 0.03 0.05 0.00 -0.04 -0.07 -0.01 -0.07 -0.10 -0.02

61 1 -0.09 -0.08 0.04 0.09 0.07 -0.03 0.17 0.14 -0.05

62 1 0.10 0.12 0.19 0.21 0.23 0.38 -0.01 -0.02 -0.03

63 1 0.11 -0.07 0.02 0.19 -0.12 0.03 -0.02 0.01 -0.00

64 1 -0.11 0.13 0.05 -0.23 0.30 0.10 0.02 -0.02 -0.01

65 1 0.16 -0.11 0.06 0.32 -0.19 0.09 -0.02 0.02 -0.01

66 1 -0.06 0.07 0.01 -0.15 0.17 0.03 0.01 -0.01 -0.00

67 1 -0.16 0.11 0.06 0.11 -0.07 -0.03 -0.30 0.18 0.09

68 1 0.06 -0.07 0.01 -0.05 0.06 -0.01 0.14 -0.16 0.03

69 1 -0.10 -0.12 0.19 0.07 0.08 -0.13 -0.20 -0.22 0.35

70 1 -0.11 0.07 0.02 0.07 -0.04 -0.01 -0.18 0.11 0.03

71 1 0.11 -0.13 0.05 -0.08 0.10 -0.03 0.22 -0.28 0.09

72 1 0.09 0.08 0.04 -0.14 -0.12 -0.05 -0.13 -0.11 -0.04

73 1 -0.03 -0.05 0.00 0.05 0.08 -0.01 0.06 0.09 -0.02

74 1 0.07 -0.06 0.12 -0.11 0.09 -0.17 -0.11 0.09 -0.17

75 1 0.07 0.06 0.01 -0.09 -0.07 -0.01 -0.07 -0.07 -0.01

76 1 -0.06 -0.09 0.03 0.09 0.14 -0.05 0.09 0.15 -0.05

77 1 0.01 0.01 -0.00 0.05 -0.00 0.00 0.00 -0.00 -0.00

78 1 -0.01 -0.01 -0.00 0.01 0.00 -0.00 -0.05 0.00 0.00

136 137 138

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Frequencies -- 1104.8745 1108.7675 1161.7539

Red. masses -- 1.5837 1.4577 2.4704

Frc consts -- 1.1391 1.0559 1.9645

IR Inten -- 18.2452 29.4168 0.0297

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.00 -0.00 0.01 -0.03 0.01 0.02 -0.02 0.00

2 6 -0.01 -0.00 0.00 0.01 0.01 -0.00 -0.10 -0.02 0.01

3 7 0.00 0.00 -0.00 -0.00 0.02 -0.01 -0.03 -0.01 0.00

4 6 -0.01 0.01 -0.00 -0.01 0.01 -0.00 -0.10 0.00 -0.01

5 6 0.00 -0.01 0.00 -0.01 -0.03 0.01 0.01 0.03 -0.00

6 6 -0.01 0.01 0.01 -0.03 0.03 0.00 0.04 0.01 0.00

7 6 -0.01 0.00 -0.00 -0.02 0.01 -0.00 0.04 -0.08 0.01

8 7 0.00 0.00 -0.00 0.02 0.00 0.00 -0.00 0.01 0.00

9 6 0.01 0.00 0.00 -0.01 -0.01 -0.00 -0.03 -0.09 -0.01

10 6 0.00 -0.01 0.00 0.03 -0.03 0.01 -0.03 0.01 -0.00

11 6 0.01 0.01 0.00 0.02 0.03 0.01 0.02 0.02 0.00

12 6 0.00 -0.00 -0.00 0.02 0.03 0.00 0.04 -0.01 0.00

13 6 0.01 0.00 -0.00 0.01 0.01 -0.00 0.03 0.09 -0.01

14 6 0.00 -0.01 -0.00 -0.03 0.03 0.01 0.03 -0.01 -0.00

15 6 0.01 0.01 -0.00 -0.02 -0.03 0.01 -0.02 -0.02 0.00

16 6 -0.01 0.00 0.00 0.02 -0.01 -0.00 -0.04 0.08 0.01

17 7 0.00 0.00 0.00 -0.02 -0.00 0.00 0.00 -0.01 0.00

18 6 -0.01 0.01 -0.01 0.03 -0.03 0.00 -0.04 -0.01 0.00

19 6 -0.01 0.01 0.00 0.01 -0.01 -0.00 0.10 -0.00 -0.01

20 6 0.00 -0.01 -0.00 0.01 0.03 0.01 -0.01 -0.03 -0.00

21 6 0.00 -0.00 0.00 -0.01 0.03 0.01 -0.02 0.02 0.00

22 6 -0.01 -0.00 -0.00 -0.01 -0.01 -0.00 0.10 0.02 0.01

23 7 0.00 0.00 0.00 0.00 -0.02 -0.01 0.03 0.01 0.00

24 6 0.00 -0.00 0.00 -0.02 -0.03 0.00 -0.04 0.01 0.00

25 6 0.03 -0.02 -0.03 0.02 -0.01 -0.01 0.06 0.07 0.00

26 6 -0.06 -0.04 0.02 -0.03 -0.02 0.01 0.01 0.01 -0.00

27 6 0.00 0.04 0.03 0.00 0.02 0.02 -0.01 -0.03 -0.01

28 6 0.03 -0.02 -0.05 0.02 -0.01 -0.02 0.01 0.01 0.00

29 6 -0.05 -0.01 0.03 -0.02 -0.01 0.02 -0.03 -0.02 0.01

30 6 0.03 0.07 0.03 0.02 0.03 0.01 0.00 0.01 0.00

31 6 0.00 0.00 0.00 -0.01 -0.01 -0.02 0.01 -0.01 -0.00

32 6 -0.00 -0.00 -0.00 -0.00 0.02 0.01 -0.01 0.03 0.01

33 6 -0.01 0.00 -0.00 0.03 -0.01 0.01 0.01 -0.01 0.00

34 6 0.01 -0.00 0.00 -0.02 -0.01 -0.00 0.07 -0.06 -0.00

35 6 0.00 -0.01 -0.00 -0.02 0.03 0.01 0.00 -0.00 -0.00

36 6 -0.01 0.00 -0.00 0.02 -0.00 0.01 -0.03 0.01 -0.01

37 6 0.01 -0.00 -0.00 0.02 0.01 -0.00 -0.07 0.06 -0.00

38 6 0.00 -0.01 0.00 0.02 -0.03 0.01 -0.00 0.00 -0.00

39 6 -0.01 0.00 0.00 -0.02 0.00 0.01 0.03 -0.01 -0.01

40 6 0.00 0.00 -0.00 0.01 0.01 -0.02 -0.01 0.01 -0.00

41 6 -0.00 -0.00 0.00 0.00 -0.02 0.01 0.01 -0.03 0.01

42 6 -0.01 0.00 0.00 -0.03 0.01 0.01 -0.01 0.01 0.00

43 6 0.03 -0.02 0.03 -0.02 0.01 -0.01 -0.06 -0.07 0.00

44 6 0.03 0.07 -0.03 -0.02 -0.03 0.01 -0.00 -0.01 0.00

45 6 -0.05 -0.01 -0.03 0.02 0.01 0.02 0.03 0.02 0.01

46 6 0.03 -0.02 0.05 -0.02 0.01 -0.02 -0.01 -0.01 0.00

47 6 0.00 0.04 -0.03 -0.00 -0.02 0.02 0.01 0.03 -0.01

48 6 -0.06 -0.04 -0.02 0.03 0.02 0.01 -0.01 -0.01 -0.00

49 1 0.03 0.02 -0.00 0.03 -0.02 0.00 0.13 0.07 -0.02

50 1 0.03 -0.03 0.01 -0.03 -0.02 0.00 0.12 -0.04 0.02

51 1 -0.05 -0.09 -0.02 -0.16 -0.33 -0.06 0.07 0.16 0.02

52 1 -0.03 0.05 -0.01 -0.20 0.30 -0.05 -0.09 0.15 -0.02

53 1 -0.05 -0.09 0.02 0.16 0.33 -0.06 -0.07 -0.16 0.02

54 1 -0.03 0.05 0.01 0.20 -0.30 -0.05 0.09 -0.15 -0.02

55 1 0.03 -0.03 -0.01 0.03 0.02 0.00 -0.12 0.04 0.02

56 1 0.03 0.02 0.00 -0.03 0.02 0.00 -0.13 -0.07 -0.02

57 1 -0.15 -0.27 -0.09 -0.07 -0.15 -0.05 -0.01 -0.06 -0.04

58 1 0.14 0.12 -0.02 0.05 0.05 -0.01 -0.09 -0.08 0.02

59 1 0.20 -0.16 -0.31 0.10 -0.08 -0.15 -0.00 0.02 0.02

60 1 -0.10 -0.17 -0.03 -0.06 -0.09 -0.02 -0.06 -0.12 -0.03

61 1 0.25 0.20 -0.07 0.13 0.09 -0.03 -0.07 -0.03 0.03

62 1 0.02 0.02 0.03 -0.08 -0.08 -0.14 -0.00 -0.02 -0.02

63 1 0.00 -0.00 -0.00 -0.06 0.04 -0.01 -0.10 0.06 -0.02

64 1 -0.02 0.03 0.01 0.08 -0.13 -0.04 -0.02 0.06 0.03

65 1 0.02 -0.01 0.00 -0.12 0.06 -0.03 -0.07 0.02 -0.03

66 1 -0.02 0.02 0.01 0.06 -0.07 -0.01 -0.08 0.11 0.03

67 1 0.02 -0.01 -0.00 0.12 -0.06 -0.03 0.07 -0.02 -0.03

68 1 -0.02 0.02 -0.01 -0.06 0.07 -0.01 0.08 -0.11 0.03

69 1 0.02 0.02 -0.03 0.08 0.08 -0.14 0.00 0.02 -0.02

70 1 0.00 -0.00 0.00 0.06 -0.04 -0.01 0.10 -0.06 -0.02

71 1 -0.02 0.03 -0.01 -0.08 0.13 -0.04 0.02 -0.06 0.03

72 1 0.25 0.20 0.07 -0.13 -0.09 -0.03 0.07 0.03 0.03

73 1 -0.10 -0.17 0.03 0.06 0.09 -0.02 0.06 0.12 -0.03

74 1 0.20 -0.16 0.31 -0.10 0.08 -0.15 0.00 -0.02 0.02

75 1 0.14 0.12 0.02 -0.05 -0.05 -0.01 0.09 0.08 0.02

76 1 -0.15 -0.27 0.09 0.07 0.15 -0.05 0.01 0.06 -0.04

77 1 0.05 0.01 -0.00 -0.00 0.03 -0.01 0.48 0.03 -0.00

78 1 0.05 0.01 0.00 0.00 -0.03 -0.01 -0.48 -0.03 -0.00

139 140 141

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Frequencies -- 1174.3725 1174.3964 1176.1272

Red. masses -- 1.0973 1.0980 1.0991

Frc consts -- 0.8916 0.8923 0.8957

IR Inten -- 0.6240 0.0259 0.8470

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 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.03 0.02 -0.01

28 6 -0.00 0.00 0.00 0.00 0.00 0.00 -0.02 0.02 0.03

29 6 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.01 -0.03 -0.01

30 6 0.00 0.00 -0.00 0.00 0.00 0.00 0.01 0.00 -0.00

31 6 0.02 0.02 0.04 0.02 0.02 0.03 -0.00 -0.00 -0.00

32 6 -0.03 0.01 -0.01 -0.03 0.01 -0.01 0.00 -0.00 0.00

33 6 0.00 -0.01 -0.00 0.00 -0.01 -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 -0.01 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

36 6 0.02 -0.03 -0.01 0.01 -0.02 -0.01 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 -0.01 0.00 0.00 0.01 -0.00 -0.00 -0.00 0.00 0.00

39 6 0.01 -0.02 0.01 -0.01 0.03 -0.01 0.00 0.00 -0.00

40 6 0.02 0.02 -0.03 -0.02 -0.02 0.03 -0.00 -0.00 0.00

41 6 -0.03 0.01 0.01 0.03 -0.01 -0.01 0.00 -0.00 -0.00

42 6 0.00 -0.01 0.00 -0.00 0.01 -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 0.01 0.00 0.00

45 6 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.01 -0.03 0.01

46 6 -0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.02 0.02 -0.03

47 6 0.00 0.00 0.00 0.00 0.00 -0.00 0.03 0.02 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 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.04 -0.10 -0.05

58 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.28 0.16 -0.12

59 1 -0.00 0.00 0.00 0.00 0.00 0.00 -0.24 0.19 0.36

60 1 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.11 -0.31 -0.14

61 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.10 0.06 -0.05

62 1 0.21 0.23 0.37 0.19 0.22 0.34 -0.00 -0.00 -0.00

63 1 -0.32 0.12 -0.13 -0.30 0.12 -0.12 0.00 -0.00 0.00

64 1 0.06 -0.11 -0.05 0.06 -0.10 -0.05 -0.00 0.00 0.00

65 1 -0.10 0.04 -0.05 -0.09 0.04 -0.05 0.00 -0.00 0.00

66 1 0.16 -0.29 -0.14 0.14 -0.27 -0.13 -0.00 0.00 0.00

67 1 -0.09 0.04 0.04 0.10 -0.04 -0.05 0.00 -0.00 -0.00

68 1 0.15 -0.27 0.13 -0.16 0.29 -0.14 -0.00 0.00 -0.00

69 1 0.19 0.22 -0.34 -0.21 -0.23 0.37 -0.00 -0.00 0.00

70 1 -0.30 0.11 0.12 0.33 -0.12 -0.13 0.00 -0.00 -0.00

71 1 0.06 -0.10 0.05 -0.06 0.11 -0.05 -0.00 0.00 -0.00

72 1 0.00 0.00 0.00 0.00 0.00 0.00 0.10 0.06 0.05

73 1 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.11 -0.31 0.14

74 1 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.24 0.19 -0.36

75 1 0.00 0.00 0.00 0.00 0.00 0.00 0.28 0.16 0.12

76 1 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.04 -0.10 0.05

77 1 0.00 0.00 -0.00 0.01 0.00 -0.00 -0.00 0.00 -0.00

78 1 0.00 0.00 0.00 -0.01 -0.00 -0.00 -0.00 0.00 0.00

142 143 144

A A A

Frequencies -- 1176.1470 1191.0847 1199.1359

Red. masses -- 1.0997 5.0000 1.3803

Frc consts -- 0.8963 4.1793 1.1694

IR Inten -- 0.0379 86.6623 519.9674

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.00 -0.00 -0.03 0.00 -0.00 0.00 -0.01 0.00

2 6 0.00 -0.00 -0.00 -0.06 0.01 -0.01 -0.05 -0.01 0.00

3 7 0.00 0.00 0.00 0.00 -0.05 0.01 -0.01 -0.00 0.00

4 6 0.00 0.00 0.00 0.05 0.02 -0.01 -0.04 0.00 -0.00

5 6 -0.00 -0.00 0.00 0.03 0.01 -0.00 0.00 0.01 -0.00

6 6 -0.00 -0.00 -0.00 0.04 0.01 0.01 0.03 -0.02 0.00

7 6 0.00 0.00 0.00 -0.16 -0.16 -0.03 0.03 -0.01 0.01

8 7 0.00 -0.00 -0.00 -0.01 0.19 0.00 -0.02 0.00 -0.01

9 6 -0.00 0.00 -0.00 0.18 -0.14 0.03 0.03 0.01 0.01

10 6 0.00 -0.00 0.00 -0.08 0.04 -0.01 -0.02 0.01 -0.00

11 6 -0.00 -0.00 -0.00 0.07 0.05 0.01 -0.02 -0.01 -0.00

12 6 -0.00 -0.00 0.00 -0.04 0.01 0.01 0.02 0.02 -0.00

13 6 0.00 -0.00 -0.00 0.18 -0.14 -0.03 0.03 0.01 -0.01

14 6 -0.00 0.00 0.00 -0.08 0.04 0.01 -0.02 0.01 0.00

15 6 0.00 0.00 -0.00 0.07 0.05 -0.01 -0.02 -0.01 0.00

16 6 -0.00 -0.00 0.00 -0.16 -0.16 0.03 0.03 -0.01 -0.01

17 7 -0.00 0.00 -0.00 -0.01 0.19 -0.00 -0.02 0.00 0.01

18 6 0.00 0.00 -0.00 0.04 0.01 -0.01 0.03 -0.02 -0.00

19 6 -0.00 -0.00 0.00 0.05 0.02 0.01 -0.04 0.00 0.00

20 6 0.00 0.00 0.00 0.03 0.01 0.00 0.00 0.01 0.00

21 6 0.00 -0.00 -0.00 -0.03 0.00 0.00 0.00 -0.01 -0.00

22 6 -0.00 0.00 -0.00 -0.06 0.01 0.01 -0.05 -0.01 -0.00

23 7 -0.00 -0.00 0.00 0.00 -0.05 -0.01 -0.01 -0.00 -0.00

24 6 0.00 0.00 0.00 -0.04 0.01 -0.01 0.02 0.02 0.00

25 6 0.00 -0.00 -0.00 -0.01 -0.00 -0.02 0.01 0.02 -0.00

26 6 -0.00 -0.01 -0.00 0.01 0.02 0.01 0.01 0.02 0.01

27 6 0.03 0.02 -0.01 -0.01 -0.01 0.00 -0.02 -0.02 0.00

28 6 -0.02 0.02 0.03 -0.00 -0.00 -0.00 -0.00 -0.00 0.00

29 6 -0.01 -0.03 -0.01 -0.00 -0.01 -0.00 -0.01 -0.02 -0.00

30 6 0.01 0.00 -0.00 0.00 0.01 0.00 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 0.00 -0.00 -0.00 0.02 -0.01 0.01 -0.02 0.01 -0.00

33 6 -0.00 0.00 0.00 -0.01 0.02 0.02 0.02 -0.03 -0.01

34 6 -0.00 0.00 -0.00 0.01 -0.01 -0.02 0.01 -0.01 0.00

35 6 -0.00 0.00 0.00 -0.01 0.01 0.00 0.03 -0.01 0.01

36 6 0.00 -0.00 0.00 0.00 -0.01 -0.01 -0.02 0.02 0.01

37 6 0.00 -0.00 -0.00 0.01 -0.01 0.02 0.01 -0.01 -0.00

38 6 0.00 -0.00 0.00 -0.01 0.01 -0.00 0.03 -0.01 -0.01

39 6 -0.00 0.00 0.00 0.00 -0.01 0.01 -0.02 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 -0.00 0.00 -0.00 0.02 -0.01 -0.01 -0.02 0.01 0.00

42 6 0.00 -0.00 0.00 -0.01 0.02 -0.02 0.02 -0.03 0.01

43 6 -0.00 0.00 -0.00 -0.01 -0.00 0.02 0.01 0.02 0.00

44 6 -0.01 -0.00 -0.00 0.00 0.01 -0.00 0.02 0.01 0.01

45 6 0.01 0.03 -0.01 -0.00 -0.01 0.00 -0.01 -0.02 0.00

46 6 0.02 -0.02 0.03 -0.00 -0.00 0.00 -0.00 -0.00 -0.00

47 6 -0.03 -0.02 -0.01 -0.01 -0.01 -0.00 -0.02 -0.02 -0.00

48 6 0.00 0.01 -0.00 0.01 0.02 -0.01 0.01 0.02 -0.01

49 1 -0.00 -0.00 0.00 -0.01 0.03 -0.01 0.04 0.02 -0.01

50 1 -0.00 -0.00 0.00 0.01 0.03 -0.00 0.04 -0.01 0.01

51 1 0.00 -0.00 0.00 -0.22 -0.17 -0.06 -0.01 0.03 0.00

52 1 0.00 -0.00 0.00 0.25 -0.15 0.06 0.01 -0.04 0.00

53 1 -0.00 0.00 0.00 -0.22 -0.17 0.06 -0.01 0.03 -0.00

54 1 -0.00 0.00 0.00 0.25 -0.15 -0.06 0.01 -0.04 -0.00

55 1 0.00 0.00 0.00 0.01 0.03 0.00 0.04 -0.01 -0.01

56 1 0.00 0.00 0.00 -0.01 0.03 0.01 0.04 0.02 0.01

57 1 -0.04 -0.10 -0.05 0.05 0.15 0.06 0.06 0.17 0.08

58 1 0.29 0.16 -0.12 -0.10 -0.05 0.04 -0.18 -0.11 0.07

59 1 -0.24 0.19 0.36 -0.02 0.01 0.02 -0.01 0.00 0.01

60 1 -0.11 -0.30 -0.14 -0.04 -0.10 -0.05 -0.07 -0.18 -0.08

61 1 0.10 0.06 -0.05 0.05 0.04 -0.03 0.13 0.08 -0.06

62 1 0.00 0.00 0.00 0.02 0.01 0.02 -0.01 -0.00 -0.01

63 1 0.00 -0.00 0.00 0.12 -0.04 0.05 -0.23 0.09 -0.09

64 1 0.00 -0.00 -0.00 -0.08 0.17 0.07 0.11 -0.20 -0.09

65 1 0.00 -0.00 0.00 -0.08 0.04 -0.04 0.19 -0.08 0.09

66 1 0.00 -0.00 -0.00 0.06 -0.11 -0.05 -0.13 0.22 0.10

67 1 -0.00 0.00 0.00 -0.08 0.04 0.04 0.19 -0.08 -0.09

68 1 -0.00 0.00 -0.00 0.06 -0.11 0.05 -0.13 0.22 -0.10

69 1 -0.00 -0.00 0.00 0.02 0.01 -0.02 -0.01 -0.00 0.01

70 1 -0.00 0.00 0.00 0.12 -0.04 -0.05 -0.23 0.09 0.09

71 1 -0.00 0.00 -0.00 -0.08 0.17 -0.07 0.11 -0.20 0.09

72 1 -0.10 -0.06 -0.05 0.05 0.04 0.03 0.13 0.08 0.06

73 1 0.11 0.31 -0.14 -0.04 -0.10 0.05 -0.07 -0.18 0.08

74 1 0.24 -0.19 0.36 -0.02 0.01 -0.02 -0.01 0.00 -0.01

75 1 -0.29 -0.16 -0.12 -0.10 -0.05 -0.04 -0.18 -0.11 -0.07

76 1 0.04 0.10 -0.05 0.05 0.15 -0.06 0.06 0.17 -0.08

77 1 -0.01 -0.00 -0.00 0.01 -0.05 0.02 0.26 0.02 0.00

78 1 0.01 0.00 -0.00 0.01 -0.05 -0.02 0.26 0.02 -0.00

145 146 147

A A A

Frequencies -- 1200.7507 1201.0768 1201.3085

Red. masses -- 1.1362 1.1349 1.1974

Frc consts -- 0.9652 0.9646 1.0181

IR Inten -- 0.0078 0.0002 41.6760

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 0.01 -0.00 0.00

2 6 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.01 -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 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.01 -0.00 0.00

5 6 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.01 -0.00 0.00

6 6 0.00 -0.00 0.00 0.00 0.00 0.00 -0.01 -0.00 -0.00

7 6 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.02 0.02 0.01

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 -0.00 0.00 0.00 0.00 -0.02 0.01 -0.00

10 6 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.01 -0.00 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 -0.02 0.01 0.00

14 6 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.01 -0.00 -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 0.02 0.02 -0.01

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 0.00 -0.00 -0.00 0.00 -0.01 -0.00 0.00

19 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.01 -0.00 -0.00

20 6 0.00 0.00 0.00 0.00 0.00 -0.00 -0.01 -0.00 -0.00

21 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.01 -0.00 -0.00

22 6 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.01 -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 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.01 0.00 0.00

25 6 -0.00 -0.00 -0.00 -0.01 -0.01 -0.00 -0.00 -0.00 0.00

26 6 0.00 0.00 0.00 0.01 0.03 0.02 0.01 0.03 0.01

27 6 -0.00 0.00 0.00 -0.03 -0.02 0.01 -0.02 -0.01 0.01

28 6 -0.00 -0.00 -0.00 -0.01 -0.01 -0.00 -0.00 -0.00 -0.00

29 6 0.00 -0.00 -0.00 -0.01 -0.03 -0.01 -0.01 -0.02 -0.01

30 6 0.00 0.00 -0.00 0.03 0.02 -0.02 0.03 0.02 -0.01

31 6 -0.01 0.01 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

32 6 -0.03 0.01 -0.01 0.00 -0.00 0.00 0.02 -0.01 0.01

33 6 0.02 -0.03 -0.02 -0.00 0.00 0.00 -0.01 0.02 0.01

34 6 -0.01 0.01 0.00 -0.00 0.00 0.00 0.00 -0.00 0.00

35 6 0.04 -0.01 0.02 -0.00 0.00 -0.00 -0.02 0.01 -0.01

36 6 -0.01 0.03 0.01 0.00 -0.00 -0.00 0.01 -0.02 -0.01

37 6 0.01 -0.01 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00

38 6 -0.04 0.01 0.02 0.00 -0.00 -0.00 -0.02 0.01 0.01

39 6 0.01 -0.03 0.01 -0.00 0.00 -0.00 0.01 -0.02 0.01

40 6 0.01 -0.01 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

41 6 0.03 -0.01 -0.01 -0.00 0.00 0.00 0.02 -0.01 -0.01

42 6 -0.02 0.03 -0.02 0.00 -0.00 0.00 -0.01 0.02 -0.01

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 -0.03 -0.02 -0.02 0.03 0.02 0.01

45 6 -0.00 0.00 -0.00 0.01 0.03 -0.01 -0.01 -0.02 0.01

46 6 0.00 0.00 -0.00 0.01 0.01 -0.00 -0.00 -0.00 0.00

47 6 0.00 -0.00 0.00 0.03 0.01 0.01 -0.02 -0.01 -0.01

48 6 -0.00 -0.00 0.00 -0.01 -0.03 0.02 0.01 0.03 -0.01

49 1 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.01 -0.00 0.00

50 1 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.01 -0.00 0.00

51 1 -0.01 -0.01 -0.00 0.00 0.00 0.00 0.03 0.03 0.01

52 1 0.00 -0.00 -0.00 0.01 -0.01 0.00 -0.03 0.02 -0.01

53 1 0.01 0.01 -0.00 -0.00 -0.00 0.00 0.03 0.03 -0.01

54 1 -0.00 0.00 -0.00 -0.01 0.01 0.00 -0.03 0.02 0.01

55 1 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.01 -0.00 -0.00

56 1 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.01 -0.00 -0.00

57 1 0.01 0.02 0.01 0.12 0.32 0.15 0.09 0.23 0.11

58 1 -0.01 -0.00 0.00 -0.28 -0.15 0.12 -0.22 -0.13 0.09

59 1 -0.00 -0.00 0.00 -0.00 -0.01 -0.00 0.00 -0.01 -0.01

60 1 -0.00 -0.01 -0.01 -0.10 -0.28 -0.13 -0.08 -0.22 -0.10

61 1 0.02 0.01 -0.01 0.29 0.17 -0.13 0.23 0.13 -0.10

62 1 -0.01 0.00 -0.01 0.00 -0.00 -0.00 0.00 -0.00 -0.00

63 1 -0.28 0.11 -0.12 0.02 -0.01 0.01 0.18 -0.07 0.08

64 1 0.16 -0.30 -0.15 -0.01 0.01 0.01 -0.10 0.17 0.09

65 1 0.31 -0.13 0.14 -0.01 0.01 -0.01 -0.20 0.08 -0.09

66 1 -0.15 0.28 0.13 0.01 -0.02 -0.01 0.10 -0.18 -0.08

67 1 -0.31 0.13 0.14 0.01 -0.01 -0.01 -0.20 0.08 0.09

68 1 0.15 -0.28 0.13 -0.01 0.02 -0.01 0.10 -0.18 0.08

69 1 0.01 -0.00 -0.01 -0.00 0.00 -0.00 0.00 -0.00 0.00

70 1 0.28 -0.11 -0.12 -0.02 0.01 0.01 0.18 -0.07 -0.08

71 1 -0.16 0.30 -0.15 0.01 -0.01 0.01 -0.10 0.17 -0.09

72 1 -0.02 -0.01 -0.01 -0.29 -0.17 -0.13 0.23 0.13 0.10

73 1 0.00 0.01 -0.01 0.10 0.28 -0.13 -0.08 -0.22 0.10

74 1 0.00 0.00 0.00 0.00 0.01 -0.00 0.00 -0.01 0.01

75 1 0.01 0.00 0.01 0.28 0.15 0.12 -0.22 -0.13 -0.09

76 1 -0.01 -0.02 0.01 -0.12 -0.32 0.15 0.09 0.23 -0.11

77 1 -0.02 -0.00 -0.00 -0.02 -0.00 0.00 0.01 0.01 -0.00

78 1 0.02 0.00 -0.00 0.02 0.00 0.00 0.01 0.01 0.00

148 149 150

A A A

Frequencies -- 1204.0055 1246.3652 1246.4761

Red. masses -- 1.7150 1.6143 3.9732

Frc consts -- 1.4647 1.4775 3.6371

IR Inten -- 719.8537 0.0351 10.8549

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 -0.02 0.00 -0.03 -0.01 0.00 0.06 -0.02 0.01

2 6 -0.07 -0.01 0.00 0.03 -0.09 0.02 0.09 -0.02 0.01

3 7 -0.02 -0.00 -0.00 -0.02 -0.00 -0.00 -0.01 0.07 -0.02

4 6 -0.07 -0.00 -0.00 0.02 0.10 -0.02 -0.08 -0.01 0.00

5 6 0.00 0.02 -0.00 -0.03 -0.00 -0.00 -0.06 -0.02 0.00

6 6 0.04 -0.04 0.00 -0.01 0.01 0.00 -0.08 -0.02 -0.01

7 6 0.06 -0.01 0.01 0.04 -0.02 0.01 0.02 -0.11 0.00

8 7 -0.03 -0.00 -0.01 -0.00 -0.00 -0.00 0.01 0.06 0.00

9 6 0.05 0.03 0.01 -0.03 -0.02 -0.01 -0.03 -0.10 -0.01

10 6 -0.03 0.01 -0.01 -0.01 -0.01 -0.00 -0.05 -0.00 -0.01

11 6 -0.03 -0.02 -0.01 0.01 -0.00 0.00 0.05 -0.00 0.01

12 6 0.03 0.04 -0.00 -0.01 -0.01 -0.00 0.08 0.00 -0.01

13 6 0.05 0.03 -0.01 0.03 0.03 -0.01 -0.03 -0.10 0.01

14 6 -0.03 0.01 0.01 0.01 0.01 -0.00 -0.05 -0.00 0.01

15 6 -0.03 -0.02 0.01 -0.01 0.00 0.00 0.05 -0.00 -0.01

16 6 0.06 -0.01 -0.01 -0.04 0.02 0.01 0.02 -0.11 -0.00

17 7 -0.03 -0.00 0.01 0.00 0.00 -0.00 0.01 0.06 -0.00

18 6 0.04 -0.04 -0.00 0.01 -0.01 0.00 -0.08 -0.02 0.01

19 6 -0.07 -0.00 0.00 -0.02 -0.10 -0.02 -0.08 -0.01 -0.00

20 6 0.00 0.02 0.00 0.03 0.00 -0.00 -0.06 -0.02 -0.00

21 6 0.01 -0.02 -0.00 0.03 0.01 0.00 0.06 -0.02 -0.01

22 6 -0.07 -0.01 -0.00 -0.03 0.09 0.02 0.09 -0.02 -0.01

23 7 -0.02 -0.00 0.00 0.02 0.00 -0.00 -0.01 0.07 0.02

24 6 0.03 0.04 0.00 0.01 0.01 -0.00 0.08 0.00 0.01

25 6 0.03 0.04 -0.00 -0.01 -0.01 -0.00 0.10 0.13 0.02

26 6 -0.00 -0.01 -0.01 -0.00 -0.00 0.00 0.01 0.01 -0.00

27 6 0.01 -0.00 -0.01 -0.00 0.00 0.00 -0.00 -0.04 -0.03

28 6 0.00 0.01 0.00 0.00 -0.00 -0.00 0.00 0.01 0.00

29 6 -0.01 0.01 0.01 0.00 0.00 -0.00 -0.04 -0.02 0.02

30 6 -0.01 -0.01 0.01 -0.00 -0.00 0.00 0.03 0.02 -0.01

31 6 0.01 -0.01 -0.00 0.00 0.00 0.00 -0.00 0.01 0.00

32 6 0.01 0.01 0.01 -0.00 -0.00 -0.00 0.01 -0.03 -0.03

33 6 -0.00 0.01 0.01 -0.00 0.00 -0.00 -0.01 0.01 -0.01

34 6 0.03 -0.03 0.00 -0.01 0.01 0.00 -0.10 0.10 0.03

35 6 -0.02 0.01 -0.01 -0.00 0.00 -0.00 -0.03 0.01 -0.01

36 6 -0.00 -0.01 -0.01 0.00 -0.00 0.00 0.04 -0.01 0.02

37 6 0.03 -0.03 -0.00 0.01 -0.01 0.00 -0.10 0.10 -0.03

38 6 -0.02 0.01 0.01 0.00 -0.00 -0.00 -0.03 0.01 0.01

39 6 -0.00 -0.01 0.01 -0.00 0.00 0.00 0.04 -0.01 -0.02

40 6 0.01 -0.01 0.00 -0.00 -0.00 0.00 -0.01 0.01 -0.00

41 6 0.01 0.01 -0.01 0.00 0.00 -0.00 0.01 -0.03 0.03

42 6 -0.00 0.01 -0.01 0.00 -0.00 -0.00 -0.01 0.01 0.01

43 6 0.03 0.04 0.00 0.01 0.01 -0.00 0.10 0.13 -0.02

44 6 -0.01 -0.01 -0.01 0.00 0.00 0.00 0.03 0.02 0.01

45 6 -0.01 0.01 -0.01 -0.00 -0.00 -0.00 -0.04 -0.02 -0.02

46 6 0.00 0.01 -0.00 -0.00 0.00 -0.00 0.00 0.01 -0.00

47 6 0.01 -0.00 0.01 0.00 -0.00 0.00 -0.00 -0.04 0.03

48 6 -0.00 -0.01 0.01 0.00 0.00 0.00 0.01 0.01 0.00

49 1 0.06 0.03 -0.01 0.30 0.27 -0.07 0.06 -0.02 0.01

50 1 0.06 -0.02 0.01 0.33 -0.23 0.08 0.01 -0.08 0.02

51 1 -0.01 0.05 -0.00 0.07 0.12 0.02 0.11 0.25 0.04

52 1 -0.01 -0.04 -0.00 -0.09 0.12 -0.02 -0.13 0.21 -0.03

53 1 -0.01 0.05 0.00 -0.07 -0.12 0.02 0.11 0.25 -0.04

54 1 -0.01 -0.04 0.00 0.09 -0.12 -0.02 -0.13 0.21 0.03

55 1 0.06 -0.02 -0.01 -0.33 0.23 0.08 0.01 -0.08 -0.02

56 1 0.06 0.03 0.01 -0.30 -0.27 -0.07 0.06 -0.02 -0.01

57 1 -0.06 -0.17 -0.09 0.00 0.01 0.00 -0.05 -0.19 -0.09

58 1 0.10 0.04 -0.05 0.01 0.01 -0.00 -0.12 -0.11 0.02

59 1 -0.00 0.01 0.01 -0.00 0.00 0.00 0.02 -0.00 -0.02

60 1 0.03 0.10 0.06 0.01 0.01 0.00 -0.07 -0.10 -0.01

61 1 -0.19 -0.10 0.08 0.01 0.00 -0.00 -0.13 -0.06 0.06

62 1 0.00 -0.01 -0.01 -0.00 -0.00 -0.00 -0.02 -0.01 -0.02

63 1 0.11 -0.03 0.05 0.01 -0.01 0.00 0.12 -0.08 0.02

64 1 -0.09 0.17 0.09 0.00 -0.01 -0.00 0.07 -0.19 -0.09

65 1 -0.22 0.08 -0.10 -0.00 0.00 -0.00 0.10 -0.04 0.05

66 1 0.05 -0.12 -0.06 0.01 -0.01 -0.00 0.07 -0.07 -0.00

67 1 -0.22 0.08 0.10 0.00 -0.00 -0.00 0.10 -0.04 -0.05

68 1 0.05 -0.12 0.06 -0.01 0.01 -0.00 0.07 -0.07 0.00

69 1 0.00 -0.01 0.01 0.00 0.00 -0.00 -0.02 -0.01 0.02

70 1 0.11 -0.03 -0.05 -0.01 0.01 0.00 0.12 -0.08 -0.02

71 1 -0.09 0.17 -0.09 -0.00 0.01 -0.00 0.07 -0.19 0.09

72 1 -0.19 -0.10 -0.08 -0.01 -0.00 -0.00 -0.13 -0.06 -0.06

73 1 0.03 0.10 -0.06 -0.01 -0.01 0.00 -0.07 -0.10 0.01

74 1 -0.00 0.01 -0.01 0.00 -0.00 0.00 0.02 -0.00 0.02

75 1 0.10 0.04 0.05 -0.01 -0.01 -0.00 -0.12 -0.11 -0.02

76 1 -0.06 -0.17 0.09 -0.00 -0.01 0.00 -0.05 -0.19 0.09

77 1 0.44 0.03 -0.00 -0.31 -0.02 0.00 -0.03 0.07 -0.02

78 1 0.44 0.03 0.00 0.31 0.02 0.00 -0.03 0.07 0.02

151 152 153

A A A

Frequencies -- 1251.8296 1257.2457 1261.5414

Red. masses -- 2.6417 4.8300 2.6049

Frc consts -- 2.4391 4.4982 2.4426

IR Inten -- 24.4458 0.1236 44.0144

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 -0.01 0.00 -0.02 -0.00 0.00 -0.02 -0.02 0.00

2 6 0.01 -0.08 0.02 -0.05 0.02 -0.01 0.01 -0.09 0.02

3 7 -0.01 -0.01 0.00 0.00 -0.03 0.01 -0.05 -0.00 -0.00

4 6 0.01 0.08 -0.02 0.05 0.02 -0.01 0.00 0.09 -0.02

5 6 -0.02 0.01 -0.00 0.03 0.00 0.00 -0.03 0.01 -0.00

6 6 0.00 -0.05 0.01 0.06 0.09 0.00 0.06 0.03 0.01

7 6 -0.07 -0.07 -0.02 0.08 0.10 0.02 0.08 0.03 0.02

8 7 0.09 -0.00 0.02 -0.10 -0.01 -0.02 -0.07 -0.00 -0.01

9 6 -0.08 0.08 -0.02 0.09 -0.09 0.02 0.08 -0.02 0.02

10 6 0.02 0.03 0.00 -0.01 -0.03 -0.00 -0.03 -0.01 -0.01

11 6 0.01 -0.02 0.00 -0.02 0.03 -0.00 -0.03 0.01 -0.01

12 6 -0.02 0.04 -0.01 -0.08 0.08 -0.00 0.06 -0.02 -0.00

13 6 -0.08 0.08 0.02 -0.09 0.09 0.02 0.08 -0.02 -0.02

14 6 0.02 0.03 -0.00 0.01 0.03 -0.00 -0.03 -0.01 0.01

15 6 0.01 -0.02 -0.00 0.02 -0.03 -0.00 -0.03 0.01 0.01

16 6 -0.07 -0.07 0.02 -0.08 -0.10 0.02 0.08 0.03 -0.02

17 7 0.09 -0.00 -0.02 0.10 0.01 -0.02 -0.07 -0.00 0.01

18 6 0.00 -0.05 -0.01 -0.06 -0.09 0.00 0.06 0.03 -0.01

19 6 0.01 0.08 0.02 -0.05 -0.02 -0.01 0.00 0.09 0.02

20 6 -0.02 0.01 0.00 -0.03 -0.00 0.00 -0.03 0.01 0.00

21 6 -0.03 -0.01 -0.00 0.02 0.00 0.00 -0.02 -0.02 -0.00

22 6 0.01 -0.08 -0.02 0.05 -0.02 -0.01 0.01 -0.09 -0.02

23 7 -0.01 -0.01 -0.00 -0.00 0.03 0.01 -0.05 -0.00 0.00

24 6 -0.02 0.04 0.01 0.08 -0.08 -0.00 0.06 -0.02 0.00

25 6 0.05 0.04 -0.03 -0.13 -0.15 0.00 -0.06 -0.07 -0.01

26 6 0.00 0.02 0.01 -0.01 -0.03 -0.01 -0.01 -0.01 0.00

27 6 -0.01 -0.02 -0.01 0.01 0.05 0.03 0.00 0.02 0.02

28 6 0.00 0.00 -0.00 -0.01 -0.01 -0.00 -0.00 -0.00 -0.00

29 6 -0.01 0.00 0.01 0.05 0.02 -0.03 0.02 0.01 -0.01

30 6 0.00 0.00 0.01 -0.03 -0.02 0.00 -0.02 -0.01 0.01

31 6 0.01 -0.00 0.00 0.01 -0.01 0.00 -0.00 0.00 0.00

32 6 -0.01 0.02 0.01 -0.02 0.05 0.03 0.00 -0.02 -0.02

33 6 0.01 -0.02 -0.01 0.02 -0.03 -0.01 -0.01 0.01 -0.00

34 6 0.07 -0.05 0.02 0.14 -0.13 0.00 -0.06 0.06 0.01

35 6 0.00 -0.00 -0.01 0.03 -0.01 0.00 -0.02 0.01 -0.01

36 6 -0.02 -0.00 -0.02 -0.05 0.01 -0.03 0.02 -0.01 0.01

37 6 0.07 -0.05 -0.02 -0.14 0.13 0.00 -0.06 0.06 -0.01

38 6 0.00 -0.00 0.01 -0.03 0.01 0.00 -0.02 0.01 0.01

39 6 -0.02 -0.00 0.02 0.05 -0.01 -0.03 0.02 -0.01 -0.01

40 6 0.01 -0.00 -0.00 -0.01 0.01 0.00 -0.00 0.00 -0.00

41 6 -0.01 0.02 -0.01 0.02 -0.05 0.03 0.00 -0.02 0.02

42 6 0.01 -0.02 0.01 -0.02 0.03 -0.01 -0.01 0.01 0.00

43 6 0.05 0.04 0.03 0.13 0.15 0.00 -0.06 -0.07 0.01

44 6 0.00 0.00 -0.01 0.03 0.02 0.00 -0.02 -0.01 -0.01

45 6 -0.01 0.00 -0.01 -0.05 -0.02 -0.03 0.02 0.01 0.01

46 6 0.00 0.00 0.00 0.01 0.01 -0.00 -0.00 -0.00 0.00

47 6 -0.01 -0.02 0.01 -0.01 -0.05 0.03 0.00 0.02 -0.02

48 6 0.00 0.02 -0.01 0.01 0.03 -0.01 -0.01 -0.01 -0.00

49 1 0.28 0.25 -0.07 -0.05 -0.02 0.01 0.30 0.25 -0.06

50 1 0.32 -0.20 0.07 0.03 0.01 0.00 0.33 -0.21 0.07

51 1 0.04 0.06 0.01 -0.06 -0.10 -0.02 -0.04 -0.02 -0.01

52 1 0.07 -0.09 0.01 -0.07 0.10 -0.02 -0.04 0.01 -0.01

53 1 0.04 0.06 -0.01 0.06 0.10 -0.02 -0.04 -0.02 0.01

54 1 0.07 -0.09 -0.01 0.07 -0.10 -0.02 -0.04 0.01 0.01

55 1 0.32 -0.20 -0.07 -0.03 -0.01 0.00 0.33 -0.21 -0.07

56 1 0.28 0.25 0.07 0.05 0.02 0.01 0.30 0.25 0.06

57 1 -0.01 -0.00 -0.01 0.04 0.15 0.07 0.02 0.08 0.04

58 1 -0.03 -0.03 0.00 0.14 0.12 -0.02 0.07 0.06 -0.01

59 1 -0.01 0.01 0.01 -0.00 -0.01 -0.00 -0.01 0.00 0.01

60 1 -0.04 -0.07 -0.02 0.10 0.16 0.03 0.04 0.07 0.01

61 1 -0.10 -0.04 0.04 0.19 0.08 -0.08 0.06 0.03 -0.03

62 1 -0.00 -0.01 -0.01 0.00 -0.01 -0.00 -0.01 -0.00 -0.01

63 1 -0.05 0.04 -0.00 -0.15 0.11 -0.02 0.09 -0.05 0.02

64 1 -0.02 0.04 0.02 -0.07 0.16 0.08 0.03 -0.09 -0.04

65 1 -0.13 0.03 -0.05 -0.19 0.05 -0.08 0.06 -0.02 0.02

66 1 -0.06 0.06 0.01 -0.12 0.13 0.02 0.05 -0.05 -0.01

67 1 -0.13 0.03 0.05 0.19 -0.05 -0.08 0.06 -0.02 -0.02

68 1 -0.06 0.06 -0.01 0.12 -0.13 0.02 0.05 -0.05 0.01

69 1 -0.00 -0.01 0.01 -0.00 0.01 -0.00 -0.01 -0.00 0.01

70 1 -0.05 0.04 0.00 0.15 -0.11 -0.02 0.09 -0.05 -0.02

71 1 -0.02 0.04 -0.02 0.07 -0.16 0.08 0.03 -0.09 0.04

72 1 -0.10 -0.04 -0.04 -0.19 -0.08 -0.08 0.06 0.03 0.03

73 1 -0.04 -0.07 0.02 -0.10 -0.16 0.03 0.04 0.07 -0.01

74 1 -0.01 0.01 -0.01 0.00 0.01 -0.00 -0.01 0.00 -0.01

75 1 -0.03 -0.03 -0.00 -0.14 -0.12 -0.02 0.07 0.06 0.01

76 1 -0.01 -0.00 0.01 -0.04 -0.15 0.07 0.02 0.08 -0.04

77 1 -0.24 -0.02 0.00 0.02 -0.03 0.02 -0.21 -0.01 -0.00

78 1 -0.24 -0.02 -0.00 -0.02 0.03 0.02 -0.21 -0.01 0.00

154 155 156

A A A

Frequencies -- 1284.6312 1294.3202 1313.3304

Red. masses -- 8.2973 3.2810 3.2554

Frc consts -- 8.0676 3.2385 3.3083

IR Inten -- 3.2187 0.0009 3.4870

Atom AN X Y Z X Y Z X Y Z

1 6 0.09 0.04 -0.01 -0.00 -0.02 0.00 -0.00 -0.05 0.01

2 6 0.14 -0.09 0.03 -0.04 -0.03 0.01 -0.01 0.09 -0.02

3 7 -0.01 0.13 -0.03 -0.05 -0.00 -0.00 0.00 -0.05 0.01

4 6 -0.12 -0.11 0.03 -0.04 0.03 -0.01 0.00 0.09 -0.02

5 6 -0.09 0.03 -0.01 -0.01 0.02 -0.00 0.01 -0.05 0.01

6 6 -0.05 -0.04 -0.02 0.12 -0.03 0.02 0.01 0.10 -0.01

7 6 0.24 0.06 0.05 -0.07 -0.00 -0.01 0.03 -0.06 0.01

8 7 -0.19 -0.01 -0.04 -0.00 0.05 0.00 0.00 -0.03 0.00

9 6 0.24 -0.03 0.05 0.07 0.01 0.01 -0.02 -0.06 -0.01

10 6 -0.08 -0.03 -0.02 0.03 0.03 0.01 -0.08 -0.03 -0.02

11 6 -0.08 0.02 -0.02 -0.03 0.02 -0.01 0.08 -0.02 0.02

12 6 0.05 -0.04 -0.01 0.11 0.04 -0.02 -0.02 0.10 -0.01

13 6 -0.24 0.03 0.05 -0.07 -0.01 0.01 -0.02 -0.06 0.01

14 6 0.08 0.03 -0.02 -0.03 -0.03 0.01 -0.08 -0.03 0.02

15 6 0.08 -0.02 -0.02 0.03 -0.02 -0.01 0.08 -0.02 -0.02

16 6 -0.24 -0.06 0.05 0.07 0.00 -0.01 0.03 -0.06 -0.01

17 7 0.19 0.01 -0.04 0.00 -0.05 0.00 0.00 -0.03 -0.00

18 6 0.05 0.04 -0.02 -0.12 0.03 0.02 0.01 0.10 0.01

19 6 0.12 0.11 0.03 0.04 -0.03 -0.01 0.00 0.09 0.02

20 6 0.09 -0.03 -0.01 0.01 -0.02 -0.00 0.01 -0.05 -0.01

21 6 -0.09 -0.04 -0.01 0.00 0.02 0.00 -0.00 -0.05 -0.01

22 6 -0.14 0.09 0.03 0.04 0.03 0.01 -0.01 0.09 0.02

23 7 0.01 -0.13 -0.03 0.05 0.00 -0.00 0.00 -0.05 -0.01

24 6 -0.05 0.04 -0.01 -0.11 -0.04 -0.02 -0.02 0.10 0.01

25 6 0.01 0.08 0.08 0.01 -0.07 -0.09 -0.08 -0.03 0.05

26 6 0.00 -0.02 -0.02 0.00 0.03 0.03 -0.01 -0.04 -0.02

27 6 0.03 -0.00 -0.03 -0.03 -0.00 0.03 0.03 0.03 -0.00

28 6 -0.01 0.01 0.02 0.02 -0.01 -0.03 -0.01 0.01 0.02

29 6 -0.02 -0.04 -0.01 0.02 0.04 0.01 0.01 -0.02 -0.03

30 6 0.04 0.01 -0.03 -0.04 -0.01 0.03 0.01 -0.00 -0.01

31 6 0.01 0.01 0.02 0.01 0.02 0.03 0.01 0.01 0.02

32 6 -0.03 -0.01 -0.03 -0.04 -0.00 -0.03 -0.03 0.02 -0.01

33 6 -0.00 -0.02 -0.02 0.01 -0.03 -0.03 0.01 -0.04 -0.02

34 6 -0.02 0.08 0.08 0.00 0.07 0.09 0.08 -0.01 0.06

35 6 -0.04 0.01 -0.03 -0.05 0.01 -0.03 -0.01 -0.00 -0.02

36 6 0.03 -0.03 -0.01 0.03 -0.04 -0.01 -0.00 -0.03 -0.03

37 6 0.02 -0.08 0.08 -0.00 -0.07 0.09 0.08 -0.01 -0.06

38 6 0.04 -0.01 -0.03 0.05 -0.01 -0.03 -0.01 -0.00 0.02

39 6 -0.03 0.03 -0.01 -0.03 0.04 -0.01 -0.00 -0.03 0.03

40 6 -0.01 -0.01 0.02 -0.01 -0.02 0.03 0.01 0.01 -0.02

41 6 0.03 0.01 -0.03 0.04 0.00 -0.03 -0.03 0.02 0.01

42 6 0.00 0.02 -0.02 -0.01 0.03 -0.03 0.01 -0.04 0.02

43 6 -0.01 -0.08 0.08 -0.01 0.07 -0.09 -0.08 -0.03 -0.05

44 6 -0.04 -0.01 -0.03 0.04 0.01 0.03 0.01 -0.00 0.01

45 6 0.02 0.04 -0.01 -0.02 -0.04 0.01 0.01 -0.02 0.03

46 6 0.01 -0.01 0.02 -0.02 0.01 -0.03 -0.01 0.01 -0.02

47 6 -0.03 0.00 -0.03 0.03 0.00 0.03 0.03 0.03 0.00

48 6 -0.00 0.02 -0.02 -0.00 -0.03 0.03 -0.01 -0.04 0.02

49 1 -0.00 -0.04 0.02 0.13 0.09 -0.02 0.02 -0.05 0.01

50 1 -0.00 -0.03 0.01 0.14 -0.07 0.02 -0.01 -0.04 0.01

51 1 -0.08 -0.01 -0.01 -0.15 -0.25 -0.04 0.16 0.34 0.05

52 1 -0.09 0.01 -0.02 0.18 -0.22 0.04 -0.20 0.32 -0.04

53 1 0.08 0.01 -0.01 0.15 0.25 -0.04 0.16 0.34 -0.05

54 1 0.09 -0.01 -0.02 -0.18 0.22 0.04 -0.20 0.32 0.04

55 1 0.00 0.03 0.01 -0.14 0.07 0.02 -0.01 -0.04 -0.01

56 1 0.00 0.04 0.02 -0.13 -0.09 -0.02 0.02 -0.05 -0.01

57 1 -0.04 -0.18 -0.09 0.04 0.17 0.08 -0.01 -0.03 -0.02

58 1 -0.12 -0.09 0.03 0.12 0.09 -0.04 -0.01 0.01 0.01

59 1 0.02 -0.02 -0.03 -0.03 0.02 0.04 0.01 -0.01 -0.02

60 1 -0.00 0.02 0.02 -0.01 -0.04 -0.03 0.07 0.12 0.04

61 1 0.05 0.01 -0.02 -0.09 -0.03 0.04 0.14 0.06 -0.06

62 1 -0.02 -0.02 -0.03 -0.02 -0.02 -0.04 -0.01 -0.01 -0.02

63 1 0.13 -0.07 0.04 0.13 -0.07 0.04 0.01 0.01 0.01

64 1 0.07 -0.18 -0.08 0.06 -0.17 -0.08 0.01 -0.03 -0.02

65 1 -0.05 0.00 -0.03 -0.10 0.02 -0.05 -0.15 0.04 -0.06

66 1 0.00 0.02 0.02 -0.02 0.05 0.03 -0.08 0.11 0.04

67 1 0.05 -0.00 -0.03 0.10 -0.02 -0.05 -0.15 0.04 0.06

68 1 -0.00 -0.02 0.02 0.02 -0.05 0.03 -0.08 0.11 -0.04

69 1 0.02 0.02 -0.03 0.02 0.02 -0.04 -0.01 -0.01 0.02

70 1 -0.13 0.07 0.04 -0.13 0.07 0.04 0.01 0.01 -0.01

71 1 -0.07 0.18 -0.08 -0.06 0.17 -0.08 0.01 -0.03 0.02

72 1 -0.05 -0.01 -0.02 0.09 0.03 0.04 0.14 0.06 0.06

73 1 0.00 -0.02 0.02 0.01 0.04 -0.03 0.07 0.12 -0.04

74 1 -0.02 0.02 -0.03 0.03 -0.02 0.04 0.01 -0.01 0.02

75 1 0.12 0.09 0.03 -0.12 -0.09 -0.04 -0.01 0.01 -0.01

76 1 0.04 0.18 -0.09 -0.04 -0.17 0.08 -0.01 -0.03 0.02

77 1 -0.01 0.13 -0.04 0.15 0.01 -0.00 0.01 -0.05 0.02

78 1 0.01 -0.13 -0.04 -0.15 -0.01 -0.00 0.01 -0.05 -0.02

157 158 159

A A A

Frequencies -- 1315.7720 1318.8439 1320.8846

Red. masses -- 4.3800 4.2769 5.4365

Frc consts -- 4.4677 4.3829 5.5885

IR Inten -- 57.6555 1.0277 0.2091

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 0.01 -0.01 -0.02 0.04 -0.01 -0.04 -0.00 -0.00

2 6 -0.02 0.01 0.00 -0.02 -0.06 0.02 -0.05 0.01 -0.00

3 7 -0.01 0.00 -0.00 0.00 0.02 -0.00 0.00 -0.03 0.01

4 6 -0.02 -0.03 0.00 0.03 -0.06 0.02 0.05 0.02 0.00

5 6 0.01 -0.00 0.00 0.01 0.04 -0.01 0.04 0.00 0.00

6 6 0.03 0.02 0.01 0.01 -0.05 -0.01 0.01 -0.00 -0.01

7 6 -0.04 0.02 -0.01 -0.02 0.02 -0.00 -0.06 -0.03 -0.01

8 7 0.02 0.00 0.00 -0.00 0.02 0.00 0.05 0.00 0.01

9 6 -0.03 -0.02 -0.01 0.02 0.02 0.00 -0.07 0.02 -0.01

10 6 0.02 0.01 0.01 0.04 0.02 0.01 0.02 0.01 0.00

11 6 0.01 0.00 0.00 -0.05 0.02 -0.01 0.02 -0.01 0.00

12 6 0.03 -0.03 -0.01 -0.01 -0.05 -0.01 -0.02 0.00 -0.01

13 6 -0.03 -0.02 0.01 0.02 0.02 -0.00 0.07 -0.02 -0.01

14 6 0.02 0.01 -0.01 0.04 0.02 -0.01 -0.02 -0.01 0.00

15 6 0.01 0.00 -0.00 -0.05 0.02 0.01 -0.02 0.01 0.00

16 6 -0.04 0.02 0.01 -0.02 0.02 0.00 0.06 0.03 -0.01

17 7 0.02 0.00 -0.00 -0.00 0.02 0.00 -0.05 -0.00 0.01

18 6 0.03 0.02 -0.01 0.01 -0.05 0.01 -0.01 0.00 -0.01

19 6 -0.02 -0.03 -0.00 0.03 -0.06 -0.02 -0.05 -0.02 0.00

20 6 0.01 -0.00 -0.00 0.01 0.04 0.01 -0.04 -0.00 0.00

21 6 0.01 0.01 0.01 -0.02 0.04 0.01 0.04 0.00 -0.00

22 6 -0.02 0.01 -0.00 -0.02 -0.06 -0.02 0.05 -0.01 -0.00

23 7 -0.01 0.00 0.00 0.00 0.02 0.00 -0.00 0.03 0.01

24 6 0.03 -0.03 0.01 -0.01 -0.05 0.01 0.02 -0.00 -0.01

25 6 0.07 -0.09 -0.12 -0.08 0.09 0.12 -0.11 0.08 0.13

26 6 0.01 0.06 0.04 -0.01 -0.07 -0.04 -0.02 -0.08 -0.05

27 6 -0.07 -0.03 0.04 0.08 0.04 -0.04 0.09 0.04 -0.04

28 6 0.04 -0.03 -0.06 -0.04 0.03 0.06 -0.04 0.04 0.07

29 6 0.03 0.08 0.04 -0.03 -0.09 -0.04 -0.02 -0.09 -0.05

30 6 -0.07 -0.03 0.04 0.08 0.03 -0.04 0.08 0.03 -0.05

31 6 0.04 0.04 0.06 0.03 0.03 0.05 0.04 0.05 0.07

32 6 -0.09 0.02 -0.05 -0.07 0.02 -0.04 -0.10 0.03 -0.04

33 6 0.02 -0.07 -0.05 0.02 -0.06 -0.04 0.03 -0.09 -0.05

34 6 0.06 0.11 0.14 0.06 0.08 0.10 0.10 0.09 0.14

35 6 -0.09 0.02 -0.05 -0.07 0.01 -0.04 -0.08 0.02 -0.05

36 6 0.04 -0.08 -0.04 0.03 -0.07 -0.03 0.04 -0.09 -0.05

37 6 0.06 0.11 -0.14 0.06 0.08 -0.10 -0.10 -0.09 0.14

38 6 -0.09 0.02 0.05 -0.07 0.01 0.04 0.08 -0.02 -0.05

39 6 0.04 -0.08 0.04 0.03 -0.07 0.03 -0.04 0.09 -0.05

40 6 0.04 0.04 -0.06 0.03 0.03 -0.05 -0.04 -0.05 0.07

41 6 -0.09 0.02 0.05 -0.07 0.02 0.04 0.10 -0.03 -0.04

42 6 0.02 -0.07 0.05 0.02 -0.06 0.04 -0.03 0.09 -0.05

43 6 0.07 -0.09 0.12 -0.08 0.09 -0.12 0.11 -0.08 0.13

44 6 -0.07 -0.03 -0.04 0.08 0.03 0.04 -0.08 -0.03 -0.05

45 6 0.03 0.08 -0.04 -0.03 -0.09 0.04 0.02 0.09 -0.05

46 6 0.04 -0.03 0.06 -0.04 0.03 -0.06 0.04 -0.04 0.07

47 6 -0.07 -0.03 -0.04 0.08 0.04 0.04 -0.09 -0.04 -0.04

48 6 0.01 0.06 -0.04 -0.01 -0.07 0.04 0.02 0.08 -0.05

49 1 -0.09 -0.07 0.02 -0.02 0.05 -0.01 -0.01 0.03 -0.01

50 1 -0.10 0.07 -0.03 0.03 0.04 -0.01 -0.00 0.04 -0.01

51 1 -0.02 -0.05 -0.01 -0.12 -0.23 -0.04 0.03 0.03 0.01

52 1 0.01 0.00 -0.00 0.15 -0.22 0.04 0.03 -0.01 0.01

53 1 -0.02 -0.05 0.01 -0.12 -0.23 0.04 -0.03 -0.03 0.01

54 1 0.01 0.00 0.00 0.15 -0.22 -0.04 -0.03 0.01 0.01

55 1 -0.10 0.07 0.03 0.03 0.04 0.01 0.00 -0.04 -0.01

56 1 -0.09 -0.07 -0.02 -0.02 0.05 0.01 0.01 -0.03 -0.01

57 1 0.05 0.17 0.09 -0.04 -0.14 -0.08 -0.04 -0.14 -0.08

58 1 0.16 0.11 -0.06 -0.16 -0.10 0.06 -0.16 -0.09 0.06

59 1 -0.03 0.03 0.05 0.04 -0.03 -0.06 0.04 -0.03 -0.06

60 1 -0.05 -0.13 -0.06 0.06 0.14 0.06 0.08 0.18 0.07

61 1 -0.12 -0.05 0.07 0.11 0.05 -0.07 0.15 0.07 -0.08

62 1 -0.03 -0.03 -0.06 -0.02 -0.03 -0.05 -0.03 -0.04 -0.06

63 1 0.20 -0.09 0.07 0.15 -0.07 0.05 0.16 -0.07 0.06

64 1 0.08 -0.18 -0.10 0.05 -0.11 -0.06 0.05 -0.12 -0.07

65 1 -0.13 0.04 -0.08 -0.10 0.03 -0.06 -0.16 0.05 -0.09

66 1 -0.07 0.13 0.06 -0.06 0.11 0.05 -0.11 0.17 0.07

67 1 -0.13 0.04 0.08 -0.10 0.03 0.06 0.16 -0.05 -0.09

68 1 -0.07 0.13 -0.06 -0.06 0.11 -0.05 0.11 -0.17 0.07

69 1 -0.03 -0.03 0.06 -0.02 -0.03 0.05 0.03 0.04 -0.06

70 1 0.20 -0.09 -0.07 0.15 -0.07 -0.05 -0.16 0.07 0.06

71 1 0.08 -0.18 0.10 0.05 -0.11 0.06 -0.05 0.12 -0.07

72 1 -0.12 -0.05 -0.07 0.11 0.05 0.07 -0.15 -0.07 -0.08

73 1 -0.05 -0.13 0.06 0.06 0.14 -0.06 -0.08 -0.18 0.07

74 1 -0.03 0.03 -0.05 0.04 -0.03 0.06 -0.04 0.03 -0.06

75 1 0.16 0.11 0.06 -0.16 -0.10 -0.06 0.16 0.09 0.06

76 1 0.05 0.17 -0.09 -0.04 -0.14 0.08 0.04 0.14 -0.08

77 1 0.16 0.01 -0.00 -0.01 0.02 -0.01 -0.00 -0.03 0.01

78 1 0.16 0.01 0.00 -0.01 0.02 0.01 0.00 0.03 0.01

160 161 162

A A A

Frequencies -- 1324.1336 1333.6371 1354.9120

Red. masses -- 5.4298 3.3257 2.9376

Frc consts -- 5.6091 3.4850 3.1773

IR Inten -- 0.0008 0.0000 421.1326

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 -0.03 0.01 0.02 0.01 -0.01 0.01 0.00 -0.00

2 6 -0.05 -0.00 0.01 -0.02 0.04 -0.00 -0.03 0.00 0.00

3 7 -0.04 -0.00 0.00 0.02 0.00 0.00 -0.04 -0.00 -0.00

4 6 -0.05 -0.01 -0.01 -0.01 -0.04 0.00 -0.03 -0.01 -0.00

5 6 0.01 0.03 -0.01 0.02 -0.01 0.01 0.01 0.00 0.00

6 6 0.15 0.10 -0.00 0.00 0.13 -0.00 0.09 0.04 0.01

7 6 -0.02 -0.03 0.01 0.03 -0.01 0.01 -0.08 -0.02 -0.01

8 7 0.00 -0.03 0.00 0.01 -0.07 -0.00 0.07 0.00 0.01

9 6 0.02 -0.03 -0.01 -0.03 -0.02 -0.01 -0.09 0.01 -0.01

10 6 -0.01 0.01 0.00 -0.07 -0.03 -0.02 0.02 0.02 0.01

11 6 0.01 0.01 0.00 0.07 -0.02 0.02 0.02 -0.02 0.01

12 6 0.16 -0.08 0.00 0.02 -0.13 0.00 0.10 -0.03 -0.01

13 6 -0.02 0.03 -0.01 0.03 0.02 -0.01 -0.09 0.01 0.01

14 6 0.01 -0.01 0.00 0.07 0.03 -0.02 0.02 0.02 -0.01

15 6 -0.01 -0.01 0.00 -0.07 0.02 0.02 0.02 -0.02 -0.01

16 6 0.02 0.03 0.01 -0.03 0.01 0.01 -0.08 -0.02 0.01

17 7 -0.00 0.03 0.00 -0.01 0.07 -0.00 0.07 0.00 -0.01

18 6 -0.15 -0.10 -0.00 -0.00 -0.13 -0.00 0.09 0.04 -0.01

19 6 0.05 0.01 -0.01 0.01 0.04 0.00 -0.03 -0.01 0.00

20 6 -0.01 -0.03 -0.01 -0.02 0.01 0.01 0.01 0.00 -0.00

21 6 -0.01 0.03 0.01 -0.02 -0.01 -0.01 0.01 0.00 0.00

22 6 0.05 0.00 0.01 0.02 -0.04 -0.00 -0.03 0.00 -0.00

23 7 0.04 0.00 0.00 -0.02 -0.00 0.00 -0.04 -0.00 0.00

24 6 -0.16 0.08 0.00 -0.02 0.13 0.00 0.10 -0.03 0.01

25 6 -0.16 -0.04 0.09 -0.00 -0.08 -0.04 -0.04 -0.03 -0.00

26 6 -0.02 -0.09 -0.04 0.01 0.03 0.02 -0.03 -0.07 -0.02

27 6 0.06 0.06 -0.01 -0.04 -0.01 0.03 0.03 0.03 0.00

28 6 -0.03 0.03 0.05 0.03 -0.02 -0.04 -0.03 0.02 0.05

29 6 0.01 -0.06 -0.06 0.03 0.05 0.01 -0.00 -0.03 -0.02

30 6 0.03 0.01 -0.02 -0.06 -0.03 0.02 0.03 0.03 -0.01

31 6 -0.03 -0.03 -0.05 0.02 0.02 0.04 -0.03 -0.04 -0.06

32 6 0.07 -0.05 0.01 -0.04 0.00 -0.03 0.03 -0.03 -0.00

33 6 -0.03 0.08 0.04 0.01 -0.03 -0.01 -0.05 0.07 0.03

34 6 -0.15 0.02 -0.08 -0.02 0.09 0.04 -0.04 0.03 0.01

35 6 0.03 -0.00 0.02 -0.06 0.02 -0.02 0.05 -0.03 0.01

36 6 0.00 0.06 0.05 0.04 -0.04 -0.01 -0.01 0.03 0.02

37 6 0.15 -0.02 -0.08 0.02 -0.09 0.04 -0.04 0.03 -0.01

38 6 -0.03 0.00 0.02 0.06 -0.02 -0.02 0.05 -0.03 -0.01

39 6 -0.00 -0.06 0.05 -0.04 0.04 -0.01 -0.01 0.03 -0.02

40 6 0.03 0.03 -0.05 -0.02 -0.02 0.04 -0.03 -0.04 0.06

41 6 -0.07 0.05 0.01 0.04 -0.00 -0.03 0.03 -0.03 0.00

42 6 0.03 -0.08 0.04 -0.01 0.03 -0.01 -0.05 0.07 -0.03

43 6 0.16 0.04 0.09 0.00 0.08 -0.04 -0.04 -0.03 0.00

44 6 -0.03 -0.01 -0.02 0.06 0.03 0.02 0.03 0.03 0.01

45 6 -0.01 0.06 -0.06 -0.03 -0.05 0.01 -0.00 -0.03 0.02

46 6 0.03 -0.03 0.05 -0.03 0.02 -0.04 -0.03 0.02 -0.05

47 6 -0.06 -0.06 -0.01 0.04 0.01 0.03 0.03 0.03 -0.00

48 6 0.02 0.09 -0.04 -0.01 -0.03 0.02 -0.03 -0.07 0.02

49 1 0.07 0.02 -0.01 -0.12 -0.10 0.03 -0.02 -0.02 0.01

50 1 0.07 -0.01 0.01 -0.14 0.09 -0.03 -0.02 0.02 -0.01

51 1 -0.03 -0.02 -0.01 0.16 0.33 0.05 0.01 -0.00 0.00

52 1 0.03 -0.01 0.01 -0.21 0.31 -0.05 0.01 -0.00 0.00

53 1 0.03 0.02 -0.01 -0.16 -0.33 0.05 0.01 -0.00 -0.00

54 1 -0.03 0.01 0.01 0.21 -0.31 -0.05 0.01 -0.00 -0.00

55 1 -0.07 0.01 0.01 0.14 -0.09 -0.03 -0.02 0.02 0.01

56 1 -0.07 -0.02 -0.01 0.12 0.10 0.03 -0.02 -0.02 -0.01

57 1 0.01 0.02 -0.01 0.02 0.05 0.03 0.08 0.24 0.12

58 1 -0.02 0.02 0.03 0.10 0.08 -0.03 0.10 0.07 -0.03

59 1 0.03 -0.01 -0.04 -0.02 0.02 0.04 0.06 -0.05 -0.10

60 1 0.12 0.23 0.08 0.02 0.00 -0.01 0.01 -0.01 -0.01

61 1 0.21 0.10 -0.10 0.08 0.03 -0.02 -0.13 -0.06 0.06

62 1 0.02 0.02 0.04 -0.02 -0.02 -0.03 0.07 0.07 0.13

63 1 0.01 -0.03 -0.02 0.12 -0.06 0.03 0.14 -0.07 0.04

64 1 0.02 -0.05 -0.01 0.03 -0.05 -0.03 0.14 -0.29 -0.14

65 1 0.20 -0.06 0.10 0.08 -0.02 0.02 -0.19 0.07 -0.09

66 1 0.14 -0.19 -0.06 0.01 0.00 0.01 -0.01 0.04 0.02

67 1 -0.20 0.06 0.10 -0.08 0.02 0.02 -0.19 0.07 0.09

68 1 -0.14 0.19 -0.06 -0.01 -0.00 0.01 -0.01 0.04 -0.02

69 1 -0.02 -0.02 0.04 0.02 0.02 -0.03 0.07 0.07 -0.13

70 1 -0.01 0.03 -0.02 -0.12 0.06 0.03 0.14 -0.07 -0.04

71 1 -0.02 0.05 -0.01 -0.03 0.05 -0.03 0.14 -0.29 0.14

72 1 -0.21 -0.10 -0.10 -0.08 -0.03 -0.02 -0.13 -0.06 -0.06

73 1 -0.12 -0.23 0.08 -0.02 -0.00 -0.01 0.01 -0.01 0.01

74 1 -0.03 0.01 -0.04 0.02 -0.02 0.04 0.06 -0.05 0.10

75 1 0.02 -0.02 0.03 -0.10 -0.08 -0.03 0.10 0.07 0.03

76 1 -0.01 -0.02 -0.01 -0.02 -0.05 0.03 0.08 0.24 -0.12

77 1 0.14 0.01 -0.00 0.02 0.00 0.00 0.23 0.01 0.00

78 1 -0.14 -0.01 -0.00 -0.02 -0.00 0.00 0.23 0.01 -0.00

163 164 165

A A A

Frequencies -- 1359.4776 1359.6629 1360.7039

Red. masses -- 1.5071 1.4913 1.4610

Frc consts -- 1.6411 1.6243 1.5938

IR Inten -- 2.2935 1.8979 0.0129

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 0.00 0.00 -0.00

2 6 0.00 0.01 -0.00 -0.01 -0.00 0.00 -0.00 0.00 -0.00

3 7 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 0.00

4 6 -0.01 0.01 -0.00 0.01 -0.00 0.00 -0.00 -0.00 -0.00

5 6 -0.00 -0.01 0.00 0.01 0.00 -0.00 0.00 -0.00 0.00

6 6 -0.00 0.00 0.01 -0.00 -0.00 -0.00 -0.01 0.01 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 -0.01 -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 -0.01 -0.01 -0.00

11 6 0.00 -0.00 0.00 0.00 -0.00 0.00 0.02 -0.01 0.00

12 6 0.00 -0.00 0.00 -0.00 -0.00 -0.01 -0.01 -0.01 -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 0.01 0.01 -0.00

15 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.02 0.01 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 0.01 -0.00

18 6 -0.00 0.00 -0.01 0.00 0.00 -0.00 0.01 -0.01 0.00

19 6 -0.01 0.01 0.00 -0.01 0.00 0.00 0.00 0.00 -0.00

20 6 -0.00 -0.01 -0.00 -0.01 -0.00 -0.00 -0.00 0.00 0.00

21 6 0.01 -0.01 -0.00 0.01 -0.00 -0.00 -0.00 -0.00 -0.00

22 6 0.00 0.01 0.00 0.01 0.00 0.00 0.00 -0.00 -0.00

23 7 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00

24 6 0.00 -0.00 -0.00 0.00 0.00 -0.01 0.01 0.01 -0.00

25 6 0.01 -0.01 -0.02 -0.01 0.01 0.02 0.01 -0.02 -0.02

26 6 -0.03 -0.05 -0.02 0.02 0.04 0.01 -0.03 -0.05 -0.02

27 6 0.01 0.01 -0.00 -0.01 -0.01 -0.00 0.01 0.01 0.00

28 6 -0.03 0.02 0.05 0.02 -0.02 -0.04 -0.03 0.02 0.04

29 6 -0.01 -0.02 -0.00 0.01 0.01 0.00 -0.01 -0.01 -0.00

30 6 0.05 0.04 -0.01 -0.04 -0.03 0.01 0.04 0.04 -0.01

31 6 0.02 0.02 0.04 -0.03 -0.03 -0.05 -0.02 -0.02 -0.04

32 6 -0.01 0.01 -0.00 0.01 -0.01 0.00 0.01 -0.01 -0.00

33 6 0.03 -0.04 -0.01 -0.04 0.05 0.02 -0.03 0.04 0.01

34 6 -0.01 -0.01 -0.02 0.01 0.01 0.02 0.01 0.01 0.02

35 6 -0.04 0.03 -0.01 0.05 -0.03 0.01 0.04 -0.02 0.01

36 6 0.01 -0.01 -0.00 -0.01 0.01 0.00 -0.01 0.01 0.00

37 6 -0.01 -0.01 0.02 -0.01 -0.01 0.02 -0.01 -0.01 0.02

38 6 -0.04 0.02 0.01 -0.05 0.03 0.01 -0.04 0.02 0.01

39 6 0.01 -0.01 0.00 0.01 -0.01 0.00 0.01 -0.01 0.00

40 6 0.02 0.02 -0.04 0.03 0.03 -0.05 0.02 0.02 -0.04

41 6 -0.01 0.01 0.00 -0.01 0.01 0.00 -0.01 0.01 -0.00

42 6 0.03 -0.04 0.01 0.04 -0.05 0.02 0.03 -0.04 0.01

43 6 0.01 -0.01 0.02 0.01 -0.01 0.02 -0.01 0.02 -0.02

44 6 0.05 0.04 0.01 0.04 0.03 0.01 -0.04 -0.04 -0.01

45 6 -0.01 -0.02 0.00 -0.01 -0.01 0.00 0.01 0.01 -0.00

46 6 -0.03 0.02 -0.05 -0.03 0.02 -0.04 0.03 -0.02 0.04

47 6 0.01 0.01 0.00 0.01 0.01 -0.00 -0.01 -0.01 0.00

48 6 -0.03 -0.05 0.02 -0.02 -0.04 0.01 0.03 0.05 -0.02

49 1 0.00 -0.01 0.00 0.00 0.01 -0.00 -0.03 -0.02 0.01

50 1 -0.00 -0.01 0.00 -0.01 0.02 -0.00 -0.03 0.01 -0.01

51 1 0.01 0.02 0.00 0.00 0.01 0.00 0.03 0.07 0.01

52 1 -0.01 0.02 -0.00 -0.00 0.00 0.00 -0.04 0.06 -0.01

53 1 0.01 0.02 -0.00 -0.00 -0.01 0.00 -0.03 -0.07 0.01

54 1 -0.01 0.02 0.00 0.00 -0.00 0.00 0.04 -0.06 -0.01

55 1 -0.00 -0.01 -0.00 0.01 -0.02 -0.00 0.03 -0.01 -0.01

56 1 0.00 -0.01 -0.00 -0.00 -0.01 -0.00 0.03 0.02 0.01

57 1 0.09 0.27 0.14 -0.08 -0.23 -0.12 0.09 0.27 0.14

58 1 0.12 0.08 -0.05 -0.10 -0.06 0.04 0.13 0.08 -0.05

59 1 0.09 -0.07 -0.14 -0.07 0.06 0.11 0.09 -0.07 -0.13

60 1 -0.05 -0.13 -0.05 0.04 0.11 0.04 -0.05 -0.13 -0.06

61 1 -0.26 -0.14 0.13 0.21 0.11 -0.10 -0.25 -0.14 0.12

62 1 -0.06 -0.07 -0.11 0.08 0.08 0.14 0.06 0.07 0.11

63 1 -0.11 0.05 -0.04 0.13 -0.06 0.05 0.12 -0.05 0.04

64 1 -0.11 0.21 0.11 0.13 -0.25 -0.13 0.11 -0.21 -0.11

65 1 0.23 -0.09 0.11 -0.28 0.10 -0.13 -0.22 0.08 -0.11

66 1 0.06 -0.10 -0.04 -0.07 0.12 0.05 -0.06 0.10 0.04

67 1 0.23 -0.08 -0.11 0.28 -0.10 -0.13 0.22 -0.08 -0.11

68 1 0.06 -0.10 0.04 0.07 -0.12 0.05 0.06 -0.10 0.04

69 1 -0.06 -0.07 0.11 -0.08 -0.08 0.14 -0.06 -0.07 0.11

70 1 -0.11 0.05 0.04 -0.13 0.06 0.05 -0.12 0.05 0.04

71 1 -0.10 0.21 -0.11 -0.13 0.26 -0.14 -0.11 0.21 -0.11

72 1 -0.26 -0.14 -0.13 -0.22 -0.12 -0.11 0.25 0.14 0.12

73 1 -0.05 -0.13 0.05 -0.04 -0.11 0.05 0.05 0.13 -0.06

74 1 0.09 -0.07 0.14 0.07 -0.06 0.11 -0.09 0.07 -0.13

75 1 0.12 0.07 0.05 0.10 0.06 0.04 -0.13 -0.08 -0.05

76 1 0.09 0.27 -0.14 0.08 0.23 -0.12 -0.09 -0.27 0.14

77 1 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.01 -0.00 0.00

78 1 0.00 -0.00 -0.00 0.00 0.00 0.00 0.01 0.00 0.00

166 167 168

A A A

Frequencies -- 1363.5640 1378.5103 1388.9625

Red. masses -- 1.9726 6.0948 3.3374

Frc consts -- 2.1609 6.8238 3.7935

IR Inten -- 352.5802 349.7240 0.0001

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 -0.00 -0.00 -0.23 -0.08 0.02 -0.01 -0.12 0.03

2 6 -0.02 -0.00 0.00 -0.08 0.11 -0.02 -0.10 0.09 -0.02

3 7 -0.03 -0.00 -0.00 0.00 -0.10 0.02 0.19 0.01 0.00

4 6 -0.02 -0.00 -0.00 0.07 0.12 -0.02 -0.09 -0.09 0.02

5 6 0.00 0.00 0.00 0.24 -0.05 0.02 -0.03 0.11 -0.03

6 6 0.07 0.03 0.00 -0.11 -0.09 -0.01 0.01 -0.01 0.00

7 6 -0.06 -0.03 -0.01 0.01 0.05 -0.00 -0.01 0.01 -0.00

8 7 0.05 0.00 0.01 -0.00 0.01 0.00 -0.00 0.01 -0.00

9 6 -0.06 0.02 -0.01 -0.02 0.05 0.00 0.01 0.01 0.00

10 6 0.01 0.02 0.00 -0.00 -0.02 -0.00 -0.00 -0.00 -0.00

11 6 0.02 -0.02 0.00 0.00 -0.02 0.00 0.00 -0.00 0.00

12 6 0.07 -0.02 0.00 0.12 -0.08 -0.00 0.01 0.01 -0.00

13 6 -0.06 0.02 0.01 -0.02 0.05 -0.00 -0.01 -0.01 0.00

14 6 0.01 0.02 -0.00 -0.00 -0.02 0.00 0.00 0.00 -0.00

15 6 0.02 -0.02 -0.00 0.00 -0.02 -0.00 -0.00 0.00 0.00

16 6 -0.06 -0.03 0.01 0.01 0.05 0.00 0.01 -0.01 -0.00

17 7 0.05 0.00 -0.01 -0.00 0.01 -0.00 0.00 -0.01 -0.00

18 6 0.07 0.03 -0.00 -0.11 -0.09 0.01 -0.01 0.01 0.00

19 6 -0.02 -0.00 0.00 0.07 0.12 0.02 0.09 0.09 0.02

20 6 0.00 0.00 -0.00 0.24 -0.05 -0.02 0.03 -0.11 -0.03

21 6 0.01 -0.00 0.00 -0.23 -0.08 -0.02 0.01 0.12 0.03

22 6 -0.02 -0.00 -0.00 -0.08 0.11 0.02 0.10 -0.09 -0.02

23 7 -0.03 -0.00 0.00 0.00 -0.10 -0.02 -0.19 -0.01 0.00

24 6 0.07 -0.02 -0.00 0.12 -0.08 0.00 -0.01 -0.01 -0.00

25 6 -0.05 -0.01 0.02 0.04 0.06 0.01 0.01 0.00 -0.00

26 6 0.02 0.02 0.01 0.01 0.02 0.01 0.00 0.01 0.00

27 6 0.00 0.01 0.00 0.00 -0.01 -0.02 -0.00 -0.00 -0.00

28 6 0.02 -0.01 -0.03 -0.00 -0.00 -0.00 0.00 -0.00 -0.00

29 6 0.01 -0.00 -0.01 -0.02 -0.00 0.01 -0.00 0.00 0.00

30 6 -0.04 -0.03 0.01 0.02 0.01 -0.01 0.00 0.00 -0.00

31 6 0.02 0.02 0.03 0.00 -0.00 0.00 0.00 0.00 0.00

32 6 0.00 -0.00 -0.00 -0.00 -0.02 -0.02 -0.00 0.00 0.00

33 6 0.02 -0.02 -0.01 -0.01 0.02 0.01 0.00 -0.00 -0.00

34 6 -0.05 0.00 -0.02 -0.05 0.05 0.00 0.01 -0.00 0.00

35 6 -0.05 0.03 -0.01 -0.02 0.01 -0.01 0.00 -0.00 0.00

36 6 0.01 0.00 0.01 0.02 -0.00 0.01 -0.00 -0.00 -0.00

37 6 -0.05 0.00 0.02 -0.05 0.05 -0.00 -0.01 0.00 0.00

38 6 -0.05 0.03 0.01 -0.02 0.01 0.01 -0.00 0.00 0.00

39 6 0.01 0.00 -0.01 0.02 -0.00 -0.01 0.00 0.00 -0.00

40 6 0.02 0.02 -0.03 0.00 -0.00 -0.00 -0.00 -0.00 0.00

41 6 0.00 -0.00 0.00 -0.00 -0.02 0.02 0.00 -0.00 0.00

42 6 0.02 -0.02 0.01 -0.01 0.02 -0.01 -0.00 0.00 -0.00

43 6 -0.05 -0.01 -0.02 0.04 0.06 -0.01 -0.01 -0.00 -0.00

44 6 -0.04 -0.03 -0.01 0.02 0.01 0.01 -0.00 -0.00 -0.00

45 6 0.01 -0.00 0.01 -0.02 -0.00 -0.01 0.00 -0.00 0.00

46 6 0.02 -0.01 0.03 -0.00 -0.00 0.00 -0.00 0.00 -0.00

47 6 0.00 0.01 -0.00 0.00 -0.01 0.02 0.00 0.00 -0.00

48 6 0.02 0.02 -0.01 0.01 0.02 -0.01 -0.00 -0.01 0.00

49 1 -0.00 -0.01 0.00 0.15 0.25 -0.07 0.21 0.06 -0.01

50 1 0.00 0.00 -0.00 -0.19 0.23 -0.08 0.22 -0.04 0.02

51 1 0.00 0.01 0.00 0.05 0.06 0.01 0.01 0.01 -0.00

52 1 0.01 -0.01 0.00 -0.05 0.05 -0.01 -0.01 0.01 -0.00

53 1 0.00 0.01 -0.00 0.05 0.06 -0.01 -0.01 -0.01 -0.00

54 1 0.01 -0.01 -0.00 -0.05 0.05 0.01 0.01 -0.01 -0.00

55 1 0.00 0.00 0.00 -0.19 0.23 0.08 -0.22 0.04 0.02

56 1 -0.00 -0.01 -0.00 0.15 0.25 0.07 -0.21 -0.06 -0.01

57 1 -0.06 -0.16 -0.09 -0.03 -0.10 -0.05 -0.00 -0.02 -0.01

58 1 -0.08 -0.04 0.04 -0.07 -0.06 0.02 -0.00 -0.00 -0.00

59 1 -0.07 0.06 0.10 -0.01 -0.00 0.01 0.00 -0.00 -0.00

60 1 0.07 0.15 0.06 -0.04 -0.05 -0.01 -0.01 -0.02 -0.00

61 1 0.23 0.13 -0.11 -0.06 -0.03 0.02 -0.02 -0.01 0.01

62 1 -0.07 -0.08 -0.12 0.00 -0.01 -0.00 0.00 0.00 0.00

63 1 -0.11 0.04 -0.05 0.07 -0.05 0.01 -0.00 0.00 0.00

64 1 -0.10 0.19 0.11 0.04 -0.08 -0.04 -0.01 0.01 0.01

65 1 0.28 -0.11 0.14 0.08 -0.03 0.03 -0.02 0.01 -0.01

66 1 0.10 -0.16 -0.06 0.05 -0.06 -0.01 -0.01 0.01 0.00

67 1 0.28 -0.11 -0.14 0.08 -0.03 -0.03 0.02 -0.01 -0.01

68 1 0.10 -0.16 0.06 0.05 -0.06 0.01 0.01 -0.01 0.00

69 1 -0.07 -0.08 0.12 0.00 -0.01 0.00 -0.00 -0.00 0.00

70 1 -0.11 0.04 0.05 0.07 -0.05 -0.01 0.00 -0.00 0.00

71 1 -0.10 0.19 -0.11 0.04 -0.08 0.04 0.01 -0.01 0.01

72 1 0.23 0.13 0.11 -0.06 -0.03 -0.02 0.02 0.01 0.01

73 1 0.07 0.15 -0.06 -0.04 -0.05 0.01 0.01 0.02 -0.00

74 1 -0.07 0.06 -0.11 -0.01 -0.00 -0.01 -0.00 0.00 -0.00

75 1 -0.08 -0.04 -0.04 -0.07 -0.06 -0.02 0.00 0.00 -0.00

76 1 -0.06 -0.16 0.09 -0.03 -0.10 0.05 0.00 0.02 -0.01

77 1 0.16 0.01 -0.00 0.01 -0.10 0.04 -0.54 -0.04 0.00

78 1 0.16 0.01 0.00 0.01 -0.10 -0.04 0.54 0.04 0.00

169 170 171

A A A

Frequencies -- 1396.5880 1411.1841 1411.3255

Red. masses -- 5.9532 7.7967 4.1869

Frc consts -- 6.8413 9.1481 4.9135

IR Inten -- 0.7202 0.2928 450.6893

Atom AN X Y Z X Y Z X Y Z

1 6 -0.24 -0.06 0.01 0.10 -0.11 0.03 -0.02 -0.14 0.04

2 6 -0.09 0.04 -0.01 0.01 0.29 -0.07 -0.12 0.11 -0.03

3 7 0.00 -0.06 0.01 0.01 -0.14 0.03 0.19 0.01 0.00

4 6 0.08 0.06 -0.01 -0.05 0.29 -0.07 -0.10 -0.13 0.03

5 6 0.25 -0.02 0.01 -0.08 -0.13 0.03 -0.03 0.14 -0.04

6 6 -0.12 -0.06 -0.01 -0.01 -0.02 0.00 0.03 0.01 0.00

7 6 0.08 0.07 0.01 0.11 -0.10 0.02 -0.01 0.01 -0.00

8 7 -0.07 -0.00 -0.01 -0.04 -0.00 -0.01 0.00 -0.00 0.00

9 6 0.08 -0.07 0.01 0.10 0.12 0.02 -0.01 -0.01 0.00

10 6 -0.01 -0.03 -0.00 -0.04 0.02 -0.01 -0.01 0.02 -0.00

11 6 -0.02 0.03 -0.00 -0.04 -0.03 -0.01 0.00 -0.02 0.00

12 6 0.13 -0.04 -0.01 0.02 -0.02 0.00 0.04 -0.01 -0.00

13 6 -0.08 0.07 0.01 -0.10 -0.12 0.02 -0.01 -0.01 -0.00

14 6 0.01 0.03 -0.00 0.04 -0.02 -0.01 -0.01 0.02 0.00

15 6 0.02 -0.03 -0.00 0.04 0.03 -0.01 0.00 -0.02 -0.00

16 6 -0.08 -0.07 0.01 -0.11 0.10 0.02 -0.01 0.01 0.00

17 7 0.07 0.00 -0.01 0.04 0.00 -0.01 0.00 -0.00 -0.00

18 6 0.12 0.06 -0.01 0.01 0.02 0.00 0.03 0.01 -0.00

19 6 -0.08 -0.06 -0.01 0.05 -0.29 -0.07 -0.10 -0.13 -0.03

20 6 -0.25 0.02 0.01 0.08 0.13 0.03 -0.03 0.14 0.04

21 6 0.24 0.06 0.01 -0.10 0.11 0.03 -0.02 -0.14 -0.04

22 6 0.09 -0.04 -0.01 -0.01 -0.29 -0.07 -0.12 0.11 0.03

23 7 -0.00 0.06 0.01 -0.00 0.14 0.03 0.19 0.01 -0.00

24 6 -0.13 0.04 -0.01 -0.02 0.02 0.00 0.04 -0.01 0.00

25 6 0.04 0.03 -0.00 -0.00 0.01 -0.00 -0.00 -0.01 -0.00

26 6 0.00 0.02 0.01 0.00 0.00 0.01 0.00 -0.00 -0.00

27 6 -0.01 -0.02 -0.01 0.01 0.00 -0.01 -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 -0.01 0.01 0.02 -0.01 -0.01 -0.00 0.00 0.00 0.00

30 6 0.02 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 0.00

32 6 0.01 -0.01 -0.01 -0.01 0.00 -0.01 -0.00 -0.00 -0.00

33 6 -0.01 0.02 0.00 -0.00 0.01 0.01 0.00 0.00 0.00

34 6 -0.05 0.03 -0.00 -0.00 0.01 -0.00 -0.00 0.01 0.00

35 6 -0.02 0.00 -0.01 -0.01 0.01 -0.00 -0.00 0.00 -0.00

36 6 0.01 0.01 0.02 0.01 -0.01 -0.00 0.00 -0.00 -0.00

37 6 0.05 -0.03 -0.00 0.00 -0.01 -0.00 -0.00 0.01 -0.00

38 6 0.02 -0.00 -0.01 0.01 -0.01 -0.00 -0.00 0.00 0.00

39 6 -0.01 -0.01 0.02 -0.01 0.01 -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 -0.01 0.01 -0.01 0.01 -0.00 -0.01 -0.00 -0.00 0.00

42 6 0.01 -0.02 0.00 0.00 -0.01 0.01 0.00 0.00 -0.00

43 6 -0.04 -0.03 -0.00 0.00 -0.01 -0.00 -0.00 -0.01 0.00

44 6 -0.02 -0.01 -0.01 -0.01 -0.01 -0.00 -0.00 -0.00 -0.00

45 6 0.01 -0.01 0.02 0.01 0.01 -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 0.01 0.02 -0.01 -0.01 -0.00 -0.01 -0.00 -0.00 -0.00

48 6 -0.00 -0.02 0.01 -0.00 -0.00 0.01 0.00 -0.00 0.00

49 1 0.15 0.29 -0.08 -0.03 -0.26 0.07 0.25 0.07 -0.02

50 1 -0.17 0.26 -0.08 0.04 -0.25 0.07 0.25 -0.02 0.02

51 1 -0.02 -0.05 -0.01 -0.03 0.07 -0.00 -0.02 -0.01 -0.01

52 1 -0.01 0.03 -0.00 -0.03 -0.06 -0.01 -0.04 0.03 -0.01

53 1 0.02 0.05 -0.01 0.03 -0.07 -0.00 -0.02 -0.01 0.01

54 1 0.01 -0.03 -0.00 0.03 0.06 -0.01 -0.04 0.03 0.01

55 1 0.17 -0.26 -0.08 -0.04 0.25 0.07 0.25 -0.03 -0.02

56 1 -0.15 -0.29 -0.08 0.03 0.26 0.07 0.25 0.07 0.02

57 1 -0.01 -0.04 -0.02 -0.02 -0.04 -0.02 0.00 0.01 0.00

58 1 -0.01 -0.02 -0.00 -0.05 -0.03 0.02 0.01 0.01 -0.01

59 1 0.01 -0.02 -0.03 -0.02 0.01 0.03 0.00 -0.00 -0.00

60 1 -0.05 -0.09 -0.03 0.00 0.02 0.01 0.00 -0.00 -0.00

61 1 -0.08 -0.05 0.04 -0.01 0.00 0.00 0.00 -0.00 0.00

62 1 -0.01 -0.02 -0.03 0.02 0.02 0.03 0.00 0.00 0.00

63 1 0.01 -0.02 -0.01 0.05 -0.02 0.02 0.01 -0.01 0.00

64 1 0.01 -0.04 -0.01 0.03 -0.04 -0.02 0.00 -0.01 -0.00

65 1 0.10 -0.04 0.04 0.01 0.00 0.01 0.00 0.00 -0.00

66 1 0.06 -0.09 -0.03 -0.01 0.02 0.01 0.00 -0.00 0.00

67 1 -0.10 0.04 0.04 -0.01 -0.00 0.01 0.00 0.00 0.00

68 1 -0.06 0.09 -0.03 0.01 -0.02 0.01 0.00 -0.00 -0.00

69 1 0.01 0.02 -0.03 -0.02 -0.02 0.03 0.00 0.00 -0.00

70 1 -0.01 0.02 -0.01 -0.05 0.02 0.02 0.01 -0.01 -0.00

71 1 -0.01 0.04 -0.01 -0.03 0.04 -0.02 0.00 -0.01 0.00

72 1 0.08 0.05 0.04 0.01 -0.00 0.00 0.00 -0.00 -0.00

73 1 0.05 0.09 -0.03 -0.00 -0.02 0.01 0.00 -0.00 0.00

74 1 -0.01 0.02 -0.03 0.02 -0.01 0.03 0.00 -0.00 0.00

75 1 0.01 0.02 -0.00 0.05 0.03 0.02 0.01 0.01 0.00

76 1 0.01 0.04 -0.02 0.02 0.04 -0.02 0.00 0.01 -0.00

77 1 0.01 -0.06 0.04 0.03 -0.14 0.06 -0.47 -0.03 -0.00

78 1 -0.01 0.06 0.04 -0.03 0.14 0.06 -0.48 -0.03 0.00

172 173 174

A A A

Frequencies -- 1416.4372 1427.5365 1463.9425

Red. masses -- 3.7487 3.5747 3.0221

Frc consts -- 4.4313 4.2920 3.8160

IR Inten -- 120.0354 0.0001 10.0103

Atom AN X Y Z X Y Z X Y Z

1 6 0.07 -0.06 0.02 -0.00 0.01 -0.00 0.08 0.00 0.00

2 6 0.03 0.15 -0.04 -0.01 -0.02 0.00 -0.03 0.05 -0.01

3 7 0.01 -0.06 0.01 -0.01 -0.00 -0.00 0.00 -0.03 0.01

4 6 -0.05 0.14 -0.04 -0.01 0.02 -0.00 0.03 0.05 -0.01

5 6 -0.06 -0.06 0.01 0.01 -0.01 0.00 -0.08 -0.01 0.00

6 6 0.01 -0.01 0.00 0.05 -0.09 0.01 0.02 -0.08 0.01

7 6 0.09 -0.06 0.02 -0.14 0.07 -0.03 -0.06 0.06 -0.01

8 7 -0.00 0.02 0.00 -0.00 0.04 0.00 -0.00 0.01 0.00

9 6 -0.08 -0.07 -0.02 0.13 0.09 0.03 0.05 0.08 0.02

10 6 0.10 0.07 0.03 -0.12 -0.08 -0.03 -0.04 -0.03 -0.01

11 6 -0.11 0.05 -0.03 0.12 -0.06 0.03 0.04 -0.03 0.01

12 6 -0.00 -0.01 0.00 0.04 0.09 -0.01 -0.00 -0.08 0.02

13 6 -0.08 -0.07 0.02 -0.13 -0.09 0.03 0.05 0.08 -0.02

14 6 0.10 0.07 -0.03 0.12 0.08 -0.03 -0.04 -0.03 0.01

15 6 -0.11 0.05 0.03 -0.12 0.06 0.03 0.04 -0.03 -0.01

16 6 0.09 -0.06 -0.02 0.14 -0.07 -0.03 -0.06 0.06 0.01

17 7 -0.00 0.02 -0.00 0.00 -0.04 0.00 -0.00 0.01 -0.00

18 6 0.01 -0.01 -0.00 -0.05 0.09 0.01 0.02 -0.08 -0.01

19 6 -0.05 0.14 0.04 0.01 -0.02 -0.00 0.03 0.05 0.01

20 6 -0.06 -0.06 -0.01 -0.01 0.01 0.00 -0.08 -0.01 -0.00

21 6 0.07 -0.06 -0.02 0.00 -0.01 -0.00 0.08 0.00 -0.00

22 6 0.03 0.15 0.04 0.01 0.02 0.00 -0.03 0.05 0.01

23 7 0.01 -0.06 -0.01 0.01 0.00 -0.00 0.00 -0.03 -0.01

24 6 -0.00 -0.01 -0.00 -0.04 -0.09 -0.01 -0.00 -0.08 -0.02

25 6 -0.00 0.00 -0.00 -0.00 0.02 -0.00 0.03 -0.01 -0.04

26 6 -0.00 0.00 0.00 -0.00 0.00 0.01 -0.03 -0.01 0.02

27 6 0.01 0.00 -0.00 0.02 0.01 -0.01 0.05 0.04 -0.01

28 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.01 -0.02 -0.02

29 6 -0.01 -0.01 -0.00 -0.01 -0.02 -0.00 -0.03 -0.04 -0.00

30 6 0.00 0.00 0.00 0.01 0.01 0.00 0.01 0.03 0.02

31 6 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.01 -0.02 -0.03

32 6 -0.01 0.00 -0.00 0.02 -0.01 0.01 -0.06 0.04 -0.01

33 6 -0.00 0.00 0.00 -0.00 -0.00 -0.01 0.04 -0.00 0.03

34 6 -0.00 0.01 -0.00 0.00 -0.02 0.00 -0.03 -0.02 -0.05

35 6 -0.00 0.00 0.00 0.01 -0.01 -0.00 -0.02 0.04 0.02

36 6 0.01 -0.01 -0.00 -0.01 0.02 0.00 0.05 -0.05 -0.00

37 6 -0.00 0.01 0.00 -0.00 0.02 0.00 -0.03 -0.02 0.05

38 6 -0.00 0.00 -0.00 -0.01 0.01 -0.00 -0.02 0.04 -0.02

39 6 0.01 -0.01 0.00 0.01 -0.02 0.00 0.05 -0.05 0.00

40 6 -0.00 -0.00 0.00 0.00 -0.00 0.00 -0.01 -0.02 0.03

41 6 -0.01 0.00 0.00 -0.02 0.01 0.01 -0.06 0.04 0.01

42 6 -0.00 0.00 -0.00 0.00 0.00 -0.01 0.04 -0.00 -0.03

43 6 -0.00 0.00 0.00 0.00 -0.02 -0.00 0.03 -0.01 0.04

44 6 0.00 0.00 -0.00 -0.01 -0.01 0.00 0.01 0.03 -0.02

45 6 -0.01 -0.01 0.00 0.01 0.02 -0.00 -0.03 -0.04 0.00

46 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.01 -0.02 0.02

47 6 0.01 0.00 0.00 -0.02 -0.01 -0.01 0.05 0.04 0.01

48 6 -0.00 0.00 -0.00 0.00 -0.00 0.01 -0.03 -0.01 -0.02

49 1 -0.00 -0.14 0.04 -0.02 -0.00 0.00 -0.07 -0.14 0.04

50 1 0.03 -0.14 0.04 -0.03 0.01 -0.01 0.09 -0.13 0.04

51 1 -0.16 -0.36 -0.05 0.16 0.38 0.06 0.06 0.13 0.02

52 1 0.21 -0.34 0.05 -0.21 0.35 -0.05 -0.08 0.12 -0.02

53 1 -0.16 -0.36 0.05 -0.16 -0.38 0.06 0.06 0.13 -0.02

54 1 0.21 -0.34 -0.05 0.21 -0.35 -0.05 -0.08 0.12 0.02

55 1 0.03 -0.14 -0.04 0.03 -0.01 -0.01 0.09 -0.13 -0.04

56 1 -0.00 -0.14 -0.04 0.02 0.00 0.00 -0.07 -0.14 -0.04

57 1 -0.01 -0.02 -0.01 -0.02 -0.04 -0.02 -0.03 0.01 0.03

58 1 -0.03 -0.02 0.01 -0.08 -0.04 0.03 -0.17 -0.08 0.09

59 1 -0.01 0.01 0.02 -0.04 0.03 0.06 -0.12 0.09 0.17

60 1 0.00 0.02 0.01 0.01 0.04 0.02 0.03 0.13 0.08

61 1 -0.01 0.00 0.00 0.00 0.01 -0.00 -0.05 0.00 0.04

62 1 0.01 0.01 0.02 -0.04 -0.04 -0.06 0.13 0.13 0.22

63 1 0.03 -0.01 0.01 -0.09 0.03 -0.04 0.21 -0.06 0.11

64 1 0.02 -0.02 -0.01 -0.03 0.03 0.01 0.03 0.03 0.04

65 1 0.01 0.00 0.00 0.00 -0.01 0.00 0.07 0.01 0.06

66 1 -0.01 0.02 0.01 0.02 -0.05 -0.03 -0.05 0.16 0.10

67 1 0.01 0.00 -0.00 -0.00 0.01 0.00 0.07 0.01 -0.06

68 1 -0.01 0.02 -0.01 -0.02 0.05 -0.03 -0.05 0.16 -0.10

69 1 0.01 0.01 -0.02 0.04 0.04 -0.06 0.13 0.13 -0.22

70 1 0.03 -0.01 -0.01 0.09 -0.03 -0.04 0.21 -0.06 -0.11

71 1 0.02 -0.02 0.01 0.03 -0.03 0.01 0.03 0.03 -0.04

72 1 -0.01 0.00 -0.00 -0.00 -0.01 -0.00 -0.05 0.00 -0.04

73 1 0.00 0.02 -0.01 -0.01 -0.04 0.02 0.03 0.13 -0.08

74 1 -0.01 0.01 -0.02 0.04 -0.03 0.06 -0.12 0.09 -0.17

75 1 -0.03 -0.02 -0.01 0.08 0.04 0.03 -0.17 -0.08 -0.09

76 1 -0.01 -0.02 0.01 0.02 0.04 -0.02 -0.03 0.01 -0.03

77 1 -0.01 -0.06 0.03 0.01 0.00 -0.00 0.00 -0.04 0.01

78 1 -0.01 -0.06 -0.03 -0.01 -0.00 -0.00 0.00 -0.04 -0.01

175 176 177

A A A

Frequencies -- 1474.0951 1474.2691 1476.9558

Red. masses -- 2.2233 2.2321 2.2500

Frc consts -- 2.8464 2.8583 2.8918

IR Inten -- 25.8768 10.4958 1.8615

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 0.01 -0.00 -0.00 -0.01 0.01 -0.00 -0.00 0.00 0.00

3 7 -0.00 0.00 -0.00 0.00 -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 -0.01 -0.00 0.00 0.00 -0.00 0.00

6 6 0.00 -0.02 0.01 -0.01 -0.02 0.01 -0.02 0.02 0.01

7 6 -0.01 0.03 -0.00 -0.01 0.03 -0.00 0.02 0.00 0.00

8 7 -0.00 0.00 -0.00 -0.01 0.00 -0.00 -0.00 -0.01 -0.00

9 6 0.01 -0.02 -0.00 0.01 -0.02 -0.00 -0.02 -0.02 -0.00

10 6 -0.00 -0.01 0.00 -0.00 -0.01 -0.00 0.01 0.00 0.00

11 6 0.00 0.01 0.00 0.00 0.01 0.00 -0.01 0.01 -0.00

12 6 0.01 -0.00 0.01 -0.01 0.00 -0.01 -0.01 -0.02 -0.00

13 6 -0.01 0.02 -0.00 0.01 -0.02 0.00 0.02 0.02 -0.00

14 6 0.00 0.01 0.00 -0.00 -0.01 0.00 -0.01 -0.00 0.00

15 6 -0.00 -0.01 0.00 0.00 0.01 -0.00 0.01 -0.01 -0.00

16 6 0.01 -0.03 -0.00 -0.01 0.03 0.00 -0.02 -0.00 0.00

17 7 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.01 -0.00

18 6 -0.00 0.02 0.01 -0.01 -0.02 -0.01 0.02 -0.02 0.01

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 -0.01 -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 -0.01 0.00 -0.00 -0.01 0.01 0.00 0.00 -0.00 0.00

23 7 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.01 -0.00 -0.00

24 6 -0.01 0.00 0.01 -0.01 0.00 0.01 0.01 0.02 -0.00

25 6 0.03 -0.02 -0.04 0.04 -0.03 -0.06 0.05 -0.04 -0.07

26 6 -0.03 -0.01 0.02 -0.04 -0.02 0.02 -0.06 -0.03 0.03

27 6 0.04 0.04 -0.00 0.06 0.06 -0.00 0.06 0.07 -0.00

28 6 0.02 -0.01 -0.03 0.03 -0.02 -0.04 0.03 -0.02 -0.05

29 6 -0.03 -0.04 -0.00 -0.05 -0.06 -0.01 -0.06 -0.08 -0.01

30 6 0.01 0.03 0.02 0.01 0.05 0.02 0.02 0.06 0.03

31 6 -0.03 -0.03 -0.05 0.02 0.02 0.04 0.02 0.02 0.03

32 6 -0.07 0.06 -0.00 0.06 -0.05 0.00 0.04 -0.03 0.00

33 6 0.06 -0.02 0.03 -0.05 0.01 -0.02 -0.03 0.01 -0.02

34 6 -0.04 -0.05 -0.07 0.04 0.04 0.05 0.03 0.03 0.04

35 6 -0.02 0.05 0.03 0.02 -0.04 -0.02 0.01 -0.03 -0.02

36 6 0.07 -0.07 -0.01 -0.05 0.05 0.00 -0.04 0.04 0.00

37 6 0.04 0.05 -0.07 0.04 0.04 -0.06 -0.03 -0.03 0.04

38 6 0.02 -0.05 0.03 0.02 -0.04 0.02 -0.01 0.03 -0.02

39 6 -0.07 0.07 -0.01 -0.06 0.05 -0.00 0.04 -0.04 0.00

40 6 0.03 0.03 -0.05 0.02 0.02 -0.04 -0.02 -0.02 0.03

41 6 0.07 -0.06 -0.00 0.06 -0.05 -0.00 -0.04 0.03 0.00

42 6 -0.06 0.02 0.03 -0.05 0.01 0.02 0.03 -0.01 -0.02

43 6 -0.03 0.02 -0.04 0.04 -0.03 0.06 -0.05 0.04 -0.07

44 6 -0.01 -0.03 0.02 0.01 0.05 -0.02 -0.02 -0.06 0.03

45 6 0.03 0.04 -0.00 -0.05 -0.06 0.01 0.06 0.08 -0.01

46 6 -0.02 0.01 -0.03 0.03 -0.02 0.04 -0.03 0.02 -0.05

47 6 -0.04 -0.04 -0.00 0.06 0.06 0.00 -0.06 -0.07 -0.00

48 6 0.03 0.01 0.02 -0.04 -0.02 -0.02 0.06 0.03 0.03

49 1 0.01 0.01 -0.00 -0.01 -0.02 0.01 -0.01 -0.01 0.00

50 1 -0.00 0.00 -0.00 0.01 -0.01 0.00 -0.02 0.01 -0.00

51 1 0.01 -0.00 0.00 0.01 -0.00 0.00 -0.01 -0.03 -0.00

52 1 -0.00 0.02 -0.00 -0.00 0.03 -0.00 0.01 -0.02 0.00

53 1 -0.01 0.00 0.00 0.01 -0.00 -0.00 0.01 0.03 -0.00

54 1 0.00 -0.02 -0.00 -0.00 0.03 0.00 -0.01 0.02 0.00

55 1 0.00 -0.00 -0.00 0.01 -0.01 -0.00 0.02 -0.01 -0.00

56 1 -0.01 -0.01 -0.00 -0.01 -0.02 -0.01 0.01 0.01 0.00

57 1 -0.02 0.04 0.05 -0.02 0.06 0.07 -0.02 0.09 0.09

58 1 -0.14 -0.06 0.08 -0.20 -0.08 0.11 -0.22 -0.09 0.13

59 1 -0.11 0.09 0.17 -0.16 0.13 0.24 -0.19 0.15 0.30

60 1 0.03 0.13 0.08 0.04 0.19 0.12 0.05 0.24 0.15

61 1 -0.05 0.00 0.05 -0.08 0.00 0.07 -0.09 0.00 0.09

62 1 0.16 0.18 0.29 -0.13 -0.14 -0.23 -0.09 -0.10 -0.17

63 1 0.24 -0.06 0.14 -0.19 0.05 -0.11 -0.13 0.03 -0.08

64 1 0.01 0.08 0.09 -0.01 -0.07 -0.07 -0.00 -0.06 -0.05

65 1 0.09 0.02 0.09 -0.08 -0.01 -0.07 -0.05 -0.01 -0.05

66 1 -0.08 0.22 0.14 0.06 -0.18 -0.11 0.05 -0.13 -0.08

67 1 -0.09 -0.02 0.09 -0.08 -0.01 0.07 0.05 0.01 -0.05

68 1 0.08 -0.22 0.14 0.06 -0.18 0.11 -0.05 0.13 -0.08

69 1 -0.16 -0.18 0.29 -0.13 -0.14 0.23 0.09 0.10 -0.17

70 1 -0.24 0.06 0.14 -0.19 0.05 0.11 0.13 -0.03 -0.08

71 1 -0.01 -0.08 0.08 -0.01 -0.07 0.07 0.00 0.06 -0.05

72 1 0.05 -0.00 0.05 -0.08 0.00 -0.07 0.09 -0.00 0.09

73 1 -0.03 -0.13 0.08 0.04 0.19 -0.12 -0.05 -0.24 0.15

74 1 0.11 -0.09 0.17 -0.16 0.13 -0.24 0.19 -0.15 0.30

75 1 0.14 0.06 0.08 -0.20 -0.08 -0.11 0.22 0.09 0.13

76 1 0.02 -0.04 0.05 -0.02 0.06 -0.07 0.02 -0.09 0.09

77 1 0.00 0.00 0.00 -0.02 -0.01 0.00 -0.02 -0.00 0.00

78 1 -0.00 -0.00 0.00 -0.02 -0.01 -0.00 0.02 0.00 0.00

178 179 180

A A A

Frequencies -- 1482.0767 1509.7584 1522.0750

Red. masses -- 3.0979 4.9607 7.8208

Frc consts -- 4.0092 6.6620 10.6751

IR Inten -- 0.2762 2.2270 225.2594

Atom AN X Y Z X Y Z X Y Z

1 6 0.09 0.01 -0.00 -0.13 -0.05 0.01 0.05 0.04 -0.01

2 6 -0.09 0.04 -0.01 0.19 0.01 -0.00 -0.26 -0.08 0.02

3 7 0.00 -0.04 0.01 -0.00 0.04 -0.01 -0.01 -0.02 0.01

4 6 0.08 0.05 -0.01 -0.19 -0.02 -0.01 0.29 -0.06 0.03

5 6 -0.09 -0.00 -0.00 0.14 -0.03 0.01 -0.07 0.05 -0.02

6 6 -0.01 -0.07 -0.00 0.06 0.07 0.00 -0.18 0.10 -0.02

7 6 -0.04 0.04 -0.01 0.02 -0.09 0.01 0.08 -0.04 0.02

8 7 -0.00 0.01 0.00 0.02 -0.00 0.00 0.00 -0.02 -0.00

9 6 0.03 0.05 0.01 0.01 0.10 0.01 -0.09 -0.10 -0.02

10 6 -0.02 -0.02 -0.01 -0.01 0.10 -0.00 0.04 0.01 0.01

11 6 0.02 -0.02 0.01 0.00 -0.10 -0.00 -0.03 0.03 -0.01

12 6 0.02 -0.07 -0.00 -0.07 0.06 -0.00 0.17 0.15 -0.02

13 6 0.03 0.05 -0.01 -0.01 -0.10 0.01 -0.09 -0.10 0.02

14 6 -0.02 -0.02 0.01 0.01 -0.10 -0.00 0.04 0.01 -0.01

15 6 0.02 -0.02 -0.01 -0.00 0.10 -0.00 -0.03 0.03 0.01

16 6 -0.04 0.04 0.01 -0.02 0.09 0.01 0.08 -0.04 -0.02

17 7 -0.00 0.01 -0.00 -0.02 0.00 0.00 0.00 -0.02 0.00

18 6 -0.01 -0.07 0.00 -0.06 -0.07 0.00 -0.18 0.10 0.02

19 6 0.08 0.05 0.01 0.19 0.02 -0.01 0.29 -0.06 -0.03

20 6 -0.09 -0.00 0.00 -0.14 0.03 0.01 -0.07 0.05 0.02

21 6 0.09 0.01 0.00 0.13 0.05 0.01 0.05 0.04 0.01

22 6 -0.09 0.04 0.01 -0.19 -0.01 -0.00 -0.26 -0.08 -0.02

23 7 0.00 -0.04 -0.01 0.00 -0.04 -0.01 -0.01 -0.02 -0.01

24 6 0.02 -0.07 0.00 0.07 -0.06 -0.00 0.17 0.15 0.02

25 6 -0.04 0.04 0.05 0.01 0.00 -0.00 0.02 -0.03 -0.02

26 6 0.04 0.03 -0.01 -0.01 -0.03 -0.02 -0.02 0.00 0.01

27 6 -0.04 -0.05 -0.01 -0.03 -0.00 0.02 0.03 0.02 -0.01

28 6 -0.03 0.02 0.04 0.02 0.02 -0.00 0.01 -0.02 -0.03

29 6 0.04 0.06 0.01 -0.00 -0.03 -0.02 -0.02 0.01 0.02

30 6 -0.01 -0.04 -0.03 -0.03 -0.00 0.02 0.02 0.02 -0.01

31 6 0.02 0.02 0.03 -0.02 0.01 -0.00 -0.01 -0.02 -0.03

32 6 0.04 -0.04 -0.01 0.03 0.00 0.02 -0.02 0.02 0.00

33 6 -0.04 0.02 -0.01 0.01 -0.03 -0.02 0.02 -0.00 0.01

34 6 0.03 0.04 0.04 -0.01 0.00 -0.00 -0.02 -0.03 -0.02

35 6 0.01 -0.04 -0.02 0.03 0.00 0.02 -0.02 0.02 -0.00

36 6 -0.04 0.05 0.01 0.01 -0.03 -0.02 0.02 -0.00 0.01

37 6 0.03 0.04 -0.04 0.01 -0.00 -0.00 -0.02 -0.03 0.02

38 6 0.01 -0.04 0.02 -0.03 -0.00 0.02 -0.02 0.02 0.00

39 6 -0.04 0.05 -0.01 -0.01 0.03 -0.02 0.02 -0.00 -0.01

40 6 0.02 0.02 -0.03 0.02 -0.01 -0.00 -0.01 -0.02 0.03

41 6 0.04 -0.04 0.01 -0.03 -0.00 0.02 -0.02 0.02 -0.00

42 6 -0.04 0.02 0.01 -0.01 0.03 -0.02 0.02 -0.00 -0.01

43 6 -0.04 0.04 -0.05 -0.01 -0.00 -0.00 0.02 -0.03 0.02

44 6 -0.01 -0.04 0.03 0.03 0.00 0.02 0.02 0.02 0.01

45 6 0.04 0.06 -0.01 0.00 0.03 -0.02 -0.02 0.01 -0.02

46 6 -0.03 0.02 -0.04 -0.02 -0.02 -0.00 0.01 -0.02 0.03

47 6 -0.04 -0.05 0.01 0.03 0.00 0.02 0.03 0.02 0.01

48 6 0.04 0.03 0.01 0.01 0.03 -0.02 -0.02 0.00 -0.01

49 1 -0.10 -0.16 0.04 0.17 0.21 -0.06 -0.14 -0.11 0.04

50 1 0.12 -0.14 0.05 -0.19 0.18 -0.06 0.21 -0.11 0.05

51 1 0.03 0.07 0.01 -0.08 0.02 -0.02 -0.03 -0.09 -0.01

52 1 -0.04 0.06 -0.01 -0.08 -0.03 -0.02 0.05 -0.07 0.01

53 1 0.03 0.07 -0.01 0.08 -0.02 -0.02 -0.03 -0.09 0.01

54 1 -0.04 0.06 0.01 0.08 0.03 -0.02 0.05 -0.07 -0.01

55 1 0.12 -0.14 -0.05 0.19 -0.18 -0.06 0.21 -0.11 -0.05

56 1 -0.10 -0.16 -0.04 -0.17 -0.21 -0.06 -0.14 -0.11 -0.04

57 1 -0.00 -0.10 -0.08 0.05 0.12 0.05 -0.02 -0.01 0.02

58 1 0.13 0.04 -0.09 0.09 0.07 -0.03 -0.10 -0.05 0.05

59 1 0.14 -0.12 -0.22 0.01 0.03 0.02 -0.07 0.03 0.08

60 1 -0.05 -0.19 -0.12 0.05 0.12 0.05 -0.03 -0.02 0.01

61 1 0.05 -0.01 -0.06 0.09 0.07 -0.03 -0.10 -0.05 0.06

62 1 -0.10 -0.12 -0.19 -0.01 0.03 0.02 0.06 0.05 0.10

63 1 -0.11 0.01 -0.07 -0.11 0.06 -0.03 0.08 -0.02 0.05

64 1 0.02 -0.09 -0.07 -0.07 0.12 0.05 0.00 0.02 0.04

65 1 -0.04 -0.02 -0.05 -0.11 0.06 -0.03 0.08 -0.03 0.06

66 1 0.07 -0.16 -0.10 -0.07 0.12 0.05 0.01 0.02 0.03

67 1 -0.04 -0.02 0.05 0.11 -0.06 -0.03 0.08 -0.03 -0.06

68 1 0.07 -0.16 0.10 0.07 -0.12 0.05 0.01 0.02 -0.03

69 1 -0.10 -0.12 0.19 0.01 -0.03 0.02 0.06 0.05 -0.10

70 1 -0.11 0.01 0.07 0.11 -0.06 -0.03 0.08 -0.02 -0.05

71 1 0.02 -0.09 0.07 0.07 -0.12 0.05 0.00 0.02 -0.04

72 1 0.05 -0.01 0.06 -0.09 -0.07 -0.03 -0.10 -0.05 -0.06

73 1 -0.05 -0.19 0.12 -0.05 -0.12 0.05 -0.03 -0.02 -0.01

74 1 0.14 -0.12 0.22 -0.01 -0.03 0.02 -0.07 0.03 -0.08

75 1 0.13 0.04 0.09 -0.09 -0.07 -0.03 -0.10 -0.05 -0.05

76 1 -0.00 -0.10 0.08 -0.05 -0.12 0.05 -0.02 -0.01 -0.02

77 1 0.00 -0.05 0.01 -0.00 0.05 -0.01 0.04 -0.02 0.00

78 1 0.00 -0.05 -0.01 0.00 -0.05 -0.01 0.04 -0.02 -0.00

181 182 183

A A A

Frequencies -- 1525.8149 1526.6381 1527.8424

Red. masses -- 2.3322 2.2636 2.3608

Frc consts -- 3.1990 3.1083 3.2469

IR Inten -- 0.8344 0.0345 21.0399

Atom AN X Y Z X Y Z X Y Z

1 6 -0.01 -0.02 0.00 -0.02 -0.02 0.01 -0.02 -0.02 0.01

2 6 0.01 0.01 -0.00 0.03 0.02 -0.01 0.04 0.01 -0.00

3 7 -0.02 -0.00 0.00 -0.01 0.00 -0.00 -0.02 0.01 -0.00

4 6 0.01 -0.00 0.00 0.00 -0.02 0.01 -0.01 -0.02 0.00

5 6 -0.01 0.01 -0.00 -0.00 0.02 -0.01 -0.00 0.02 -0.00

6 6 0.02 -0.03 0.00 -0.01 -0.01 -0.00 0.04 0.00 0.00

7 6 -0.03 0.05 -0.01 -0.00 -0.00 -0.00 -0.02 0.03 -0.00

8 7 0.00 0.00 0.00 0.00 0.00 0.00 0.00 -0.01 -0.00

9 6 -0.01 -0.05 -0.00 0.00 0.01 0.00 -0.01 -0.03 -0.00

10 6 0.01 -0.01 0.00 -0.00 0.00 -0.00 0.00 -0.02 0.00

11 6 0.01 0.01 0.00 0.00 -0.01 0.00 0.00 0.02 0.00

12 6 0.03 0.01 -0.00 -0.03 0.03 0.00 -0.02 0.03 -0.00

13 6 -0.01 -0.05 0.00 -0.00 -0.01 0.00 -0.01 -0.03 0.00

14 6 0.01 -0.01 -0.00 0.00 -0.00 -0.00 0.00 -0.02 -0.00

15 6 0.01 0.01 -0.00 -0.00 0.01 0.00 0.00 0.02 -0.00

16 6 -0.03 0.05 0.01 0.00 0.00 -0.00 -0.02 0.03 0.00

17 7 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.01 0.00

18 6 0.02 -0.03 -0.00 0.01 0.01 -0.00 0.04 0.00 -0.00

19 6 0.01 -0.00 -0.00 -0.00 0.02 0.01 -0.01 -0.02 -0.00

20 6 -0.01 0.01 0.00 0.00 -0.02 -0.01 -0.00 0.02 0.00

21 6 -0.01 -0.02 -0.00 0.02 0.02 0.01 -0.02 -0.02 -0.01

22 6 0.01 0.01 0.00 -0.03 -0.02 -0.01 0.04 0.01 0.00

23 7 -0.02 -0.00 -0.00 0.01 -0.00 -0.00 -0.02 0.01 0.00

24 6 0.03 0.01 0.00 0.03 -0.03 0.00 -0.02 0.03 0.00

25 6 -0.03 -0.02 0.00 0.03 0.04 0.00 -0.06 -0.07 -0.00

26 6 0.00 0.03 0.02 -0.00 -0.03 -0.03 0.00 0.06 0.05

27 6 0.03 0.01 -0.02 -0.04 -0.01 0.03 0.07 0.02 -0.05

28 6 -0.02 -0.02 0.00 0.02 0.03 0.00 -0.04 -0.05 0.00

29 6 0.01 0.04 0.02 -0.00 -0.04 -0.03 0.01 0.08 0.05

30 6 0.02 0.00 -0.02 -0.03 -0.01 0.02 0.06 0.01 -0.05

31 6 -0.05 0.04 -0.00 0.05 -0.04 0.00 0.02 -0.02 -0.00

32 6 0.08 -0.01 0.05 -0.08 0.01 -0.05 -0.04 0.01 -0.02

33 6 0.01 -0.06 -0.05 -0.01 0.06 0.05 -0.00 0.03 0.02

34 6 -0.07 0.06 -0.00 0.07 -0.06 -0.00 0.04 -0.04 -0.00

35 6 0.06 0.00 0.05 -0.06 0.00 -0.05 -0.03 0.00 -0.02

36 6 0.03 -0.08 -0.05 -0.02 0.07 0.05 -0.01 0.04 0.03

37 6 -0.07 0.06 0.00 -0.07 0.06 -0.00 0.04 -0.04 0.00

38 6 0.06 0.00 -0.05 0.06 -0.00 -0.05 -0.03 0.00 0.02

39 6 0.03 -0.08 0.05 0.02 -0.07 0.05 -0.01 0.04 -0.03

40 6 -0.05 0.04 0.00 -0.05 0.04 0.00 0.02 -0.02 0.00

41 6 0.08 -0.01 -0.05 0.08 -0.01 -0.05 -0.04 0.01 0.02

42 6 0.01 -0.06 0.05 0.01 -0.06 0.05 -0.00 0.03 -0.02

43 6 -0.03 -0.02 -0.00 -0.03 -0.04 0.00 -0.06 -0.07 0.00

44 6 0.02 0.00 0.02 0.03 0.01 0.02 0.06 0.01 0.05

45 6 0.01 0.04 -0.02 0.00 0.04 -0.03 0.01 0.08 -0.05

46 6 -0.02 -0.02 -0.00 -0.02 -0.03 0.00 -0.04 -0.05 -0.00

47 6 0.03 0.01 0.02 0.04 0.01 0.03 0.07 0.02 0.05

48 6 0.00 0.03 -0.02 0.00 0.03 -0.03 0.00 0.06 -0.05

49 1 0.04 0.02 -0.01 0.06 0.04 -0.01 0.06 0.04 -0.01

50 1 0.04 -0.02 0.01 0.03 -0.00 0.00 0.02 0.00 0.00

51 1 0.01 -0.01 0.00 -0.00 0.01 -0.00 0.01 -0.01 0.00

52 1 0.00 0.02 0.00 -0.01 0.01 -0.00 0.01 0.01 0.00

53 1 0.01 -0.01 -0.00 0.00 -0.01 -0.00 0.01 -0.01 -0.00

54 1 0.00 0.02 -0.00 0.01 -0.01 -0.00 0.01 0.01 -0.00

55 1 0.04 -0.02 -0.01 -0.03 0.00 0.00 0.02 0.00 -0.00

56 1 0.04 0.02 0.01 -0.05 -0.04 -0.01 0.06 0.04 0.01

57 1 -0.05 -0.12 -0.05 0.07 0.14 0.05 -0.12 -0.25 -0.10

58 1 -0.10 -0.07 0.03 0.13 0.08 -0.04 -0.23 -0.15 0.08

59 1 -0.01 -0.03 -0.02 0.03 0.03 0.00 -0.04 -0.06 -0.01

60 1 -0.05 -0.12 -0.05 0.06 0.13 0.05 -0.11 -0.25 -0.10

61 1 -0.09 -0.07 0.03 0.12 0.09 -0.04 -0.22 -0.16 0.07

62 1 -0.05 0.06 0.01 0.05 -0.05 -0.00 0.03 -0.02 0.00

63 1 -0.25 0.12 -0.08 0.24 -0.12 0.08 0.13 -0.06 0.04

64 1 -0.16 0.24 0.10 0.15 -0.23 -0.09 0.08 -0.11 -0.05

65 1 -0.25 0.13 -0.08 0.24 -0.13 0.09 0.13 -0.07 0.05

66 1 -0.15 0.24 0.10 0.14 -0.23 -0.09 0.07 -0.11 -0.04

67 1 -0.25 0.13 0.08 -0.24 0.13 0.09 0.13 -0.07 -0.05

68 1 -0.15 0.24 -0.10 -0.14 0.23 -0.09 0.07 -0.11 0.04

69 1 -0.05 0.06 -0.01 -0.05 0.05 -0.00 0.03 -0.02 -0.00

70 1 -0.25 0.12 0.08 -0.24 0.12 0.08 0.13 -0.06 -0.04

71 1 -0.16 0.24 -0.10 -0.15 0.23 -0.09 0.08 -0.11 0.05

72 1 -0.09 -0.07 -0.03 -0.12 -0.09 -0.04 -0.22 -0.16 -0.07

73 1 -0.05 -0.12 0.05 -0.06 -0.13 0.05 -0.11 -0.25 0.10

74 1 -0.01 -0.03 0.02 -0.03 -0.03 0.00 -0.04 -0.06 0.01

75 1 -0.10 -0.07 -0.03 -0.13 -0.08 -0.04 -0.23 -0.15 -0.08

76 1 -0.05 -0.12 0.05 -0.07 -0.14 0.05 -0.12 -0.25 0.10

77 1 0.06 0.00 0.00 0.06 0.01 -0.00 0.07 0.01 -0.00

78 1 0.06 0.00 -0.00 -0.06 -0.01 -0.00 0.07 0.01 0.00

184 185 186

A A A

Frequencies -- 1529.2363 1529.7550 1538.4653

Red. masses -- 2.4396 3.8550 3.3731

Frc consts -- 3.3613 5.3152 4.7038

IR Inten -- 0.1491 10.5411 0.0024

Atom AN X Y Z X Y Z X Y Z

1 6 -0.02 -0.00 -0.00 -0.05 -0.09 0.03 0.06 0.12 -0.03

2 6 0.04 -0.01 0.00 0.09 0.08 -0.02 -0.10 -0.12 0.03

3 7 0.00 0.01 -0.00 -0.09 -0.01 -0.00 0.10 0.01 0.00

4 6 -0.05 -0.00 -0.00 0.09 -0.06 0.02 -0.12 0.10 -0.03

5 6 0.03 -0.01 0.00 -0.06 0.08 -0.02 0.07 -0.11 0.03

6 6 0.04 0.04 0.00 0.01 -0.09 0.00 0.03 -0.02 0.00

7 6 0.00 -0.02 0.00 -0.06 0.11 -0.02 0.01 -0.03 0.00

8 7 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.03 0.00

9 6 -0.00 0.01 0.00 -0.04 -0.11 -0.01 -0.01 -0.04 -0.00

10 6 0.00 0.03 0.00 0.02 -0.09 0.00 0.01 0.01 0.00

11 6 0.00 -0.02 -0.00 0.01 0.09 0.00 -0.01 0.01 -0.00

12 6 -0.03 0.02 0.00 -0.01 0.07 -0.00 0.02 0.02 -0.00

13 6 0.00 -0.01 0.00 -0.04 -0.11 0.01 0.01 0.04 -0.00

14 6 -0.00 -0.03 0.00 0.02 -0.09 -0.00 -0.01 -0.01 0.00

15 6 -0.00 0.02 -0.00 0.01 0.09 -0.00 0.01 -0.01 -0.00

16 6 -0.00 0.02 0.00 -0.06 0.11 0.02 -0.01 0.03 0.00

17 7 -0.00 0.00 0.00 0.00 0.00 0.00 0.00 -0.03 0.00

18 6 -0.04 -0.04 0.00 0.01 -0.09 -0.00 -0.03 0.02 0.00

19 6 0.05 0.00 -0.00 0.09 -0.06 -0.02 0.12 -0.10 -0.03

20 6 -0.03 0.01 0.00 -0.06 0.08 0.02 -0.07 0.11 0.03

21 6 0.02 0.00 -0.00 -0.05 -0.09 -0.03 -0.06 -0.12 -0.03

22 6 -0.04 0.01 0.00 0.09 0.08 0.02 0.10 0.12 0.03

23 7 -0.00 -0.01 -0.00 -0.09 -0.01 0.00 -0.10 -0.01 0.00

24 6 0.03 -0.02 0.00 -0.01 0.07 0.00 -0.02 -0.02 -0.00

25 6 -0.06 -0.08 -0.00 0.03 0.05 0.00 0.01 0.02 0.00

26 6 -0.00 0.06 0.05 0.00 -0.03 -0.03 0.01 -0.01 -0.01

27 6 0.08 0.03 -0.05 -0.04 -0.02 0.02 -0.02 -0.01 0.01

28 6 -0.04 -0.05 -0.00 0.01 0.03 0.01 0.01 0.01 0.00

29 6 0.01 0.07 0.05 0.00 -0.03 -0.03 -0.00 -0.02 -0.01

30 6 0.06 0.01 -0.05 -0.04 -0.02 0.02 -0.01 -0.00 0.01

31 6 0.02 -0.02 -0.00 0.00 -0.01 -0.01 0.01 -0.01 -0.00

32 6 -0.04 0.01 -0.02 -0.02 0.01 -0.01 -0.02 0.01 -0.01

33 6 -0.00 0.03 0.02 0.00 0.01 0.01 0.00 0.01 0.01

34 6 0.04 -0.04 -0.00 0.02 -0.02 -0.00 0.01 -0.02 -0.00

35 6 -0.03 0.00 -0.02 -0.02 0.01 -0.01 -0.01 -0.00 -0.01

36 6 -0.01 0.04 0.03 0.00 0.01 0.01 -0.01 0.02 0.01

37 6 -0.04 0.04 -0.00 0.02 -0.02 0.00 -0.01 0.02 -0.00

38 6 0.03 -0.00 -0.02 -0.02 0.01 0.01 0.01 0.00 -0.01

39 6 0.01 -0.04 0.03 0.00 0.01 -0.01 0.01 -0.02 0.01

40 6 -0.02 0.02 -0.00 0.00 -0.01 0.01 -0.01 0.01 -0.00

41 6 0.04 -0.01 -0.02 -0.02 0.01 0.01 0.02 -0.01 -0.01

42 6 0.00 -0.03 0.02 0.00 0.01 -0.01 -0.00 -0.01 0.01

43 6 0.06 0.08 -0.00 0.03 0.05 -0.00 -0.01 -0.02 0.00

44 6 -0.06 -0.01 -0.05 -0.04 -0.02 -0.02 0.01 0.00 0.01

45 6 -0.01 -0.07 0.05 0.00 -0.03 0.03 0.00 0.02 -0.01

46 6 0.04 0.05 -0.00 0.01 0.03 -0.01 -0.01 -0.01 0.00

47 6 -0.08 -0.03 -0.05 -0.04 -0.02 -0.02 0.02 0.01 0.01

48 6 0.00 -0.06 0.05 0.00 -0.03 0.03 -0.01 0.01 -0.01

49 1 0.02 0.03 -0.01 0.22 0.11 -0.03 -0.26 -0.13 0.04

50 1 -0.05 0.04 -0.01 0.23 -0.08 0.03 -0.28 0.09 -0.04

51 1 -0.02 -0.00 -0.01 0.08 -0.02 0.02 -0.02 -0.04 -0.01

52 1 -0.02 -0.01 -0.01 0.07 0.04 0.02 0.02 -0.04 0.01

53 1 0.02 0.00 -0.01 0.08 -0.02 -0.02 0.02 0.04 -0.01

54 1 0.02 0.01 -0.01 0.07 0.04 -0.02 -0.02 0.04 0.01

55 1 0.05 -0.04 -0.01 0.23 -0.08 -0.03 0.28 -0.09 -0.04

56 1 -0.02 -0.03 -0.01 0.22 0.11 0.03 0.27 0.13 0.04

57 1 -0.12 -0.25 -0.10 0.06 0.12 0.04 0.02 0.03 0.01

58 1 -0.23 -0.15 0.08 0.13 0.08 -0.05 0.05 0.03 -0.02

59 1 -0.05 -0.06 0.00 0.04 0.01 -0.03 0.02 0.01 -0.01

60 1 -0.11 -0.24 -0.10 0.06 0.11 0.04 0.02 0.05 0.02

61 1 -0.22 -0.16 0.08 0.13 0.09 -0.06 0.04 0.03 -0.02

62 1 0.03 -0.03 0.00 0.02 0.00 0.02 0.02 -0.01 0.01

63 1 0.13 -0.06 0.04 0.05 -0.02 0.02 0.06 -0.02 0.02

64 1 0.08 -0.11 -0.05 0.03 -0.04 -0.01 0.02 -0.03 -0.01

65 1 0.12 -0.07 0.04 0.06 -0.03 0.03 0.04 -0.02 0.02

66 1 0.07 -0.12 -0.05 0.03 -0.03 -0.01 0.03 -0.04 -0.02

67 1 -0.12 0.07 0.04 0.06 -0.03 -0.03 -0.04 0.02 0.02

68 1 -0.07 0.12 -0.05 0.03 -0.03 0.01 -0.03 0.04 -0.02

69 1 -0.03 0.03 0.00 0.02 0.00 -0.02 -0.02 0.01 0.01

70 1 -0.13 0.06 0.04 0.05 -0.02 -0.02 -0.06 0.02 0.02

71 1 -0.08 0.11 -0.05 0.03 -0.04 0.01 -0.02 0.03 -0.01

72 1 0.22 0.16 0.08 0.13 0.09 0.06 -0.04 -0.03 -0.02

73 1 0.11 0.24 -0.10 0.06 0.11 -0.04 -0.02 -0.05 0.02

74 1 0.05 0.06 0.00 0.04 0.01 0.03 -0.02 -0.01 -0.01

75 1 0.23 0.15 0.08 0.13 0.08 0.05 -0.05 -0.03 -0.02

76 1 0.12 0.25 -0.10 0.06 0.12 -0.04 -0.02 -0.03 0.01

77 1 -0.02 0.01 -0.00 0.35 0.02 0.00 -0.44 -0.03 -0.00

78 1 0.02 -0.01 -0.00 0.35 0.02 -0.00 0.44 0.03 -0.00

187 188 189

A A A

Frequencies -- 1551.4928 1572.2711 1578.7226

Red. masses -- 6.0980 6.5388 5.6503

Frc consts -- 8.6485 9.5236 8.2973

IR Inten -- 673.4083 0.6942 52.7368

Atom AN X Y Z X Y Z X Y Z

1 6 0.03 0.07 -0.02 0.03 -0.00 0.00 -0.03 -0.06 0.02

2 6 -0.06 -0.09 0.02 0.01 0.04 -0.01 0.09 0.07 -0.02

3 7 0.05 0.00 0.00 -0.00 -0.02 0.00 -0.07 -0.01 -0.00

4 6 -0.08 0.09 -0.02 -0.01 0.03 -0.00 0.10 -0.06 0.02

5 6 0.04 -0.07 0.02 -0.03 -0.00 -0.00 -0.04 0.05 -0.02

6 6 0.06 -0.16 0.01 0.03 -0.11 0.01 -0.07 0.05 -0.01

7 6 -0.05 0.21 -0.01 -0.04 0.19 -0.01 0.03 0.00 0.01

8 7 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

9 6 -0.02 -0.21 -0.01 -0.01 -0.19 -0.01 0.03 0.00 0.01

10 6 0.01 0.13 0.01 0.01 0.27 0.01 0.00 0.27 0.01

11 6 0.03 -0.13 0.01 0.05 -0.27 0.01 0.04 -0.27 0.00

12 6 0.03 0.16 -0.01 -0.02 -0.11 0.01 -0.06 -0.06 0.01

13 6 -0.02 -0.21 0.01 0.01 0.19 -0.01 0.03 0.00 -0.01

14 6 0.01 0.13 -0.01 -0.01 -0.27 0.01 0.00 0.27 -0.01

15 6 0.03 -0.13 -0.01 -0.05 0.26 0.01 0.04 -0.27 -0.00

16 6 -0.05 0.21 0.01 0.04 -0.19 -0.01 0.03 0.00 -0.01

17 7 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

18 6 0.06 -0.16 -0.01 -0.03 0.11 0.01 -0.07 0.05 0.01

19 6 -0.08 0.09 0.02 0.01 -0.03 -0.00 0.10 -0.06 -0.02

20 6 0.04 -0.07 -0.02 0.03 0.00 -0.00 -0.04 0.05 0.02

21 6 0.03 0.07 0.02 -0.03 0.00 0.00 -0.03 -0.06 -0.02

22 6 -0.06 -0.09 -0.02 -0.01 -0.04 -0.01 0.09 0.07 0.02

23 7 0.05 0.00 -0.00 0.00 0.02 0.00 -0.07 -0.01 0.00

24 6 0.03 0.16 0.01 0.02 0.11 0.01 -0.06 -0.06 -0.01

25 6 0.01 0.04 0.00 0.01 0.02 -0.00 0.00 -0.01 0.00

26 6 0.01 -0.00 -0.01 -0.00 0.00 0.00 -0.01 -0.01 -0.00

27 6 -0.01 -0.01 0.00 0.01 -0.00 -0.01 0.00 0.01 0.00

28 6 -0.01 0.02 0.02 -0.01 0.00 0.01 0.01 -0.01 -0.02

29 6 0.01 -0.01 -0.01 0.01 0.00 -0.00 -0.00 0.01 0.01

30 6 -0.02 -0.01 0.01 -0.01 -0.01 0.01 0.01 0.00 -0.01

31 6 -0.00 -0.02 -0.02 0.01 0.01 0.02 0.00 0.01 0.02

32 6 -0.01 0.01 -0.00 -0.01 -0.00 -0.01 0.01 -0.01 -0.00

33 6 0.01 0.00 0.01 0.00 0.00 0.00 -0.01 0.01 0.00

34 6 0.02 -0.04 -0.00 -0.01 0.02 -0.00 0.00 0.01 -0.00

35 6 -0.02 0.01 -0.01 0.01 -0.01 0.01 0.01 -0.00 0.01

36 6 0.01 0.01 0.01 -0.01 0.00 -0.01 -0.00 -0.01 -0.01

37 6 0.02 -0.04 0.00 0.01 -0.02 -0.00 0.00 0.01 0.00

38 6 -0.02 0.01 0.01 -0.01 0.01 0.01 0.01 -0.00 -0.01

39 6 0.01 0.01 -0.01 0.01 -0.00 -0.01 -0.00 -0.01 0.01

40 6 -0.00 -0.02 0.02 -0.01 -0.01 0.02 0.00 0.01 -0.02

41 6 -0.01 0.01 0.00 0.01 0.00 -0.01 0.01 -0.01 0.00

42 6 0.01 0.00 -0.01 -0.00 -0.00 0.00 -0.01 0.01 -0.00

43 6 0.01 0.04 -0.00 -0.01 -0.02 -0.00 0.00 -0.01 -0.00

44 6 -0.02 -0.01 -0.01 0.01 0.01 0.01 0.01 0.00 0.01

45 6 0.01 -0.01 0.01 -0.01 -0.00 -0.00 -0.00 0.01 -0.01

46 6 -0.01 0.02 -0.02 0.01 -0.00 0.01 0.01 -0.01 0.02

47 6 -0.01 -0.01 -0.00 -0.01 0.00 -0.01 0.00 0.01 -0.00

48 6 0.01 -0.00 0.01 0.00 -0.00 0.00 -0.01 -0.01 0.00

49 1 -0.15 -0.06 0.02 -0.01 -0.04 0.01 0.13 0.07 -0.02

50 1 -0.16 0.04 -0.02 0.02 -0.04 0.01 0.14 -0.05 0.02

51 1 -0.17 -0.13 -0.05 -0.29 -0.15 -0.08 -0.27 -0.07 -0.07

52 1 -0.19 0.12 -0.05 -0.32 0.12 -0.08 -0.28 0.04 -0.07

53 1 -0.17 -0.13 0.05 0.29 0.15 -0.08 -0.27 -0.07 0.07

54 1 -0.19 0.12 0.05 0.32 -0.12 -0.08 -0.28 0.04 0.07

55 1 -0.16 0.04 0.02 -0.02 0.04 0.01 0.14 -0.05 -0.02

56 1 -0.15 -0.06 -0.02 0.01 0.04 0.01 0.13 0.07 0.02

57 1 0.01 0.01 -0.01 -0.01 -0.01 -0.00 0.01 0.02 0.02

58 1 0.04 0.02 -0.02 -0.01 -0.01 -0.00 -0.02 -0.00 0.02

59 1 0.03 -0.01 -0.04 0.02 -0.02 -0.03 -0.03 0.01 0.03

60 1 0.02 0.02 -0.00 0.00 -0.01 -0.01 -0.01 -0.01 0.00

61 1 0.06 0.04 -0.04 0.03 0.02 -0.02 -0.02 -0.02 0.01

62 1 0.03 0.02 0.04 -0.01 -0.02 -0.03 -0.02 -0.02 -0.03

63 1 0.04 -0.01 0.02 0.01 -0.01 -0.00 -0.02 -0.00 -0.02

64 1 0.01 -0.01 0.01 0.01 -0.01 -0.00 0.01 -0.02 -0.02

65 1 0.06 -0.03 0.04 -0.03 0.02 -0.03 -0.02 0.01 -0.01

66 1 0.02 -0.02 0.00 -0.00 -0.01 -0.01 -0.02 0.01 -0.00

67 1 0.06 -0.03 -0.04 0.03 -0.02 -0.03 -0.02 0.01 0.01

68 1 0.02 -0.02 -0.00 0.00 0.01 -0.01 -0.02 0.01 0.00

69 1 0.03 0.02 -0.04 0.01 0.02 -0.03 -0.02 -0.02 0.03

70 1 0.04 -0.01 -0.02 -0.01 0.01 -0.00 -0.02 -0.00 0.02

71 1 0.01 -0.01 -0.01 -0.01 0.01 -0.00 0.01 -0.02 0.02

72 1 0.06 0.04 0.04 -0.03 -0.02 -0.02 -0.02 -0.02 -0.01

73 1 0.02 0.02 0.00 -0.00 0.01 -0.01 -0.01 -0.01 -0.00

74 1 0.03 -0.01 0.04 -0.02 0.02 -0.03 -0.03 0.01 -0.03

75 1 0.04 0.02 0.02 0.01 0.01 -0.00 -0.02 -0.00 -0.02

76 1 0.01 0.01 0.01 0.01 0.01 -0.00 0.01 0.02 -0.02

77 1 -0.29 -0.02 -0.00 0.01 -0.02 0.01 0.27 0.02 0.00

78 1 -0.29 -0.02 0.00 -0.01 0.02 0.01 0.27 0.02 -0.00

190 191 192

A A A

Frequencies -- 1584.5068 1615.0723 1615.3460

Red. masses -- 8.6750 5.2338 5.2801

Frc consts -- 12.8324 8.0437 8.1175

IR Inten -- 0.2493 0.1959 3.5730

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 -0.04 0.01 -0.00 0.00 -0.00 0.00 -0.00 0.00

2 6 0.17 0.09 -0.02 -0.00 -0.01 0.00 0.01 0.01 -0.00

3 7 -0.00 -0.01 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00

4 6 -0.18 0.07 -0.02 0.01 0.00 0.00 -0.00 0.00 -0.00

5 6 0.03 -0.03 0.01 -0.00 0.00 -0.00 -0.00 0.00 -0.00

6 6 0.16 -0.16 0.03 0.00 0.00 -0.01 0.00 0.00 -0.00

7 6 -0.09 0.15 -0.02 -0.00 -0.01 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 -0.06 -0.15 -0.02 0.01 0.01 0.00 0.01 0.01 0.00

10 6 0.02 -0.21 -0.00 -0.00 0.00 0.00 -0.00 0.01 0.00

11 6 -0.01 0.21 0.00 0.00 -0.00 -0.00 0.00 -0.01 -0.00

12 6 -0.14 -0.17 0.03 0.01 0.02 0.01 -0.02 -0.03 -0.01

13 6 0.06 0.15 -0.02 -0.01 -0.01 0.00 0.01 0.01 -0.00

14 6 -0.02 0.21 -0.00 0.00 -0.00 0.00 -0.00 0.01 -0.00

15 6 0.01 -0.21 0.00 -0.00 0.00 -0.00 0.00 -0.01 0.00

16 6 0.09 -0.15 -0.02 0.00 0.01 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 -0.16 0.16 0.03 -0.00 -0.00 -0.01 0.00 0.00 0.00

19 6 0.18 -0.07 -0.02 -0.01 -0.00 0.00 -0.00 0.00 0.00

20 6 -0.03 0.03 0.01 0.00 -0.00 -0.00 -0.00 0.00 0.00

21 6 0.03 0.04 0.01 0.00 -0.00 -0.00 0.00 -0.00 -0.00

22 6 -0.17 -0.09 -0.02 0.00 0.01 0.00 0.01 0.01 0.00

23 7 0.00 0.01 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00

24 6 0.14 0.17 0.03 -0.01 -0.02 0.01 -0.02 -0.03 0.01

25 6 0.00 0.01 -0.02 -0.05 0.04 0.07 -0.01 0.01 0.01

26 6 0.01 0.02 0.01 0.01 -0.06 -0.05 0.00 -0.01 -0.01

27 6 0.02 -0.01 -0.02 -0.06 0.01 0.06 -0.01 0.00 0.01

28 6 -0.03 0.02 0.05 0.07 -0.06 -0.11 0.01 -0.01 -0.02

29 6 0.02 -0.00 -0.02 -0.03 0.05 0.06 -0.01 0.01 0.01

30 6 -0.03 -0.02 0.02 0.07 0.01 -0.05 0.01 0.00 -0.01

31 6 0.03 0.03 0.05 0.09 0.10 0.17 -0.11 -0.13 -0.20

32 6 -0.02 -0.01 -0.02 -0.08 -0.04 -0.09 0.09 0.04 0.11

33 6 -0.01 0.02 0.01 -0.00 0.09 0.08 0.00 -0.11 -0.09

34 6 -0.00 0.01 -0.02 -0.07 -0.08 -0.11 0.08 0.09 0.13

35 6 0.03 -0.01 0.02 0.09 0.01 0.08 -0.11 -0.01 -0.09

36 6 -0.02 -0.01 -0.02 -0.03 -0.08 -0.09 0.03 0.10 0.11

37 6 0.00 -0.01 -0.02 0.07 0.08 -0.11 0.08 0.09 -0.13

38 6 -0.03 0.01 0.02 -0.09 -0.01 0.08 -0.11 -0.01 0.09

39 6 0.02 0.01 -0.02 0.03 0.08 -0.09 0.03 0.10 -0.11

40 6 -0.03 -0.03 0.05 -0.09 -0.10 0.17 -0.11 -0.13 0.20

41 6 0.02 0.01 -0.02 0.08 0.04 -0.09 0.09 0.04 -0.11

42 6 0.01 -0.02 0.01 0.00 -0.09 0.08 0.00 -0.11 0.09

43 6 -0.00 -0.01 -0.02 0.05 -0.04 0.07 -0.01 0.01 -0.01

44 6 0.03 0.02 0.02 -0.07 -0.01 -0.05 0.01 0.00 0.01

45 6 -0.02 0.00 -0.02 0.03 -0.05 0.06 -0.01 0.01 -0.01

46 6 0.03 -0.02 0.05 -0.07 0.06 -0.11 0.01 -0.01 0.02

47 6 -0.02 0.01 -0.02 0.06 -0.01 0.06 -0.01 0.00 -0.01

48 6 -0.01 -0.02 0.01 -0.01 0.06 -0.05 0.00 -0.01 0.01

49 1 0.09 0.04 -0.01 0.00 0.00 -0.00 0.00 -0.00 0.00

50 1 -0.09 0.03 -0.02 0.01 -0.00 0.00 0.00 -0.00 0.00

51 1 0.19 -0.01 0.04 -0.01 -0.00 -0.00 -0.01 -0.00 -0.00

52 1 0.19 0.03 0.04 -0.00 -0.00 -0.00 -0.01 -0.00 -0.00

53 1 -0.19 0.01 0.04 0.01 0.00 -0.00 -0.01 -0.00 0.00

54 1 -0.19 -0.03 0.04 0.00 0.00 -0.00 -0.01 -0.00 0.00

55 1 0.09 -0.03 -0.02 -0.01 0.00 0.00 0.00 -0.00 -0.00

56 1 -0.09 -0.04 -0.01 -0.00 -0.00 -0.00 0.00 -0.00 -0.00

57 1 -0.03 -0.05 -0.03 0.07 0.10 0.02 0.01 0.02 0.00

58 1 -0.00 -0.03 -0.02 0.05 0.08 0.02 0.01 0.02 0.00

59 1 0.06 -0.05 -0.09 -0.11 0.09 0.16 -0.02 0.02 0.03

60 1 0.02 -0.01 -0.03 -0.07 -0.05 0.02 -0.01 -0.01 0.00

61 1 0.06 0.04 -0.04 -0.10 -0.09 0.02 -0.02 -0.02 0.00

62 1 -0.05 -0.06 -0.09 -0.14 -0.15 -0.24 0.16 0.18 0.29

63 1 0.01 -0.03 -0.02 0.08 -0.11 -0.03 -0.10 0.13 0.04

64 1 0.04 -0.05 -0.03 0.12 -0.14 -0.03 -0.15 0.16 0.03

65 1 -0.06 0.04 -0.04 -0.16 0.11 -0.03 0.19 -0.13 0.03

66 1 -0.02 -0.01 -0.03 -0.12 0.07 -0.03 0.14 -0.08 0.03

67 1 0.06 -0.04 -0.04 0.16 -0.11 -0.03 0.19 -0.13 -0.03

68 1 0.02 0.01 -0.03 0.12 -0.07 -0.03 0.14 -0.08 -0.03

69 1 0.05 0.06 -0.09 0.14 0.15 -0.24 0.16 0.18 -0.29

70 1 -0.01 0.03 -0.02 -0.08 0.11 -0.03 -0.10 0.13 -0.04

71 1 -0.04 0.05 -0.03 -0.12 0.14 -0.03 -0.15 0.16 -0.03

72 1 -0.06 -0.04 -0.04 0.10 0.09 0.02 -0.02 -0.02 -0.00

73 1 -0.02 0.01 -0.03 0.07 0.05 0.02 -0.01 -0.01 -0.00

74 1 -0.06 0.05 -0.09 0.11 -0.09 0.16 -0.02 0.02 -0.03

75 1 0.00 0.03 -0.02 -0.05 -0.08 0.02 0.01 0.02 -0.00

76 1 0.03 0.05 -0.03 -0.07 -0.10 0.02 0.01 0.02 -0.00

77 1 0.00 -0.00 0.01 0.00 0.00 -0.00 0.01 -0.00 0.00

78 1 -0.00 0.00 0.01 -0.00 -0.00 -0.00 0.01 -0.00 -0.00

193 194 195

A A A

Frequencies -- 1616.1883 1617.1635 1639.5781

Red. masses -- 5.2660 5.4584 5.5300

Frc consts -- 8.1042 8.4106 8.7587

IR Inten -- 4.0299 4.3369 2.6335

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 -0.01 0.00

2 6 -0.00 -0.00 0.00 -0.03 -0.02 0.00 0.01 0.01 0.00

3 7 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.01 -0.00 0.00

4 6 -0.01 0.01 -0.00 0.03 -0.02 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 0.02 -0.02 -0.01 -0.04 0.04 0.00 -0.00 -0.00 -0.00

7 6 -0.01 0.01 -0.00 0.02 -0.03 0.00 -0.00 0.00 -0.00

8 7 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.01 -0.00

9 6 -0.00 -0.01 -0.00 0.01 0.03 0.00 -0.00 -0.02 0.00

10 6 0.00 -0.01 -0.00 -0.00 0.02 -0.00 0.00 0.01 0.00

11 6 0.00 0.01 -0.00 -0.00 -0.02 -0.00 0.00 -0.01 0.00

12 6 0.00 0.01 0.00 0.03 0.04 -0.00 0.01 -0.01 -0.00

13 6 -0.00 -0.01 0.00 -0.01 -0.03 0.00 -0.00 -0.02 -0.00

14 6 0.00 -0.01 0.00 0.00 -0.02 -0.00 0.00 0.01 -0.00

15 6 0.00 0.01 0.00 0.00 0.02 -0.00 0.00 -0.01 -0.00

16 6 -0.01 0.01 0.00 -0.02 0.03 0.00 -0.00 0.00 0.00

17 7 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.01 0.00

18 6 0.02 -0.02 0.01 0.04 -0.04 0.00 -0.00 -0.00 0.00

19 6 -0.01 0.01 0.00 -0.03 0.02 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 -0.01 -0.00

22 6 -0.00 -0.00 -0.00 0.03 0.02 0.00 0.01 0.01 -0.00

23 7 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.01 -0.00 -0.00

24 6 0.00 0.01 -0.00 -0.03 -0.04 -0.00 0.01 -0.01 0.00

25 6 -0.10 0.07 0.13 0.08 -0.07 -0.11 0.01 0.01 0.00

26 6 0.02 -0.10 -0.09 -0.01 0.09 0.08 -0.01 -0.02 -0.01

27 6 -0.10 0.02 0.11 0.08 -0.02 -0.09 0.02 0.01 -0.00

28 6 0.13 -0.10 -0.20 -0.11 0.09 0.17 -0.01 -0.01 -0.00

29 6 -0.05 0.08 0.11 0.04 -0.07 -0.10 0.01 0.02 0.01

30 6 0.12 0.01 -0.09 -0.09 -0.01 0.08 -0.02 -0.01 0.00

31 6 0.01 0.01 0.02 0.06 0.07 0.11 0.08 -0.07 -0.00

32 6 -0.01 -0.00 -0.01 -0.05 -0.02 -0.06 -0.17 0.11 -0.04

33 6 -0.00 0.01 0.01 -0.00 0.06 0.05 0.13 -0.16 -0.05

34 6 -0.01 -0.01 -0.01 -0.05 -0.05 -0.07 -0.10 0.09 0.00

35 6 0.01 0.00 0.01 0.06 0.01 0.05 0.17 -0.11 0.04

36 6 -0.00 -0.01 -0.01 -0.01 -0.06 -0.06 -0.12 0.16 0.04

37 6 -0.01 -0.01 0.01 0.05 0.05 -0.07 -0.10 0.09 -0.00

38 6 0.01 0.00 -0.01 -0.06 -0.01 0.05 0.17 -0.11 -0.04

39 6 -0.00 -0.01 0.01 0.01 0.06 -0.06 -0.12 0.16 -0.04

40 6 0.01 0.01 -0.02 -0.06 -0.07 0.11 0.08 -0.07 0.00

41 6 -0.01 -0.00 0.01 0.05 0.02 -0.06 -0.17 0.11 0.04

42 6 -0.00 0.01 -0.01 0.00 -0.06 0.05 0.13 -0.16 0.05

43 6 -0.10 0.07 -0.13 -0.08 0.07 -0.11 0.01 0.01 -0.00

44 6 0.12 0.01 0.09 0.09 0.01 0.08 -0.02 -0.01 -0.00

45 6 -0.05 0.08 -0.11 -0.04 0.07 -0.10 0.01 0.02 -0.01

46 6 0.13 -0.10 0.20 0.11 -0.09 0.17 -0.01 -0.01 0.00

47 6 -0.10 0.02 -0.11 -0.08 0.02 -0.09 0.02 0.01 0.00

48 6 0.02 -0.10 0.09 0.01 -0.09 0.08 -0.01 -0.02 0.01

49 1 -0.00 -0.00 0.00 -0.01 0.00 -0.00 0.01 0.00 -0.00

50 1 -0.00 -0.00 0.00 0.01 0.00 -0.00 0.00 0.00 0.00

51 1 0.01 0.00 0.00 -0.02 0.01 -0.00 -0.01 -0.01 -0.00

52 1 0.01 0.00 0.00 -0.02 -0.01 -0.00 -0.01 0.00 -0.00

53 1 0.01 0.00 -0.00 0.02 -0.01 -0.00 -0.01 -0.01 0.00

54 1 0.01 0.00 -0.00 0.02 0.01 -0.00 -0.01 0.00 0.00

55 1 -0.00 -0.00 -0.00 -0.01 -0.00 -0.00 0.00 0.00 -0.00

56 1 -0.00 -0.00 -0.00 0.01 -0.00 -0.00 0.01 0.00 0.00

57 1 0.12 0.18 0.04 -0.10 -0.15 -0.03 0.01 0.03 0.02

58 1 0.09 0.14 0.04 -0.07 -0.12 -0.03 -0.02 -0.01 0.01

59 1 -0.19 0.15 0.29 0.16 -0.13 -0.24 -0.01 -0.01 0.00

60 1 -0.13 -0.09 0.04 0.11 0.08 -0.03 -0.00 -0.02 -0.01

61 1 -0.17 -0.16 0.03 0.14 0.13 -0.02 0.02 0.01 -0.01

62 1 -0.02 -0.02 -0.03 -0.09 -0.09 -0.15 0.09 -0.07 0.00

63 1 0.01 -0.01 -0.00 0.05 -0.07 -0.02 0.21 -0.04 0.13

64 1 0.02 -0.02 -0.00 0.08 -0.09 -0.02 -0.07 0.22 0.15

65 1 -0.02 0.01 -0.00 -0.10 0.07 -0.01 -0.23 0.05 -0.14

66 1 -0.01 0.01 -0.00 -0.08 0.05 -0.01 0.07 -0.20 -0.13

67 1 -0.02 0.01 0.00 0.10 -0.07 -0.01 -0.23 0.05 0.14

68 1 -0.01 0.01 0.00 0.08 -0.05 -0.01 0.07 -0.20 0.13

69 1 -0.02 -0.02 0.03 0.09 0.09 -0.15 0.09 -0.07 -0.00

70 1 0.01 -0.01 0.00 -0.05 0.07 -0.02 0.21 -0.04 -0.13

71 1 0.02 -0.02 0.00 -0.08 0.09 -0.02 -0.07 0.22 -0.15

72 1 -0.17 -0.16 -0.03 -0.14 -0.13 -0.02 0.02 0.01 0.01

73 1 -0.13 -0.09 -0.04 -0.11 -0.08 -0.03 -0.00 -0.02 0.01

74 1 -0.19 0.15 -0.29 -0.16 0.13 -0.24 -0.01 -0.01 -0.00

75 1 0.09 0.14 -0.04 0.07 0.12 -0.03 -0.02 -0.01 -0.01

76 1 0.12 0.18 -0.04 0.10 0.15 -0.03 0.01 0.03 -0.02

77 1 -0.01 -0.00 0.00 -0.00 0.00 -0.00 0.01 0.00 0.00

78 1 -0.01 -0.00 -0.00 0.00 -0.00 -0.00 0.01 0.00 -0.00

196 197 198

A A A

Frequencies -- 1639.6778 1640.4362 1640.5248

Red. masses -- 5.5328 5.5290 5.5337

Frc consts -- 8.7643 8.7663 8.7747

IR Inten -- 0.0027 3.8827 0.0011

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 0.00 0.00 0.00 0.01 0.00 -0.00

3 7 -0.01 -0.00 -0.00 -0.01 -0.00 -0.00 -0.01 -0.00 -0.00

4 6 0.01 -0.00 0.00 0.01 -0.00 -0.00 0.01 -0.00 -0.00

5 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

6 6 -0.00 0.01 -0.00 0.01 0.01 0.00 0.02 0.00 0.00

7 6 0.00 -0.00 0.00 -0.00 0.02 0.00 -0.01 0.02 0.00

8 7 0.00 -0.01 0.00 -0.00 -0.00 -0.00 -0.00 -0.01 -0.00

9 6 0.00 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 0.01 0.00 0.00 0.01 0.00

11 6 -0.00 0.00 -0.00 0.00 -0.01 0.00 0.00 -0.01 0.00

12 6 0.02 -0.00 -0.00 0.00 0.00 0.00 -0.01 -0.01 0.00

13 6 -0.00 -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 0.01 -0.00 -0.00 -0.01 0.00

15 6 0.00 -0.00 -0.00 0.00 -0.01 -0.00 -0.00 0.01 0.00

16 6 -0.00 0.00 0.00 -0.00 0.02 -0.00 0.01 -0.02 0.00

17 7 -0.00 0.01 0.00 -0.00 -0.00 0.00 0.00 0.01 -0.00

18 6 0.00 -0.01 -0.00 0.01 0.01 -0.00 -0.02 -0.00 0.00

19 6 -0.01 0.00 0.00 0.01 -0.00 0.00 -0.01 0.00 -0.00

20 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

21 6 0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00 0.00

22 6 -0.01 -0.00 0.00 0.00 0.00 -0.00 -0.01 -0.00 -0.00

23 7 0.01 0.00 -0.00 -0.01 -0.00 0.00 0.01 0.00 -0.00

24 6 -0.02 0.00 -0.00 0.00 0.00 -0.00 0.01 0.01 0.00

25 6 -0.01 -0.01 -0.00 -0.09 -0.11 -0.01 -0.09 -0.11 -0.01

26 6 0.01 0.02 0.01 0.11 0.18 0.05 0.11 0.18 0.05

27 6 -0.02 -0.01 0.00 -0.15 -0.13 0.03 -0.15 -0.13 0.03

28 6 0.01 0.01 0.00 0.06 0.08 0.01 0.06 0.08 0.01

29 6 -0.01 -0.02 -0.01 -0.10 -0.17 -0.05 -0.10 -0.17 -0.05

30 6 0.02 0.01 -0.00 0.15 0.13 -0.03 0.15 0.13 -0.03

31 6 0.08 -0.07 -0.00 0.01 -0.01 0.00 -0.01 0.01 -0.00

32 6 -0.17 0.11 -0.04 -0.02 0.01 -0.00 0.02 -0.01 0.01

33 6 0.13 -0.16 -0.04 0.01 -0.02 -0.00 -0.01 0.02 0.00

34 6 -0.10 0.09 0.00 -0.01 0.01 -0.00 0.01 -0.01 0.00

35 6 0.17 -0.11 0.04 0.02 -0.01 0.00 -0.02 0.01 -0.01

36 6 -0.12 0.16 0.04 -0.01 0.02 0.00 0.01 -0.02 -0.00

37 6 0.10 -0.09 0.00 -0.01 0.01 0.00 -0.01 0.01 0.00

38 6 -0.17 0.11 0.04 0.02 -0.01 -0.00 0.02 -0.01 -0.01

39 6 0.12 -0.16 0.04 -0.01 0.02 -0.00 -0.01 0.02 -0.00

40 6 -0.08 0.07 -0.00 0.01 -0.01 -0.00 0.01 -0.01 -0.00

41 6 0.17 -0.11 -0.04 -0.02 0.01 0.00 -0.02 0.01 0.01

42 6 -0.13 0.16 -0.04 0.01 -0.02 0.00 0.01 -0.02 0.00

43 6 0.01 0.01 -0.00 -0.09 -0.11 0.01 0.09 0.11 -0.01

44 6 -0.02 -0.01 -0.00 0.15 0.13 0.03 -0.15 -0.13 -0.03

45 6 0.01 0.02 -0.01 -0.10 -0.17 0.05 0.10 0.17 -0.05

46 6 -0.01 -0.01 0.00 0.06 0.08 -0.01 -0.06 -0.08 0.01

47 6 0.02 0.01 0.00 -0.15 -0.13 -0.03 0.15 0.13 0.03

48 6 -0.01 -0.02 0.01 0.11 0.18 -0.05 -0.11 -0.18 0.05

49 1 0.01 0.00 -0.00 0.00 0.00 -0.00 0.01 0.00 -0.00

50 1 0.01 -0.00 0.00 0.01 -0.00 0.00 0.00 -0.00 0.00

51 1 0.01 0.01 0.00 -0.01 -0.00 -0.00 -0.01 -0.00 -0.00

52 1 0.00 -0.00 0.00 -0.01 0.01 -0.00 -0.01 0.01 -0.00

53 1 -0.01 -0.01 0.00 -0.01 -0.00 0.00 0.01 0.00 -0.00

54 1 -0.00 0.00 0.00 -0.01 0.01 0.00 0.01 -0.01 -0.00

55 1 -0.01 0.00 0.00 0.01 -0.00 -0.00 -0.00 0.00 0.00

56 1 -0.01 -0.00 -0.00 0.00 0.00 0.00 -0.01 -0.00 -0.00

57 1 -0.01 -0.03 -0.02 -0.04 -0.23 -0.15 -0.04 -0.23 -0.16

58 1 0.02 0.01 -0.01 0.20 0.07 -0.13 0.21 0.07 -0.13

59 1 0.01 0.01 -0.00 0.08 0.08 -0.01 0.08 0.08 -0.01

60 1 0.01 0.02 0.01 0.04 0.21 0.14 0.04 0.21 0.14

61 1 -0.02 -0.01 0.02 -0.21 -0.08 0.14 -0.21 -0.08 0.14

62 1 0.09 -0.07 -0.00 0.01 -0.01 -0.00 -0.01 0.01 0.00

63 1 0.21 -0.04 0.13 0.02 -0.00 0.01 -0.02 0.01 -0.01

64 1 -0.07 0.22 0.15 -0.01 0.02 0.02 0.01 -0.02 -0.02

65 1 -0.23 0.05 -0.14 -0.02 0.01 -0.02 0.03 -0.01 0.02

66 1 0.06 -0.20 -0.13 0.01 -0.02 -0.01 -0.01 0.02 0.01

67 1 0.23 -0.05 -0.14 -0.02 0.01 0.01 -0.03 0.01 0.02

68 1 -0.06 0.20 -0.13 0.01 -0.02 0.01 0.01 -0.02 0.01

69 1 -0.09 0.07 -0.00 0.01 -0.01 0.00 0.01 -0.01 0.00

70 1 -0.21 0.04 0.13 0.02 -0.00 -0.01 0.02 -0.01 -0.01

71 1 0.07 -0.22 0.15 -0.01 0.02 -0.02 -0.01 0.02 -0.02

72 1 0.02 0.01 0.02 -0.21 -0.08 -0.14 0.21 0.08 0.14

73 1 -0.01 -0.02 0.01 0.04 0.21 -0.14 -0.04 -0.21 0.14

74 1 -0.01 -0.01 -0.00 0.08 0.08 0.01 -0.08 -0.08 -0.01

75 1 -0.02 -0.01 -0.01 0.20 0.07 0.13 -0.20 -0.07 -0.13

76 1 0.01 0.03 -0.02 -0.04 -0.23 0.16 0.04 0.23 -0.15

77 1 0.02 0.00 -0.00 0.02 0.00 -0.00 0.02 0.00 0.00

78 1 -0.02 -0.00 -0.00 0.02 0.00 0.00 -0.02 -0.00 0.00

199 200 201

A A A

Frequencies -- 3173.6915 3173.6955 3173.7826

Red. masses -- 1.0864 1.0864 1.0865

Frc consts -- 6.4471 6.4471 6.4479

IR Inten -- 5.2872 0.1104 4.6346

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 0.00 0.00 -0.00

27 6 -0.00 0.03 0.02 0.00 -0.02 -0.02 -0.00 0.00 0.00

28 6 -0.02 -0.03 -0.00 0.02 0.03 0.00 -0.00 -0.00 -0.00

29 6 0.02 0.00 -0.02 -0.02 -0.00 0.02 0.00 0.00 -0.00

30 6 -0.00 0.01 0.01 0.00 -0.01 -0.01 -0.00 0.00 0.00

31 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.03 0.02 0.00

32 6 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.02 -0.02

33 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 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 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.01 -0.01

36 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.02 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 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.01 0.01

39 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.02 0.00 -0.02

40 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.03 0.02 -0.00

41 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.02 0.02

42 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 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 0.00 -0.00

45 6 0.02 0.00 0.02 0.02 0.00 0.02 0.00 0.00 0.00

46 6 -0.02 -0.03 0.00 -0.02 -0.03 0.00 -0.00 -0.00 0.00

47 6 -0.00 0.02 -0.02 -0.00 0.02 -0.02 -0.00 0.00 -0.00

48 6 0.01 -0.00 0.01 0.01 -0.00 0.01 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 -0.12 -0.00 0.10 0.10 0.00 -0.09 -0.00 -0.00 0.00

58 1 0.04 -0.29 -0.28 -0.04 0.26 0.25 0.00 -0.00 -0.00

59 1 0.29 0.33 0.01 -0.25 -0.30 -0.01 0.00 0.00 0.00

60 1 -0.29 -0.01 0.25 0.25 0.01 -0.22 -0.00 -0.00 0.00

61 1 0.02 -0.12 -0.12 -0.02 0.11 0.10 0.00 -0.00 -0.00

62 1 0.00 -0.00 -0.00 -0.02 0.02 0.00 0.32 -0.29 -0.01

63 1 -0.00 0.00 0.00 0.00 -0.02 -0.02 -0.00 0.28 0.26

64 1 -0.00 -0.00 -0.00 0.01 0.00 0.01 -0.11 -0.01 -0.10

65 1 0.00 0.00 0.00 -0.00 -0.01 -0.01 0.00 0.11 0.10

66 1 0.00 0.00 0.00 0.02 0.00 0.02 -0.28 -0.03 -0.25

67 1 0.00 -0.00 0.00 0.00 0.01 -0.01 0.00 0.10 -0.09

68 1 0.00 0.00 -0.00 -0.02 -0.00 0.02 -0.27 -0.03 0.24

69 1 -0.00 0.00 -0.00 0.02 -0.02 0.00 0.31 -0.28 0.00

70 1 0.00 -0.00 0.00 -0.00 0.02 -0.02 -0.00 0.27 -0.25

71 1 0.00 0.00 -0.00 -0.01 -0.00 0.01 -0.11 -0.01 0.09

72 1 0.02 -0.11 0.10 0.02 -0.12 0.11 0.00 -0.00 0.00

73 1 -0.25 -0.01 -0.22 -0.28 -0.01 -0.25 -0.00 -0.00 -0.00

74 1 0.25 0.30 -0.01 0.28 0.33 -0.01 0.00 0.00 -0.00

75 1 0.04 -0.26 0.25 0.04 -0.29 0.28 0.00 -0.00 0.00

76 1 -0.10 -0.00 -0.09 -0.11 -0.00 -0.10 -0.00 -0.00 -0.00

77 1 -0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

78 1 -0.00 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

202 203 204

A A A

Frequencies -- 3173.7876 3180.7276 3180.7307

Red. masses -- 1.0865 1.0886 1.0886

Frc consts -- 6.4479 6.4888 6.4888

IR Inten -- 0.0057 7.9764 5.9840

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 0.02 -0.00 -0.01 0.01 -0.00 -0.01

27 6 -0.00 0.00 0.00 -0.00 0.03 0.03 -0.00 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 0.00 0.00 -0.00 -0.03 -0.00 0.03 -0.03 -0.00 0.02

30 6 -0.00 0.00 0.00 0.00 -0.02 -0.02 0.00 -0.02 -0.02

31 6 0.03 -0.02 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00

32 6 -0.00 0.02 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 -0.02 -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 0.02 0.00 -0.02 0.00 0.00 -0.00 0.00 0.00 -0.00

40 6 -0.03 0.02 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00

41 6 0.00 -0.02 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 -0.00 0.00 -0.00 0.02 -0.02 0.00 -0.02 0.02

45 6 -0.00 -0.00 -0.00 0.03 0.00 0.02 -0.03 -0.00 -0.03

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 -0.02 0.02 -0.00 0.03 -0.03

48 6 -0.00 0.00 -0.00 -0.01 0.00 -0.01 0.02 -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 -0.01 -0.00 0.01 -0.18 -0.01 0.16 -0.16 -0.01 0.14

58 1 0.00 -0.02 -0.02 0.05 -0.32 -0.31 0.04 -0.29 -0.28

59 1 0.02 0.02 0.00 0.00 0.00 0.00 0.00 0.00 0.00

60 1 -0.02 -0.00 0.02 0.33 0.02 -0.29 0.30 0.01 -0.26

61 1 0.00 -0.01 -0.01 -0.03 0.22 0.21 -0.03 0.20 0.19

62 1 -0.31 0.28 0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00

63 1 0.00 -0.27 -0.25 0.00 0.01 0.01 0.00 -0.00 -0.00

64 1 0.11 0.01 0.09 -0.01 -0.00 -0.00 0.00 0.00 0.00

65 1 -0.00 -0.10 -0.09 0.00 -0.01 -0.00 -0.00 0.00 0.00

66 1 0.27 0.03 0.24 0.01 0.00 0.01 -0.00 -0.00 -0.00

67 1 0.00 0.11 -0.10 -0.00 0.01 -0.00 -0.00 0.00 -0.00

68 1 -0.27 -0.03 0.25 -0.01 -0.00 0.01 -0.00 -0.00 0.00

69 1 0.32 -0.28 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00

70 1 -0.00 0.28 -0.26 -0.00 -0.01 0.01 0.00 -0.00 0.00

71 1 -0.11 -0.01 0.10 0.01 0.00 -0.00 0.00 0.00 -0.00

72 1 -0.00 0.01 -0.01 0.03 -0.20 0.19 -0.03 0.22 -0.21

73 1 0.02 0.00 0.02 -0.30 -0.01 -0.26 0.33 0.02 0.29

74 1 -0.02 -0.02 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

75 1 -0.00 0.02 -0.02 -0.04 0.29 -0.28 0.05 -0.32 0.31

76 1 0.01 0.00 0.01 0.16 0.01 0.14 -0.18 -0.01 -0.16

77 1 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

78 1 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

205 206 207

A A A

Frequencies -- 3181.1122 3181.1145 3190.1132

Red. masses -- 1.0887 1.0887 1.0919

Frc consts -- 6.4910 6.4910 6.5470

IR Inten -- 10.0224 6.5487 2.2716

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 -0.02 -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 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.03 -0.03 -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 -0.03 -0.03

31 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.00 0.00 0.00

32 6 -0.00 -0.03 -0.03 -0.00 -0.03 -0.02 0.00 0.00 0.00

33 6 0.02 0.00 0.01 0.01 0.00 0.01 -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 0.02 0.02 0.00 0.01 0.01 0.00 0.00 0.00

36 6 -0.03 -0.00 -0.03 -0.03 -0.00 -0.02 -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 0.02 -0.02 -0.00 -0.00 0.00

39 6 0.03 0.00 -0.02 -0.03 -0.00 0.03 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 0.03 -0.02 -0.00 -0.03 0.03 -0.00 -0.00 0.00

42 6 -0.01 -0.00 0.01 0.02 0.00 -0.01 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 0.03 -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 -0.00

47 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.01 -0.01

48 6 0.00 -0.00 0.00 0.00 -0.00 0.00 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 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.24 0.01 -0.21

58 1 -0.00 0.01 0.01 0.00 -0.00 -0.00 -0.02 0.12 0.11

59 1 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.30 0.35 0.01

60 1 -0.01 -0.00 0.01 0.00 0.00 -0.00 0.03 -0.00 -0.03

61 1 0.00 -0.01 -0.01 -0.00 0.00 0.00 -0.05 0.31 0.29

62 1 -0.01 0.00 -0.00 -0.01 0.00 -0.00 0.02 -0.01 -0.00

63 1 0.00 0.33 0.30 0.00 0.30 0.28 -0.00 -0.00 -0.00

64 1 -0.19 -0.02 -0.17 -0.17 -0.02 -0.15 0.01 0.00 0.01

65 1 0.00 -0.19 -0.18 0.00 -0.17 -0.16 0.00 -0.01 -0.01

66 1 0.34 0.04 0.30 0.31 0.03 0.28 0.00 0.00 0.00

67 1 -0.00 0.17 -0.16 0.00 -0.19 0.18 -0.00 0.01 -0.01

68 1 -0.31 -0.03 0.28 0.34 0.04 -0.30 -0.00 -0.00 0.00

69 1 0.01 -0.00 -0.00 -0.01 0.00 0.00 -0.02 0.01 -0.00

70 1 -0.00 -0.30 0.28 0.00 0.33 -0.30 0.00 0.00 -0.00

71 1 0.17 0.02 -0.15 -0.19 -0.02 0.17 -0.01 -0.00 0.01

72 1 -0.00 0.01 -0.01 -0.00 0.00 -0.00 0.04 -0.29 0.28

73 1 0.01 0.00 0.01 0.00 0.00 0.00 -0.03 0.00 -0.03

74 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.28 -0.33 0.01

75 1 0.00 -0.01 0.01 0.00 -0.00 0.00 0.02 -0.11 0.11

76 1 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.23 -0.01 -0.20

77 1 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00

78 1 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00 0.00

208 209 210

A A A

Frequencies -- 3190.1273 3190.7577 3190.7670

Red. masses -- 1.0919 1.0919 1.0920

Frc consts -- 6.5472 6.5499 6.5501

IR Inten -- 67.5777 0.0507 76.2774

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 -0.02 -0.00 0.02 0.00 -0.00 -0.00 0.00 -0.00 -0.00

27 6 0.00 -0.01 -0.01 -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 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00

30 6 0.00 -0.03 -0.02 -0.00 0.00 0.00 -0.00 0.00 0.00

31 6 -0.00 0.00 0.00 -0.03 0.03 0.00 -0.03 0.03 0.00

32 6 0.00 -0.00 -0.00 0.00 0.01 0.01 0.00 0.01 0.01

33 6 -0.00 -0.00 -0.00 -0.02 -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 0.00 0.00 0.00 0.02 0.02 0.00 0.02 0.02

36 6 -0.00 -0.00 -0.00 -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 0.00 -0.00 -0.00 -0.02 0.02 0.00 0.02 -0.02

39 6 -0.00 -0.00 0.00 0.01 0.00 -0.01 -0.01 -0.00 0.01

40 6 -0.00 0.00 -0.00 0.03 -0.03 0.00 -0.03 0.03 -0.00

41 6 0.00 -0.00 -0.00 -0.00 -0.01 0.01 0.00 0.01 -0.01

42 6 -0.00 -0.00 0.00 0.02 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 -0.03 0.03 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 -0.03 -0.03 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

47 6 0.00 -0.01 0.01 0.00 -0.00 0.00 -0.00 0.00 -0.00

48 6 -0.02 -0.00 -0.02 -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 0.23 0.01 -0.20 -0.01 -0.00 0.01 -0.00 -0.00 0.00

58 1 -0.02 0.11 0.11 0.00 -0.01 -0.01 0.00 -0.00 -0.00

59 1 0.28 0.33 0.01 -0.01 -0.02 -0.00 -0.00 -0.00 -0.00

60 1 0.03 -0.00 -0.03 -0.00 0.00 0.00 0.00 0.00 -0.00

61 1 -0.04 0.29 0.28 0.00 -0.01 -0.01 0.00 -0.00 -0.00

62 1 0.00 -0.00 -0.00 0.35 -0.31 -0.01 0.34 -0.30 -0.01

63 1 -0.00 0.00 0.00 -0.00 -0.09 -0.09 -0.00 -0.09 -0.09

64 1 0.00 0.00 0.00 0.26 0.03 0.23 0.26 0.03 0.23

65 1 -0.00 -0.00 -0.00 0.00 -0.27 -0.25 0.00 -0.26 -0.24

66 1 0.00 0.00 0.00 0.09 0.01 0.08 0.09 0.01 0.08

67 1 -0.00 -0.00 0.00 -0.00 0.26 -0.24 0.00 -0.27 0.25

68 1 0.00 0.00 -0.00 -0.09 -0.01 0.08 0.09 0.01 -0.09

69 1 0.00 -0.00 0.00 -0.34 0.30 -0.01 0.35 -0.31 0.01

70 1 -0.00 -0.00 0.00 0.00 0.09 -0.09 -0.00 -0.09 0.09

71 1 0.00 0.00 -0.00 -0.26 -0.03 0.23 0.26 0.03 -0.23

72 1 -0.05 0.31 -0.29 -0.00 0.01 -0.01 0.00 -0.00 0.00

73 1 0.03 -0.00 0.03 0.00 -0.00 0.00 0.00 0.00 0.00

74 1 0.30 0.35 -0.01 0.01 0.02 -0.00 -0.00 -0.00 0.00

75 1 -0.02 0.12 -0.11 -0.00 0.01 -0.01 0.00 -0.00 0.00

76 1 0.24 0.01 0.21 0.01 0.00 0.01 -0.00 -0.00 -0.00

77 1 -0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

78 1 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

211 212 213

A A A

Frequencies -- 3196.4713 3196.4776 3197.2114

Red. masses -- 1.0942 1.0942 1.0940

Frc consts -- 6.5869 6.5870 6.5890

IR Inten -- 43.6111 38.5059 53.2509

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 -0.00 0.03 -0.03 -0.00 0.02 0.00 0.00 -0.00

27 6 -0.00 0.01 0.01 -0.00 0.01 0.01 0.00 -0.00 -0.00

28 6 -0.00 -0.01 -0.00 -0.00 -0.01 -0.00 0.00 0.00 0.00

29 6 -0.02 -0.00 0.02 -0.02 -0.00 0.02 0.00 0.00 -0.00

30 6 -0.00 0.03 0.02 -0.00 0.02 0.02 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 -0.02 -0.01

33 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.03 -0.00 -0.03

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 -0.03 -0.03

36 6 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.02 -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 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.03 -0.02

39 6 0.00 0.00 -0.00 -0.00 0.00 0.00 0.02 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 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.02 -0.01

42 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.03 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 -0.02 0.02 -0.00 0.03 -0.02 -0.00 0.00 -0.00

45 6 0.02 0.00 0.02 -0.02 -0.00 -0.02 -0.00 -0.00 -0.00

46 6 0.00 0.01 -0.00 -0.00 -0.01 0.00 -0.00 -0.00 0.00

47 6 0.00 -0.01 0.01 -0.00 0.01 -0.01 -0.00 0.00 -0.00

48 6 0.03 0.00 0.02 -0.03 -0.00 -0.03 -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 0.01 -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 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.01 0.00 0.00

54 1 0.01 0.00 -0.00 -0.01 -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 0.34 0.02 -0.30 0.33 0.02 -0.29 -0.02 -0.00 0.01

58 1 0.02 -0.14 -0.13 0.02 -0.14 -0.13 -0.00 0.01 0.01

59 1 0.06 0.08 0.00 0.06 0.07 0.00 -0.00 -0.00 -0.00

60 1 0.24 0.01 -0.21 0.23 0.01 -0.20 -0.01 -0.00 0.01

61 1 0.04 -0.29 -0.27 0.04 -0.28 -0.26 -0.00 0.01 0.01

62 1 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

63 1 -0.00 0.01 0.01 0.00 0.00 0.00 -0.00 0.18 0.17

64 1 0.02 0.00 0.01 0.00 0.00 0.00 0.33 0.04 0.29

65 1 -0.00 0.02 0.01 -0.00 0.00 0.00 -0.00 0.32 0.29

66 1 0.01 0.00 0.01 -0.00 -0.00 -0.00 0.19 0.02 0.17

67 1 0.00 -0.02 0.01 -0.00 0.00 -0.00 0.00 -0.31 0.28

68 1 -0.01 -0.00 0.01 0.00 0.00 -0.00 -0.18 -0.02 0.16

69 1 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

70 1 0.00 -0.01 0.01 0.00 0.00 -0.00 0.00 -0.18 0.16

71 1 -0.02 -0.00 0.01 0.00 0.00 -0.00 -0.32 -0.03 0.28

72 1 -0.04 0.28 -0.26 0.04 -0.29 0.27 0.00 -0.01 0.01

73 1 -0.23 -0.01 -0.20 0.24 0.01 0.21 0.01 0.00 0.01

74 1 -0.06 -0.07 0.00 0.06 0.08 -0.00 0.00 0.00 -0.00

75 1 -0.02 0.14 -0.13 0.02 -0.14 0.13 0.00 -0.01 0.01

76 1 -0.33 -0.02 -0.29 0.34 0.02 0.30 0.02 0.00 0.01

77 1 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00

78 1 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00

214 215 216

A A A

Frequencies -- 3197.2159 3201.9934 3202.0305

Red. masses -- 1.0940 1.0977 1.0977

Frc consts -- 6.5891 6.6308 6.6309

IR Inten -- 33.6646 0.7327 64.2177

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 -0.02 -0.00 0.02 -0.02 -0.00 0.02

27 6 -0.00 -0.00 0.00 -0.00 0.02 0.02 -0.00 0.02 0.02

28 6 0.00 0.00 0.00 0.02 0.02 0.00 0.02 0.02 0.00

29 6 0.00 0.00 -0.00 0.02 0.00 -0.02 0.02 0.00 -0.02

30 6 0.00 -0.00 -0.00 0.00 -0.02 -0.01 0.00 -0.02 -0.02

31 6 0.00 0.00 0.00 0.01 -0.00 -0.00 -0.00 0.00 0.00

32 6 0.00 -0.02 -0.01 -0.00 -0.01 -0.00 0.00 0.00 0.00

33 6 -0.03 -0.00 -0.02 -0.01 -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 -0.03 -0.02 -0.00 0.01 0.00 0.00 -0.00 -0.00

36 6 -0.02 -0.00 -0.01 0.01 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 -0.03 0.03 0.00 -0.01 0.00 0.00 -0.00 0.00

39 6 -0.02 -0.00 0.01 -0.01 -0.00 0.00 -0.00 -0.00 0.00

40 6 0.00 0.00 -0.00 -0.01 0.00 -0.00 -0.00 0.00 -0.00

41 6 0.00 -0.02 0.01 0.00 0.01 -0.00 0.00 0.00 -0.00

42 6 -0.03 -0.00 0.03 0.01 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 0.02 -0.01 0.00 -0.02 0.02

45 6 0.00 0.00 0.00 -0.02 -0.00 -0.02 0.02 0.00 0.02

46 6 0.00 0.00 -0.00 -0.02 -0.02 0.00 0.02 0.02 -0.00

47 6 -0.00 -0.00 0.00 0.00 -0.02 0.02 -0.00 0.02 -0.02

48 6 0.00 0.00 0.00 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 -0.01 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 -0.01 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 -0.00 -0.00 0.00 0.26 0.01 -0.23 0.27 0.01 -0.23

58 1 0.00 -0.00 -0.00 0.03 -0.23 -0.22 0.04 -0.23 -0.22

59 1 -0.00 -0.00 -0.00 -0.21 -0.25 -0.01 -0.22 -0.25 -0.01

60 1 -0.00 -0.00 0.00 -0.22 -0.01 0.19 -0.22 -0.01 0.19

61 1 -0.00 0.00 0.00 -0.02 0.17 0.17 -0.03 0.18 0.17

62 1 0.00 -0.00 -0.00 -0.06 0.05 0.00 0.02 -0.02 -0.00

63 1 -0.00 0.18 0.16 0.00 0.06 0.05 -0.00 -0.02 -0.02

64 1 0.32 0.03 0.28 0.06 0.01 0.05 -0.02 -0.00 -0.02

65 1 -0.00 0.31 0.29 0.00 -0.06 -0.05 -0.00 0.02 0.02

66 1 0.18 0.02 0.16 -0.06 -0.01 -0.05 0.02 0.00 0.02

67 1 -0.00 0.32 -0.29 -0.00 0.06 -0.05 -0.00 0.02 -0.02

68 1 0.19 0.02 -0.17 0.06 0.01 -0.05 0.02 0.00 -0.01

69 1 0.00 -0.00 0.00 0.06 -0.05 0.00 0.02 -0.02 0.00

70 1 -0.00 0.18 -0.17 -0.00 -0.06 0.05 -0.00 -0.02 0.02

71 1 0.33 0.04 -0.29 -0.06 -0.01 0.05 -0.02 -0.00 0.02

72 1 -0.00 0.00 -0.00 0.02 -0.17 0.16 -0.03 0.18 -0.17

73 1 -0.00 -0.00 -0.00 0.22 0.01 0.19 -0.22 -0.01 -0.20

74 1 -0.00 -0.00 0.00 0.21 0.25 -0.01 -0.22 -0.25 0.01

75 1 -0.00 0.00 -0.00 -0.03 0.22 -0.21 0.04 -0.23 0.22

76 1 -0.00 -0.00 -0.00 -0.26 -0.01 -0.23 0.27 0.01 0.23

77 1 -0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

78 1 -0.00 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

217 218 219

A A A

Frequencies -- 3202.3822 3202.3899 3243.2211

Red. masses -- 1.0976 1.0976 1.0897

Frc consts -- 6.6322 6.6323 6.7530

IR Inten -- 50.2371 0.0529 0.0007

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 -0.04 0.02 -0.01

11 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.03 0.03 0.01

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 0.04 -0.02 -0.01

15 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.03 -0.03 0.01

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 0.01 0.00 -0.01 0.00 -0.00 -0.00

27 6 0.00 -0.00 -0.00 0.00 -0.01 -0.01 0.00 0.00 -0.00

28 6 -0.00 -0.00 -0.00 -0.00 -0.01 -0.00 -0.00 -0.00 0.00

29 6 -0.00 -0.00 0.00 -0.01 -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 -0.02 0.02 0.00 0.02 -0.02 -0.00 -0.00 -0.00 -0.00

32 6 0.00 0.02 0.02 -0.00 -0.02 -0.02 0.00 -0.00 0.00

33 6 0.02 0.00 0.02 -0.02 -0.00 -0.02 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 -0.02 -0.02 -0.00 0.02 0.02 -0.00 0.00 0.00

36 6 -0.02 -0.00 -0.02 0.02 0.00 0.02 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 -0.02 0.02 0.00 -0.02 0.02 0.00 -0.00 0.00

39 6 -0.02 -0.00 0.02 -0.02 -0.00 0.02 -0.00 -0.00 0.00

40 6 -0.02 0.02 -0.00 -0.02 0.02 -0.00 0.00 0.00 -0.00

41 6 0.00 0.02 -0.02 0.00 0.02 -0.02 -0.00 0.00 0.00

42 6 0.02 0.00 -0.02 0.02 0.00 -0.02 -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 0.01 -0.00 0.00 0.00 0.00

47 6 0.00 -0.00 0.00 -0.00 0.01 -0.00 -0.00 -0.00 -0.00

48 6 0.00 0.00 0.00 -0.01 -0.00 -0.01 -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 0.42 -0.29 0.10

52 1 0.00 0.00 0.00 0.00 0.00 0.00 -0.35 -0.32 -0.10

53 1 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.41 0.28 0.10

54 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.34 0.31 -0.10

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 -0.02 -0.00 0.02 -0.07 -0.00 0.06 -0.00 -0.00 0.00

58 1 -0.00 0.02 0.02 -0.01 0.06 0.05 -0.00 0.00 0.00

59 1 0.02 0.02 0.00 0.05 0.06 0.00 0.00 0.00 0.00

60 1 0.02 0.00 -0.01 0.06 0.00 -0.05 -0.00 -0.00 0.00

61 1 0.00 -0.01 -0.01 0.01 -0.05 -0.04 -0.00 0.01 0.01

62 1 0.24 -0.21 -0.00 -0.23 0.20 0.00 0.00 -0.00 -0.00

63 1 -0.00 -0.23 -0.21 0.00 0.22 0.20 -0.00 -0.00 0.00

64 1 -0.24 -0.03 -0.21 0.23 0.02 0.20 -0.00 -0.00 -0.00

65 1 -0.00 0.24 0.22 0.00 -0.22 -0.20 0.00 -0.01 -0.01

66 1 0.23 0.03 0.21 -0.22 -0.02 -0.20 -0.00 -0.00 -0.00

67 1 -0.00 0.23 -0.21 -0.00 0.23 -0.21 -0.00 0.01 -0.01

68 1 0.23 0.03 -0.20 0.23 0.03 -0.20 0.00 0.00 -0.00

69 1 0.24 -0.21 0.00 0.24 -0.21 0.00 -0.00 0.00 -0.00

70 1 -0.00 -0.22 0.20 -0.00 -0.22 0.20 0.00 0.00 -0.00

71 1 -0.24 -0.03 0.21 -0.23 -0.02 0.21 0.00 0.00 -0.00

72 1 0.00 -0.01 0.01 -0.01 0.04 -0.04 0.00 -0.01 0.01

73 1 0.02 0.00 0.02 -0.06 -0.00 -0.05 0.00 0.00 0.00

74 1 0.02 0.02 -0.00 -0.05 -0.06 0.00 -0.00 -0.00 0.00

75 1 -0.00 0.02 -0.02 0.01 -0.06 0.05 0.00 -0.00 0.00

76 1 -0.02 -0.00 -0.02 0.07 0.00 0.06 0.00 0.00 0.00

77 1 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00

78 1 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00

220 221 222

A A A

Frequencies -- 3243.2443 3256.9207 3256.9822

Red. masses -- 1.0897 1.0924 1.0924

Frc consts -- 6.7532 6.8270 6.8276

IR Inten -- 3.9682 0.0019 11.6808

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.00 0.00 0.02 -0.03 0.01 -0.02 0.03 -0.01

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 0.04 -0.01 -0.02 -0.04 0.01

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 -0.01 -0.00 0.00 -0.00 0.00 -0.00 0.00

11 6 0.03 0.03 0.01 0.00 0.00 0.00 0.00 0.00 0.00

12 6 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

13 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

14 6 -0.04 0.02 0.01 0.00 -0.00 -0.00 0.00 -0.00 -0.00

15 6 0.03 0.03 -0.01 -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 -0.02 -0.04 -0.01 -0.02 -0.04 -0.01

21 6 0.00 -0.00 -0.00 -0.02 0.03 0.01 -0.02 0.03 0.01

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 -0.00 0.00 -0.00 -0.29 0.33 -0.10 0.30 -0.34 0.10

50 1 0.00 0.00 -0.00 -0.29 -0.43 0.11 0.30 0.44 -0.12

51 1 0.41 -0.28 0.10 0.01 -0.00 0.00 -0.01 0.01 -0.00

52 1 -0.34 -0.31 -0.10 -0.00 -0.00 -0.00 -0.01 -0.01 -0.00

53 1 0.42 -0.29 -0.10 -0.01 0.00 0.00 -0.01 0.01 0.00

54 1 -0.35 -0.32 0.10 0.00 0.00 -0.00 -0.01 -0.01 0.00

55 1 0.00 0.00 0.00 0.30 0.44 0.12 0.29 0.43 0.11

56 1 -0.00 0.00 0.00 0.30 -0.34 -0.10 0.29 -0.33 -0.10

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 0.01 0.01 -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 0.01 0.01 -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 0.01 -0.01 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 0.01 -0.01 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 1 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

78 1 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

223 224 225

A A A

Frequencies -- 3261.1582 3261.2007 3269.9377

Red. masses -- 1.1048 1.1048 1.1012

Frc consts -- 6.9230 6.9231 6.9372

IR Inten -- 26.3928 1.1356 9.3667

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.03 -0.03 0.01

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 -0.02 -0.03 0.01

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 -0.03 0.03 -0.01 0.03 -0.03 0.01 0.00 -0.00 0.00

11 6 -0.03 -0.03 -0.01 0.03 0.03 0.01 -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 -0.03 0.03 0.01 -0.03 0.03 0.01 0.00 -0.00 -0.00

15 6 -0.03 -0.03 0.01 -0.03 -0.03 0.01 -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 -0.02 -0.03 -0.01

21 6 -0.00 0.00 0.00 -0.00 0.00 0.00 0.03 -0.04 -0.01

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 -0.01 0.01 -0.00 -0.34 0.38 -0.11

50 1 0.01 0.01 -0.00 0.00 0.01 -0.00 0.25 0.36 -0.10

51 1 0.39 -0.27 0.10 -0.38 0.27 -0.09 -0.00 0.00 -0.00

52 1 0.37 0.34 0.11 -0.37 -0.34 -0.11 0.00 0.00 0.00

53 1 0.38 -0.27 -0.09 0.39 -0.27 -0.10 -0.00 0.00 0.00

54 1 0.37 0.34 -0.11 0.37 0.34 -0.11 0.00 0.00 -0.00

55 1 0.01 0.01 0.00 -0.00 -0.01 -0.00 0.26 0.37 0.10

56 1 0.01 -0.01 -0.00 0.01 -0.01 -0.00 -0.35 0.40 0.12

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 1 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

78 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

226 227 228

A A A

Frequencies -- 3269.9780 3588.9215 3592.1327

Red. masses -- 1.1012 1.0829 1.0826

Frc consts -- 6.9374 8.2183 8.2301

IR Inten -- 0.2178 16.1006 301.5427

Atom AN X Y Z X Y Z X Y Z

1 6 0.03 -0.04 0.01 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 -0.05 0.01 0.00 -0.05 0.01

4 6 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

5 6 -0.02 -0.03 0.01 -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 0.02 0.03 0.01 0.00 -0.00 -0.00 -0.00 0.00 0.00

21 6 -0.03 0.03 0.01 -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 0.05 0.01 0.00 -0.05 -0.01

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 -0.35 0.39 -0.12 0.00 0.00 -0.00 0.00 0.00 -0.00

50 1 0.26 0.37 -0.10 -0.00 0.00 -0.00 -0.00 0.00 -0.00

51 1 0.01 -0.01 0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00

52 1 0.01 0.01 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

53 1 -0.01 0.01 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00

54 1 -0.01 -0.01 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

55 1 -0.25 -0.36 -0.10 0.00 -0.00 -0.00 -0.00 0.00 0.00

56 1 0.34 -0.38 -0.11 -0.00 -0.00 -0.00 0.00 0.00 0.00

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 1 -0.00 0.00 -0.00 -0.05 0.69 -0.15 -0.04 0.68 -0.15

78 1 0.00 -0.00 -0.00 0.05 -0.68 -0.15 -0.05 0.69 0.15

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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 1 and mass 1.00783

Atom 78 has atomic number 1 and mass 1.00783

Molecular mass: 614.24705 amu.

Principal axes and moments of inertia in atomic units:

1 2 3

Eigenvalues -- \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

X 1.00000 -0.00083 -0.00000

Y 0.00083 1.00000 0.00000

Z 0.00000 -0.00000 1.00000

This molecule is an asymmetric top.

Rotational symmetry number 1.

Warning -- assumption of classical behavior for rotation

may cause significant error

Rotational temperatures (Kelvin) 0.00282 0.00280 0.00144

Rotational constants (GHZ): 0.05879 0.05826 0.03009

Zero-point vibrational energy 1611948.1 (Joules/Mol)

385.26485 (Kcal/Mol)

Warning -- explicit consideration of 56 degrees of freedom as

vibrations may cause significant error

Vibrational temperatures: 9.88 33.85 36.52 39.86 51.68

(Kelvin) 59.18 65.27 76.90 78.13 81.83

87.92 117.09 119.99 132.76 134.50

143.82 164.41 198.34 236.47 257.66

265.90 268.95 291.24 313.42 319.43

319.68 356.68 358.40 368.30 405.85

416.40 442.57 447.36 459.98 478.97

535.24 545.77 552.57 575.89 596.05

598.06 603.18 603.79 611.33 617.75

639.51 712.34 722.27 743.70 744.61

763.91 820.47 820.79 833.54 834.56

884.38 913.69 913.84 915.45 916.19

934.62 948.04 951.99 963.76 970.89

974.27 985.88 993.52 1024.64 1025.36

1027.20 1027.89 1034.06 1042.14 1052.65

1054.37 1097.87 1100.81 1106.78 1108.03

1134.39 1140.04 1152.69 1158.14 1165.77

1217.30 1229.81 1233.04 1233.54 1235.03

1236.43 1236.46 1259.71 1259.80 1275.69

1290.85 1291.57 1296.78 1335.88 1336.31

1353.32 1353.73 1356.33 1356.89 1392.95

1411.38 1411.40 1411.65 1414.03 1414.13

1415.08 1442.62 1442.84 1444.97 1445.06

1454.61 1455.29 1465.53 1465.57 1466.58

1467.76 1471.03 1497.23 1507.64 1511.72

1516.29 1517.79 1518.73 1535.13 1548.72

1556.97 1582.26 1586.02 1588.56 1588.56

1589.67 1595.27 1671.50 1689.66 1689.69

1692.18 1692.21 1713.70 1725.29 1727.61

1728.08 1728.41 1732.29 1793.24 1793.40

1801.10 1808.89 1815.07 1848.30 1862.24

1889.59 1893.10 1897.52 1900.46 1905.13

1918.80 1949.41 1955.98 1956.25 1957.75

1961.86 1983.37 1998.40 2009.38 2030.38

2030.58 2037.93 2053.90 2106.28 2120.89

2121.14 2125.01 2132.38 2172.20 2189.92

2195.30 2196.49 2198.22 2200.23 2200.97

2213.51 2232.25 2262.14 2271.43 2279.75

2323.73 2324.12 2325.33 2326.73 2358.98

2359.13 2360.22 2360.35 4566.23 4566.23

4566.36 4566.37 4576.35 4576.36 4576.91

4576.91 4589.86 4589.88 4590.78 4590.80

4599.00 4599.01 4600.07 4600.07 4606.95

4607.00 4607.51 4607.52 4666.27 4666.30

4685.98 4686.07 4692.07 4692.13 4704.71

4704.76 5163.65 5168.27

Zero-point correction= 0.613959 (Hartree/Particle)

Thermal correction to Energy= 0.650892

Thermal correction to Enthalpy= 0.651836

Thermal correction to Gibbs Free Energy= 0.540591

Sum of electronic and zero-point Energies= -1913.719359

Sum of electronic and thermal Energies= -1913.682426

Sum of electronic and thermal Enthalpies= -1913.681482

Sum of electronic and thermal Free Energies= -1913.792726

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 408.441 150.400 234.134

Electronic 0.000 0.000 2.183

Translational 0.889 2.981 45.129

Rotational 0.889 2.981 39.275

Vibrational 406.663 144.439 147.547

Vibration 1 0.593 1.987 8.758

Vibration 2 0.593 1.985 6.312

Vibration 3 0.593 1.985 6.161

Vibration 4 0.593 1.984 5.987

Vibration 5 0.594 1.982 5.472

Vibration 6 0.594 1.981 5.204

Vibration 7 0.595 1.979 5.010

Vibration 8 0.596 1.976 4.686

Vibration 9 0.596 1.976 4.654

Vibration 10 0.596 1.975 4.563

Vibration 11 0.597 1.973 4.421

Vibration 12 0.600 1.962 3.857

Vibration 13 0.600 1.961 3.809

Vibration 14 0.602 1.955 3.611

Vibration 15 0.602 1.954 3.586

Vibration 16 0.604 1.949 3.455

Vibration 17 0.607 1.938 3.195

Vibration 18 0.614 1.916 2.833

Vibration 19 0.623 1.886 2.499

Vibration 20 0.629 1.868 2.338

Vibration 21 0.631 1.861 2.279

Vibration 22 0.632 1.858 2.258

Vibration 23 0.639 1.836 2.111

Vibration 24 0.646 1.814 1.977

Vibration 25 0.648 1.808 1.943

Vibration 26 0.648 1.807 1.941

Vibration 27 0.662 1.766 1.745

Vibration 28 0.662 1.764 1.737

Vibration 29 0.666 1.753 1.689

Vibration 30 0.681 1.707 1.521

Vibration 31 0.686 1.693 1.477

Vibration 32 0.697 1.659 1.375

Vibration 33 0.700 1.653 1.357

Vibration 34 0.706 1.636 1.312

Vibration 35 0.715 1.610 1.246

Vibration 36 0.744 1.530 1.071

Vibration 37 0.749 1.514 1.042

Vibration 38 0.753 1.504 1.023

Vibration 39 0.766 1.470 0.962

Vibration 40 0.778 1.439 0.912

Vibration 41 0.779 1.436 0.907

Vibration 42 0.782 1.428 0.895

Vibration 43 0.782 1.428 0.893

Vibration 44 0.787 1.416 0.875

Vibration 45 0.791 1.406 0.861

Vibration 46 0.804 1.373 0.813

Vibration 47 0.851 1.261 0.670

Vibration 48 0.857 1.246 0.653

Vibration 49 0.872 1.213 0.617

Vibration 50 0.873 1.211 0.616

Vibration 51 0.886 1.182 0.585

Vibration 52 0.926 1.096 0.504

Vibration 53 0.927 1.095 0.503

Vibration 54 0.936 1.076 0.487

Vibration 55 0.937 1.074 0.485

Vibration 56 0.974 1.001 0.425

Q Log10(Q) Ln(Q)

Total Bot 0.221706-248 -248.654222 -572.547506

Total V=0 0.557872D+34 33.746534 77.704267

Vib (Bot) 0.144474-265 -265.840211 -612.119707

Vib (Bot) 1 0.301768D+02 1.479673 3.407073

Vib (Bot) 2 0.880360D+01 0.944660 2.175160

Vib (Bot) 3 0.815900D+01 0.911637 2.099122

Vib (Bot) 4 0.747389D+01 0.873547 2.011415

Vib (Bot) 5 0.576227D+01 0.760594 1.751331

Vib (Bot) 6 0.502976D+01 0.701547 1.615372

Vib (Bot) 7 0.455876D+01 0.658846 1.517050

Vib (Bot) 8 0.386662D+01 0.587331 1.352380

Vib (Bot) 9 0.380507D+01 0.580362 1.336333

Vib (Bot) 10 0.363200D+01 0.560146 1.289784

Vib (Bot) 11 0.337900D+01 0.528789 1.217581

Vib (Bot) 12 0.253001D+01 0.403121 0.928222

Vib (Bot) 13 0.246806D+01 0.392355 0.903432

Vib (Bot) 14 0.222739D+01 0.347796 0.800830

Vib (Bot) 15 0.219803D+01 0.342034 0.787563

Vib (Bot) 16 0.205304D+01 0.312398 0.719324

Vib (Bot) 17 0.179071D+01 0.253024 0.582610

Vib (Bot) 18 0.147586D+01 0.169045 0.389241

Vib (Bot) 19 0.122837D+01 0.089331 0.205691

Vib (Bot) 20 0.112192D+01 0.049960 0.115038

Vib (Bot) 21 0.108497D+01 0.035418 0.081554

Vib (Bot) 22 0.107186D+01 0.030138 0.069395

Vib (Bot) 23 0.984116D+00 -0.006954 -0.016012

Vib (Bot) 24 0.908850D+00 -0.041508 -0.095575

Vib (Bot) 25 0.890204D+00 -0.050511 -0.116305

Vib (Bot) 26 0.889421D+00 -0.050893 -0.117185

Vib (Bot) 27 0.788052D+00 -0.103445 -0.238192

Vib (Bot) 28 0.783838D+00 -0.105774 -0.243553

Vib (Bot) 29 0.760255D+00 -0.119040 -0.274101

Vib (Bot) 30 0.680841D+00 -0.166954 -0.384427

Vib (Bot) 31 0.660974D+00 -0.179816 -0.414041

Vib (Bot) 32 0.615580D+00 -0.210716 -0.485190

Vib (Bot) 33 0.607824D+00 -0.216222 -0.497870

Vib (Bot) 34 0.588091D+00 -0.230555 -0.530873

Vib (Bot) 35 0.560257D+00 -0.251613 -0.579360

Vib (Bot) 36 0.488715D+00 -0.310944 -0.715975

Vib (Bot) 37 0.476873D+00 -0.321597 -0.740505

Vib (Bot) 38 0.469440D+00 -0.328420 -0.756214

Vib (Bot) 39 0.445215D+00 -0.351430 -0.809198

Vib (Bot) 40 0.425689D+00 -0.370907 -0.854046

Vib (Bot) 41 0.423812D+00 -0.372827 -0.858466

Vib (Bot) 42 0.419079D+00 -0.377704 -0.869697

Vib (Bot) 43 0.418522D+00 -0.378282 -0.871026

Vib (Bot) 44 0.411697D+00 -0.385422 -0.887467

Vib (Bot) 45 0.406014D+00 -0.391459 -0.901368

Vib (Bot) 46 0.387534D+00 -0.411690 -0.947952

Vib (Bot) 47 0.333400D+00 -0.477035 -1.098413

Vib (Bot) 48 0.326812D+00 -0.485702 -1.118371

Vib (Bot) 49 0.313163D+00 -0.504230 -1.161032

Vib (Bot) 50 0.312597D+00 -0.505015 -1.162840

Vib (Bot) 51 0.300949D+00 -0.521507 -1.200814

Vib (Bot) 52 0.269823D+00 -0.568922 -1.309991

Vib (Bot) 53 0.269656D+00 -0.569190 -1.310609

Vib (Bot) 54 0.263199D+00 -0.579717 -1.334847

Vib (Bot) 55 0.262693D+00 -0.580552 -1.336770

Vib (Bot) 56 0.239250D+00 -0.621148 -1.430245

Vib (V=0) 0.363534D+17 16.560546 38.132065

Vib (V=0) 1 0.306809D+02 1.486868 3.423641

Vib (V=0) 2 0.931778D+01 0.969313 2.231925

Vib (V=0) 3 0.867431D+01 0.938235 2.160366

Vib (V=0) 4 0.799059D+01 0.902579 2.078265

Vib (V=0) 5 0.628392D+01 0.798231 1.837994

Vib (V=0) 6 0.555455D+01 0.744649 1.714618

Vib (V=0) 7 0.508609D+01 0.706384 1.626510

Vib (V=0) 8 0.439881D+01 0.643335 1.481334

Vib (V=0) 9 0.433778D+01 0.637267 1.467362

Vib (V=0) 10 0.416626D+01 0.619746 1.427018

Vib (V=0) 11 0.391580D+01 0.592820 1.365019

Vib (V=0) 12 0.307894D+01 0.488401 1.124585

Vib (V=0) 13 0.301820D+01 0.479747 1.104659

Vib (V=0) 14 0.278282D+01 0.444485 1.023465

Vib (V=0) 15 0.275418D+01 0.439993 1.013121

Vib (V=0) 16 0.261305D+01 0.417148 0.960519

Vib (V=0) 17 0.235920D+01 0.372765 0.858323

Vib (V=0) 18 0.205826D+01 0.313499 0.721859

Vib (V=0) 19 0.182624D+01 0.261557 0.602257

Vib (V=0) 20 0.172829D+01 0.237616 0.547132

Vib (V=0) 21 0.169464D+01 0.229077 0.527470

Vib (V=0) 22 0.168274D+01 0.226018 0.520426

Vib (V=0) 23 0.160385D+01 0.205164 0.472407

Vib (V=0) 24 0.153731D+01 0.186761 0.430033

Vib (V=0) 25 0.152101D+01 0.182132 0.419375

Vib (V=0) 26 0.152033D+01 0.181937 0.418926

Vib (V=0) 27 0.143329D+01 0.156333 0.359971

Vib (V=0) 28 0.142973D+01 0.155255 0.357487

Vib (V=0) 29 0.140994D+01 0.149200 0.343546

Vib (V=0) 30 0.134472D+01 0.128630 0.296182

Vib (V=0) 31 0.132879D+01 0.123455 0.284266

Vib (V=0) 32 0.129306D+01 0.111618 0.257009

Vib (V=0) 33 0.128705D+01 0.109596 0.252354

Vib (V=0) 34 0.127191D+01 0.104458 0.240523

Vib (V=0) 35 0.125092D+01 0.097231 0.223883

Vib (V=0) 36 0.119917D+01 0.078882 0.181632

Vib (V=0) 37 0.119095D+01 0.075892 0.174749

Vib (V=0) 38 0.118584D+01 0.074025 0.170450

Vib (V=0) 39 0.116949D+01 0.067996 0.156567

Vib (V=0) 40 0.115667D+01 0.063208 0.145542

Vib (V=0) 41 0.115545D+01 0.062752 0.144491

Vib (V=0) 42 0.115240D+01 0.061604 0.141848

Vib (V=0) 43 0.115204D+01 0.061469 0.141537

Vib (V=0) 44 0.114768D+01 0.059822 0.137746

Vib (V=0) 45 0.114409D+01 0.058459 0.134606

Vib (V=0) 46 0.113260D+01 0.054076 0.124516

Vib (V=0) 47 0.110096D+01 0.041772 0.096184

Vib (V=0) 48 0.109733D+01 0.040338 0.092882

Vib (V=0) 49 0.108998D+01 0.037417 0.086155

Vib (V=0) 50 0.108968D+01 0.037297 0.085880

Vib (V=0) 51 0.108358D+01 0.034863 0.080274

Vib (V=0) 52 0.106816D+01 0.028636 0.065936

Vib (V=0) 53 0.106808D+01 0.028604 0.065862

Vib (V=0) 54 0.106504D+01 0.027367 0.063015

Vib (V=0) 55 0.106481D+01 0.027271 0.062794

Vib (V=0) 56 0.105429D+01 0.022961 0.052870

Electronic 0.300000D+01 0.477121 1.098612

Translational 0.598370D+09 8.776970 20.209720

Rotational 0.854865D+08 7.931898 18.263869

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000000467 -0.000000097 -0.000000236

2 6 0.000000343 -0.000000151 -0.000000551

3 7 0.000000484 0.000000465 -0.000000289

4 6 -0.000000208 0.000000170 0.000000015

5 6 -0.000000112 -0.000000027 -0.000000397

6 6 -0.000000221 -0.000000176 -0.000000436

7 6 -0.000000845 -0.000000006 0.000000278

8 7 0.000000227 0.000000010 -0.000000428

9 6 0.000000124 0.000000042 0.000000149

10 6 -0.000000529 0.000000004 0.000000021

11 6 -0.000000428 0.000000148 -0.000000445

12 6 0.000000015 0.000000055 0.000000185

13 6 -0.000000045 0.000000039 -0.000000242

14 6 0.000000568 0.000000180 -0.000000081

15 6 0.000000436 -0.000000080 0.000000476

16 6 0.000000810 -0.000000057 -0.000000303

17 7 -0.000000046 -0.000000348 0.000000400

18 6 0.000000158 -0.000000066 0.000000551

19 6 0.000000284 0.000000261 -0.000000441

20 6 -0.000000068 -0.000000085 0.000000450

21 6 -0.000000464 0.000000088 0.000000243

22 6 -0.000000134 -0.000000018 0.000000734

23 7 -0.000000195 0.000000377 0.000000413

24 6 -0.000000188 0.000000155 -0.000000066

25 6 -0.000000665 0.000000010 -0.000000601

26 6 0.000000022 -0.000000435 -0.000000028

27 6 -0.000000691 0.000000170 -0.000000731

28 6 -0.000000234 -0.000000052 -0.000000327

29 6 -0.000000828 0.000000267 -0.000000464

30 6 -0.000000263 -0.000000175 -0.000000147

31 6 0.000000193 0.000000039 -0.000000504

32 6 0.000000389 0.000000093 -0.000000625

33 6 -0.000000059 -0.000000121 -0.000000275

34 6 0.000000573 -0.000000425 -0.000000608

35 6 0.000000449 0.000000049 0.000000043

36 6 0.000000937 -0.000000102 -0.000000779

37 6 -0.000000470 -0.000000333 0.000000276

38 6 -0.000000583 -0.000000079 -0.000000052

39 6 -0.000000868 0.000000050 0.000000575

40 6 -0.000000199 0.000000008 0.000000652

41 6 -0.000000302 0.000000244 0.000000552

42 6 -0.000000087 -0.000000199 0.000000440

43 6 0.000000560 0.000000010 0.000000678

44 6 0.000000243 -0.000000308 0.000000252

45 6 0.000000866 0.000000418 0.000000547

46 6 0.000000250 -0.000000007 0.000000246

47 6 0.000000683 0.000000223 0.000000748

48 6 -0.000000131 -0.000000388 -0.000000051

49 1 0.000000003 0.000000038 -0.000000322

50 1 -0.000000086 0.000000208 -0.000000502

51 1 -0.000000346 0.000000066 0.000000177

52 1 -0.000000267 0.000000001 -0.000000235

53 1 0.000000353 0.000000084 -0.000000165

54 1 0.000000287 0.000000054 0.000000198

55 1 0.000000202 0.000000101 0.000000604

56 1 -0.000000136 -0.000000085 0.000000384

57 1 -0.000000420 0.000000059 -0.000000424

58 1 -0.000000410 -0.000000007 -0.000000545

59 1 -0.000000654 -0.000000010 -0.000000735

60 1 -0.000000508 -0.000000080 -0.000000425

61 1 -0.000000282 -0.000000053 -0.000000196

62 1 0.000000697 -0.000000012 -0.000000609

63 1 0.000000404 0.000000020 -0.000000583

64 1 0.000000397 0.000000124 -0.000000397

65 1 0.000000399 -0.000000012 -0.000000277

66 1 0.000000552 0.000000044 -0.000000392

67 1 -0.000000353 0.000000037 0.000000238

68 1 -0.000000575 0.000000067 0.000000407

69 1 -0.000000665 0.000000035 0.000000609

70 1 -0.000000411 0.000000021 0.000000629

71 1 -0.000000428 0.000000051 0.000000410

72 1 0.000000367 0.000000064 0.000000201

73 1 0.000000524 -0.000000056 0.000000425

74 1 0.000000661 0.000000026 0.000000751

75 1 0.000000431 -0.000000001 0.000000544

76 1 0.000000389 0.000000014 0.000000411

77 1 -0.000001492 -0.000000009 -0.000000336

78 1 0.000001144 -0.000000629 0.000000338

-------------------------------------------------------------------

Cartesian Forces: Max 0.000001492 RMS 0.000000394

Red2BG is reusing G-inverse.

Leave Link 716 at Fri Aug 30 06:16:25 2019, MaxMem= 4294967296 cpu: 3.0

(Enter /home/kira/g09/l9999.exe)

1\1\ WCSS.PL-BEM-DHCP-129-94-99-158\Freq\UB3LYP\6-311G(d)\C44H30N4(3)\

KIRA\30-Aug-2019\0\\#p opt=(GDIIS,calcall) b3lyp/6-311G\* scrf=(solvent

=dmso,smd) empiricaldispersion=gd3bj\\TPP3C1\\0,3\C,4.1725298959,-0.56

15738676,0.681874205\C,2.883025116,-0.2117855976,1.1195049579\N,2.1148

842407,-0.017983141,-0.0048793894\C,2.8732153054,-0.199025199,-1.13789

87145\C,4.166483617,-0.553075461,-0.7156292098\C,2.4193938081,-0.01673

96723,-2.4898935034\C,1.084440939,0.1097420288,-2.8832175668\N,-0.0083

848792,-0.0566485425,-2.0674057893\C,-1.1066856448,0.0951159434,-2.877

0033604\C,-0.6928300639,0.4217702598,-4.240404813\C,0.6588460294,0.431

9039503,-4.2438363082\C,2.4393565579,-0.0416925732,2.4758945786\C,1.10

67086579,0.0963757588,2.8769989131\C,0.6924973062,0.4226017796,4.24039

51825\C,-0.659188974,0.4312644668,4.2438262064\C,-1.0844327475,0.10861

84784,2.8832127653\N,0.0085735731,-0.0565960925,2.0674034191\C,-2.4192

473854,-0.0193313001,2.489893589\C,-2.8728644918,-0.2021369753,1.13790

03271\C,-4.165698243,-0.5577759997,0.7156383123\C,-4.1717335599,-0.566

3096401,-0.6818657714\C,-2.8826581441,-0.2149535608,-1.1195023483\N,-2

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8299\C,3.4740270682,-0.9420861752,4.5743950071\C,4.4696324532,-0.92929

71116,5.547244155\C,-3.5012992272,-0.0313203877,-3.5117704369\C,-3.472

8167764,-0.9460412173,-4.574370667\C,-4.4684484409,-0.9344392017,-5.54

72071878\C,-5.5038199446,-0.0035657063,-5.4790844285\C,-5.541953595,0.

9117248383,-4.4269269234\C,-4.5554340014,0.8923264894,-3.4462476984\C,

-3.4777639904,0.0193943472,3.5291640279\C,-3.4632287297,-0.885132297,4

.6005853819\C,-4.4583712765,-0.8477052346,5.5735524769\C,-5.4774922378

,0.1002237201,5.4975668472\C,-5.50091803,1.0061674529,4.4369506601\C,-

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31685885\H,4.9942279476,-0.7819788763,-1.3671904292\H,-1.3522442824,0.

6390597584,-5.0664837567\H,1.3107260835,0.6582814816,-5.0733554251\H,1

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.802759782,-1.3231587066\H,4.5348024741,1.6737591703,-2.6356713397\H,6

.2859585622,1.757342594,-4.373956335\H,6.2503505304,0.1387680405,-6.25

81847229\H,4.4397736787,-1.5566629651,-6.3902546459\H,2.6793336783,-1.

6267691878,-4.6583505688\H,6.2771335099,0.0155965641,6.2399395473\H,6.

339737726,1.6500753184,4.3700211557\H,4.5850418609,1.613698132,2.63308

3205\H,2.6764805839,-1.6745220267,4.6255040982\H,4.4383657662,-1.65038

49235,6.3572175014\H,-2.6744235736,-1.6775547516,-4.6254656248\H,-4.43

63534817,-1.6555146044,-6.3571592267\H,-6.2770571617,0.0083298756,-6.2

399064883\H,-6.3415403921,1.6427879625,-4.3700344041\H,-4.5867847891,1

.6084998473,-2.6331136297\H,-2.677342719,-1.6296312431,4.6583701134\H,

-4.4378854438,-1.5615475387,6.3902487209\H,-6.2504228307,0.1317841304,

6.2581385494\H,-6.2878785016,1.7503007665,4.3738963275\H,-4.5366032421

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1.125666249,0.1880770847,-0.0018609427\\Version=ES64L-G09RevE.01\State

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MSF=3.939e-07\ZeroPoint=0.6139586\Thermal=0.6508917\Dipole=-0.0003529,

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,-0.0071276,0.0149226,-0.0051308,-0.4108653,0.1471244,-0.0078154,0.124

2284,-1.2280494,0.2377909,0.0123369,0.4122092,-0.0587483,0.0887246,0.1

52973,0.0011237,-0.0057293,-0.3365765,0.0327546,0.0702715,-0.7435427,-

0.0445384,-0.1943126,-0.1000649,-0.008735,-0.1065096,0.435818,0.073895

2,-0.0652942,0.7476131,0.0378711,-0.1963522,-0.0895221,0.039537,-0.105

7408,0.4381255,0.8024079,-0.0784862,-0.6457007,-0.2061239,-0.0125679,0

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,-0.0700419,-0.7436597,0.0447794,-0.1943347,0.0992936,-0.008865,0.1065

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0000005,0.,-0.00000004,0.00000032,0.00000009,-0.00000021,0.00000050,0.

00000035,-0.00000007,-0.00000018,0.00000027,0.,0.00000024,-0.00000035,

-0.00000008,0.00000016,-0.00000029,-0.00000005,-0.00000020,-0.00000020

,-0.00000010,-0.00000060,0.00000014,0.00000008,-0.00000038,0.00000042,

-0.00000006,0.00000042,0.00000041,0.,0.00000054,0.00000065,0.00000001,

0.00000074,0.00000051,0.00000008,0.00000042,0.00000028,0.00000005,0.00

000020,-0.00000070,0.00000001,0.00000061,-0.00000040,-0.00000002,0.000

00058,-0.00000040,-0.00000012,0.00000040,-0.00000040,0.00000001,0.0000

0028,-0.00000055,-0.00000004,0.00000039,0.00000035,-0.00000004,-0.0000

0024,0.00000057,-0.00000007,-0.00000041,0.00000066,-0.00000004,-0.0000

0061,0.00000041,-0.00000002,-0.00000063,0.00000043,-0.00000005,-0.0000

0041,-0.00000037,-0.00000006,-0.00000020,-0.00000052,0.00000006,-0.000

00042,-0.00000066,-0.00000003,-0.00000075,-0.00000043,0.,-0.00000054,-

0.00000039,-0.00000001,-0.00000041,0.00000149,0.,0.00000034,-0.0000011

4,0.00000063,-0.00000034\\\@

The best way to pay for a lovely moment is to enjoy it.

-- Richard Bach

Job cpu time: 74 days 17 hours 3 minutes 10.0 seconds.

File lengths (MBytes): RWF= 13334 Int= 0 D2E= 0 Chk= 118 Scr= 1

Normal termination of Gaussian 09 at Fri Aug 30 06:16:27 2019.