Entering Gaussian System, Link 0=g09

Initial command:

/apps/gaussian/g09d01/g09/l1.exe "/srv/scratch/z5105842/Gau-670.inp" -scrdir="/srv/scratch/z5105842/"

Entering Link 1 = /apps/gaussian/g09d01/g09/l1.exe PID= 688.

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Cite this work as:

Gaussian 09, Revision D.01,

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

5-Jul-2019

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

%nprocshared=12

Will use up to 12 processors via shared memory.

%mem=10GB

%chk=ZnOMPC3.chk

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

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

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

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

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

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

4//1;

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

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

7//1,2,3,16;

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

2/9=110/2;

99//99;

2/9=110/2;

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

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

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

7//1,2,3,16;

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

2/9=110/2;

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

99/9=1/99;

Leave Link 1 at Fri Jul 5 23:09:35 2019, MaxMem= 1342177280 cpu: 0.8

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

-------

ZnOMPC3

-------

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C -1.1279 2.81043 0.08876

N 0. 2.04326 -0.00094

C 1.1279 2.81043 0.08876

C 0.71026 4.20714 0.26664

C -0.71026 4.20714 0.26664

N 2.39495 2.39495 0.

C 2.81043 1.1279 -0.08876

N 2.04326 0. 0.00094

C 2.81043 -1.1279 -0.08876

C 4.20714 -0.71026 -0.26664

C 4.20714 0.71026 -0.26664

N -2.39495 2.39495 0.

C -4.20714 0.71026 -0.26664

C -4.20714 -0.71026 -0.26664

C -2.81043 -1.1279 -0.08876

N -2.04326 0. 0.00094

C -2.81043 1.1279 -0.08876

N -2.39495 -2.39495 0.

N 0. -2.04326 -0.00094

C -1.1279 -2.81043 0.08876

C -0.71026 -4.20714 0.26664

C 0.71026 -4.20714 0.26664

C 1.1279 -2.81043 0.08876

N 2.39495 -2.39495 0.

Zn 0. 0. 0.

C -5.40344 1.43438 -0.42797

C -6.58814 0.70173 -0.57679

C -6.58814 -0.70173 -0.57679

C -5.40344 -1.43438 -0.42797

C 1.43438 -5.40344 0.42797

C 0.70173 -6.58814 0.57679

C -0.70173 -6.58814 0.57679

C -1.43438 -5.40344 0.42797

C 5.40344 1.43438 -0.42797

C 6.58814 0.70173 -0.57679

C 6.58814 -0.70173 -0.57679

C 5.40344 -1.43438 -0.42797

C -1.43438 5.40344 0.42797

C -0.70173 6.58814 0.57679

C 0.70173 6.58814 0.57679

C 1.43438 5.40344 0.42797

H 7.53526 1.21173 -0.70248

H 7.53526 -1.21173 -0.70248

H 1.21173 7.53526 0.70248

H -1.21173 7.53526 0.70248

H -7.53526 1.21173 -0.70248

H -7.53526 -1.21173 -0.70248

H -1.21173 -7.53526 0.70248

H 1.21173 -7.53526 0.70248

O 2.7898 5.33817 0.43769

O -2.7898 5.33817 0.43769

O 5.33817 2.7898 -0.43769

O 5.33817 -2.7898 -0.43769

O 2.7898 -5.33817 0.43769

O -2.7898 -5.33817 0.43769

O -5.33817 -2.7898 -0.43769

O -5.33817 2.7898 -0.43769

C 3.5237 6.55914 0.54283

H 3.31611 7.07228 1.48926

H 3.3022 7.22932 -0.29639

H 4.57584 6.27198 0.5107

C 6.55914 3.5237 -0.54283

H 7.07228 3.31611 -1.48926

H 7.22932 3.3022 0.29639

H 6.27198 4.57584 -0.5107

C 6.55914 -3.5237 -0.54283

H 7.22932 -3.3022 0.29639

H 7.07228 -3.31611 -1.48926

H 6.27198 -4.57584 -0.5107

C -3.5237 6.55914 0.54283

H -3.3022 7.22932 -0.29639

H -3.31611 7.07228 1.48926

H -4.57584 6.27198 0.5107

C -6.55914 3.5237 -0.54283

H -7.22932 3.3022 0.29639

H -7.07228 3.31611 -1.48926

H -6.27198 4.57584 -0.5107

C -6.55914 -3.5237 -0.54283

H -7.07228 -3.31611 -1.48926

H -7.22932 -3.3022 0.29639

H -6.27198 -4.57584 -0.5107

C -3.5237 -6.55914 0.54283

H -3.31611 -7.07228 1.48926

H -3.3022 -7.22932 -0.29639

H -4.57584 -6.27198 0.5107

C 3.5237 -6.55914 0.54283

H 3.3022 -7.22932 -0.29639

H 3.31611 -7.07228 1.48926

H 4.57584 -6.27198 0.5107

NAtoms= 89 NQM= 89 NQMF= 0 NMMI= 0 NMMIF= 0

NMic= 0 NMicF= 0.

Isotopes and Nuclear Properties:

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

in nuclear magnetons)

Atom 1 2 3 4 5 6 7 8 9 10

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

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

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

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

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

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

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

Atom 11 12 13 14 15 16 17 18 19 20

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

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

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

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

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

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

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

Atom 21 22 23 24 25 26 27 28 29 30

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

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

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

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

AtZNuc= 6.0000000 6.0000000 6.0000000 7.0000000 30.0000000 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 1 1 1 1 1 1 1 1 16

AtmWgt= 12.0000000 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 15.9949146

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

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

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

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

AtZNuc= 6.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 8.0000000

Atom 51 52 53 54 55 56 57 58 59 60

IAtWgt= 16 16 16 16 16 16 16 12 1 1

AtmWgt= 15.9949146 15.9949146 15.9949146 15.9949146 15.9949146 15.9949146 15.9949146 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= 8.0000000 8.0000000 8.0000000 8.0000000 8.0000000 8.0000000 8.0000000 6.0000000 1.0000000 1.0000000

Atom 61 62 63 64 65 66 67 68 69 70

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

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

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

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

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

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

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

Atom 71 72 73 74 75 76 77 78 79 80

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

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

NucSpn= 1 1 1 0 1 1 1 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= 2.7928460 2.7928460 2.7928460 0.0000000 2.7928460 2.7928460 2.7928460 0.0000000 2.7928460 2.7928460

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

Atom 81 82 83 84 85 86 87 88 89

IAtWgt= 1 12 1 1 1 12 1 1 1

AtmWgt= 1.0078250 12.0000000 1.0078250 1.0078250 1.0078250 12.0000000 1.0078250 1.0078250 1.0078250

NucSpn= 1 0 1 1 1 0 1 1 1

AtZEff= 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

NMagM= 2.7928460 0.0000000 2.7928460 2.7928460 2.7928460 0.0000000 2.7928460 2.7928460 2.7928460

AtZNuc= 1.0000000 6.0000000 1.0000000 1.0000000 1.0000000 6.0000000 1.0000000 1.0000000 1.0000000

Leave Link 101 at Fri Jul 5 23:09:36 2019, MaxMem= 1342177280 cpu: 3.0

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Initialization pass.

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

! Initial Parameters !

! (Angstroms and Degrees) !

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

! Name Definition Value Derivative Info. !

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

! R1 R(1,2) 1.367 estimate D2E/DX2 !

! R2 R(1,5) 1.4686 estimate D2E/DX2 !

! R3 R(1,12) 1.3364 estimate D2E/DX2 !

! R4 R(2,3) 1.367 estimate D2E/DX2 !

! R5 R(2,25) 2.0433 estimate D2E/DX2 !

! R6 R(3,4) 1.4686 estimate D2E/DX2 !

! R7 R(3,6) 1.3364 estimate D2E/DX2 !

! R8 R(4,5) 1.4205 estimate D2E/DX2 !

! R9 R(4,41) 1.4077 estimate D2E/DX2 !

! R10 R(5,38) 1.4077 estimate D2E/DX2 !

! R11 R(6,7) 1.3364 estimate D2E/DX2 !

! R12 R(7,8) 1.367 estimate D2E/DX2 !

! R13 R(7,11) 1.4686 estimate D2E/DX2 !

! R14 R(8,9) 1.367 estimate D2E/DX2 !

! R15 R(8,25) 2.0433 estimate D2E/DX2 !

! R16 R(9,10) 1.4686 estimate D2E/DX2 !

! R17 R(9,24) 1.3364 estimate D2E/DX2 !

! R18 R(10,11) 1.4205 estimate D2E/DX2 !

! R19 R(10,37) 1.4077 estimate D2E/DX2 !

! R20 R(11,34) 1.4077 estimate D2E/DX2 !

! R21 R(12,17) 1.3364 estimate D2E/DX2 !

! R22 R(13,14) 1.4205 estimate D2E/DX2 !

! R23 R(13,17) 1.4686 estimate D2E/DX2 !

! R24 R(13,26) 1.4077 estimate D2E/DX2 !

! R25 R(14,15) 1.4686 estimate D2E/DX2 !

! R26 R(14,29) 1.4077 estimate D2E/DX2 !

! R27 R(15,16) 1.367 estimate D2E/DX2 !

! R28 R(15,18) 1.3364 estimate D2E/DX2 !

! R29 R(16,17) 1.367 estimate D2E/DX2 !

! R30 R(16,25) 2.0433 estimate D2E/DX2 !

! R31 R(18,20) 1.3364 estimate D2E/DX2 !

! R32 R(19,20) 1.367 estimate D2E/DX2 !

! R33 R(19,23) 1.367 estimate D2E/DX2 !

! R34 R(19,25) 2.0433 estimate D2E/DX2 !

! R35 R(20,21) 1.4686 estimate D2E/DX2 !

! R36 R(21,22) 1.4205 estimate D2E/DX2 !

! R37 R(21,33) 1.4077 estimate D2E/DX2 !

! R38 R(22,23) 1.4686 estimate D2E/DX2 !

! R39 R(22,30) 1.4077 estimate D2E/DX2 !

! R40 R(23,24) 1.3364 estimate D2E/DX2 !

! R41 R(26,27) 1.4009 estimate D2E/DX2 !

! R42 R(26,57) 1.357 estimate D2E/DX2 !

! R43 R(27,28) 1.4035 estimate D2E/DX2 !

! R44 R(27,46) 1.083 estimate D2E/DX2 !

! R45 R(28,29) 1.4009 estimate D2E/DX2 !

! R46 R(28,47) 1.083 estimate D2E/DX2 !

! R47 R(29,56) 1.357 estimate D2E/DX2 !

! R48 R(30,31) 1.4009 estimate D2E/DX2 !

! R49 R(30,54) 1.357 estimate D2E/DX2 !

! R50 R(31,32) 1.4035 estimate D2E/DX2 !

! R51 R(31,49) 1.083 estimate D2E/DX2 !

! R52 R(32,33) 1.4009 estimate D2E/DX2 !

! R53 R(32,48) 1.083 estimate D2E/DX2 !

! R54 R(33,55) 1.357 estimate D2E/DX2 !

! R55 R(34,35) 1.4009 estimate D2E/DX2 !

! R56 R(34,52) 1.357 estimate D2E/DX2 !

! R57 R(35,36) 1.4035 estimate D2E/DX2 !

! R58 R(35,42) 1.083 estimate D2E/DX2 !

! R59 R(36,37) 1.4009 estimate D2E/DX2 !

! R60 R(36,43) 1.083 estimate D2E/DX2 !

! R61 R(37,53) 1.357 estimate D2E/DX2 !

! R62 R(38,39) 1.4009 estimate D2E/DX2 !

! R63 R(38,51) 1.357 estimate D2E/DX2 !

! R64 R(39,40) 1.4035 estimate D2E/DX2 !

! R65 R(39,45) 1.083 estimate D2E/DX2 !

! R66 R(40,41) 1.4009 estimate D2E/DX2 !

! R67 R(40,44) 1.083 estimate D2E/DX2 !

! R68 R(41,50) 1.357 estimate D2E/DX2 !

! R69 R(50,58) 1.4284 estimate D2E/DX2 !

! R70 R(51,70) 1.4284 estimate D2E/DX2 !

! R71 R(52,62) 1.4284 estimate D2E/DX2 !

! R72 R(53,66) 1.4284 estimate D2E/DX2 !

! R73 R(54,86) 1.4284 estimate D2E/DX2 !

! R74 R(55,82) 1.4284 estimate D2E/DX2 !

! R75 R(56,78) 1.4284 estimate D2E/DX2 !

! R76 R(57,74) 1.4284 estimate D2E/DX2 !

! R77 R(58,59) 1.0964 estimate D2E/DX2 !

! R78 R(58,60) 1.0966 estimate D2E/DX2 !

! R79 R(58,61) 1.0911 estimate D2E/DX2 !

! R80 R(62,63) 1.0964 estimate D2E/DX2 !

! R81 R(62,64) 1.0966 estimate D2E/DX2 !

! R82 R(62,65) 1.0911 estimate D2E/DX2 !

! R83 R(66,67) 1.0966 estimate D2E/DX2 !

! R84 R(66,68) 1.0964 estimate D2E/DX2 !

! R85 R(66,69) 1.0911 estimate D2E/DX2 !

! R86 R(70,71) 1.0966 estimate D2E/DX2 !

! R87 R(70,72) 1.0964 estimate D2E/DX2 !

! R88 R(70,73) 1.0911 estimate D2E/DX2 !

! R89 R(74,75) 1.0966 estimate D2E/DX2 !

! R90 R(74,76) 1.0964 estimate D2E/DX2 !

! R91 R(74,77) 1.0911 estimate D2E/DX2 !

! R92 R(78,79) 1.0964 estimate D2E/DX2 !

! R93 R(78,80) 1.0966 estimate D2E/DX2 !

! R94 R(78,81) 1.0911 estimate D2E/DX2 !

! R95 R(82,83) 1.0964 estimate D2E/DX2 !

! R96 R(82,84) 1.0966 estimate D2E/DX2 !

! R97 R(82,85) 1.0911 estimate D2E/DX2 !

! R98 R(86,87) 1.0966 estimate D2E/DX2 !

! R99 R(86,88) 1.0964 estimate D2E/DX2 !

! R100 R(86,89) 1.0911 estimate D2E/DX2 !

! A1 A(2,1,5) 107.8803 estimate D2E/DX2 !

! A2 A(2,1,12) 127.1164 estimate D2E/DX2 !

! A3 A(5,1,12) 124.9838 estimate D2E/DX2 !

! A4 A(1,2,3) 111.1928 estimate D2E/DX2 !

! A5 A(1,2,25) 124.1364 estimate D2E/DX2 !

! A6 A(3,2,25) 124.1364 estimate D2E/DX2 !

! A7 A(2,3,4) 107.8803 estimate D2E/DX2 !

! A8 A(2,3,6) 127.1164 estimate D2E/DX2 !

! A9 A(4,3,6) 124.9838 estimate D2E/DX2 !

! A10 A(3,4,5) 106.5215 estimate D2E/DX2 !

! A11 A(3,4,41) 132.5184 estimate D2E/DX2 !

! A12 A(5,4,41) 120.9583 estimate D2E/DX2 !

! A13 A(1,5,4) 106.5215 estimate D2E/DX2 !

! A14 A(1,5,38) 132.5184 estimate D2E/DX2 !

! A15 A(4,5,38) 120.9583 estimate D2E/DX2 !

! A16 A(3,6,7) 126.4382 estimate D2E/DX2 !

! A17 A(6,7,8) 127.1164 estimate D2E/DX2 !

! A18 A(6,7,11) 124.9838 estimate D2E/DX2 !

! A19 A(8,7,11) 107.8803 estimate D2E/DX2 !

! A20 A(7,8,9) 111.1928 estimate D2E/DX2 !

! A21 A(7,8,25) 124.1364 estimate D2E/DX2 !

! A22 A(9,8,25) 124.1364 estimate D2E/DX2 !

! A23 A(8,9,10) 107.8803 estimate D2E/DX2 !

! A24 A(8,9,24) 127.1164 estimate D2E/DX2 !

! A25 A(10,9,24) 124.9838 estimate D2E/DX2 !

! A26 A(9,10,11) 106.5215 estimate D2E/DX2 !

! A27 A(9,10,37) 132.5184 estimate D2E/DX2 !

! A28 A(11,10,37) 120.9583 estimate D2E/DX2 !

! A29 A(7,11,10) 106.5215 estimate D2E/DX2 !

! A30 A(7,11,34) 132.5184 estimate D2E/DX2 !

! A31 A(10,11,34) 120.9583 estimate D2E/DX2 !

! A32 A(1,12,17) 126.4382 estimate D2E/DX2 !

! A33 A(14,13,17) 106.5215 estimate D2E/DX2 !

! A34 A(14,13,26) 120.9583 estimate D2E/DX2 !

! A35 A(17,13,26) 132.5184 estimate D2E/DX2 !

! A36 A(13,14,15) 106.5215 estimate D2E/DX2 !

! A37 A(13,14,29) 120.9583 estimate D2E/DX2 !

! A38 A(15,14,29) 132.5184 estimate D2E/DX2 !

! A39 A(14,15,16) 107.8803 estimate D2E/DX2 !

! A40 A(14,15,18) 124.9838 estimate D2E/DX2 !

! A41 A(16,15,18) 127.1164 estimate D2E/DX2 !

! A42 A(15,16,17) 111.1928 estimate D2E/DX2 !

! A43 A(15,16,25) 124.1364 estimate D2E/DX2 !

! A44 A(17,16,25) 124.1364 estimate D2E/DX2 !

! A45 A(12,17,13) 124.9838 estimate D2E/DX2 !

! A46 A(12,17,16) 127.1164 estimate D2E/DX2 !

! A47 A(13,17,16) 107.8803 estimate D2E/DX2 !

! A48 A(15,18,20) 126.4382 estimate D2E/DX2 !

! A49 A(20,19,23) 111.1928 estimate D2E/DX2 !

! A50 A(20,19,25) 124.1364 estimate D2E/DX2 !

! A51 A(23,19,25) 124.1364 estimate D2E/DX2 !

! A52 A(18,20,19) 127.1164 estimate D2E/DX2 !

! A53 A(18,20,21) 124.9838 estimate D2E/DX2 !

! A54 A(19,20,21) 107.8803 estimate D2E/DX2 !

! A55 A(20,21,22) 106.5215 estimate D2E/DX2 !

! A56 A(20,21,33) 132.5184 estimate D2E/DX2 !

! A57 A(22,21,33) 120.9583 estimate D2E/DX2 !

! A58 A(21,22,23) 106.5215 estimate D2E/DX2 !

! A59 A(21,22,30) 120.9583 estimate D2E/DX2 !

! A60 A(23,22,30) 132.5184 estimate D2E/DX2 !

! A61 A(19,23,22) 107.8803 estimate D2E/DX2 !

! A62 A(19,23,24) 127.1164 estimate D2E/DX2 !

! A63 A(22,23,24) 124.9838 estimate D2E/DX2 !

! A64 A(9,24,23) 126.4382 estimate D2E/DX2 !

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

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

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

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

! A69 A(13,26,27) 117.5063 estimate D2E/DX2 !

! A70 A(13,26,57) 118.278 estimate D2E/DX2 !

! A71 A(27,26,57) 124.2146 estimate D2E/DX2 !

! A72 A(26,27,28) 121.5335 estimate D2E/DX2 !

! A73 A(26,27,46) 120.3724 estimate D2E/DX2 !

! A74 A(28,27,46) 118.0929 estimate D2E/DX2 !

! A75 A(27,28,29) 121.5335 estimate D2E/DX2 !

! A76 A(27,28,47) 118.0929 estimate D2E/DX2 !

! A77 A(29,28,47) 120.3724 estimate D2E/DX2 !

! A78 A(14,29,28) 117.5063 estimate D2E/DX2 !

! A79 A(14,29,56) 118.278 estimate D2E/DX2 !

! A80 A(28,29,56) 124.2146 estimate D2E/DX2 !

! A81 A(22,30,31) 117.5063 estimate D2E/DX2 !

! A82 A(22,30,54) 118.278 estimate D2E/DX2 !

! A83 A(31,30,54) 124.2146 estimate D2E/DX2 !

! A84 A(30,31,32) 121.5335 estimate D2E/DX2 !

! A85 A(30,31,49) 120.3724 estimate D2E/DX2 !

! A86 A(32,31,49) 118.0929 estimate D2E/DX2 !

! A87 A(31,32,33) 121.5335 estimate D2E/DX2 !

! A88 A(31,32,48) 118.0929 estimate D2E/DX2 !

! A89 A(33,32,48) 120.3724 estimate D2E/DX2 !

! A90 A(21,33,32) 117.5063 estimate D2E/DX2 !

! A91 A(21,33,55) 118.278 estimate D2E/DX2 !

! A92 A(32,33,55) 124.2146 estimate D2E/DX2 !

! A93 A(11,34,35) 117.5063 estimate D2E/DX2 !

! A94 A(11,34,52) 118.278 estimate D2E/DX2 !

! A95 A(35,34,52) 124.2146 estimate D2E/DX2 !

! A96 A(34,35,36) 121.5335 estimate D2E/DX2 !

! A97 A(34,35,42) 120.3724 estimate D2E/DX2 !

! A98 A(36,35,42) 118.0929 estimate D2E/DX2 !

! A99 A(35,36,37) 121.5335 estimate D2E/DX2 !

! A100 A(35,36,43) 118.0929 estimate D2E/DX2 !

! A101 A(37,36,43) 120.3724 estimate D2E/DX2 !

! A102 A(10,37,36) 117.5063 estimate D2E/DX2 !

! A103 A(10,37,53) 118.278 estimate D2E/DX2 !

! A104 A(36,37,53) 124.2146 estimate D2E/DX2 !

! A105 A(5,38,39) 117.5063 estimate D2E/DX2 !

! A106 A(5,38,51) 118.278 estimate D2E/DX2 !

! A107 A(39,38,51) 124.2146 estimate D2E/DX2 !

! A108 A(38,39,40) 121.5335 estimate D2E/DX2 !

! A109 A(38,39,45) 120.3724 estimate D2E/DX2 !

! A110 A(40,39,45) 118.0929 estimate D2E/DX2 !

! A111 A(39,40,41) 121.5335 estimate D2E/DX2 !

! A112 A(39,40,44) 118.0929 estimate D2E/DX2 !

! A113 A(41,40,44) 120.3724 estimate D2E/DX2 !

! A114 A(4,41,40) 117.5063 estimate D2E/DX2 !

! A115 A(4,41,50) 118.278 estimate D2E/DX2 !

! A116 A(40,41,50) 124.2146 estimate D2E/DX2 !

! A117 A(41,50,58) 118.2022 estimate D2E/DX2 !

! A118 A(38,51,70) 118.2022 estimate D2E/DX2 !

! A119 A(34,52,62) 118.2022 estimate D2E/DX2 !

! A120 A(37,53,66) 118.2022 estimate D2E/DX2 !

! A121 A(30,54,86) 118.2022 estimate D2E/DX2 !

! A122 A(33,55,82) 118.2022 estimate D2E/DX2 !

! A123 A(29,56,78) 118.2022 estimate D2E/DX2 !

! A124 A(26,57,74) 118.2022 estimate D2E/DX2 !

! A125 A(50,58,59) 111.4881 estimate D2E/DX2 !

! A126 A(50,58,60) 111.2406 estimate D2E/DX2 !

! A127 A(50,58,61) 105.5635 estimate D2E/DX2 !

! A128 A(59,58,60) 109.6538 estimate D2E/DX2 !

! A129 A(59,58,61) 109.3393 estimate D2E/DX2 !

! A130 A(60,58,61) 109.4561 estimate D2E/DX2 !

! A131 A(52,62,63) 111.4881 estimate D2E/DX2 !

! A132 A(52,62,64) 111.2406 estimate D2E/DX2 !

! A133 A(52,62,65) 105.5635 estimate D2E/DX2 !

! A134 A(63,62,64) 109.6538 estimate D2E/DX2 !

! A135 A(63,62,65) 109.3393 estimate D2E/DX2 !

! A136 A(64,62,65) 109.4561 estimate D2E/DX2 !

! A137 A(53,66,67) 111.2406 estimate D2E/DX2 !

! A138 A(53,66,68) 111.4881 estimate D2E/DX2 !

! A139 A(53,66,69) 105.5635 estimate D2E/DX2 !

! A140 A(67,66,68) 109.6538 estimate D2E/DX2 !

! A141 A(67,66,69) 109.4561 estimate D2E/DX2 !

! A142 A(68,66,69) 109.3393 estimate D2E/DX2 !

! A143 A(51,70,71) 111.2406 estimate D2E/DX2 !

! A144 A(51,70,72) 111.4881 estimate D2E/DX2 !

! A145 A(51,70,73) 105.5635 estimate D2E/DX2 !

! A146 A(71,70,72) 109.6538 estimate D2E/DX2 !

! A147 A(71,70,73) 109.4561 estimate D2E/DX2 !

! A148 A(72,70,73) 109.3393 estimate D2E/DX2 !

! A149 A(57,74,75) 111.2406 estimate D2E/DX2 !

! A150 A(57,74,76) 111.4881 estimate D2E/DX2 !

! A151 A(57,74,77) 105.5635 estimate D2E/DX2 !

! A152 A(75,74,76) 109.6538 estimate D2E/DX2 !

! A153 A(75,74,77) 109.4561 estimate D2E/DX2 !

! A154 A(76,74,77) 109.3393 estimate D2E/DX2 !

! A155 A(56,78,79) 111.4881 estimate D2E/DX2 !

! A156 A(56,78,80) 111.2406 estimate D2E/DX2 !

! A157 A(56,78,81) 105.5635 estimate D2E/DX2 !

! A158 A(79,78,80) 109.6538 estimate D2E/DX2 !

! A159 A(79,78,81) 109.3393 estimate D2E/DX2 !

! A160 A(80,78,81) 109.4561 estimate D2E/DX2 !

! A161 A(55,82,83) 111.4881 estimate D2E/DX2 !

! A162 A(55,82,84) 111.2406 estimate D2E/DX2 !

! A163 A(55,82,85) 105.5635 estimate D2E/DX2 !

! A164 A(83,82,84) 109.6538 estimate D2E/DX2 !

! A165 A(83,82,85) 109.3393 estimate D2E/DX2 !

! A166 A(84,82,85) 109.4561 estimate D2E/DX2 !

! A167 A(54,86,87) 111.2406 estimate D2E/DX2 !

! A168 A(54,86,88) 111.4881 estimate D2E/DX2 !

! A169 A(54,86,89) 105.5635 estimate D2E/DX2 !

! A170 A(87,86,88) 109.6538 estimate D2E/DX2 !

! A171 A(87,86,89) 109.4561 estimate D2E/DX2 !

! A172 A(88,86,89) 109.3393 estimate D2E/DX2 !

! A173 L(2,25,19,16,-1) 180.0 estimate D2E/DX2 !

! A174 L(8,25,16,19,-1) 180.0 estimate D2E/DX2 !

! A175 L(2,25,19,16,-2) 179.9474 estimate D2E/DX2 !

! A176 L(8,25,16,19,-2) 179.9474 estimate D2E/DX2 !

! D1 D(5,1,2,3) -0.5937 estimate D2E/DX2 !

! D2 D(5,1,2,25) 171.3091 estimate D2E/DX2 !

! D3 D(12,1,2,3) 177.8538 estimate D2E/DX2 !

! D4 D(12,1,2,25) -10.2433 estimate D2E/DX2 !

! D5 D(2,1,5,4) 0.3499 estimate D2E/DX2 !

! D6 D(2,1,5,38) -179.159 estimate D2E/DX2 !

! D7 D(12,1,5,4) -178.1391 estimate D2E/DX2 !

! D8 D(12,1,5,38) 2.352 estimate D2E/DX2 !

! D9 D(2,1,12,17) 5.7083 estimate D2E/DX2 !

! D10 D(5,1,12,17) -176.0951 estimate D2E/DX2 !

! D11 D(1,2,3,4) 0.5937 estimate D2E/DX2 !

! D12 D(1,2,3,6) -177.8538 estimate D2E/DX2 !

! D13 D(25,2,3,4) -171.3091 estimate D2E/DX2 !

! D14 D(25,2,3,6) 10.2433 estimate D2E/DX2 !

! D15 D(1,2,25,8) -175.4091 estimate D2E/DX2 !

! D16 D(1,2,25,16) 4.5383 estimate D2E/DX2 !

! D17 D(3,2,25,8) -4.5383 estimate D2E/DX2 !

! D18 D(3,2,25,16) 175.4091 estimate D2E/DX2 !

! D19 D(2,3,4,5) -0.3499 estimate D2E/DX2 !

! D20 D(2,3,4,41) 179.159 estimate D2E/DX2 !

! D21 D(6,3,4,5) 178.1391 estimate D2E/DX2 !

! D22 D(6,3,4,41) -2.352 estimate D2E/DX2 !

! D23 D(2,3,6,7) -5.7083 estimate D2E/DX2 !

! D24 D(4,3,6,7) 176.0951 estimate D2E/DX2 !

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

! D26 D(3,4,5,38) 179.5779 estimate D2E/DX2 !

! D27 D(41,4,5,1) -179.5779 estimate D2E/DX2 !

! D28 D(41,4,5,38) 0.0 estimate D2E/DX2 !

! D29 D(3,4,41,40) -179.9505 estimate D2E/DX2 !

! D30 D(3,4,41,50) -0.3311 estimate D2E/DX2 !

! D31 D(5,4,41,40) -0.4996 estimate D2E/DX2 !

! D32 D(5,4,41,50) 179.1198 estimate D2E/DX2 !

! D33 D(1,5,38,39) 179.9505 estimate D2E/DX2 !

! D34 D(1,5,38,51) 0.3311 estimate D2E/DX2 !

! D35 D(4,5,38,39) 0.4996 estimate D2E/DX2 !

! D36 D(4,5,38,51) -179.1198 estimate D2E/DX2 !

! D37 D(3,6,7,8) -5.7083 estimate D2E/DX2 !

! D38 D(3,6,7,11) 176.0951 estimate D2E/DX2 !

! D39 D(6,7,8,9) -177.8538 estimate D2E/DX2 !

! D40 D(6,7,8,25) 10.2433 estimate D2E/DX2 !

! D41 D(11,7,8,9) 0.5937 estimate D2E/DX2 !

! D42 D(11,7,8,25) -171.3091 estimate D2E/DX2 !

! D43 D(6,7,11,10) 178.1391 estimate D2E/DX2 !

! D44 D(6,7,11,34) -2.352 estimate D2E/DX2 !

! D45 D(8,7,11,10) -0.3499 estimate D2E/DX2 !

! D46 D(8,7,11,34) 179.159 estimate D2E/DX2 !

! D47 D(7,8,9,10) -0.5937 estimate D2E/DX2 !

! D48 D(7,8,9,24) 177.8538 estimate D2E/DX2 !

! D49 D(25,8,9,10) 171.3091 estimate D2E/DX2 !

! D50 D(25,8,9,24) -10.2433 estimate D2E/DX2 !

! D51 D(7,8,25,2) -4.5383 estimate D2E/DX2 !

! D52 D(7,8,25,19) 175.4091 estimate D2E/DX2 !

! D53 D(9,8,25,2) -175.4091 estimate D2E/DX2 !

! D54 D(9,8,25,19) 4.5383 estimate D2E/DX2 !

! D55 D(8,9,10,11) 0.3499 estimate D2E/DX2 !

! D56 D(8,9,10,37) -179.159 estimate D2E/DX2 !

! D57 D(24,9,10,11) -178.1391 estimate D2E/DX2 !

! D58 D(24,9,10,37) 2.352 estimate D2E/DX2 !

! D59 D(8,9,24,23) 5.7083 estimate D2E/DX2 !

! D60 D(10,9,24,23) -176.0951 estimate D2E/DX2 !

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

! D62 D(9,10,11,34) -179.5779 estimate D2E/DX2 !

! D63 D(37,10,11,7) 179.5779 estimate D2E/DX2 !

! D64 D(37,10,11,34) 0.0 estimate D2E/DX2 !

! D65 D(9,10,37,36) 179.9505 estimate D2E/DX2 !

! D66 D(9,10,37,53) 0.3311 estimate D2E/DX2 !

! D67 D(11,10,37,36) 0.4996 estimate D2E/DX2 !

! D68 D(11,10,37,53) -179.1198 estimate D2E/DX2 !

! D69 D(7,11,34,35) -179.9505 estimate D2E/DX2 !

! D70 D(7,11,34,52) -0.3311 estimate D2E/DX2 !

! D71 D(10,11,34,35) -0.4996 estimate D2E/DX2 !

! D72 D(10,11,34,52) 179.1198 estimate D2E/DX2 !

! D73 D(1,12,17,13) -176.0951 estimate D2E/DX2 !

! D74 D(1,12,17,16) 5.7083 estimate D2E/DX2 !

! D75 D(17,13,14,15) 0.0 estimate D2E/DX2 !

! D76 D(17,13,14,29) -179.5779 estimate D2E/DX2 !

! D77 D(26,13,14,15) 179.5779 estimate D2E/DX2 !

! D78 D(26,13,14,29) 0.0 estimate D2E/DX2 !

! D79 D(14,13,17,12) -178.1391 estimate D2E/DX2 !

! D80 D(14,13,17,16) 0.3499 estimate D2E/DX2 !

! D81 D(26,13,17,12) 2.352 estimate D2E/DX2 !

! D82 D(26,13,17,16) -179.159 estimate D2E/DX2 !

! D83 D(14,13,26,27) 0.4996 estimate D2E/DX2 !

! D84 D(14,13,26,57) -179.1198 estimate D2E/DX2 !

! D85 D(17,13,26,27) 179.9505 estimate D2E/DX2 !

! D86 D(17,13,26,57) 0.3311 estimate D2E/DX2 !

! D87 D(13,14,15,16) -0.3499 estimate D2E/DX2 !

! D88 D(13,14,15,18) 178.1391 estimate D2E/DX2 !

! D89 D(29,14,15,16) 179.159 estimate D2E/DX2 !

! D90 D(29,14,15,18) -2.352 estimate D2E/DX2 !

! D91 D(13,14,29,28) -0.4996 estimate D2E/DX2 !

! D92 D(13,14,29,56) 179.1198 estimate D2E/DX2 !

! D93 D(15,14,29,28) -179.9505 estimate D2E/DX2 !

! D94 D(15,14,29,56) -0.3311 estimate D2E/DX2 !

! D95 D(14,15,16,17) 0.5937 estimate D2E/DX2 !

! D96 D(14,15,16,25) -171.3091 estimate D2E/DX2 !

! D97 D(18,15,16,17) -177.8538 estimate D2E/DX2 !

! D98 D(18,15,16,25) 10.2433 estimate D2E/DX2 !

! D99 D(14,15,18,20) 176.0951 estimate D2E/DX2 !

! D100 D(16,15,18,20) -5.7083 estimate D2E/DX2 !

! D101 D(15,16,17,12) 177.8538 estimate D2E/DX2 !

! D102 D(15,16,17,13) -0.5937 estimate D2E/DX2 !

! D103 D(25,16,17,12) -10.2433 estimate D2E/DX2 !

! D104 D(25,16,17,13) 171.3091 estimate D2E/DX2 !

! D105 D(15,16,25,2) 175.4091 estimate D2E/DX2 !

! D106 D(15,16,25,19) -4.5383 estimate D2E/DX2 !

! D107 D(17,16,25,2) 4.5383 estimate D2E/DX2 !

! D108 D(17,16,25,19) -175.4091 estimate D2E/DX2 !

! D109 D(15,18,20,19) -5.7083 estimate D2E/DX2 !

! D110 D(15,18,20,21) 176.0951 estimate D2E/DX2 !

! D111 D(23,19,20,18) -177.8538 estimate D2E/DX2 !

! D112 D(23,19,20,21) 0.5937 estimate D2E/DX2 !

! D113 D(25,19,20,18) 10.2433 estimate D2E/DX2 !

! D114 D(25,19,20,21) -171.3091 estimate D2E/DX2 !

! D115 D(20,19,23,22) -0.5937 estimate D2E/DX2 !

! D116 D(20,19,23,24) 177.8538 estimate D2E/DX2 !

! D117 D(25,19,23,22) 171.3091 estimate D2E/DX2 !

! D118 D(25,19,23,24) -10.2433 estimate D2E/DX2 !

! D119 D(20,19,25,8) 175.4091 estimate D2E/DX2 !

! D120 D(20,19,25,16) -4.5383 estimate D2E/DX2 !

! D121 D(23,19,25,8) 4.5383 estimate D2E/DX2 !

! D122 D(23,19,25,16) -175.4091 estimate D2E/DX2 !

! D123 D(18,20,21,22) 178.1391 estimate D2E/DX2 !

! D124 D(18,20,21,33) -2.352 estimate D2E/DX2 !

! D125 D(19,20,21,22) -0.3499 estimate D2E/DX2 !

! D126 D(19,20,21,33) 179.159 estimate D2E/DX2 !

! D127 D(20,21,22,23) 0.0 estimate D2E/DX2 !

! D128 D(20,21,22,30) 179.5779 estimate D2E/DX2 !

! D129 D(33,21,22,23) -179.5779 estimate D2E/DX2 !

! D130 D(33,21,22,30) 0.0 estimate D2E/DX2 !

! D131 D(20,21,33,32) -179.9505 estimate D2E/DX2 !

! D132 D(20,21,33,55) -0.3311 estimate D2E/DX2 !

! D133 D(22,21,33,32) -0.4996 estimate D2E/DX2 !

! D134 D(22,21,33,55) 179.1198 estimate D2E/DX2 !

! D135 D(21,22,23,19) 0.3499 estimate D2E/DX2 !

! D136 D(21,22,23,24) -178.1391 estimate D2E/DX2 !

! D137 D(30,22,23,19) -179.159 estimate D2E/DX2 !

! D138 D(30,22,23,24) 2.352 estimate D2E/DX2 !

! D139 D(21,22,30,31) 0.4996 estimate D2E/DX2 !

! D140 D(21,22,30,54) -179.1198 estimate D2E/DX2 !

! D141 D(23,22,30,31) 179.9505 estimate D2E/DX2 !

! D142 D(23,22,30,54) 0.3311 estimate D2E/DX2 !

! D143 D(19,23,24,9) 5.7083 estimate D2E/DX2 !

! D144 D(22,23,24,9) -176.0951 estimate D2E/DX2 !

! D145 D(13,26,27,28) -0.5026 estimate D2E/DX2 !

! D146 D(13,26,27,46) 179.9051 estimate D2E/DX2 !

! D147 D(57,26,27,28) 179.0921 estimate D2E/DX2 !

! D148 D(57,26,27,46) -0.5002 estimate D2E/DX2 !

! D149 D(13,26,57,74) -177.3154 estimate D2E/DX2 !

! D150 D(27,26,57,74) 3.0928 estimate D2E/DX2 !

! D151 D(26,27,28,29) 0.0 estimate D2E/DX2 !

! D152 D(26,27,28,47) -179.6012 estimate D2E/DX2 !

! D153 D(46,27,28,29) 179.6012 estimate D2E/DX2 !

! D154 D(46,27,28,47) 0.0 estimate D2E/DX2 !

! D155 D(27,28,29,14) 0.5026 estimate D2E/DX2 !

! D156 D(27,28,29,56) -179.0921 estimate D2E/DX2 !

! D157 D(47,28,29,14) -179.9051 estimate D2E/DX2 !

! D158 D(47,28,29,56) 0.5002 estimate D2E/DX2 !

! D159 D(14,29,56,78) 177.3154 estimate D2E/DX2 !

! D160 D(28,29,56,78) -3.0928 estimate D2E/DX2 !

! D161 D(22,30,31,32) -0.5026 estimate D2E/DX2 !

! D162 D(22,30,31,49) 179.9051 estimate D2E/DX2 !

! D163 D(54,30,31,32) 179.0921 estimate D2E/DX2 !

! D164 D(54,30,31,49) -0.5002 estimate D2E/DX2 !

! D165 D(22,30,54,86) -177.3154 estimate D2E/DX2 !

! D166 D(31,30,54,86) 3.0928 estimate D2E/DX2 !

! D167 D(30,31,32,33) 0.0 estimate D2E/DX2 !

! D168 D(30,31,32,48) -179.6012 estimate D2E/DX2 !

! D169 D(49,31,32,33) 179.6012 estimate D2E/DX2 !

! D170 D(49,31,32,48) 0.0 estimate D2E/DX2 !

! D171 D(31,32,33,21) 0.5026 estimate D2E/DX2 !

! D172 D(31,32,33,55) -179.0921 estimate D2E/DX2 !

! D173 D(48,32,33,21) -179.9051 estimate D2E/DX2 !

! D174 D(48,32,33,55) 0.5002 estimate D2E/DX2 !

! D175 D(21,33,55,82) 177.3154 estimate D2E/DX2 !

! D176 D(32,33,55,82) -3.0928 estimate D2E/DX2 !

! D177 D(11,34,35,36) 0.5026 estimate D2E/DX2 !

! D178 D(11,34,35,42) -179.9051 estimate D2E/DX2 !

! D179 D(52,34,35,36) -179.0921 estimate D2E/DX2 !

! D180 D(52,34,35,42) 0.5002 estimate D2E/DX2 !

! D181 D(11,34,52,62) 177.3154 estimate D2E/DX2 !

! D182 D(35,34,52,62) -3.0928 estimate D2E/DX2 !

! D183 D(34,35,36,37) 0.0 estimate D2E/DX2 !

! D184 D(34,35,36,43) 179.6012 estimate D2E/DX2 !

! D185 D(42,35,36,37) -179.6012 estimate D2E/DX2 !

! D186 D(42,35,36,43) 0.0 estimate D2E/DX2 !

! D187 D(35,36,37,10) -0.5026 estimate D2E/DX2 !

! D188 D(35,36,37,53) 179.0921 estimate D2E/DX2 !

! D189 D(43,36,37,10) 179.9051 estimate D2E/DX2 !

! D190 D(43,36,37,53) -0.5002 estimate D2E/DX2 !

! D191 D(10,37,53,66) -177.3154 estimate D2E/DX2 !

! D192 D(36,37,53,66) 3.0928 estimate D2E/DX2 !

! D193 D(5,38,39,40) -0.5026 estimate D2E/DX2 !

! D194 D(5,38,39,45) 179.9051 estimate D2E/DX2 !

! D195 D(51,38,39,40) 179.0921 estimate D2E/DX2 !

! D196 D(51,38,39,45) -0.5002 estimate D2E/DX2 !

! D197 D(5,38,51,70) -177.3154 estimate D2E/DX2 !

! D198 D(39,38,51,70) 3.0928 estimate D2E/DX2 !

! D199 D(38,39,40,41) 0.0 estimate D2E/DX2 !

! D200 D(38,39,40,44) -179.6012 estimate D2E/DX2 !

! D201 D(45,39,40,41) 179.6012 estimate D2E/DX2 !

! D202 D(45,39,40,44) 0.0 estimate D2E/DX2 !

! D203 D(39,40,41,4) 0.5026 estimate D2E/DX2 !

! D204 D(39,40,41,50) -179.0921 estimate D2E/DX2 !

! D205 D(44,40,41,4) -179.9051 estimate D2E/DX2 !

! D206 D(44,40,41,50) 0.5002 estimate D2E/DX2 !

! D207 D(4,41,50,58) 177.3154 estimate D2E/DX2 !

! D208 D(40,41,50,58) -3.0928 estimate D2E/DX2 !

! D209 D(41,50,58,59) 62.5083 estimate D2E/DX2 !

! D210 D(41,50,58,60) -60.2312 estimate D2E/DX2 !

! D211 D(41,50,58,61) -178.8656 estimate D2E/DX2 !

! D212 D(38,51,70,71) 60.2312 estimate D2E/DX2 !

! D213 D(38,51,70,72) -62.5083 estimate D2E/DX2 !

! D214 D(38,51,70,73) 178.8656 estimate D2E/DX2 !

! D215 D(34,52,62,63) 62.5083 estimate D2E/DX2 !

! D216 D(34,52,62,64) -60.2312 estimate D2E/DX2 !

! D217 D(34,52,62,65) -178.8656 estimate D2E/DX2 !

! D218 D(37,53,66,67) 60.2312 estimate D2E/DX2 !

! D219 D(37,53,66,68) -62.5083 estimate D2E/DX2 !

! D220 D(37,53,66,69) 178.8656 estimate D2E/DX2 !

! D221 D(30,54,86,87) 60.2312 estimate D2E/DX2 !

! D222 D(30,54,86,88) -62.5083 estimate D2E/DX2 !

! D223 D(30,54,86,89) 178.8656 estimate D2E/DX2 !

! D224 D(33,55,82,83) 62.5083 estimate D2E/DX2 !

! D225 D(33,55,82,84) -60.2312 estimate D2E/DX2 !

! D226 D(33,55,82,85) -178.8656 estimate D2E/DX2 !

! D227 D(29,56,78,79) 62.5083 estimate D2E/DX2 !

! D228 D(29,56,78,80) -60.2312 estimate D2E/DX2 !

! D229 D(29,56,78,81) -178.8656 estimate D2E/DX2 !

! D230 D(26,57,74,75) 60.2312 estimate D2E/DX2 !

! D231 D(26,57,74,76) -62.5083 estimate D2E/DX2 !

! D232 D(26,57,74,77) 178.8656 estimate D2E/DX2 !

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

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

Number of steps in this run= 518 maximum allowed number of steps= 534.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 5 23:09:36 2019, MaxMem= 1342177280 cpu: 0.2

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

Stoichiometry C40H32N8O8Zn(3)

Framework group D2D[O(Zn),2SGD(N2),X(C40H32N4O8)]

Deg. of freedom 32

Full point group D2D NOp 8

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -1.127903 2.810434 0.088758

2 7 0 0.000000 2.043265 -0.000938

3 6 0 1.127903 2.810434 0.088758

4 6 0 0.710261 4.207143 0.266641

5 6 0 -0.710261 4.207143 0.266641

6 7 0 2.394950 2.394950 0.000000

7 6 0 2.810434 1.127903 -0.088758

8 7 0 2.043265 0.000000 0.000938

9 6 0 2.810434 -1.127903 -0.088758

10 6 0 4.207143 -0.710261 -0.266641

11 6 0 4.207143 0.710261 -0.266641

12 7 0 -2.394950 2.394950 0.000000

13 6 0 -4.207143 0.710261 -0.266641

14 6 0 -4.207143 -0.710261 -0.266641

15 6 0 -2.810434 -1.127903 -0.088758

16 7 0 -2.043265 0.000000 0.000938

17 6 0 -2.810434 1.127903 -0.088758

18 7 0 -2.394950 -2.394950 0.000000

19 7 0 0.000000 -2.043265 -0.000938

20 6 0 -1.127903 -2.810434 0.088758

21 6 0 -0.710261 -4.207143 0.266641

22 6 0 0.710261 -4.207143 0.266641

23 6 0 1.127903 -2.810434 0.088758

24 7 0 2.394950 -2.394950 0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.403443 1.434382 -0.427965

27 6 0 -6.588145 0.701729 -0.576793

28 6 0 -6.588145 -0.701729 -0.576793

29 6 0 -5.403443 -1.434382 -0.427965

30 6 0 1.434382 -5.403443 0.427965

31 6 0 0.701729 -6.588145 0.576793

32 6 0 -0.701729 -6.588145 0.576793

33 6 0 -1.434382 -5.403443 0.427965

34 6 0 5.403443 1.434382 -0.427965

35 6 0 6.588145 0.701729 -0.576793

36 6 0 6.588145 -0.701729 -0.576793

37 6 0 5.403443 -1.434382 -0.427965

38 6 0 -1.434382 5.403443 0.427965

39 6 0 -0.701729 6.588145 0.576793

40 6 0 0.701729 6.588145 0.576793

41 6 0 1.434382 5.403443 0.427965

42 1 0 7.535264 1.211725 -0.702477

43 1 0 7.535264 -1.211725 -0.702477

44 1 0 1.211725 7.535264 0.702477

45 1 0 -1.211725 7.535264 0.702477

46 1 0 -7.535264 1.211725 -0.702477

47 1 0 -7.535264 -1.211725 -0.702477

48 1 0 -1.211725 -7.535264 0.702477

49 1 0 1.211725 -7.535264 0.702477

50 8 0 2.789800 5.338171 0.437687

51 8 0 -2.789800 5.338171 0.437687

52 8 0 5.338171 2.789800 -0.437687

53 8 0 5.338171 -2.789800 -0.437687

54 8 0 2.789800 -5.338171 0.437687

55 8 0 -2.789800 -5.338171 0.437687

56 8 0 -5.338171 -2.789800 -0.437687

57 8 0 -5.338171 2.789800 -0.437687

58 6 0 3.523697 6.559137 0.542829

59 1 0 3.316115 7.072282 1.489258

60 1 0 3.302204 7.229319 -0.296388

61 1 0 4.575837 6.271977 0.510699

62 6 0 6.559137 3.523697 -0.542829

63 1 0 7.072282 3.316115 -1.489258

64 1 0 7.229319 3.302204 0.296388

65 1 0 6.271977 4.575837 -0.510699

66 6 0 6.559137 -3.523697 -0.542829

67 1 0 7.229319 -3.302204 0.296388

68 1 0 7.072282 -3.316115 -1.489258

69 1 0 6.271977 -4.575837 -0.510699

70 6 0 -3.523697 6.559137 0.542829

71 1 0 -3.302204 7.229319 -0.296388

72 1 0 -3.316115 7.072282 1.489258

73 1 0 -4.575837 6.271977 0.510699

74 6 0 -6.559137 3.523697 -0.542829

75 1 0 -7.229319 3.302204 0.296388

76 1 0 -7.072282 3.316115 -1.489258

77 1 0 -6.271977 4.575837 -0.510699

78 6 0 -6.559137 -3.523697 -0.542829

79 1 0 -7.072282 -3.316115 -1.489258

80 1 0 -7.229319 -3.302204 0.296388

81 1 0 -6.271977 -4.575837 -0.510699

82 6 0 -3.523697 -6.559137 0.542829

83 1 0 -3.316115 -7.072282 1.489258

84 1 0 -3.302204 -7.229319 -0.296388

85 1 0 -4.575837 -6.271977 0.510699

86 6 0 3.523697 -6.559137 0.542829

87 1 0 3.302204 -7.229319 -0.296388

88 1 0 3.316115 -7.072282 1.489258

89 1 0 4.575837 -6.271977 0.510699

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

Rotational constants (GHZ): 0.0441201 0.0441201 0.0223223

Leave Link 202 at Fri Jul 5 23:09:36 2019, MaxMem= 1342177280 cpu: 0.2

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

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

Centers: 25

S 1 1.00

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

S 1 1.00

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

S 1 1.00

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

P 1 1.00

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

P 1 1.00

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

D 3 1.00

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

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

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

D 1 1.00

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

D 1 1.00

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

\*\*\*\*

Centers: 42 43 44 45 46 47 48 49 59 60

Centers: 61 63 64 65 67 68 69 71 72 73

Centers: 75 76 77 79 80 81 83 84 85 87

Centers: 88 89 1 3 4 5 7 9 10 11

Centers: 13 14 15 17 20 21 22 23 26 27

Centers: 28 29 30 31 32 33 34 35 36 37

Centers: 38 39 40 41 58 62 66 70 74 78

Centers: 82 86 2 6 8 12 16 18 19 24

Centers: 50 51 52 53 54 55 56 57

6-311G\*

\*\*\*\*

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

Pseudopotential Parameters

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

Center Atomic Valence Angular Power

Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

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

1 6

No pseudopotential on this center.

2 7

No pseudopotential on this center.

3 6

No pseudopotential on this center.

4 6

No pseudopotential on this center.

5 6

No pseudopotential on this center.

6 7

No pseudopotential on this center.

7 6

No pseudopotential on this center.

8 7

No pseudopotential on this center.

9 6

No pseudopotential on this center.

10 6

No pseudopotential on this center.

11 6

No pseudopotential on this center.

12 7

No pseudopotential on this center.

13 6

No pseudopotential on this center.

14 6

No pseudopotential on this center.

15 6

No pseudopotential on this center.

16 7

No pseudopotential on this center.

17 6

No pseudopotential on this center.

18 7

No pseudopotential on this center.

19 7

No pseudopotential on this center.

20 6

No pseudopotential on this center.

21 6

No pseudopotential on this center.

22 6

No pseudopotential on this center.

23 6

No pseudopotential on this center.

24 7

No pseudopotential on this center.

25 30 12

F and up

1 386.7379660 -18.00000000 0.00000000

2 72.8587359 -124.35274030 0.00000000

2 15.9066170 -30.66018220 0.00000000

2 4.3502340 -10.63589890 0.00000000

2 1.2842199 -0.76836230 0.00000000

S - F

0 19.0867858 3.00000000 0.00000000

1 5.0231080 22.52342250 0.00000000

2 1.2701744 48.44659420 0.00000000

2 1.0671287 -44.55601190 0.00000000

2 0.9264190 12.99839580 0.00000000

P - F

0 43.4927750 5.00000000 0.00000000

1 20.8692669 20.74355890 0.00000000

2 21.7118378 90.30271580 0.00000000

2 6.3616915 74.66103160 0.00000000

2 1.2291195 9.88944240 0.00000000

D - F

2 13.5851800 -4.84903590 0.00000000

2 9.8373050 3.69133790 0.00000000

2 0.8373113 -0.50373190 0.00000000

26 6

No pseudopotential on this center.

27 6

No pseudopotential on this center.

28 6

No pseudopotential on this center.

29 6

No pseudopotential on this center.

30 6

No pseudopotential on this center.

31 6

No pseudopotential on this center.

32 6

No pseudopotential on this center.

33 6

No pseudopotential on this center.

34 6

No pseudopotential on this center.

35 6

No pseudopotential on this center.

36 6

No pseudopotential on this center.

37 6

No pseudopotential on this center.

38 6

No pseudopotential on this center.

39 6

No pseudopotential on this center.

40 6

No pseudopotential on this center.

41 6

No pseudopotential on this center.

42 1

No pseudopotential on this center.

43 1

No pseudopotential on this center.

44 1

No pseudopotential on this center.

45 1

No pseudopotential on this center.

46 1

No pseudopotential on this center.

47 1

No pseudopotential on this center.

48 1

No pseudopotential on this center.

49 1

No pseudopotential on this center.

50 8

No pseudopotential on this center.

51 8

No pseudopotential on this center.

52 8

No pseudopotential on this center.

53 8

No pseudopotential on this center.

54 8

No pseudopotential on this center.

55 8

No pseudopotential on this center.

56 8

No pseudopotential on this center.

57 8

No pseudopotential on this center.

58 6

No pseudopotential on this center.

59 1

No pseudopotential on this center.

60 1

No pseudopotential on this center.

61 1

No pseudopotential on this center.

62 6

No pseudopotential on this center.

63 1

No pseudopotential on this center.

64 1

No pseudopotential on this center.

65 1

No pseudopotential on this center.

66 6

No pseudopotential on this center.

67 1

No pseudopotential on this center.

68 1

No pseudopotential on this center.

69 1

No pseudopotential on this center.

70 6

No pseudopotential on this center.

71 1

No pseudopotential on this center.

72 1

No pseudopotential on this center.

73 1

No pseudopotential on this center.

74 6

No pseudopotential on this center.

75 1

No pseudopotential on this center.

76 1

No pseudopotential on this center.

77 1

No pseudopotential on this center.

78 6

No pseudopotential on this center.

79 1

No pseudopotential on this center.

80 1

No pseudopotential on this center.

81 1

No pseudopotential on this center.

82 6

No pseudopotential on this center.

83 1

No pseudopotential on this center.

84 1

No pseudopotential on this center.

85 1

No pseudopotential on this center.

86 6

No pseudopotential on this center.

87 1

No pseudopotential on this center.

88 1

No pseudopotential on this center.

89 1

No pseudopotential on this center.

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

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

There are 313 symmetry adapted cartesian basis functions of A1 symmetry.

There are 284 symmetry adapted cartesian basis functions of A2 symmetry.

There are 295 symmetry adapted cartesian basis functions of B1 symmetry.

There are 295 symmetry adapted cartesian basis functions of B2 symmetry.

There are 295 symmetry adapted basis functions of A1 symmetry.

There are 271 symmetry adapted basis functions of A2 symmetry.

There are 281 symmetry adapted basis functions of B1 symmetry.

There are 281 symmetry adapted basis functions of B2 symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8019.9293694116 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= 89 NActive= 89 NUniq= 13 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2274359222 Hartrees.

Nuclear repulsion after empirical dispersion term = 8019.7019334894 Hartrees.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6354

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.14D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 320

GePol: Fraction of low-weight points (<1% of avg) = 5.04%

GePol: Cavity surface area = 703.536 Ang\*\*2

GePol: Cavity volume = 802.514 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0089181925 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8019.6930152969 Hartrees.

Leave Link 301 at Fri Jul 5 23:09:37 2019, MaxMem= 1342177280 cpu: 1.6

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44149 LenP2D= 110838.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 2.81D-05 NBF= 295 271 281 281

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 295 271 281 281

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= 1124 1124 1140 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Fri Jul 5 23:09:39 2019, MaxMem= 1342177280 cpu: 24.2

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 5 23:09:40 2019, MaxMem= 1342177280 cpu: 2.8

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

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -2650.01194682113

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

(E)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Beta Orbitals:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

(A2)

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

Leave Link 401 at Fri Jul 5 23:09:44 2019, MaxMem= 1342177280 cpu: 49.6

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4274597 IEndB= 4274597 NGot= 1342177280 MDV= 1339329480

LenX= 1339329480 LenY= 1337919324

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:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

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

IRaf= 450000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 121119948.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.77D-15 for 6325.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.51D-15 for 2376 407.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.55D-15 for 6325.

Iteration 1 A^-1\*A deviation from orthogonality is 9.06D-12 for 4971 4917.

E= -2648.71421467518

DIIS: error= 9.57D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2648.71421467518 IErMin= 1 ErrMin= 9.57D-02

ErrMax= 9.57D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.98D+00 BMatP= 5.98D+00

IDIUse=3 WtCom= 4.26D-02 WtEn= 9.57D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.015 Goal= None Shift= 0.000

Gap= 0.032 Goal= None Shift= 0.000

GapD= 0.015 DampG=0.250 DampE=0.250 DampFc=0.1250 IDamp=-1.

Damping current iteration by 1.25D-01

RMSDP=2.58D-03 MaxDP=1.59D-01 OVMax= 2.80D-01

Cycle 2 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 3.23D-04 CP: 1.00D+00

E= -2648.93918872512 Delta-E= -0.224974049946 Rises=F Damp=T

DIIS: error= 6.81D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2648.93918872512 IErMin= 2 ErrMin= 6.81D-02

ErrMax= 6.81D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.46D+00 BMatP= 5.98D+00

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

Coeff-Com: -0.289D+01 0.389D+01

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

Coeff: -0.922D+00 0.192D+01

Gap= 0.023 Goal= None Shift= 0.000

Gap= 0.048 Goal= None Shift= 0.000

RMSDP=1.59D-03 MaxDP=9.08D-02 DE=-2.25D-01 OVMax= 1.46D-01

Cycle 3 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 9.66D-04 CP: 9.97D-01 3.00D+00

E= -2649.54455470522 Delta-E= -0.605365980098 Rises=F Damp=F

DIIS: error= 5.14D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.54455470522 IErMin= 3 ErrMin= 5.14D-02

ErrMax= 5.14D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.28D+00 BMatP= 3.46D+00

IDIUse=3 WtCom= 4.86D-01 WtEn= 5.14D-01

EnCoef did 100 forward-backward iterations

Coeff-Com: 0.256D+01-0.272D+01 0.116D+01

Coeff-En: 0.115D+00 0.268D-02 0.882D+00

Coeff: 0.130D+01-0.132D+01 0.102D+01

Gap= 0.029 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=7.83D-04 MaxDP=5.26D-02 DE=-6.05D-01 OVMax= 1.05D-01

Cycle 4 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 3.80D-04 CP: 9.96D-01 3.00D+00 2.91D-01

E= -2649.74246222051 Delta-E= -0.197907515283 Rises=F Damp=F

DIIS: error= 2.02D-02 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.74246222051 IErMin= 4 ErrMin= 2.02D-02

ErrMax= 2.02D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.42D-01 BMatP= 1.28D+00

IDIUse=3 WtCom= 7.98D-01 WtEn= 2.02D-01

Coeff-Com: -0.378D+00 0.483D+00 0.234D+00 0.661D+00

Coeff-En: 0.000D+00 0.000D+00 0.122D+00 0.878D+00

Coeff: -0.301D+00 0.385D+00 0.212D+00 0.705D+00

Gap= 0.029 Goal= None Shift= 0.000

Gap= 0.061 Goal= None Shift= 0.000

RMSDP=2.06D-04 MaxDP=1.28D-02 DE=-1.98D-01 OVMax= 4.38D-02

Cycle 5 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 8.08D-05 CP: 9.95D-01 3.00D+00 4.48D-01 6.98D-01

E= -2649.78544465188 Delta-E= -0.042982431378 Rises=F Damp=F

DIIS: error= 1.61D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.78544465188 IErMin= 5 ErrMin= 1.61D-03

ErrMax= 1.61D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.39D-02 BMatP= 2.42D-01

IDIUse=3 WtCom= 9.84D-01 WtEn= 1.61D-02

Coeff-Com: -0.319D+00 0.373D+00 0.636D-01 0.428D+00 0.454D+00

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

Coeff: -0.314D+00 0.367D+00 0.625D-01 0.421D+00 0.463D+00

Gap= 0.029 Goal= None Shift= 0.000

Gap= 0.062 Goal= None Shift= 0.000

RMSDP=4.31D-05 MaxDP=3.69D-03 DE=-4.30D-02 OVMax= 1.02D-02

Cycle 6 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 2.34D-05 CP: 9.95D-01 3.00D+00 4.46D-01 7.41D-01 6.00D-01

E= -2649.78841393921 Delta-E= -0.002969287323 Rises=F Damp=F

DIIS: error= 4.08D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.78841393921 IErMin= 6 ErrMin= 4.08D-04

ErrMax= 4.08D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.16D-04 BMatP= 1.39D-02

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.08D-03

Coeff-Com: -0.176D+00 0.203D+00 0.126D-01 0.189D+00 0.241D+00 0.530D+00

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

Coeff: -0.175D+00 0.202D+00 0.126D-01 0.189D+00 0.240D+00 0.532D+00

Gap= 0.029 Goal= None Shift= 0.000

Gap= 0.062 Goal= None Shift= 0.000

RMSDP=1.18D-05 MaxDP=1.05D-03 DE=-2.97D-03 OVMax= 3.44D-03

Cycle 7 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 8.81D-06 CP: 9.95D-01 3.00D+00 4.45D-01 7.42D-01 6.53D-01

CP: 7.22D-01

E= -2649.78851136307 Delta-E= -0.000097423859 Rises=F Damp=F

DIIS: error= 1.90D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.78851136307 IErMin= 7 ErrMin= 1.90D-04

ErrMax= 1.90D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.25D-05 BMatP= 4.16D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.90D-03

Coeff-Com: -0.567D-01 0.643D-01-0.612D-02 0.349D-01 0.462D-01 0.303D+00

Coeff-Com: 0.614D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.395D-01

Coeff-En: 0.960D+00

Coeff: -0.566D-01 0.642D-01-0.611D-02 0.348D-01 0.461D-01 0.303D+00

Coeff: 0.615D+00

Gap= 0.029 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=5.28D-06 MaxDP=3.88D-04 DE=-9.74D-05 OVMax= 2.62D-03

Cycle 8 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 4.41D-06 CP: 9.95D-01 3.00D+00 4.47D-01 7.44D-01 6.50D-01

CP: 8.26D-01 9.72D-01

E= -2649.78854184177 Delta-E= -0.000030478705 Rises=F Damp=F

DIIS: error= 8.89D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.78854184177 IErMin= 8 ErrMin= 8.89D-05

ErrMax= 8.89D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.27D-05 BMatP= 8.25D-05

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

Coeff-Com: 0.311D-01-0.361D-01-0.401D-02-0.385D-01-0.544D-01-0.554D-01

Coeff-Com: 0.188D+00 0.969D+00

Coeff: 0.311D-01-0.361D-01-0.401D-02-0.385D-01-0.544D-01-0.554D-01

Coeff: 0.188D+00 0.969D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=4.31D-06 MaxDP=3.98D-04 DE=-3.05D-05 OVMax= 1.80D-03

Cycle 9 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 2.83D-06 CP: 9.95D-01 3.00D+00 4.47D-01 7.46D-01 6.61D-01

CP: 8.98D-01 1.24D+00 1.22D+00

E= -2649.78855153949 Delta-E= -0.000009697718 Rises=F Damp=F

DIIS: error= 5.48D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.78855153949 IErMin= 9 ErrMin= 5.48D-05

ErrMax= 5.48D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.03D-06 BMatP= 1.27D-05

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

Coeff-Com: 0.361D-01-0.415D-01-0.140D-02-0.359D-01-0.484D-01-0.131D+00

Coeff-Com: -0.623D-01 0.683D+00 0.601D+00

Coeff: 0.361D-01-0.415D-01-0.140D-02-0.359D-01-0.484D-01-0.131D+00

Coeff: -0.623D-01 0.683D+00 0.601D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=2.31D-06 MaxDP=1.95D-04 DE=-9.70D-06 OVMax= 1.50D-03

Cycle 10 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.52D-06 CP: 9.95D-01 3.00D+00 4.47D-01 7.45D-01 6.65D-01

CP: 9.19D-01 1.34D+00 1.51D+00 8.23D-01

E= -2649.78855494555 Delta-E= -0.000003406061 Rises=F Damp=F

DIIS: error= 1.62D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -2649.78855494555 IErMin=10 ErrMin= 1.62D-05

ErrMax= 1.62D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.42D-07 BMatP= 8.03D-06

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

Coeff-Com: 0.608D-02-0.690D-02 0.187D-03-0.470D-02-0.337D-02-0.396D-01

Coeff-Com: -0.698D-01 0.591D-01 0.213D+00 0.846D+00

Coeff: 0.608D-02-0.690D-02 0.187D-03-0.470D-02-0.337D-02-0.396D-01

Coeff: -0.698D-01 0.591D-01 0.213D+00 0.846D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=8.79D-07 MaxDP=7.49D-05 DE=-3.41D-06 OVMax= 3.59D-04

Cycle 11 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 5.15D-07 CP: 9.95D-01 3.00D+00 4.47D-01 7.46D-01 6.65D-01

CP: 9.23D-01 1.37D+00 1.62D+00 9.45D-01 1.04D+00

E= -2649.78855531835 Delta-E= -0.000000372796 Rises=F Damp=F

DIIS: error= 8.95D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -2649.78855531835 IErMin=11 ErrMin= 8.95D-06

ErrMax= 8.95D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.34D-07 BMatP= 7.42D-07

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

Coeff-Com: -0.166D-02 0.197D-02 0.221D-03 0.209D-02 0.482D-02-0.383D-02

Coeff-Com: -0.271D-01-0.667D-01 0.209D-01 0.465D+00 0.604D+00

Coeff: -0.166D-02 0.197D-02 0.221D-03 0.209D-02 0.482D-02-0.383D-02

Coeff: -0.271D-01-0.667D-01 0.209D-01 0.465D+00 0.604D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=3.22D-07 MaxDP=2.51D-05 DE=-3.73D-07 OVMax= 1.58D-04

Cycle 12 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 2.27D-07 CP: 9.95D-01 3.00D+00 4.47D-01 7.46D-01 6.66D-01

CP: 9.24D-01 1.38D+00 1.64D+00 9.75D-01 1.10D+00

CP: 8.60D-01

E= -2649.78855539016 Delta-E= -0.000000071816 Rises=F Damp=F

DIIS: error= 2.85D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -2649.78855539016 IErMin=12 ErrMin= 2.85D-06

ErrMax= 2.85D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.58D-08 BMatP= 2.34D-07

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

Coeff-Com: -0.131D-02 0.151D-02 0.572D-04 0.130D-02 0.197D-02 0.371D-02

Coeff-Com: 0.175D-02-0.288D-01-0.212D-01 0.317D-01 0.182D+00 0.827D+00

Coeff: -0.131D-02 0.151D-02 0.572D-04 0.130D-02 0.197D-02 0.371D-02

Coeff: 0.175D-02-0.288D-01-0.212D-01 0.317D-01 0.182D+00 0.827D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=1.28D-07 MaxDP=9.31D-06 DE=-7.18D-08 OVMax= 5.69D-05

Cycle 13 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.02D-07 CP: 9.95D-01 3.00D+00 4.47D-01 7.46D-01 6.66D-01

CP: 9.23D-01 1.38D+00 1.64D+00 9.75D-01 1.13D+00

CP: 9.43D-01 1.12D+00

E= -2649.78855539785 Delta-E= -0.000000007689 Rises=F Damp=F

DIIS: error= 1.60D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -2649.78855539785 IErMin=13 ErrMin= 1.60D-06

ErrMax= 1.60D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.12D-09 BMatP= 1.58D-08

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

Coeff-Com: -0.247D-03 0.275D-03 0.208D-04 0.274D-03 0.936D-04 0.247D-02

Coeff-Com: 0.589D-02-0.282D-02-0.132D-01-0.697D-01-0.170D-01 0.450D+00

Coeff-Com: 0.644D+00

Coeff: -0.247D-03 0.275D-03 0.208D-04 0.274D-03 0.936D-04 0.247D-02

Coeff: 0.589D-02-0.282D-02-0.132D-01-0.697D-01-0.170D-01 0.450D+00

Coeff: 0.644D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=6.26D-08 MaxDP=3.89D-06 DE=-7.69D-09 OVMax= 3.07D-05

Cycle 14 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 3.97D-08 CP: 9.95D-01 3.00D+00 4.47D-01 7.46D-01 6.66D-01

CP: 9.24D-01 1.38D+00 1.64D+00 9.81D-01 1.13D+00

CP: 9.71D-01 1.27D+00 8.30D-01

E= -2649.78855540036 Delta-E= -0.000000002510 Rises=F Damp=F

DIIS: error= 6.28D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -2649.78855540036 IErMin=14 ErrMin= 6.28D-07

ErrMax= 6.28D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.35D-09 BMatP= 7.12D-09

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

Coeff-Com: 0.141D-03-0.168D-03 0.604D-05-0.938D-04-0.302D-03 0.673D-03

Coeff-Com: 0.261D-02 0.420D-02-0.130D-02-0.445D-01-0.519D-01 0.150D-01

Coeff-Com: 0.336D+00 0.739D+00

Coeff: 0.141D-03-0.168D-03 0.604D-05-0.938D-04-0.302D-03 0.673D-03

Coeff: 0.261D-02 0.420D-02-0.130D-02-0.445D-01-0.519D-01 0.150D-01

Coeff: 0.336D+00 0.739D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=2.86D-08 MaxDP=1.94D-06 DE=-2.51D-09 OVMax= 1.53D-05

Cycle 15 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.57D-08 CP: 9.95D-01 3.00D+00 4.47D-01 7.46D-01 6.66D-01

CP: 9.24D-01 1.38D+00 1.64D+00 9.82D-01 1.13D+00

CP: 9.93D-01 1.32D+00 9.80D-01 9.76D-01

E= -2649.78855540132 Delta-E= -0.000000000960 Rises=F Damp=F

DIIS: error= 2.31D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -2649.78855540132 IErMin=15 ErrMin= 2.31D-07

ErrMax= 2.31D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.32D-10 BMatP= 1.35D-09

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

Coeff-Com: 0.471D-04-0.553D-04-0.497D-05-0.515D-04-0.104D-03-0.694D-05

Coeff-Com: 0.353D-03 0.162D-02 0.810D-03-0.958D-02-0.163D-01-0.411D-01

Coeff-Com: 0.580D-01 0.267D+00 0.740D+00

Coeff: 0.471D-04-0.553D-04-0.497D-05-0.515D-04-0.104D-03-0.694D-05

Coeff: 0.353D-03 0.162D-02 0.810D-03-0.958D-02-0.163D-01-0.411D-01

Coeff: 0.580D-01 0.267D+00 0.740D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=9.56D-09 MaxDP=8.58D-07 DE=-9.60D-10 OVMax= 5.07D-06

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

Error on total polarization charges = 0.07297

SCF Done: E(UB3LYP) = -2649.78855540 A.U. after 15 cycles

NFock= 15 Conv=0.96D-08 -V/T= 1.9852

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0181 S= 1.0060

<L.S>= 0.000000000000E+00

KE= 2.689640846291D+03 PE=-2.231749061629D+04 EE= 8.958368199305D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.60

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0181, after 2.0002

Leave Link 502 at Fri Jul 5 23:16:05 2019, MaxMem= 1342177280 cpu: 4476.5

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

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

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Population analysis using the SCF density.

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

Orbital symmetries:

Alpha Orbitals:

Occupied (E) (E) (E) (E) (E) (E) (E) (E) (E) (E) (E) (E)

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

(E) (E) (E) (E) (E) (E) (E) (E) (E) (E) (E) (E)

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(E) (E) (E) (E) (E) (B2) (?A) (?A) (B2) (B1) (?A)

(?A) (B2) (?A) (B2) (?A) (B2) (?B) (?A) (E) (?A)

(?B) (?A) (?A) (E) (?B) (E) (?A) (E) (?A) (?A)

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Virtual (?A) (?D) (?C) (?A) (?A) (?C) (?D) (?A) (?A) (?C)

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(?A) (?A) (?I) (?J) (?A) (?A) (?J) (?J) (?K) (E)

(?K) (E) (?K) (?K) (?K) (E) (?K) (E) (E) (?K)

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(E) (E) (?K) (?K) (?K) (E) (E) (?K) (?K) (E) (E)

(?K) (A1) (B2) (E) (E) (E) (E) (E) (E) (E) (E)

(E) (E) (E) (E) (E) (E) (E) (E) (E) (E) (?K) (?K)

(E) (E) (?K) (E) (E) (E) (E) (E) (E) (A2) (E)

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

(B2) (A1) (E) (?K) (?K) (E) (E) (?K) (?K) (E)

(E) (?K) (?K) (E) (E) (E) (E) (E) (E) (E) (E)

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(?K) (B1) (E) (E) (?K) (E) (E) (E) (E) (E) (E)

(E) (E)

Beta Orbitals:

Occupied (E) (E) (E) (E) (E) (E) (E) (E) (E) (E) (E) (E)

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

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(E) (E) (E) (E) (E) (E) (E) (E) (E) (E) (E) (E)

(E) (E) (E) (E) (E) (?A) (B2) (B2) (?A) (?B) (B2)

(B2) (?A) (B2) (?A) (B2) (?A) (?B) (B2) (?A) (B2)

(?B) (B2) (B2) (?A) (?B) (?A) (B2) (?A) (B2) (B2)

(B2) (?B) (B2) (?B) (B2) (?A) (?B) (?A) (B2) (B2)

(?A) (B2) (?B) (B2) (?B) (?A) (?A) (B2) (B2) (B2)

(B2) (?A) (?B) (?A) (B2) (B2) (?B) (B2) (B2) (?B)

(?A) (B2) (B2) (?A) (?B) (?B) (B2) (B2) (?A) (B2)

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Virtual (?B) (B2) (B2) (?B) (?A) (B2) (B2) (?A) (?B) (B2)

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(B2) (B2) (?C) (?A) (?A) (?A) (B2) (B2) (?C) (?A)

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(?C) (B2) (B2) (?A) (B2) (B2) (B2) (B2) (?C) (?C)

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(B2) (B2) (?A) (?C) (B2) (?A) (B2) (B2) (B2) (?A)

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(B2) (B2) (?A) (B2) (?A) (?C) (B2) (B2) (?A) (?C)

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(B2) (B2) (?D) (B2) (B2) (?D) (?A) (E) (B2) (B2)

(?A) (B2) (B2) (?A) (?D) (B2) (?D) (B2) (E) (?D)

(?D) (B2) (B2) (?D) (?D) (?D) (B2) (B2) (B2) (B2)

(?E) (?E) (B2) (B2) (?E) (B2) (B2) (?D) (?D) (B2)

(B2) (?D) (?E) (B2) (?D) (?E) (B2) (B2) (?D) (B2)

(?E) (?D) (B2) (B2) (?E) (B2) (B2) (?E) (?D) (?E)

(B2) (B2) (?E) (?D) (B2) (B2) (B2) (B2) (?E) (?E)

(?D) (?D) (?D) (B2) (B2) (?E) (?D) (B2) (B2) (B2)

(B2) (?E) (?D) (?E) (B2) (B2) (?E) (?E) (B2) (B2)

(B2) (B2) (?D) (?E) (?E) (?D) (B2) (?D) (?D) (B2)

(B2) (B2) (?D) (B2) (B2) (?E) (?E) (?D) (B2) (B2)

(?D) (?E) (B2) (B2) (?E) (?D) (B2) (?E) (B2) (B2)

(B2) (?D) (?D) (?D) (B2) (B2) (?E) (?D) (B2) (?E)

(B2) (B2) (B2) (?D) (?D) (?E) (B2) (B2) (?E) (?D)

(B2) (B2) (?D) (?E) (B2) (?E) (B2) (B2) (?E) (B2)

(?E) (?D) (?E) (B2) (?E) (B2) (?E) (B2) (?D) (B2)

(?D) (B2) (B2) (?D) (B2) (B2) (?D) (?D) (B2) (B2)

(?E) (B2) (?E) (B2) (?E) (?D) (B2) (B2) (?E) (?D)

(B2) (B2) (?E) (?D) (?E) (B2) (B2) (?D) (B2) (?E)

(B2) (?D) (B2) (B2) (?E) (?F) (B2) (B2) (?F) (?F)

(?G) (E) (?G) (E) (?G) (?G) (?G) (?H) (?G) (?H)

(?H) (?I) (E) (?I) (E) (E) (E) (?H) (?I) (E) (?H)

(E) (?H) (E) (A2) (E) (?H) (?H) (?J) (?J) (?H)

(?J) (E) (?J) (?H) (?J) (?J) (?H) (E) (?K) (E)

(E) (?K) (E) (E) (?K) (?K) (?K) (E) (E) (?K) (?K)

(E) (E) (?K) (E) (E) (E) (E) (E) (E) (E) (E) (E)

(E) (E) (E) (E) (E) (E) (E) (E) (E) (E) (E) (?K)

(?K) (E) (E) (?K) (E) (E) (E) (E) (E) (E) (A2)

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

(B2) (A1) (E) (?K) (?K) (E) (E) (?K) (?K) (E)

(E) (?K) (?K) (E) (E) (?K) (?K) (E) (E) (?K) (?K)

(E) (?K) (E) (?K) (E) (E) (?K) (?K) (E) (?K) (E)

(?K) (E) (E) (E) (E) (E) (E) (E) (E) (E) (?K)

(E) (E) (?K) (B1) (E) (E) (?K) (E) (E) (E) (E)

(E) (E) (E) (E)

Unable to determine electronic state: an orbital has unidentified symmetry.

Alpha occ. eigenvalues -- -19.14917 -19.14917 -19.14917 -19.14916 -19.14548

Alpha occ. eigenvalues -- -19.14548 -19.14548 -19.14547 -14.30404 -14.30404

Alpha occ. eigenvalues -- -14.29899 -14.29898 -14.29477 -14.29477 -14.29477

Alpha occ. eigenvalues -- -14.29476 -10.25041 -10.25040 -10.25039 -10.25039

Alpha occ. eigenvalues -- -10.24309 -10.24309 -10.24307 -10.24307 -10.23972

Alpha occ. eigenvalues -- -10.23971 -10.23970 -10.23970 -10.23641 -10.23641

Alpha occ. eigenvalues -- -10.23639 -10.23639 -10.21054 -10.21054 -10.21054

Alpha occ. eigenvalues -- -10.21054 -10.20900 -10.20900 -10.20899 -10.20899

Alpha occ. eigenvalues -- -10.18426 -10.18426 -10.18381 -10.18381 -10.18184

Alpha occ. eigenvalues -- -10.18184 -10.18135 -10.18135 -10.17467 -10.17467

Alpha occ. eigenvalues -- -10.17422 -10.17422 -10.17310 -10.17310 -10.17262

Alpha occ. eigenvalues -- -10.17262 -1.06777 -1.06777 -1.06676 -1.06676

Alpha occ. eigenvalues -- -1.06401 -1.06401 -1.06305 -1.06305 -0.99439

Alpha occ. eigenvalues -- -0.98238 -0.97908 -0.95565 -0.92864 -0.89040

Alpha occ. eigenvalues -- -0.88925 -0.86149 -0.85251 -0.85046 -0.84655

Alpha occ. eigenvalues -- -0.84442 -0.77491 -0.76716 -0.76430 -0.76385

Alpha occ. eigenvalues -- -0.76208 -0.76184 -0.75687 -0.75680 -0.72596

Alpha occ. eigenvalues -- -0.71337 -0.71262 -0.70961 -0.70955 -0.69393

Alpha occ. eigenvalues -- -0.69272 -0.68165 -0.68120 -0.67777 -0.67727

Alpha occ. eigenvalues -- -0.63401 -0.63222 -0.61684 -0.61488 -0.61322

Alpha occ. eigenvalues -- -0.59829 -0.59606 -0.59590 -0.59554 -0.58974

Alpha occ. eigenvalues -- -0.57070 -0.56156 -0.55546 -0.55516 -0.55246

Alpha occ. eigenvalues -- -0.54915 -0.54822 -0.54666 -0.53755 -0.52926

Alpha occ. eigenvalues -- -0.52865 -0.51833 -0.51705 -0.51402 -0.51312

Alpha occ. eigenvalues -- -0.50856 -0.50707 -0.50217 -0.50128 -0.49306

Alpha occ. eigenvalues -- -0.48869 -0.47953 -0.47609 -0.47221 -0.47047

Alpha occ. eigenvalues -- -0.46785 -0.46755 -0.46346 -0.46304 -0.46296

Alpha occ. eigenvalues -- -0.46085 -0.46081 -0.45028 -0.44959 -0.44776

Alpha occ. eigenvalues -- -0.44494 -0.43775 -0.43752 -0.43589 -0.43569

Alpha occ. eigenvalues -- -0.43519 -0.43261 -0.43061 -0.41555 -0.41196

Alpha occ. eigenvalues -- -0.41077 -0.40635 -0.40502 -0.40332 -0.39556

Alpha occ. eigenvalues -- -0.39330 -0.39246 -0.38355 -0.38243 -0.38201

Alpha occ. eigenvalues -- -0.38191 -0.37909 -0.37878 -0.37754 -0.37713

Alpha occ. eigenvalues -- -0.37642 -0.36311 -0.35410 -0.35191 -0.35171

Alpha occ. eigenvalues -- -0.34480 -0.34218 -0.34014 -0.33765 -0.33323

Alpha occ. eigenvalues -- -0.33125 -0.32993 -0.32869 -0.32060 -0.31955

Alpha occ. eigenvalues -- -0.31924 -0.31382 -0.31381 -0.29627 -0.29466

Alpha occ. eigenvalues -- -0.29298 -0.29175 -0.28142 -0.25876 -0.25700

Alpha occ. eigenvalues -- -0.25585 -0.25571 -0.25245 -0.24682 -0.24634

Alpha occ. eigenvalues -- -0.24454 -0.23994 -0.23306 -0.21323 -0.21146

Alpha occ. eigenvalues -- -0.21115 -0.17954 -0.13025

Alpha virt. eigenvalues -- -0.10063 -0.05113 -0.01790 -0.00765 -0.00485

Alpha virt. eigenvalues -- -0.00381 0.01592 0.02377 0.02492 0.04073

Alpha virt. eigenvalues -- 0.04945 0.04965 0.05029 0.05290 0.05648

Alpha virt. eigenvalues -- 0.05800 0.06006 0.06093 0.06121 0.06370

Alpha virt. eigenvalues -- 0.06800 0.06860 0.07876 0.07932 0.09172

Alpha virt. eigenvalues -- 0.09177 0.09731 0.10917 0.10949 0.11030

Alpha virt. eigenvalues -- 0.11316 0.11320 0.11343 0.11428 0.11510

Alpha virt. eigenvalues -- 0.11654 0.11765 0.11964 0.12582 0.12603

Alpha virt. eigenvalues -- 0.12720 0.12850 0.12879 0.12968 0.13040

Alpha virt. eigenvalues -- 0.13159 0.13190 0.13243 0.13253 0.13283

Alpha virt. eigenvalues -- 0.16776 0.16780 0.16945 0.16946 0.17711

Alpha virt. eigenvalues -- 0.17925 0.18272 0.18396 0.18568 0.19079

Alpha virt. eigenvalues -- 0.19212 0.19269 0.19703 0.20595 0.20838

Alpha virt. eigenvalues -- 0.21041 0.21116 0.21431 0.21584 0.21628

Alpha virt. eigenvalues -- 0.22222 0.23073 0.23740 0.23954 0.24580

Alpha virt. eigenvalues -- 0.24622 0.25024 0.25133 0.25320 0.25725

Alpha virt. eigenvalues -- 0.26004 0.26461 0.26634 0.28415 0.28673

Alpha virt. eigenvalues -- 0.29027 0.29595 0.29855 0.30086 0.30238

Alpha virt. eigenvalues -- 0.30824 0.30880 0.31072 0.31984 0.32030

Alpha virt. eigenvalues -- 0.32553 0.32697 0.32758 0.32856 0.33242

Alpha virt. eigenvalues -- 0.33272 0.33323 0.33324 0.33638 0.34364

Alpha virt. eigenvalues -- 0.34536 0.34716 0.35040 0.35512 0.35517

Alpha virt. eigenvalues -- 0.35853 0.35950 0.36800 0.36809 0.37114

Alpha virt. eigenvalues -- 0.37307 0.37925 0.38045 0.38110 0.38158

Alpha virt. eigenvalues -- 0.38205 0.38478 0.38686 0.39035 0.39277

Alpha virt. eigenvalues -- 0.39383 0.39423 0.39762 0.39790 0.39806

Alpha virt. eigenvalues -- 0.39837 0.40568 0.40728 0.40889 0.41293

Alpha virt. eigenvalues -- 0.41761 0.41763 0.41846 0.41977 0.42808

Alpha virt. eigenvalues -- 0.43250 0.43264 0.43293 0.43584 0.43833

Alpha virt. eigenvalues -- 0.44127 0.44174 0.44266 0.44278 0.44569

Alpha virt. eigenvalues -- 0.45210 0.45271 0.45645 0.46043 0.46126

Alpha virt. eigenvalues -- 0.46174 0.46690 0.48025 0.48312 0.48443

Alpha virt. eigenvalues -- 0.48546 0.48791 0.49003 0.49203 0.49208

Alpha virt. eigenvalues -- 0.49466 0.49508 0.49865 0.49952 0.50016

Alpha virt. eigenvalues -- 0.50219 0.50478 0.50520 0.50616 0.51224

Alpha virt. eigenvalues -- 0.51653 0.51917 0.51948 0.51949 0.52488

Alpha virt. eigenvalues -- 0.52546 0.52945 0.52970 0.53378 0.54155

Alpha virt. eigenvalues -- 0.54331 0.54707 0.54874 0.55404 0.55441

Alpha virt. eigenvalues -- 0.55955 0.56839 0.57208 0.57268 0.57387

Alpha virt. eigenvalues -- 0.57748 0.58051 0.58077 0.58359 0.58371

Alpha virt. eigenvalues -- 0.58551 0.58841 0.59006 0.59256 0.59805

Alpha virt. eigenvalues -- 0.59885 0.60265 0.61031 0.61334 0.61475

Alpha virt. eigenvalues -- 0.61505 0.62019 0.62532 0.62711 0.62887

Alpha virt. eigenvalues -- 0.63032 0.63175 0.63323 0.63337 0.63375

Alpha virt. eigenvalues -- 0.63728 0.63770 0.64170 0.64201 0.64467

Alpha virt. eigenvalues -- 0.64674 0.64782 0.64828 0.64867 0.64910

Alpha virt. eigenvalues -- 0.65293 0.65404 0.65456 0.65767 0.67269

Alpha virt. eigenvalues -- 0.67349 0.67530 0.67815 0.68900 0.69111

Alpha virt. eigenvalues -- 0.69154 0.69604 0.69676 0.70351 0.70497

Alpha virt. eigenvalues -- 0.72036 0.72126 0.72258 0.72453 0.72470

Alpha virt. eigenvalues -- 0.73001 0.73113 0.73583 0.74765 0.74772

Alpha virt. eigenvalues -- 0.74873 0.75325 0.76129 0.76137 0.76327

Alpha virt. eigenvalues -- 0.76592 0.78104 0.78525 0.78541 0.78573

Alpha virt. eigenvalues -- 0.78864 0.79644 0.79830 0.80856 0.80914

Alpha virt. eigenvalues -- 0.80973 0.81256 0.81341 0.81352 0.81476

Alpha virt. eigenvalues -- 0.81781 0.81835 0.82408 0.83066 0.83171

Alpha virt. eigenvalues -- 0.83289 0.83991 0.85260 0.85337 0.85453

Alpha virt. eigenvalues -- 0.85518 0.86448 0.86497 0.87210 0.87293

Alpha virt. eigenvalues -- 0.87395 0.88202 0.88385 0.88389 0.90343

Alpha virt. eigenvalues -- 0.90467 0.90521 0.91692 0.92410 0.92591

Alpha virt. eigenvalues -- 0.92762 0.93152 0.93406 0.93787 0.93834

Alpha virt. eigenvalues -- 0.94785 0.94791 0.95041 0.95440 0.96158

Alpha virt. eigenvalues -- 0.96643 0.97158 0.97361 0.97401 0.98065

Alpha virt. eigenvalues -- 0.98258 0.98570 0.98686 0.99072 0.99550

Alpha virt. eigenvalues -- 0.99845 1.00172 1.01791 1.01948 1.02240

Alpha virt. eigenvalues -- 1.02543 1.04044 1.04617 1.04731 1.06507

Alpha virt. eigenvalues -- 1.06690 1.07649 1.07988 1.08188 1.08191

Alpha virt. eigenvalues -- 1.08397 1.08455 1.08617 1.10724 1.10823

Alpha virt. eigenvalues -- 1.10881 1.11151 1.11257 1.11915 1.11942

Alpha virt. eigenvalues -- 1.12030 1.13246 1.13461 1.13799 1.13825

Alpha virt. eigenvalues -- 1.14186 1.14221 1.15425 1.15666 1.16707

Alpha virt. eigenvalues -- 1.16987 1.18201 1.18312 1.18392 1.18997

Alpha virt. eigenvalues -- 1.19021 1.19329 1.19599 1.19801 1.19843

Alpha virt. eigenvalues -- 1.21712 1.22164 1.23170 1.23174 1.23197

Alpha virt. eigenvalues -- 1.23644 1.23812 1.24150 1.24307 1.25664

Alpha virt. eigenvalues -- 1.25758 1.25865 1.26582 1.26619 1.26730

Alpha virt. eigenvalues -- 1.27391 1.27781 1.28957 1.30004 1.31020

Alpha virt. eigenvalues -- 1.31198 1.31385 1.31575 1.33424 1.33436

Alpha virt. eigenvalues -- 1.33696 1.33699 1.33710 1.34899 1.34986

Alpha virt. eigenvalues -- 1.35174 1.35440 1.35970 1.36071 1.37867

Alpha virt. eigenvalues -- 1.38342 1.38770 1.38773 1.39871 1.41142

Alpha virt. eigenvalues -- 1.41606 1.44213 1.44279 1.44913 1.45017

Alpha virt. eigenvalues -- 1.46079 1.47232 1.47320 1.47626 1.47996

Alpha virt. eigenvalues -- 1.48137 1.48442 1.50636 1.50680 1.51017

Alpha virt. eigenvalues -- 1.51027 1.51425 1.51602 1.52034 1.52068

Alpha virt. eigenvalues -- 1.52111 1.52138 1.52286 1.52374 1.52464

Alpha virt. eigenvalues -- 1.52512 1.52638 1.52741 1.52835 1.52921

Alpha virt. eigenvalues -- 1.53026 1.53566 1.53864 1.54310 1.55132

Alpha virt. eigenvalues -- 1.55410 1.55418 1.55830 1.56587 1.56727

Alpha virt. eigenvalues -- 1.56986 1.57537 1.57764 1.58189 1.58922

Alpha virt. eigenvalues -- 1.59045 1.59491 1.59532 1.59720 1.60842

Alpha virt. eigenvalues -- 1.61322 1.61507 1.61659 1.61776 1.63973

Alpha virt. eigenvalues -- 1.64080 1.64792 1.64894 1.64959 1.66508

Alpha virt. eigenvalues -- 1.66556 1.66696 1.67429 1.68260 1.68660

Alpha virt. eigenvalues -- 1.68671 1.69020 1.69299 1.70327 1.71054

Alpha virt. eigenvalues -- 1.71617 1.71708 1.72208 1.72949 1.73165

Alpha virt. eigenvalues -- 1.73374 1.74282 1.74967 1.75035 1.75195

Alpha virt. eigenvalues -- 1.76717 1.77097 1.77243 1.78525 1.78891

Alpha virt. eigenvalues -- 1.79133 1.79566 1.79725 1.79822 1.80023

Alpha virt. eigenvalues -- 1.80030 1.80696 1.80779 1.81551 1.81626

Alpha virt. eigenvalues -- 1.81766 1.83517 1.83756 1.83863 1.85476

Alpha virt. eigenvalues -- 1.85537 1.87516 1.87694 1.88082 1.88494

Alpha virt. eigenvalues -- 1.88692 1.88840 1.88950 1.89693 1.89774

Alpha virt. eigenvalues -- 1.90284 1.90386 1.90510 1.91160 1.91574

Alpha virt. eigenvalues -- 1.91731 1.94651 1.95754 1.96161 1.96480

Alpha virt. eigenvalues -- 1.96585 1.97720 1.97825 1.97988 1.98112

Alpha virt. eigenvalues -- 1.98709 1.99172 1.99584 2.00741 2.00748

Alpha virt. eigenvalues -- 2.01107 2.02419 2.02940 2.05650 2.07824

Alpha virt. eigenvalues -- 2.08194 2.08533 2.08578 2.09161 2.10387

Alpha virt. eigenvalues -- 2.10622 2.11051 2.13422 2.14141 2.14315

Alpha virt. eigenvalues -- 2.15269 2.15484 2.16008 2.17008 2.19653

Alpha virt. eigenvalues -- 2.20366 2.20779 2.22376 2.22586 2.24212

Alpha virt. eigenvalues -- 2.24593 2.25075 2.25189 2.25462 2.25599

Alpha virt. eigenvalues -- 2.26213 2.26250 2.27644 2.27733 2.27831

Alpha virt. eigenvalues -- 2.28430 2.29568 2.29682 2.30702 2.31578

Alpha virt. eigenvalues -- 2.32483 2.33372 2.33462 2.33870 2.33879

Alpha virt. eigenvalues -- 2.34015 2.34050 2.34087 2.34236 2.34296

Alpha virt. eigenvalues -- 2.34424 2.34563 2.34671 2.35053 2.35784

Alpha virt. eigenvalues -- 2.35939 2.36583 2.39376 2.39644 2.39877

Alpha virt. eigenvalues -- 2.39990 2.40133 2.40314 2.42292 2.42601

Alpha virt. eigenvalues -- 2.42689 2.42700 2.43103 2.43335 2.43525

Alpha virt. eigenvalues -- 2.43545 2.46927 2.48050 2.48399 2.49171

Alpha virt. eigenvalues -- 2.49821 2.50183 2.50394 2.50404 2.50656

Alpha virt. eigenvalues -- 2.51061 2.51528 2.51729 2.53749 2.54240

Alpha virt. eigenvalues -- 2.56607 2.56965 2.57514 2.58385 2.58511

Alpha virt. eigenvalues -- 2.60419 2.61911 2.62239 2.64085 2.64288

Alpha virt. eigenvalues -- 2.64458 2.64878 2.66430 2.66557 2.66981

Alpha virt. eigenvalues -- 2.67106 2.67489 2.67773 2.68091 2.71848

Alpha virt. eigenvalues -- 2.72254 2.73031 2.73108 2.74255 2.74636

Alpha virt. eigenvalues -- 2.75039 2.75041 2.77701 2.77869 2.78590

Alpha virt. eigenvalues -- 2.78953 2.79455 2.79783 2.79907 2.80836

Alpha virt. eigenvalues -- 2.81099 2.81104 2.81157 2.82460 2.82578

Alpha virt. eigenvalues -- 2.82815 2.83644 2.84403 2.84970 2.86009

Alpha virt. eigenvalues -- 2.86054 2.86140 2.86246 2.86484 2.86590

Alpha virt. eigenvalues -- 2.87534 2.87544 2.87789 2.88823 2.90780

Alpha virt. eigenvalues -- 2.91036 2.93478 2.93645 2.94197 2.95014

Alpha virt. eigenvalues -- 2.95153 2.95333 2.95422 2.96422 2.98039

Alpha virt. eigenvalues -- 2.98377 2.98659 2.99140 2.99557 2.99745

Alpha virt. eigenvalues -- 3.00138 3.00529 3.01826 3.02065 3.02815

Alpha virt. eigenvalues -- 3.04684 3.05548 3.05655 3.06154 3.07204

Alpha virt. eigenvalues -- 3.07222 3.08563 3.10918 3.13117 3.13141

Alpha virt. eigenvalues -- 3.13370 3.13384 3.14230 3.14277 3.14518

Alpha virt. eigenvalues -- 3.14882 3.15189 3.15623 3.15636 3.15909

Alpha virt. eigenvalues -- 3.16682 3.16840 3.17263 3.17373 3.18591

Alpha virt. eigenvalues -- 3.18696 3.19353 3.19484 3.19686 3.19858

Alpha virt. eigenvalues -- 3.20095 3.20260 3.20388 3.20616 3.20819

Alpha virt. eigenvalues -- 3.21036 3.21346 3.21657 3.21775 3.22233

Alpha virt. eigenvalues -- 3.24319 3.25498 3.26062 3.26537 3.27832

Alpha virt. eigenvalues -- 3.27868 3.28375 3.28484 3.28527 3.29472

Alpha virt. eigenvalues -- 3.29642 3.30507 3.30763 3.32250 3.32318

Alpha virt. eigenvalues -- 3.34991 3.36054 3.36199 3.36837 3.37221

Alpha virt. eigenvalues -- 3.39820 3.39974 3.40408 3.40472 3.40684

Alpha virt. eigenvalues -- 3.40820 3.41229 3.42367 3.45134 3.46422

Alpha virt. eigenvalues -- 3.46885 3.48347 3.55590 3.59636 3.60105

Alpha virt. eigenvalues -- 3.60198 3.61021 3.62030 3.62383 3.67165

Alpha virt. eigenvalues -- 3.67184 3.67746 3.68116 3.75201 3.76496

Alpha virt. eigenvalues -- 3.77152 3.77318 3.77660 3.79085 3.79291

Alpha virt. eigenvalues -- 3.80696 3.82405 3.83466 3.83570 3.83606

Alpha virt. eigenvalues -- 3.87515 3.90273 3.90358 3.90393 3.92706

Alpha virt. eigenvalues -- 3.95655 3.96094 3.96341 3.97029 3.97939

Alpha virt. eigenvalues -- 3.98292 3.98305 3.98634 4.00779 4.00947

Alpha virt. eigenvalues -- 4.01313 4.01341 4.11201 4.14201 4.14578

Alpha virt. eigenvalues -- 4.16720 4.16935 4.17346 4.18360 4.20954

Alpha virt. eigenvalues -- 4.22013 4.23409 4.23838 4.25969 4.35236

Alpha virt. eigenvalues -- 4.41397 4.41421 4.42307 4.46982 4.51885

Alpha virt. eigenvalues -- 4.60743 4.60776 4.81167 4.81235 4.81889

Alpha virt. eigenvalues -- 4.81962 4.87672 4.87893 4.88157 4.88537

Alpha virt. eigenvalues -- 4.88992 4.89224 4.89489 4.89585 5.12068

Alpha virt. eigenvalues -- 5.12613 5.12799 5.16850 5.21070 5.25261

Alpha virt. eigenvalues -- 5.25447 5.25775 5.25988 5.28970 5.29078

Alpha virt. eigenvalues -- 5.29290 5.29737 5.37722 5.37759 5.55236

Alpha virt. eigenvalues -- 5.66406 5.67772 5.68138 5.68316 5.74593

Alpha virt. eigenvalues -- 5.74799 5.75181 5.75709 7.78361 7.78378

Alpha virt. eigenvalues -- 7.88916 7.95210 8.20084 11.15196 23.33864

Alpha virt. eigenvalues -- 23.36729 23.37526 23.39034 23.44092 23.44375

Alpha virt. eigenvalues -- 23.44486 23.44959 23.45186 23.45485 23.45581

Alpha virt. eigenvalues -- 23.45681 23.76631 23.77943 23.78851 23.79825

Alpha virt. eigenvalues -- 23.81267 23.81442 23.82169 23.82278 23.87714

Alpha virt. eigenvalues -- 23.87930 23.88031 23.88087 23.88908 23.89707

Alpha virt. eigenvalues -- 23.90113 23.90205 24.00719 24.00761 24.01488

Alpha virt. eigenvalues -- 24.01536 24.02184 24.02205 24.03117 24.03385

Alpha virt. eigenvalues -- 24.09527 24.09574 24.10343 24.10406 35.58308

Alpha virt. eigenvalues -- 35.61413 35.61812 35.62553 35.70365 35.71546

Alpha virt. eigenvalues -- 35.71604 35.71760 49.91481 49.91796 49.92059

Alpha virt. eigenvalues -- 49.92253 49.92349 49.92652 49.92915 49.93049

Beta occ. eigenvalues -- -19.14883 -19.14883 -19.14883 -19.14883 -19.14504

Beta occ. eigenvalues -- -19.14504 -19.14504 -19.14504 -14.30542 -14.30542

Beta occ. eigenvalues -- -14.29771 -14.29771 -14.29441 -14.29441 -14.29441

Beta occ. eigenvalues -- -14.29440 -10.24865 -10.24865 -10.24864 -10.24864

Beta occ. eigenvalues -- -10.24260 -10.24260 -10.24258 -10.24258 -10.23622

Beta occ. eigenvalues -- -10.23622 -10.23622 -10.23621 -10.23577 -10.23577

Beta occ. eigenvalues -- -10.23576 -10.23576 -10.21055 -10.21055 -10.21055

Beta occ. eigenvalues -- -10.21055 -10.20901 -10.20901 -10.20901 -10.20901

Beta occ. eigenvalues -- -10.18453 -10.18453 -10.18408 -10.18408 -10.18145

Beta occ. eigenvalues -- -10.18145 -10.18096 -10.18096 -10.17458 -10.17458

Beta occ. eigenvalues -- -10.17413 -10.17413 -10.17215 -10.17215 -10.17166

Beta occ. eigenvalues -- -10.17166 -1.06706 -1.06706 -1.06607 -1.06606

Beta occ. eigenvalues -- -1.06305 -1.06305 -1.06211 -1.06211 -0.99096

Beta occ. eigenvalues -- -0.97892 -0.97576 -0.95273 -0.92491 -0.88743

Beta occ. eigenvalues -- -0.88683 -0.86025 -0.85112 -0.84879 -0.84489

Beta occ. eigenvalues -- -0.84300 -0.77256 -0.76623 -0.76328 -0.76251

Beta occ. eigenvalues -- -0.76060 -0.76034 -0.75528 -0.75523 -0.72079

Beta occ. eigenvalues -- -0.71310 -0.71235 -0.70935 -0.70929 -0.69108

Beta occ. eigenvalues -- -0.68687 -0.68075 -0.68005 -0.67597 -0.67489

Beta occ. eigenvalues -- -0.63101 -0.62996 -0.61563 -0.61350 -0.61196

Beta occ. eigenvalues -- -0.59711 -0.59487 -0.59473 -0.59393 -0.58764

Beta occ. eigenvalues -- -0.57035 -0.56123 -0.55530 -0.55494 -0.55163

Beta occ. eigenvalues -- -0.54815 -0.54780 -0.54571 -0.53691 -0.52720

Beta occ. eigenvalues -- -0.52692 -0.51777 -0.51667 -0.51332 -0.51252

Beta occ. eigenvalues -- -0.50804 -0.50636 -0.50122 -0.50047 -0.49129

Beta occ. eigenvalues -- -0.48718 -0.47827 -0.47396 -0.46952 -0.46870

Beta occ. eigenvalues -- -0.46526 -0.46524 -0.46268 -0.46200 -0.46193

Beta occ. eigenvalues -- -0.45940 -0.45937 -0.44775 -0.44679 -0.44421

Beta occ. eigenvalues -- -0.44325 -0.43741 -0.43519 -0.43492 -0.43210

Beta occ. eigenvalues -- -0.43035 -0.43015 -0.42628 -0.41160 -0.41045

Beta occ. eigenvalues -- -0.40926 -0.40571 -0.40444 -0.40295 -0.39524

Beta occ. eigenvalues -- -0.39287 -0.39176 -0.38277 -0.38089 -0.38084

Beta occ. eigenvalues -- -0.37882 -0.37789 -0.37525 -0.37464 -0.37179

Beta occ. eigenvalues -- -0.36863 -0.35690 -0.35170 -0.34920 -0.34796

Beta occ. eigenvalues -- -0.34169 -0.34046 -0.33974 -0.33716 -0.33278

Beta occ. eigenvalues -- -0.33075 -0.32976 -0.32746 -0.31987 -0.31937

Beta occ. eigenvalues -- -0.31804 -0.30509 -0.30296 -0.29375 -0.28994

Beta occ. eigenvalues -- -0.28863 -0.28648 -0.27964 -0.25768 -0.25480

Beta occ. eigenvalues -- -0.25451 -0.25410 -0.24885 -0.24504 -0.24465

Beta occ. eigenvalues -- -0.23876 -0.23578 -0.22433 -0.20856 -0.20397

Beta occ. eigenvalues -- -0.20198

Beta virt. eigenvalues -- -0.13888 -0.09133 -0.08322 -0.03940 -0.00868

Beta virt. eigenvalues -- -0.00112 0.00197 0.00248 0.02472 0.03103

Beta virt. eigenvalues -- 0.03596 0.04165 0.04962 0.04990 0.05042

Beta virt. eigenvalues -- 0.05297 0.05967 0.06142 0.06194 0.06389

Beta virt. eigenvalues -- 0.06815 0.06858 0.06884 0.07071 0.07895

Beta virt. eigenvalues -- 0.07958 0.09194 0.09196 0.09757 0.10976

Beta virt. eigenvalues -- 0.10977 0.11160 0.11353 0.11497 0.11547

Beta virt. eigenvalues -- 0.11672 0.11782 0.12097 0.12234 0.12303

Beta virt. eigenvalues -- 0.12606 0.12618 0.12756 0.12900 0.12919

Beta virt. eigenvalues -- 0.13194 0.13214 0.13232 0.13313 0.13360

Beta virt. eigenvalues -- 0.13481 0.13743 0.16806 0.16811 0.17011

Beta virt. eigenvalues -- 0.17013 0.17979 0.18273 0.18615 0.19082

Beta virt. eigenvalues -- 0.19086 0.19122 0.19348 0.19603 0.19826

Beta virt. eigenvalues -- 0.20705 0.20935 0.21177 0.21281 0.21713

Beta virt. eigenvalues -- 0.21770 0.21842 0.22398 0.23176 0.24102

Beta virt. eigenvalues -- 0.24248 0.24856 0.24881 0.25318 0.25328

Beta virt. eigenvalues -- 0.25507 0.25859 0.26157 0.26640 0.26834

Beta virt. eigenvalues -- 0.28640 0.28895 0.29291 0.29689 0.30077

Beta virt. eigenvalues -- 0.30366 0.30377 0.30932 0.31039 0.31218

Beta virt. eigenvalues -- 0.32162 0.32206 0.32600 0.32791 0.32826

Beta virt. eigenvalues -- 0.32949 0.33295 0.33343 0.33347 0.33352

Beta virt. eigenvalues -- 0.33710 0.34572 0.34738 0.34805 0.35182

Beta virt. eigenvalues -- 0.35614 0.35629 0.35991 0.36075 0.36943

Beta virt. eigenvalues -- 0.37014 0.37375 0.37693 0.38007 0.38162

Beta virt. eigenvalues -- 0.38255 0.38305 0.38614 0.38655 0.38765

Beta virt. eigenvalues -- 0.39138 0.39458 0.39479 0.39561 0.39873

Beta virt. eigenvalues -- 0.39891 0.39896 0.39972 0.40949 0.41092

Beta virt. eigenvalues -- 0.41168 0.41439 0.41938 0.42046 0.42092

Beta virt. eigenvalues -- 0.42427 0.42947 0.43355 0.43402 0.43489

Beta virt. eigenvalues -- 0.43842 0.44227 0.44329 0.44390 0.44463

Beta virt. eigenvalues -- 0.44479 0.44650 0.45502 0.45619 0.45719

Beta virt. eigenvalues -- 0.46122 0.46211 0.46452 0.46776 0.48187

Beta virt. eigenvalues -- 0.48426 0.48652 0.48735 0.48856 0.49088

Beta virt. eigenvalues -- 0.49388 0.49526 0.49580 0.49583 0.49935

Beta virt. eigenvalues -- 0.50039 0.50104 0.50511 0.50598 0.50616

Beta virt. eigenvalues -- 0.50806 0.51302 0.51979 0.51985 0.52047

Beta virt. eigenvalues -- 0.52118 0.52690 0.52915 0.53028 0.53320

Beta virt. eigenvalues -- 0.53526 0.54353 0.54514 0.54744 0.54932

Beta virt. eigenvalues -- 0.55555 0.55598 0.56037 0.56909 0.57255

Beta virt. eigenvalues -- 0.57366 0.57502 0.57869 0.58185 0.58205

Beta virt. eigenvalues -- 0.58404 0.58466 0.58633 0.58904 0.59076

Beta virt. eigenvalues -- 0.59403 0.59864 0.59960 0.60311 0.61113

Beta virt. eigenvalues -- 0.61420 0.61568 0.61637 0.62193 0.62673

Beta virt. eigenvalues -- 0.62816 0.62949 0.63131 0.63291 0.63449

Beta virt. eigenvalues -- 0.63466 0.63478 0.63962 0.64063 0.64325

Beta virt. eigenvalues -- 0.64401 0.64572 0.64775 0.64917 0.64919

Beta virt. eigenvalues -- 0.64953 0.64985 0.65498 0.65517 0.65719

Beta virt. eigenvalues -- 0.65871 0.67444 0.67577 0.67708 0.67885

Beta virt. eigenvalues -- 0.68939 0.69229 0.69241 0.69723 0.69777

Beta virt. eigenvalues -- 0.70403 0.70574 0.72149 0.72226 0.72367

Beta virt. eigenvalues -- 0.72534 0.72589 0.72999 0.73353 0.73721

Beta virt. eigenvalues -- 0.74861 0.74873 0.75006 0.75480 0.76209

Beta virt. eigenvalues -- 0.76332 0.76437 0.76681 0.78238 0.78707

Beta virt. eigenvalues -- 0.78781 0.78806 0.78996 0.79854 0.79909

Beta virt. eigenvalues -- 0.80951 0.81045 0.81102 0.81290 0.81412

Beta virt. eigenvalues -- 0.81430 0.81620 0.81879 0.82034 0.82476

Beta virt. eigenvalues -- 0.83165 0.83305 0.83447 0.84170 0.85302

Beta virt. eigenvalues -- 0.85383 0.85523 0.85622 0.86518 0.86686

Beta virt. eigenvalues -- 0.87298 0.87362 0.87500 0.88272 0.88459

Beta virt. eigenvalues -- 0.88522 0.90412 0.90608 0.90672 0.91761

Beta virt. eigenvalues -- 0.92547 0.92754 0.92928 0.93348 0.93576

Beta virt. eigenvalues -- 0.93919 0.93958 0.94958 0.94960 0.95191

Beta virt. eigenvalues -- 0.95615 0.96254 0.96898 0.97307 0.97501

Beta virt. eigenvalues -- 0.97501 0.98220 0.98392 0.98775 0.98794

Beta virt. eigenvalues -- 0.99247 0.99666 1.00028 1.00328 1.01845

Beta virt. eigenvalues -- 1.02055 1.02302 1.02588 1.04100 1.04726

Beta virt. eigenvalues -- 1.04841 1.06684 1.06901 1.07825 1.08239

Beta virt. eigenvalues -- 1.08297 1.08341 1.08569 1.08693 1.08707

Beta virt. eigenvalues -- 1.10835 1.11068 1.11120 1.11465 1.11621

Beta virt. eigenvalues -- 1.12035 1.12324 1.12441 1.13419 1.13705

Beta virt. eigenvalues -- 1.13996 1.14146 1.14467 1.14539 1.15622

Beta virt. eigenvalues -- 1.16052 1.16993 1.17342 1.18407 1.18503

Beta virt. eigenvalues -- 1.18834 1.19165 1.19235 1.19576 1.19913

Beta virt. eigenvalues -- 1.20020 1.20038 1.21818 1.22378 1.23243

Beta virt. eigenvalues -- 1.23290 1.23395 1.23770 1.23898 1.24343

Beta virt. eigenvalues -- 1.24543 1.25722 1.25898 1.25974 1.26660

Beta virt. eigenvalues -- 1.26727 1.26818 1.27528 1.27913 1.29340

Beta virt. eigenvalues -- 1.30051 1.31179 1.31371 1.31493 1.31780

Beta virt. eigenvalues -- 1.33477 1.33492 1.33798 1.33808 1.33835

Beta virt. eigenvalues -- 1.35081 1.35106 1.35373 1.35557 1.36181

Beta virt. eigenvalues -- 1.36323 1.38156 1.38540 1.39194 1.39280

Beta virt. eigenvalues -- 1.40451 1.41229 1.42146 1.44324 1.44393

Beta virt. eigenvalues -- 1.45049 1.45133 1.46150 1.47321 1.47392

Beta virt. eigenvalues -- 1.47670 1.48065 1.48219 1.48537 1.50949

Beta virt. eigenvalues -- 1.50978 1.51481 1.51518 1.51534 1.51769

Beta virt. eigenvalues -- 1.52082 1.52143 1.52178 1.52200 1.52303

Beta virt. eigenvalues -- 1.52484 1.52552 1.52567 1.52752 1.52783

Beta virt. eigenvalues -- 1.52927 1.53005 1.53208 1.53662 1.53900

Beta virt. eigenvalues -- 1.54357 1.55244 1.55540 1.55548 1.56039

Beta virt. eigenvalues -- 1.56765 1.56863 1.57156 1.57674 1.57896

Beta virt. eigenvalues -- 1.58258 1.59050 1.59335 1.59581 1.59829

Beta virt. eigenvalues -- 1.59901 1.61342 1.61344 1.61531 1.61696

Beta virt. eigenvalues -- 1.61803 1.64329 1.64579 1.64947 1.65019

Beta virt. eigenvalues -- 1.65289 1.66540 1.66598 1.66712 1.67515

Beta virt. eigenvalues -- 1.68281 1.68721 1.68726 1.69078 1.69466

Beta virt. eigenvalues -- 1.70401 1.71169 1.71708 1.71805 1.72306

Beta virt. eigenvalues -- 1.73007 1.73268 1.73439 1.74408 1.75118

Beta virt. eigenvalues -- 1.75124 1.75308 1.76811 1.77202 1.77349

Beta virt. eigenvalues -- 1.78688 1.79067 1.79413 1.79719 1.79931

Beta virt. eigenvalues -- 1.80028 1.80218 1.80335 1.80849 1.81146

Beta virt. eigenvalues -- 1.81631 1.81959 1.82178 1.83634 1.83868

Beta virt. eigenvalues -- 1.84258 1.85580 1.85653 1.87670 1.87887

Beta virt. eigenvalues -- 1.88354 1.88629 1.88873 1.89044 1.89273

Beta virt. eigenvalues -- 1.89812 1.89892 1.90572 1.90733 1.90767

Beta virt. eigenvalues -- 1.91352 1.91744 1.91923 1.94809 1.95890

Beta virt. eigenvalues -- 1.96378 1.96745 1.96805 1.97888 1.98207

Beta virt. eigenvalues -- 1.98294 1.98538 1.98970 1.99605 1.99932

Beta virt. eigenvalues -- 2.01081 2.01203 2.01748 2.02626 2.03314

Beta virt. eigenvalues -- 2.05815 2.08012 2.08474 2.08934 2.09034

Beta virt. eigenvalues -- 2.09706 2.10624 2.10771 2.11328 2.13539

Beta virt. eigenvalues -- 2.14555 2.14581 2.15396 2.15560 2.16147

Beta virt. eigenvalues -- 2.17141 2.19684 2.20421 2.20833 2.22635

Beta virt. eigenvalues -- 2.22801 2.24271 2.24763 2.25148 2.25344

Beta virt. eigenvalues -- 2.25581 2.25911 2.26283 2.26554 2.27759

Beta virt. eigenvalues -- 2.27836 2.27905 2.28507 2.29641 2.29812

Beta virt. eigenvalues -- 2.30811 2.31676 2.32491 2.33383 2.33473

Beta virt. eigenvalues -- 2.33889 2.33897 2.34038 2.34073 2.34135

Beta virt. eigenvalues -- 2.34341 2.34441 2.34470 2.34574 2.34730

Beta virt. eigenvalues -- 2.35245 2.35801 2.35965 2.36602 2.39708

Beta virt. eigenvalues -- 2.40086 2.40159 2.40359 2.40385 2.40756

Beta virt. eigenvalues -- 2.42534 2.42706 2.42716 2.42746 2.43115

Beta virt. eigenvalues -- 2.43388 2.43663 2.44051 2.47064 2.48096

Beta virt. eigenvalues -- 2.48481 2.49219 2.49976 2.50465 2.50475

Beta virt. eigenvalues -- 2.50479 2.50765 2.51285 2.51887 2.51955

Beta virt. eigenvalues -- 2.54120 2.54309 2.56881 2.56901 2.57597

Beta virt. eigenvalues -- 2.58567 2.58572 2.60465 2.62298 2.62411

Beta virt. eigenvalues -- 2.64467 2.64817 2.64947 2.65015 2.66528

Beta virt. eigenvalues -- 2.66727 2.67501 2.67539 2.67915 2.68031

Beta virt. eigenvalues -- 2.68457 2.71942 2.72484 2.73249 2.73399

Beta virt. eigenvalues -- 2.74645 2.74960 2.75329 2.75353 2.78278

Beta virt. eigenvalues -- 2.78602 2.78986 2.79625 2.80124 2.80286

Beta virt. eigenvalues -- 2.80299 2.80892 2.81171 2.81172 2.81231

Beta virt. eigenvalues -- 2.82553 2.82687 2.83274 2.84104 2.84513

Beta virt. eigenvalues -- 2.85056 2.86067 2.86156 2.86189 2.86327

Beta virt. eigenvalues -- 2.86730 2.86931 2.87673 2.87762 2.88016

Beta virt. eigenvalues -- 2.88924 2.91422 2.91452 2.93782 2.94032

Beta virt. eigenvalues -- 2.94437 2.95097 2.95255 2.95446 2.95581

Beta virt. eigenvalues -- 2.96559 2.98419 2.98743 2.98979 2.99217

Beta virt. eigenvalues -- 2.99690 2.99818 3.00588 3.00765 3.01905

Beta virt. eigenvalues -- 3.02145 3.02885 3.04899 3.05674 3.05746

Beta virt. eigenvalues -- 3.06503 3.07306 3.07306 3.08922 3.11010

Beta virt. eigenvalues -- 3.13164 3.13187 3.13433 3.13447 3.14280

Beta virt. eigenvalues -- 3.14321 3.14590 3.14969 3.15222 3.15674

Beta virt. eigenvalues -- 3.15683 3.15965 3.16725 3.16889 3.17335

Beta virt. eigenvalues -- 3.17418 3.18649 3.18804 3.19471 3.19602

Beta virt. eigenvalues -- 3.19839 3.20018 3.20196 3.20378 3.20508

Beta virt. eigenvalues -- 3.20772 3.20886 3.21146 3.21442 3.21750

Beta virt. eigenvalues -- 3.21885 3.22285 3.24447 3.25573 3.26229

Beta virt. eigenvalues -- 3.26620 3.27859 3.27893 3.28432 3.28578

Beta virt. eigenvalues -- 3.28607 3.29540 3.29719 3.30591 3.30824

Beta virt. eigenvalues -- 3.32299 3.32382 3.35046 3.36139 3.36267

Beta virt. eigenvalues -- 3.36903 3.37316 3.39857 3.40009 3.40449

Beta virt. eigenvalues -- 3.40540 3.40743 3.40866 3.41288 3.42417

Beta virt. eigenvalues -- 3.45201 3.46471 3.46976 3.48428 3.55786

Beta virt. eigenvalues -- 3.59708 3.60166 3.60322 3.61120 3.62161

Beta virt. eigenvalues -- 3.62556 3.67268 3.67301 3.67938 3.68267

Beta virt. eigenvalues -- 3.75350 3.76575 3.77215 3.77441 3.77782

Beta virt. eigenvalues -- 3.79254 3.79436 3.80879 3.82518 3.83419

Beta virt. eigenvalues -- 3.83779 3.83968 3.87618 3.90475 3.90543

Beta virt. eigenvalues -- 3.90736 3.92874 3.95742 3.96140 3.96401

Beta virt. eigenvalues -- 3.97070 3.97994 3.98341 3.98379 3.98704

Beta virt. eigenvalues -- 4.00823 4.00998 4.01380 4.01393 4.11270

Beta virt. eigenvalues -- 4.14261 4.14680 4.16790 4.17000 4.17455

Beta virt. eigenvalues -- 4.18449 4.21014 4.22124 4.23491 4.23989

Beta virt. eigenvalues -- 4.26112 4.35459 4.41646 4.41685 4.42569

Beta virt. eigenvalues -- 4.47149 4.52002 4.60786 4.60960 4.81253

Beta virt. eigenvalues -- 4.81321 4.82081 4.82155 4.87827 4.88036

Beta virt. eigenvalues -- 4.88337 4.88710 4.89142 4.89371 4.89673

Beta virt. eigenvalues -- 4.89762 5.12296 5.12821 5.13074 5.17097

Beta virt. eigenvalues -- 5.21332 5.25297 5.25484 5.25823 5.26041

Beta virt. eigenvalues -- 5.29014 5.29120 5.29347 5.29784 5.37989

Beta virt. eigenvalues -- 5.38032 5.55535 5.66449 5.67818 5.68199

Beta virt. eigenvalues -- 5.68370 5.74635 5.74837 5.75233 5.75757

Beta virt. eigenvalues -- 7.78367 7.78397 7.88916 7.95215 8.20088

Beta virt. eigenvalues -- 11.15203 23.33925 23.36767 23.37611 23.39096

Beta virt. eigenvalues -- 23.44091 23.44374 23.44485 23.44958 23.45189

Beta virt. eigenvalues -- 23.45485 23.45581 23.45680 23.76828 23.78087

Beta virt. eigenvalues -- 23.79130 23.80045 23.81316 23.81489 23.82244

Beta virt. eigenvalues -- 23.82348 23.87813 23.87999 23.88251 23.88282

Beta virt. eigenvalues -- 23.89079 23.89913 23.90471 23.90548 24.00753

Beta virt. eigenvalues -- 24.00794 24.01553 24.01601 24.02196 24.02211

Beta virt. eigenvalues -- 24.03177 24.03439 24.09559 24.09606 24.10417

Beta virt. eigenvalues -- 24.10479 35.58303 35.61294 35.61934 35.62561

Beta virt. eigenvalues -- 35.70407 35.71565 35.71658 35.71792 49.91517

Beta virt. eigenvalues -- 49.91830 49.92099 49.92294 49.92385 49.92689

Beta virt. eigenvalues -- 49.92958 49.93089

Condensed to atoms (all electrons):

Atomic-Atomic Spin Densities.

Mulliken charges and spin densities:

1 2

1 C 0.371344 0.216803

2 N -0.678643 -0.074669

3 C 0.371344 0.216803

4 C -0.097683 0.001264

5 C -0.097683 0.001264

6 N -0.363199 0.003519

7 C 0.400263 0.113284

8 N -0.707395 0.053987

9 C 0.400263 0.113284

10 C -0.091201 -0.020451

11 C -0.091201 -0.020451

12 N -0.363199 0.003519

13 C -0.091201 -0.020451

14 C -0.091201 -0.020451

15 C 0.400263 0.113284

16 N -0.707395 0.053987

17 C 0.400263 0.113284

18 N -0.363199 0.003519

19 N -0.678643 -0.074669

20 C 0.371344 0.216803

21 C -0.097683 0.001264

22 C -0.097683 0.001264

23 C 0.371344 0.216803

24 N -0.363199 0.003519

25 Zn 1.428580 -0.000778

26 C 0.208328 0.034629

27 C -0.291681 0.027412

28 C -0.291681 0.027412

29 C 0.208328 0.034629

30 C 0.202779 0.046961

31 C -0.310895 0.067838

32 C -0.310895 0.067838

33 C 0.202779 0.046961

34 C 0.208328 0.034629

35 C -0.291681 0.027412

36 C -0.291681 0.027412

37 C 0.208328 0.034629

38 C 0.202779 0.046961

39 C -0.310895 0.067838

40 C -0.310895 0.067838

41 C 0.202779 0.046961

42 H 0.262632 -0.001714

43 H 0.262632 -0.001714

44 H 0.254499 -0.004192

45 H 0.254499 -0.004192

46 H 0.262632 -0.001714

47 H 0.262632 -0.001714

48 H 0.254499 -0.004192

49 H 0.254499 -0.004192

50 O -0.317626 0.013359

51 O -0.317626 0.013359

52 O -0.315408 0.010160

53 O -0.315408 0.010160

54 O -0.317626 0.013359

55 O -0.317626 0.013359

56 O -0.315408 0.010160

57 O -0.315408 0.010160

58 C -0.497659 -0.001471

59 H 0.228091 0.001416

60 H 0.227603 0.001262

61 H 0.251091 -0.000082

62 C -0.500238 -0.001001

63 H 0.230930 0.000858

64 H 0.230580 0.000719

65 H 0.253324 -0.000038

66 C -0.500238 -0.001001

67 H 0.230580 0.000719

68 H 0.230930 0.000858

69 H 0.253324 -0.000038

70 C -0.497659 -0.001471

71 H 0.227603 0.001262

72 H 0.228091 0.001416

73 H 0.251091 -0.000082

74 C -0.500238 -0.001001

75 H 0.230580 0.000719

76 H 0.230930 0.000858

77 H 0.253324 -0.000038

78 C -0.500238 -0.001001

79 H 0.230930 0.000858

80 H 0.230580 0.000719

81 H 0.253324 -0.000038

82 C -0.497659 -0.001471

83 H 0.228091 0.001416

84 H 0.227603 0.001262

85 H 0.251091 -0.000082

86 C -0.497659 -0.001471

87 H 0.227603 0.001262

88 H 0.228091 0.001416

89 H 0.251091 -0.000082

Sum of Mulliken charges = 0.00000 2.00000

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

1 2

1 C 0.371344 0.216803

2 N -0.678643 -0.074669

3 C 0.371344 0.216803

4 C -0.097683 0.001264

5 C -0.097683 0.001264

6 N -0.363199 0.003519

7 C 0.400263 0.113284

8 N -0.707395 0.053987

9 C 0.400263 0.113284

10 C -0.091201 -0.020451

11 C -0.091201 -0.020451

12 N -0.363199 0.003519

13 C -0.091201 -0.020451

14 C -0.091201 -0.020451

15 C 0.400263 0.113284

16 N -0.707395 0.053987

17 C 0.400263 0.113284

18 N -0.363199 0.003519

19 N -0.678643 -0.074669

20 C 0.371344 0.216803

21 C -0.097683 0.001264

22 C -0.097683 0.001264

23 C 0.371344 0.216803

24 N -0.363199 0.003519

25 Zn 1.428580 -0.000778

26 C 0.208328 0.034629

27 C -0.029049 0.025698

28 C -0.029049 0.025698

29 C 0.208328 0.034629

30 C 0.202779 0.046961

31 C -0.056396 0.063646

32 C -0.056396 0.063646

33 C 0.202779 0.046961

34 C 0.208328 0.034629

35 C -0.029049 0.025698

36 C -0.029049 0.025698

37 C 0.208328 0.034629

38 C 0.202779 0.046961

39 C -0.056396 0.063646

40 C -0.056396 0.063646

41 C 0.202779 0.046961

50 O -0.317626 0.013359

51 O -0.317626 0.013359

52 O -0.315408 0.010160

53 O -0.315408 0.010160

54 O -0.317626 0.013359

55 O -0.317626 0.013359

56 O -0.315408 0.010160

57 O -0.315408 0.010160

58 C 0.209127 0.001126

62 C 0.214595 0.000538

66 C 0.214595 0.000538

70 C 0.209127 0.001126

74 C 0.214595 0.000538

78 C 0.214595 0.000538

82 C 0.209127 0.001126

86 C 0.209127 0.001126

Electronic spatial extent (au): <R\*\*2>= 44677.7569

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0000 Y= 0.0000 Z= -0.5305 Tot= 0.5305

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

XX= -169.4102 YY= -205.9145 ZZ= -334.0968

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XX= 67.0636 YY= 30.5594 ZZ= -97.6230

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XXX= 0.0000 YYY= 0.0000 ZZZ= -1.8944 XYY= 0.0000

XXY= 0.0000 XXZ= -103.0748 XZZ= 0.0000 YZZ= 0.0000

YYZ= 82.0208 XYZ= 0.0000

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

XXXX= -19212.5021 YYYY= -20873.9731 ZZZZ= -734.1147 XXXY= 0.0000

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

ZZZY= 0.0000 XXYY= -6463.6799 XXZZ= -5103.7322 YYZZ= -5153.2009

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 8.019693015297D+03 E-N=-2.231749068141D+04 KE= 2.689640846291D+03

Symmetry A1 KE= 7.470463779869D+02

Symmetry A2 KE= 6.092262444711D+02

Symmetry B1 KE= 6.675062913647D+02

Symmetry B2 KE= 6.658619324680D+02

Isotropic Fermi Contact Couplings

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

1 C(13) 0.01480 8.31969 2.96867 2.77515

2 N(14) -0.01450 -2.34267 -0.83592 -0.78143

3 C(13) 0.01480 8.31969 2.96867 2.77515

4 C(13) -0.00705 -3.96431 -1.41456 -1.32235

5 C(13) -0.00705 -3.96431 -1.41456 -1.32235

6 N(14) -0.00134 -0.21632 -0.07719 -0.07216

7 C(13) 0.00653 3.67224 1.31035 1.22493

8 N(14) 0.00500 0.80747 0.28813 0.26934

9 C(13) 0.00653 3.67224 1.31035 1.22493

10 C(13) -0.00494 -2.77621 -0.99062 -0.92604

11 C(13) -0.00494 -2.77621 -0.99062 -0.92604

12 N(14) -0.00134 -0.21632 -0.07719 -0.07216

13 C(13) -0.00494 -2.77621 -0.99062 -0.92604

14 C(13) -0.00494 -2.77621 -0.99062 -0.92604

15 C(13) 0.00653 3.67224 1.31035 1.22493

16 N(14) 0.00500 0.80747 0.28813 0.26934

17 C(13) 0.00653 3.67224 1.31035 1.22493

18 N(14) -0.00134 -0.21632 -0.07719 -0.07216

19 N(14) -0.01450 -2.34267 -0.83592 -0.78143

20 C(13) 0.01480 8.31969 2.96867 2.77515

21 C(13) -0.00705 -3.96431 -1.41456 -1.32235

22 C(13) -0.00705 -3.96431 -1.41456 -1.32235

23 C(13) 0.01480 8.31969 2.96867 2.77515

24 N(14) -0.00134 -0.21632 -0.07719 -0.07216

25 Zn(67) 0.00000 0.00000 0.00000 0.00000

26 C(13) 0.00097 0.54245 0.19356 0.18094

27 C(13) -0.00025 -0.14280 -0.05095 -0.04763

28 C(13) -0.00025 -0.14280 -0.05095 -0.04763

29 C(13) 0.00097 0.54245 0.19356 0.18094

30 C(13) -0.00071 -0.39746 -0.14182 -0.13258

31 C(13) 0.00037 0.21025 0.07502 0.07013

32 C(13) 0.00037 0.21025 0.07502 0.07013

33 C(13) -0.00071 -0.39746 -0.14182 -0.13258

34 C(13) 0.00097 0.54245 0.19356 0.18094

35 C(13) -0.00025 -0.14280 -0.05095 -0.04763

36 C(13) -0.00025 -0.14280 -0.05095 -0.04763

37 C(13) 0.00097 0.54245 0.19356 0.18094

38 C(13) -0.00071 -0.39746 -0.14182 -0.13258

39 C(13) 0.00037 0.21025 0.07502 0.07013

40 C(13) 0.00037 0.21025 0.07502 0.07013

41 C(13) -0.00071 -0.39746 -0.14182 -0.13258

42 H(1) -0.00049 -1.08453 -0.38699 -0.36176

43 H(1) -0.00049 -1.08453 -0.38699 -0.36176

44 H(1) -0.00115 -2.58037 -0.92074 -0.86072

45 H(1) -0.00115 -2.58037 -0.92074 -0.86072

46 H(1) -0.00049 -1.08453 -0.38699 -0.36176

47 H(1) -0.00049 -1.08453 -0.38699 -0.36176

48 H(1) -0.00115 -2.58037 -0.92074 -0.86072

49 H(1) -0.00115 -2.58037 -0.92074 -0.86072

50 O(17) 0.00219 -0.66406 -0.23695 -0.22151

51 O(17) 0.00219 -0.66406 -0.23695 -0.22151

52 O(17) 0.00186 -0.56278 -0.20081 -0.18772

53 O(17) 0.00186 -0.56278 -0.20081 -0.18772

54 O(17) 0.00219 -0.66406 -0.23695 -0.22151

55 O(17) 0.00219 -0.66406 -0.23695 -0.22151

56 O(17) 0.00186 -0.56278 -0.20081 -0.18772

57 O(17) 0.00186 -0.56278 -0.20081 -0.18772

58 C(13) -0.00041 -0.22786 -0.08131 -0.07601

59 H(1) 0.00014 0.30271 0.10801 0.10097

60 H(1) 0.00006 0.13680 0.04882 0.04563

61 H(1) -0.00003 -0.06583 -0.02349 -0.02196

62 C(13) -0.00029 -0.16477 -0.05879 -0.05496

63 H(1) 0.00015 0.32689 0.11664 0.10904

64 H(1) 0.00008 0.18795 0.06706 0.06269

65 H(1) -0.00002 -0.03502 -0.01250 -0.01168

66 C(13) -0.00029 -0.16477 -0.05879 -0.05496

67 H(1) 0.00008 0.18795 0.06706 0.06269

68 H(1) 0.00015 0.32689 0.11664 0.10904

69 H(1) -0.00002 -0.03502 -0.01250 -0.01168

70 C(13) -0.00041 -0.22786 -0.08131 -0.07601

71 H(1) 0.00006 0.13680 0.04882 0.04563

72 H(1) 0.00014 0.30271 0.10801 0.10097

73 H(1) -0.00003 -0.06583 -0.02349 -0.02196

74 C(13) -0.00029 -0.16477 -0.05879 -0.05496

75 H(1) 0.00008 0.18795 0.06706 0.06269

76 H(1) 0.00015 0.32689 0.11664 0.10904

77 H(1) -0.00002 -0.03502 -0.01250 -0.01168

78 C(13) -0.00029 -0.16477 -0.05879 -0.05496

79 H(1) 0.00015 0.32689 0.11664 0.10904

80 H(1) 0.00008 0.18795 0.06706 0.06269

81 H(1) -0.00002 -0.03502 -0.01250 -0.01168

82 C(13) -0.00041 -0.22786 -0.08131 -0.07601

83 H(1) 0.00014 0.30271 0.10801 0.10097

84 H(1) 0.00006 0.13680 0.04882 0.04563

85 H(1) -0.00003 -0.06583 -0.02349 -0.02196

86 C(13) -0.00041 -0.22786 -0.08131 -0.07601

87 H(1) 0.00006 0.13680 0.04882 0.04563

88 H(1) 0.00014 0.30271 0.10801 0.10097

89 H(1) -0.00003 -0.06583 -0.02349 -0.02196

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

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

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

1 Atom -0.142144 -0.133082 0.275226

2 Atom 0.066329 0.057183 -0.123512

3 Atom -0.142144 -0.133082 0.275226

4 Atom -0.015187 -0.004913 0.020100

5 Atom -0.015187 -0.004913 0.020100

6 Atom -0.029425 -0.024359 0.053784

7 Atom -0.071017 -0.067364 0.138380

8 Atom -0.075351 -0.072925 0.148276

9 Atom -0.071017 -0.067364 0.138380

10 Atom 0.011508 0.005074 -0.016582

11 Atom 0.011508 0.005074 -0.016582

12 Atom -0.029425 -0.024359 0.053784

13 Atom 0.011508 0.005074 -0.016582

14 Atom 0.011508 0.005074 -0.016582

15 Atom -0.071017 -0.067364 0.138380

16 Atom -0.075351 -0.072925 0.148276

17 Atom -0.071017 -0.067364 0.138380

18 Atom -0.029425 -0.024359 0.053784

19 Atom 0.066329 0.057183 -0.123512

20 Atom -0.142144 -0.133082 0.275226

21 Atom -0.015187 -0.004913 0.020100

22 Atom -0.015187 -0.004913 0.020100

23 Atom -0.142144 -0.133082 0.275226

24 Atom -0.029425 -0.024359 0.053784

25 Atom 0.015915 -0.013470 -0.002446

26 Atom -0.018043 -0.021968 0.040010

27 Atom -0.015835 -0.017843 0.033678

28 Atom -0.015835 -0.017843 0.033678

29 Atom -0.018043 -0.021968 0.040010

30 Atom -0.030765 -0.024122 0.054887

31 Atom -0.042200 -0.039347 0.081547

32 Atom -0.042200 -0.039347 0.081547

33 Atom -0.030765 -0.024122 0.054887

34 Atom -0.018043 -0.021968 0.040010

35 Atom -0.015835 -0.017843 0.033678

36 Atom -0.015835 -0.017843 0.033678

37 Atom -0.018043 -0.021968 0.040010

38 Atom -0.030765 -0.024122 0.054887

39 Atom -0.042200 -0.039347 0.081547

40 Atom -0.042200 -0.039347 0.081547

41 Atom -0.030765 -0.024122 0.054887

42 Atom 0.003274 -0.001983 -0.001291

43 Atom 0.003274 -0.001983 -0.001291

44 Atom -0.004304 0.006193 -0.001890

45 Atom -0.004304 0.006193 -0.001890

46 Atom 0.003274 -0.001983 -0.001291

47 Atom 0.003274 -0.001983 -0.001291

48 Atom -0.004304 0.006193 -0.001890

49 Atom -0.004304 0.006193 -0.001890

50 Atom -0.036912 -0.034543 0.071455

51 Atom -0.036912 -0.034543 0.071455

52 Atom -0.025394 -0.028522 0.053916

53 Atom -0.025394 -0.028522 0.053916

54 Atom -0.036912 -0.034543 0.071455

55 Atom -0.036912 -0.034543 0.071455

56 Atom -0.025394 -0.028522 0.053916

57 Atom -0.025394 -0.028522 0.053916

58 Atom 0.001165 0.000468 -0.001633

59 Atom 0.000934 0.000334 -0.001268

60 Atom 0.000960 0.000607 -0.001567

61 Atom 0.001163 0.000091 -0.001255

62 Atom 0.001077 0.000427 -0.001504

63 Atom 0.000645 0.000236 -0.000881

64 Atom 0.000854 0.000247 -0.001101

65 Atom 0.000576 0.000473 -0.001049

66 Atom 0.001077 0.000427 -0.001504

67 Atom 0.000854 0.000247 -0.001101

68 Atom 0.000645 0.000236 -0.000881

69 Atom 0.000576 0.000473 -0.001049

70 Atom 0.001165 0.000468 -0.001633

71 Atom 0.000960 0.000607 -0.001567

72 Atom 0.000934 0.000334 -0.001268

73 Atom 0.001163 0.000091 -0.001255

74 Atom 0.001077 0.000427 -0.001504

75 Atom 0.000854 0.000247 -0.001101

76 Atom 0.000645 0.000236 -0.000881

77 Atom 0.000576 0.000473 -0.001049

78 Atom 0.001077 0.000427 -0.001504

79 Atom 0.000645 0.000236 -0.000881

80 Atom 0.000854 0.000247 -0.001101

81 Atom 0.000576 0.000473 -0.001049

82 Atom 0.001165 0.000468 -0.001633

83 Atom 0.000934 0.000334 -0.001268

84 Atom 0.000960 0.000607 -0.001567

85 Atom 0.001163 0.000091 -0.001255

86 Atom 0.001165 0.000468 -0.001633

87 Atom 0.000960 0.000607 -0.001567

88 Atom 0.000934 0.000334 -0.001268

89 Atom 0.001163 0.000091 -0.001255

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XY XZ YZ

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1 Atom 0.002989 0.005181 -0.052365

2 Atom 0.000000 0.000000 0.018690

3 Atom -0.002989 -0.005181 -0.052365

4 Atom 0.001305 0.000157 -0.001840

5 Atom -0.001305 -0.000157 -0.001840

6 Atom -0.001235 -0.015029 -0.017875

7 Atom 0.000348 0.024996 0.006087

8 Atom 0.000000 0.038117 0.000000

9 Atom -0.000348 0.024996 -0.006087

10 Atom -0.000556 -0.004221 0.000815

11 Atom 0.000556 -0.004221 -0.000815

12 Atom 0.001235 0.015029 -0.017875

13 Atom -0.000556 0.004221 -0.000815

14 Atom 0.000556 0.004221 0.000815

15 Atom 0.000348 -0.024996 -0.006087

16 Atom 0.000000 -0.038117 0.000000

17 Atom -0.000348 -0.024996 0.006087

18 Atom -0.001235 0.015029 0.017875

19 Atom 0.000000 0.000000 -0.018690

20 Atom -0.002989 0.005181 0.052365

21 Atom 0.001305 -0.000157 0.001840

22 Atom -0.001305 0.000157 0.001840

23 Atom 0.002989 -0.005181 0.052365

24 Atom 0.001235 -0.015029 0.017875

25 Atom 0.000000 0.000000 0.000000

26 Atom 0.001089 -0.006884 0.001016

27 Atom 0.000402 -0.007229 0.000046

28 Atom -0.000402 -0.007229 -0.000046

29 Atom -0.001089 -0.006884 -0.001016

30 Atom 0.001516 -0.001417 0.009297

31 Atom 0.000333 -0.000096 0.017061

32 Atom -0.000333 0.000096 0.017061

33 Atom -0.001516 0.001417 0.009297

34 Atom -0.001089 0.006884 0.001016

35 Atom -0.000402 0.007229 0.000046

36 Atom 0.000402 0.007229 -0.000046

37 Atom 0.001089 0.006884 -0.001016

38 Atom 0.001516 0.001417 -0.009297

39 Atom 0.000333 0.000096 -0.017061

40 Atom -0.000333 -0.000096 -0.017061

41 Atom -0.001516 -0.001417 -0.009297

42 Atom 0.001888 -0.000609 -0.000247

43 Atom -0.001888 -0.000609 0.000247

44 Atom 0.004466 0.000581 0.001075

45 Atom -0.004466 -0.000581 0.001075

46 Atom -0.001888 0.000609 -0.000247

47 Atom 0.001888 0.000609 0.000247

48 Atom 0.004466 -0.000581 -0.001075

49 Atom -0.004466 0.000581 -0.001075

50 Atom 0.002595 -0.002131 -0.006175

51 Atom -0.002595 0.002131 -0.006175

52 Atom 0.001707 0.003862 0.002103

53 Atom -0.001707 0.003862 -0.002103

54 Atom -0.002595 -0.002131 0.006175

55 Atom 0.002595 0.002131 0.006175

56 Atom 0.001707 -0.003862 -0.002103

57 Atom -0.001707 -0.003862 0.002103

58 Atom 0.001546 0.000227 0.000214

59 Atom 0.001427 0.000830 0.000802

60 Atom 0.001567 -0.000575 -0.000439

61 Atom 0.001116 0.000094 0.000164

62 Atom 0.001070 -0.000282 -0.000135

63 Atom 0.000854 -0.000621 -0.000456

64 Atom 0.000931 0.000254 0.000305

65 Atom 0.000859 -0.000210 -0.000071

66 Atom -0.001070 -0.000282 0.000135

67 Atom -0.000931 0.000254 -0.000305

68 Atom -0.000854 -0.000621 0.000456

69 Atom -0.000859 -0.000210 0.000071

70 Atom -0.001546 -0.000227 0.000214

71 Atom -0.001567 0.000575 -0.000439

72 Atom -0.001427 -0.000830 0.000802

73 Atom -0.001116 -0.000094 0.000164

74 Atom -0.001070 0.000282 -0.000135

75 Atom -0.000931 -0.000254 0.000305

76 Atom -0.000854 0.000621 -0.000456

77 Atom -0.000859 0.000210 -0.000071

78 Atom 0.001070 0.000282 0.000135

79 Atom 0.000854 0.000621 0.000456

80 Atom 0.000931 -0.000254 -0.000305

81 Atom 0.000859 0.000210 0.000071

82 Atom 0.001546 -0.000227 -0.000214

83 Atom 0.001427 -0.000830 -0.000802

84 Atom 0.001567 0.000575 0.000439

85 Atom 0.001116 -0.000094 -0.000164

86 Atom -0.001546 0.000227 -0.000214

87 Atom -0.001567 -0.000575 0.000439

88 Atom -0.001427 0.000830 -0.000802

89 Atom -0.001116 0.000094 -0.000164

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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 -0.1448 -19.427 -6.932 -6.480 0.8147 -0.5741 -0.0816

1 C(13) Bbb -0.1371 -18.400 -6.566 -6.138 0.5798 0.8092 0.0955

Bcc 0.2819 37.827 13.497 12.618 0.0112 -0.1251 0.9921

Baa -0.1254 -4.837 -1.726 -1.614 0.0000 -0.1018 0.9948

2 N(14) Bbb 0.0591 2.279 0.813 0.760 0.0000 0.9948 0.1018

Bcc 0.0663 2.558 0.913 0.853 1.0000 0.0000 0.0000

Baa -0.1448 -19.427 -6.932 -6.480 0.8147 0.5741 0.0816

3 C(13) Bbb -0.1371 -18.400 -6.566 -6.138 -0.5798 0.8092 0.0955

Bcc 0.2819 37.827 13.497 12.618 -0.0112 -0.1251 0.9921

Baa -0.0154 -2.060 -0.735 -0.687 0.9920 -0.1259 -0.0109

4 C(13) Bbb -0.0049 -0.655 -0.234 -0.218 0.1264 0.9894 0.0721

Bcc 0.0202 2.715 0.969 0.906 0.0017 -0.0729 0.9973

Baa -0.0154 -2.060 -0.735 -0.687 0.9920 0.1259 0.0109

5 C(13) Bbb -0.0049 -0.655 -0.234 -0.218 -0.1264 0.9894 0.0721

Bcc 0.0202 2.715 0.969 0.906 -0.0017 -0.0729 0.9973

Baa -0.0347 -1.338 -0.477 -0.446 0.8185 0.5201 0.2441

6 N(14) Bbb -0.0253 -0.976 -0.348 -0.326 -0.5519 0.8298 0.0826

Bcc 0.0600 2.314 0.826 0.772 -0.1596 -0.2024 0.9662

Baa -0.0740 -9.927 -3.542 -3.311 0.9914 0.0567 -0.1183

7 C(13) Bbb -0.0675 -9.061 -3.233 -3.022 -0.0597 0.9980 -0.0223

Bcc 0.1415 18.988 6.775 6.334 0.1168 0.0291 0.9927

Baa -0.0817 -3.150 -1.124 -1.051 0.9865 0.0000 -0.1635

8 N(14) Bbb -0.0729 -2.813 -1.004 -0.938 0.0000 1.0000 0.0000

Bcc 0.1546 5.962 2.128 1.989 0.1635 0.0000 0.9865

Baa -0.0740 -9.927 -3.542 -3.311 0.9914 -0.0567 -0.1183

9 C(13) Bbb -0.0675 -9.061 -3.233 -3.022 0.0597 0.9980 0.0223

Bcc 0.1415 18.988 6.775 6.334 0.1168 -0.0291 0.9927

Baa -0.0172 -2.312 -0.825 -0.771 0.1446 -0.0325 0.9889

10 C(13) Bbb 0.0050 0.676 0.241 0.225 0.0976 0.9951 0.0184

Bcc 0.0122 1.636 0.584 0.546 0.9847 -0.0938 -0.1471

Baa -0.0172 -2.312 -0.825 -0.771 0.1446 0.0325 0.9889

11 C(13) Bbb 0.0050 0.676 0.241 0.225 -0.0976 0.9951 -0.0184

Bcc 0.0122 1.636 0.584 0.546 0.9847 0.0938 -0.1471

Baa -0.0347 -1.338 -0.477 -0.446 0.8185 -0.5201 -0.2441

12 N(14) Bbb -0.0253 -0.976 -0.348 -0.326 0.5519 0.8298 0.0826

Bcc 0.0600 2.314 0.826 0.772 0.1596 -0.2024 0.9662

Baa -0.0172 -2.312 -0.825 -0.771 -0.1446 0.0325 0.9889

13 C(13) Bbb 0.0050 0.676 0.241 0.225 0.0976 0.9951 -0.0184

Bcc 0.0122 1.636 0.584 0.546 0.9847 -0.0938 0.1471

Baa -0.0172 -2.312 -0.825 -0.771 -0.1446 -0.0325 0.9889

14 C(13) Bbb 0.0050 0.676 0.241 0.225 -0.0976 0.9951 0.0184

Bcc 0.0122 1.636 0.584 0.546 0.9847 0.0938 0.1471

Baa -0.0740 -9.927 -3.542 -3.311 0.9914 0.0567 0.1183

15 C(13) Bbb -0.0675 -9.061 -3.233 -3.022 -0.0597 0.9980 0.0223

Bcc 0.1415 18.988 6.775 6.334 -0.1168 -0.0291 0.9927

Baa -0.0817 -3.150 -1.124 -1.051 0.9865 0.0000 0.1635

16 N(14) Bbb -0.0729 -2.813 -1.004 -0.938 0.0000 1.0000 0.0000

Bcc 0.1546 5.962 2.128 1.989 -0.1635 0.0000 0.9865

Baa -0.0740 -9.927 -3.542 -3.311 0.9914 -0.0567 0.1183

17 C(13) Bbb -0.0675 -9.061 -3.233 -3.022 0.0597 0.9980 -0.0223

Bcc 0.1415 18.988 6.775 6.334 -0.1168 0.0291 0.9927

Baa -0.0347 -1.338 -0.477 -0.446 0.8185 0.5201 -0.2441

18 N(14) Bbb -0.0253 -0.976 -0.348 -0.326 -0.5519 0.8298 -0.0826

Bcc 0.0600 2.314 0.826 0.772 0.1596 0.2024 0.9662

Baa -0.1254 -4.837 -1.726 -1.614 0.0000 0.1018 0.9948

19 N(14) Bbb 0.0591 2.279 0.813 0.760 0.0000 0.9948 -0.1018

Bcc 0.0663 2.558 0.913 0.853 1.0000 0.0000 0.0000

Baa -0.1448 -19.427 -6.932 -6.480 0.8147 0.5741 -0.0816

20 C(13) Bbb -0.1371 -18.400 -6.566 -6.138 -0.5798 0.8092 -0.0955

Bcc 0.2819 37.827 13.497 12.618 0.0112 0.1251 0.9921

Baa -0.0154 -2.060 -0.735 -0.687 0.9920 -0.1259 0.0109

21 C(13) Bbb -0.0049 -0.655 -0.234 -0.218 0.1264 0.9894 -0.0721

Bcc 0.0202 2.715 0.969 0.906 -0.0017 0.0729 0.9973

Baa -0.0154 -2.060 -0.735 -0.687 0.9920 0.1259 -0.0109

22 C(13) Bbb -0.0049 -0.655 -0.234 -0.218 -0.1264 0.9894 -0.0721

Bcc 0.0202 2.715 0.969 0.906 0.0017 0.0729 0.9973

Baa -0.1448 -19.427 -6.932 -6.480 0.8147 -0.5741 0.0816

23 C(13) Bbb -0.1371 -18.400 -6.566 -6.138 0.5798 0.8092 -0.0955

Bcc 0.2819 37.827 13.497 12.618 -0.0112 0.1251 0.9921

Baa -0.0347 -1.338 -0.477 -0.446 0.8185 -0.5201 0.2441

24 N(14) Bbb -0.0253 -0.976 -0.348 -0.326 0.5519 0.8298 -0.0826

Bcc 0.0600 2.314 0.826 0.772 -0.1596 0.2024 0.9662

Baa -0.0135 -0.451 -0.161 -0.150 0.0000 1.0000 0.0000

25 Zn(67) Bbb -0.0024 -0.082 -0.029 -0.027 0.0000 0.0000 1.0000

Bcc 0.0159 0.532 0.190 0.178 1.0000 0.0000 0.0000

Baa -0.0224 -3.004 -1.072 -1.002 -0.3173 0.9470 -0.0504

26 C(13) Bbb -0.0184 -2.475 -0.883 -0.825 0.9412 0.3210 0.1053

Bcc 0.0408 5.479 1.955 1.827 -0.1159 0.0141 0.9932

Baa -0.0180 -2.414 -0.861 -0.805 -0.3362 0.9406 -0.0479

27 C(13) Bbb -0.0167 -2.244 -0.801 -0.749 0.9311 0.3396 0.1332

Bcc 0.0347 4.658 1.662 1.554 -0.1416 -0.0002 0.9899

Baa -0.0180 -2.414 -0.861 -0.805 0.3362 0.9406 0.0479

28 C(13) Bbb -0.0167 -2.244 -0.801 -0.749 0.9311 -0.3396 0.1332

Bcc 0.0347 4.658 1.662 1.554 -0.1416 0.0002 0.9899

Baa -0.0224 -3.004 -1.072 -1.002 0.3173 0.9470 0.0504

29 C(13) Bbb -0.0184 -2.475 -0.883 -0.825 0.9412 -0.3210 0.1053

Bcc 0.0408 5.479 1.955 1.827 -0.1159 -0.0141 0.9932

Baa -0.0312 -4.193 -1.496 -1.398 0.9638 -0.2629 0.0442

30 C(13) Bbb -0.0247 -3.320 -1.185 -1.107 0.2663 0.9579 -0.1071

Bcc 0.0560 7.512 2.681 2.506 -0.0142 0.1150 0.9933

Baa -0.0424 -5.687 -2.029 -1.897 0.8894 -0.4527 0.0630

31 C(13) Bbb -0.0415 -5.573 -1.989 -1.859 0.4571 0.8811 -0.1218

Bcc 0.0839 11.260 4.018 3.756 -0.0004 0.1371 0.9906

Baa -0.0424 -5.687 -2.029 -1.897 0.8894 0.4527 -0.0630

32 C(13) Bbb -0.0415 -5.573 -1.989 -1.859 -0.4571 0.8811 -0.1218

Bcc 0.0839 11.260 4.018 3.756 0.0004 0.1371 0.9906

Baa -0.0312 -4.193 -1.496 -1.398 0.9638 0.2629 -0.0442

33 C(13) Bbb -0.0247 -3.320 -1.185 -1.107 -0.2663 0.9579 -0.1071

Bcc 0.0560 7.512 2.681 2.506 0.0142 0.1150 0.9933

Baa -0.0224 -3.004 -1.072 -1.002 0.3173 0.9470 -0.0504

34 C(13) Bbb -0.0184 -2.475 -0.883 -0.825 0.9412 -0.3210 -0.1053

Bcc 0.0408 5.479 1.955 1.827 0.1159 0.0141 0.9932

Baa -0.0180 -2.414 -0.861 -0.805 0.3362 0.9406 -0.0479

35 C(13) Bbb -0.0167 -2.244 -0.801 -0.749 0.9311 -0.3396 -0.1332

Bcc 0.0347 4.658 1.662 1.554 0.1416 -0.0002 0.9899

Baa -0.0180 -2.414 -0.861 -0.805 -0.3362 0.9406 0.0479

36 C(13) Bbb -0.0167 -2.244 -0.801 -0.749 0.9311 0.3396 -0.1332

Bcc 0.0347 4.658 1.662 1.554 0.1416 0.0002 0.9899

Baa -0.0224 -3.004 -1.072 -1.002 -0.3173 0.9470 0.0504

37 C(13) Bbb -0.0184 -2.475 -0.883 -0.825 0.9412 0.3210 -0.1053

Bcc 0.0408 5.479 1.955 1.827 0.1159 -0.0141 0.9932

Baa -0.0312 -4.193 -1.496 -1.398 0.9638 -0.2629 -0.0442

38 C(13) Bbb -0.0247 -3.320 -1.185 -1.107 0.2663 0.9579 0.1071

Bcc 0.0560 7.512 2.681 2.506 0.0142 -0.1150 0.9933

Baa -0.0424 -5.687 -2.029 -1.897 0.8894 -0.4527 -0.0630

39 C(13) Bbb -0.0415 -5.573 -1.989 -1.859 0.4571 0.8811 0.1218

Bcc 0.0839 11.260 4.018 3.756 0.0004 -0.1371 0.9906

Baa -0.0424 -5.687 -2.029 -1.897 0.8894 0.4527 0.0630

40 C(13) Bbb -0.0415 -5.573 -1.989 -1.859 -0.4571 0.8811 0.1218

Bcc 0.0839 11.260 4.018 3.756 -0.0004 -0.1371 0.9906

Baa -0.0312 -4.193 -1.496 -1.398 0.9638 0.2629 0.0442

41 C(13) Bbb -0.0247 -3.320 -1.185 -1.107 -0.2663 0.9579 0.1071

Bcc 0.0560 7.512 2.681 2.506 -0.0142 -0.1150 0.9933

Baa -0.0026 -1.383 -0.494 -0.461 -0.3024 0.9524 0.0389

42 H(1) Bbb -0.0014 -0.731 -0.261 -0.244 0.1298 0.0007 0.9915

Bcc 0.0040 2.115 0.755 0.705 0.9443 0.3049 -0.1238

Baa -0.0026 -1.383 -0.494 -0.461 0.3024 0.9524 -0.0389

43 H(1) Bbb -0.0014 -0.731 -0.261 -0.244 0.1298 -0.0007 0.9915

Bcc 0.0040 2.115 0.755 0.705 0.9443 -0.3049 -0.1238

Baa -0.0060 -3.177 -1.134 -1.060 0.9389 -0.3413 -0.0439

44 H(1) Bbb -0.0020 -1.083 -0.386 -0.361 -0.0006 -0.1293 0.9916

Bcc 0.0080 4.260 1.520 1.421 0.3441 0.9310 0.1216

Baa -0.0060 -3.177 -1.134 -1.060 0.9389 0.3413 0.0439

45 H(1) Bbb -0.0020 -1.083 -0.386 -0.361 0.0006 -0.1293 0.9916

Bcc 0.0080 4.260 1.520 1.421 -0.3441 0.9310 0.1216

Baa -0.0026 -1.383 -0.494 -0.461 0.3024 0.9524 0.0389

46 H(1) Bbb -0.0014 -0.731 -0.261 -0.244 -0.1298 0.0007 0.9915

Bcc 0.0040 2.115 0.755 0.705 0.9443 -0.3049 0.1238

Baa -0.0026 -1.383 -0.494 -0.461 -0.3024 0.9524 -0.0389

47 H(1) Bbb -0.0014 -0.731 -0.261 -0.244 -0.1298 -0.0007 0.9915

Bcc 0.0040 2.115 0.755 0.705 0.9443 0.3049 0.1238

Baa -0.0060 -3.177 -1.134 -1.060 0.9389 -0.3413 0.0439

48 H(1) Bbb -0.0020 -1.083 -0.386 -0.361 0.0006 0.1293 0.9916

Bcc 0.0080 4.260 1.520 1.421 0.3441 0.9310 -0.1216

Baa -0.0060 -3.177 -1.134 -1.060 0.9389 0.3413 -0.0439

49 H(1) Bbb -0.0020 -1.083 -0.386 -0.361 -0.0006 0.1293 0.9916

Bcc 0.0080 4.260 1.520 1.421 -0.3441 0.9310 -0.1216

Baa -0.0386 2.793 0.997 0.932 0.8320 -0.5546 -0.0150

50 O(17) Bbb -0.0333 2.407 0.859 0.803 0.5544 0.8301 0.0602

Bcc 0.0719 -5.200 -1.855 -1.734 -0.0209 -0.0584 0.9981

Baa -0.0386 2.793 0.997 0.932 0.8320 0.5546 0.0150

51 O(17) Bbb -0.0333 2.407 0.859 0.803 -0.5544 0.8301 0.0602

Bcc 0.0719 -5.200 -1.855 -1.734 0.0209 -0.0584 0.9981

Baa -0.0293 2.118 0.756 0.707 -0.3988 0.9170 -0.0047

52 O(17) Bbb -0.0249 1.801 0.643 0.601 0.9157 0.3979 -0.0555

Bcc 0.0542 -3.919 -1.398 -1.307 0.0490 0.0264 0.9984

Baa -0.0293 2.118 0.756 0.707 0.3988 0.9170 0.0047

53 O(17) Bbb -0.0249 1.801 0.643 0.601 0.9157 -0.3979 -0.0555

Bcc 0.0542 -3.919 -1.398 -1.307 0.0490 -0.0264 0.9984

Baa -0.0386 2.793 0.997 0.932 0.8320 0.5546 -0.0150

54 O(17) Bbb -0.0333 2.407 0.859 0.803 -0.5544 0.8301 -0.0602

Bcc 0.0719 -5.200 -1.855 -1.734 -0.0209 0.0584 0.9981

Baa -0.0386 2.793 0.997 0.932 0.8320 -0.5546 0.0150

55 O(17) Bbb -0.0333 2.407 0.859 0.803 0.5544 0.8301 -0.0602

Bcc 0.0719 -5.200 -1.855 -1.734 0.0209 0.0584 0.9981

Baa -0.0293 2.118 0.756 0.707 -0.3988 0.9170 0.0047

56 O(17) Bbb -0.0249 1.801 0.643 0.601 0.9157 0.3979 0.0555

Bcc 0.0542 -3.919 -1.398 -1.307 -0.0490 -0.0264 0.9984

Baa -0.0293 2.118 0.756 0.707 0.3988 0.9170 -0.0047

57 O(17) Bbb -0.0249 1.801 0.643 0.601 0.9157 -0.3979 0.0555

Bcc 0.0542 -3.919 -1.398 -1.307 -0.0490 0.0264 0.9984

Baa -0.0017 -0.222 -0.079 -0.074 -0.0423 -0.0695 0.9967

58 C(13) Bbb -0.0008 -0.103 -0.037 -0.034 -0.6264 0.7790 0.0277

Bcc 0.0024 0.325 0.116 0.109 0.7783 0.6232 0.0764

Baa -0.0016 -0.872 -0.311 -0.291 -0.1539 -0.2748 0.9491

59 H(1) Bbb -0.0008 -0.434 -0.155 -0.145 -0.6593 0.7440 0.1085

Bcc 0.0024 1.306 0.466 0.436 0.7360 0.6090 0.2957

Baa -0.0017 -0.906 -0.323 -0.302 0.1706 0.0713 0.9828

60 H(1) Bbb -0.0008 -0.421 -0.150 -0.141 -0.6550 0.7533 0.0590

Bcc 0.0025 1.328 0.474 0.443 0.7361 0.6538 -0.1752

Baa -0.0013 -0.680 -0.243 -0.227 0.0255 -0.1393 0.9899

61 H(1) Bbb -0.0006 -0.320 -0.114 -0.107 -0.5354 0.8343 0.1312

Bcc 0.0019 1.000 0.357 0.334 0.8442 0.5334 0.0533

Baa -0.0015 -0.206 -0.073 -0.069 0.1021 0.0130 0.9947

62 C(13) Bbb -0.0004 -0.049 -0.017 -0.016 -0.5891 0.8065 0.0499

Bcc 0.0019 0.255 0.091 0.085 0.8016 0.5911 -0.0900

Baa -0.0011 -0.600 -0.214 -0.200 0.2590 0.1565 0.9531

63 H(1) Bbb -0.0004 -0.233 -0.083 -0.078 -0.6069 0.7940 0.0346

Bcc 0.0016 0.833 0.297 0.278 0.7514 0.5874 -0.3006

Baa -0.0012 -0.624 -0.223 -0.208 -0.0369 -0.1871 0.9817

64 H(1) Bbb -0.0004 -0.222 -0.079 -0.074 -0.6028 0.7877 0.1274

Bcc 0.0016 0.846 0.302 0.282 0.7970 0.5870 0.1418

Baa -0.0011 -0.575 -0.205 -0.192 0.1436 -0.0343 0.9890

65 H(1) Bbb -0.0003 -0.173 -0.062 -0.058 -0.6700 0.7321 0.1227

Bcc 0.0014 0.748 0.267 0.250 0.7283 0.6803 -0.0822

Baa -0.0015 -0.206 -0.073 -0.069 0.1021 -0.0130 0.9947

66 C(13) Bbb -0.0004 -0.049 -0.017 -0.016 0.5891 0.8065 -0.0499

Bcc 0.0019 0.255 0.091 0.085 0.8016 -0.5911 -0.0900

Baa -0.0012 -0.624 -0.223 -0.208 -0.0369 0.1871 0.9817

67 H(1) Bbb -0.0004 -0.222 -0.079 -0.074 0.6028 0.7877 -0.1274

Bcc 0.0016 0.846 0.302 0.282 0.7970 -0.5870 0.1418

Baa -0.0011 -0.600 -0.214 -0.200 0.2590 -0.1565 0.9531

68 H(1) Bbb -0.0004 -0.233 -0.083 -0.078 0.6069 0.7940 -0.0346

Bcc 0.0016 0.833 0.297 0.278 0.7514 -0.5874 -0.3006

Baa -0.0011 -0.575 -0.205 -0.192 0.1436 0.0343 0.9890

69 H(1) Bbb -0.0003 -0.173 -0.062 -0.058 0.6700 0.7321 -0.1227

Bcc 0.0014 0.748 0.267 0.250 0.7283 -0.6803 -0.0822

Baa -0.0017 -0.222 -0.079 -0.074 0.0423 -0.0695 0.9967

70 C(13) Bbb -0.0008 -0.103 -0.037 -0.034 0.6264 0.7790 0.0277

Bcc 0.0024 0.325 0.116 0.109 0.7783 -0.6232 -0.0764

Baa -0.0017 -0.906 -0.323 -0.302 -0.1706 0.0713 0.9828

71 H(1) Bbb -0.0008 -0.421 -0.150 -0.141 0.6550 0.7533 0.0590

Bcc 0.0025 1.328 0.474 0.443 0.7361 -0.6538 0.1752

Baa -0.0016 -0.872 -0.311 -0.291 0.1539 -0.2748 0.9491

72 H(1) Bbb -0.0008 -0.434 -0.155 -0.145 0.6593 0.7440 0.1085

Bcc 0.0024 1.306 0.466 0.436 0.7360 -0.6090 -0.2957

Baa -0.0013 -0.680 -0.243 -0.227 -0.0255 -0.1393 0.9899

73 H(1) Bbb -0.0006 -0.320 -0.114 -0.107 0.5354 0.8343 0.1312

Bcc 0.0019 1.000 0.357 0.334 0.8442 -0.5334 -0.0533

Baa -0.0015 -0.206 -0.073 -0.069 -0.1021 0.0130 0.9947

74 C(13) Bbb -0.0004 -0.049 -0.017 -0.016 0.5891 0.8065 0.0499

Bcc 0.0019 0.255 0.091 0.085 0.8016 -0.5911 0.0900

Baa -0.0012 -0.624 -0.223 -0.208 0.0369 -0.1871 0.9817

75 H(1) Bbb -0.0004 -0.222 -0.079 -0.074 0.6028 0.7877 0.1274

Bcc 0.0016 0.846 0.302 0.282 0.7970 -0.5870 -0.1418

Baa -0.0011 -0.600 -0.214 -0.200 -0.2590 0.1565 0.9531

76 H(1) Bbb -0.0004 -0.233 -0.083 -0.078 0.6069 0.7940 0.0346

Bcc 0.0016 0.833 0.297 0.278 0.7514 -0.5874 0.3006

Baa -0.0011 -0.575 -0.205 -0.192 -0.1436 -0.0343 0.9890

77 H(1) Bbb -0.0003 -0.173 -0.062 -0.058 0.6700 0.7321 0.1227

Bcc 0.0014 0.748 0.267 0.250 0.7283 -0.6803 0.0822

Baa -0.0015 -0.206 -0.073 -0.069 -0.1021 -0.0130 0.9947

78 C(13) Bbb -0.0004 -0.049 -0.017 -0.016 -0.5891 0.8065 -0.0499

Bcc 0.0019 0.255 0.091 0.085 0.8016 0.5911 0.0900

Baa -0.0011 -0.600 -0.214 -0.200 -0.2590 -0.1565 0.9531

79 H(1) Bbb -0.0004 -0.233 -0.083 -0.078 -0.6069 0.7940 -0.0346

Bcc 0.0016 0.833 0.297 0.278 0.7514 0.5874 0.3006

Baa -0.0012 -0.624 -0.223 -0.208 0.0369 0.1871 0.9817

80 H(1) Bbb -0.0004 -0.222 -0.079 -0.074 -0.6028 0.7877 -0.1274

Bcc 0.0016 0.846 0.302 0.282 0.7970 0.5870 -0.1418

Baa -0.0011 -0.575 -0.205 -0.192 -0.1436 0.0343 0.9890

81 H(1) Bbb -0.0003 -0.173 -0.062 -0.058 -0.6700 0.7321 -0.1227

Bcc 0.0014 0.748 0.267 0.250 0.7283 0.6803 0.0822

Baa -0.0017 -0.222 -0.079 -0.074 0.0423 0.0695 0.9967

82 C(13) Bbb -0.0008 -0.103 -0.037 -0.034 -0.6264 0.7790 -0.0277

Bcc 0.0024 0.325 0.116 0.109 0.7783 0.6232 -0.0764

Baa -0.0016 -0.872 -0.311 -0.291 0.1539 0.2748 0.9491

83 H(1) Bbb -0.0008 -0.434 -0.155 -0.145 -0.6593 0.7440 -0.1085

Bcc 0.0024 1.306 0.466 0.436 0.7360 0.6090 -0.2957

Baa -0.0017 -0.906 -0.323 -0.302 -0.1706 -0.0713 0.9828

84 H(1) Bbb -0.0008 -0.421 -0.150 -0.141 -0.6550 0.7533 -0.0590

Bcc 0.0025 1.328 0.474 0.443 0.7361 0.6538 0.1752

Baa -0.0013 -0.680 -0.243 -0.227 -0.0255 0.1393 0.9899

85 H(1) Bbb -0.0006 -0.320 -0.114 -0.107 -0.5354 0.8343 -0.1312

Bcc 0.0019 1.000 0.357 0.334 0.8442 0.5334 -0.0533

Baa -0.0017 -0.222 -0.079 -0.074 -0.0423 0.0695 0.9967

86 C(13) Bbb -0.0008 -0.103 -0.037 -0.034 0.6264 0.7790 -0.0277

Bcc 0.0024 0.325 0.116 0.109 0.7783 -0.6232 0.0764

Baa -0.0017 -0.906 -0.323 -0.302 0.1706 -0.0713 0.9828

87 H(1) Bbb -0.0008 -0.421 -0.150 -0.141 0.6550 0.7533 -0.0590

Bcc 0.0025 1.328 0.474 0.443 0.7361 -0.6538 -0.1752

Baa -0.0016 -0.872 -0.311 -0.291 -0.1539 0.2748 0.9491

88 H(1) Bbb -0.0008 -0.434 -0.155 -0.145 0.6593 0.7440 -0.1085

Bcc 0.0024 1.306 0.466 0.436 0.7360 -0.6090 0.2957

Baa -0.0013 -0.680 -0.243 -0.227 0.0255 0.1393 0.9899

89 H(1) Bbb -0.0006 -0.320 -0.114 -0.107 0.5354 0.8343 -0.1312

Bcc 0.0019 1.000 0.357 0.334 0.8442 -0.5334 0.0533

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

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Fri Jul 5 23:16:14 2019, MaxMem= 1342177280 cpu: 93.5

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

Compute integral first derivatives.

... and contract with generalized density number 0.

Density matrix has only Abelian symmetry.

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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44149 LenP2D= 110838.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 271

Leave Link 701 at Fri Jul 5 23:16:32 2019, MaxMem= 1342177280 cpu: 214.5

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

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

Leave Link 702 at Fri Jul 5 23:16:32 2019, MaxMem= 1342177280 cpu: 0.3

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

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

Integral derivatives from FoFJK, PRISM(SPDF).

Density matrix has only Abelian symmetry.

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2800

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Petite list used in FoFCou.

Leave Link 703 at Fri Jul 5 23:17:08 2019, MaxMem= 1342177280 cpu: 425.1

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

Dipole = 1.20259358D-12 4.22772928D-13-2.08717915D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.012929772 0.008893943 0.002306497

2 7 0.000000000 0.004573590 -0.000991005

3 6 -0.012929772 0.008893943 0.002306497

4 6 0.003986287 -0.008190936 -0.000414726

5 6 -0.003986287 -0.008190936 -0.000414726

6 7 0.020842349 -0.017815155 -0.003842045

7 6 -0.009664751 0.019256459 0.002513749

8 7 -0.003395717 0.000000000 0.001297949

9 6 -0.009664751 -0.019256459 0.002513749

10 6 0.008197277 0.004306925 -0.001286826

11 6 0.008197277 -0.004306925 -0.001286826

12 7 -0.020842349 -0.017815155 -0.003842045

13 6 -0.008197277 -0.004306925 -0.001286826

14 6 -0.008197277 0.004306925 -0.001286826

15 6 0.009664751 -0.019256459 0.002513749

16 7 0.003395717 0.000000000 0.001297949

17 6 0.009664751 0.019256459 0.002513749

18 7 -0.020842349 0.017815155 -0.003842045

19 7 0.000000000 -0.004573590 -0.000991005

20 6 0.012929772 -0.008893943 0.002306497

21 6 -0.003986287 0.008190936 -0.000414726

22 6 0.003986287 0.008190936 -0.000414726

23 6 -0.012929772 -0.008893943 0.002306497

24 7 0.020842349 0.017815155 -0.003842045

25 30 0.000000000 0.000000000 -0.000237714

26 6 0.007491281 0.004627121 0.000955519

27 6 -0.002289514 -0.009188515 -0.000220397

28 6 -0.002289514 0.009188515 -0.000220397

29 6 0.007491281 -0.004627121 0.000955519

30 6 0.002519213 -0.001555091 0.000123869

31 6 0.000102560 0.001045614 -0.000254184

32 6 -0.000102560 0.001045614 -0.000254184

33 6 -0.002519213 -0.001555091 0.000123869

34 6 -0.007491281 0.004627121 0.000955519

35 6 0.002289514 -0.009188515 -0.000220397

36 6 0.002289514 0.009188515 -0.000220397

37 6 -0.007491281 -0.004627121 0.000955519

38 6 -0.002519213 0.001555091 0.000123869

39 6 -0.000102560 -0.001045614 -0.000254184

40 6 0.000102560 -0.001045614 -0.000254184

41 6 0.002519213 0.001555091 0.000123869

42 1 -0.000802594 -0.000721527 0.000085471

43 1 -0.000802594 0.000721527 0.000085471

44 1 -0.000513813 -0.000754714 -0.000066701

45 1 0.000513813 -0.000754714 -0.000066701

46 1 0.000802594 -0.000721527 0.000085471

47 1 0.000802594 0.000721527 0.000085471

48 1 0.000513813 0.000754714 -0.000066701

49 1 -0.000513813 0.000754714 -0.000066701

50 8 -0.003416357 0.001324693 0.000257987

51 8 0.003416357 0.001324693 0.000257987

52 8 0.001210858 -0.005712282 -0.000195985

53 8 0.001210858 0.005712282 -0.000195985

54 8 -0.003416357 -0.001324693 0.000257987

55 8 0.003416357 -0.001324693 0.000257987

56 8 -0.001210858 0.005712282 -0.000195985

57 8 -0.001210858 -0.005712282 -0.000195985

58 6 -0.000364291 -0.000277661 -0.000117848

59 1 0.000448391 -0.000614468 -0.001405886

60 1 0.000498906 -0.000811153 0.001299882

61 1 -0.001735854 0.000361436 0.000026973

62 6 0.000811392 0.000166380 0.000009810

63 1 -0.000755662 0.000524856 0.001470394

64 1 -0.000958381 0.000578637 -0.001322990

65 1 0.000308966 -0.001870811 -0.000016607

66 6 0.000811392 -0.000166380 0.000009810

67 1 -0.000958381 -0.000578637 -0.001322990

68 1 -0.000755662 -0.000524856 0.001470394

69 1 0.000308966 0.001870811 -0.000016607

70 6 0.000364291 -0.000277661 -0.000117848

71 1 -0.000498906 -0.000811153 0.001299882

72 1 -0.000448391 -0.000614468 -0.001405886

73 1 0.001735854 0.000361436 0.000026973

74 6 -0.000811392 0.000166380 0.000009810

75 1 0.000958381 0.000578637 -0.001322990

76 1 0.000755662 0.000524856 0.001470394

77 1 -0.000308966 -0.001870811 -0.000016607

78 6 -0.000811392 -0.000166380 0.000009810

79 1 0.000755662 -0.000524856 0.001470394

80 1 0.000958381 -0.000578637 -0.001322990

81 1 -0.000308966 0.001870811 -0.000016607

82 6 0.000364291 0.000277661 -0.000117848

83 1 -0.000448391 0.000614468 -0.001405886

84 1 -0.000498906 0.000811153 0.001299882

85 1 0.001735854 -0.000361436 0.000026973

86 6 -0.000364291 0.000277661 -0.000117848

87 1 0.000498906 0.000811153 0.001299882

88 1 0.000448391 0.000614468 -0.001405886

89 1 -0.001735854 -0.000361436 0.000026973

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

Cartesian Forces: Max 0.020842349 RMS 0.005367920

Leave Link 716 at Fri Jul 5 23:17:09 2019, MaxMem= 1342177280 cpu: 0.7

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

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

Internal Forces: Max 0.016199548 RMS 0.002462401

Search for a local minimum.

Step number 1 out of a maximum of 518

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

RMS Force = .24624D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Second derivative matrix not updated -- first step.

ITU= 0

DSYEVD-2 returned Info= 785 IAlg= 4 N= 261 NDim= 261 NE2= 5131336 trying DSYEV.

Eigenvalues --- 0.01316 0.01316 0.01316 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01544 0.01554

Eigenvalues --- 0.01565 0.01565 0.01578 0.01596 0.01617

Eigenvalues --- 0.01617 0.01707 0.01710 0.01710 0.01715

Eigenvalues --- 0.01724 0.01827 0.01840 0.01856 0.01856

Eigenvalues --- 0.01877 0.01908 0.01918 0.01919 0.01919

Eigenvalues --- 0.01922 0.01989 0.01989 0.02021 0.02021

Eigenvalues --- 0.02021 0.02021 0.02053 0.02053 0.02053

Eigenvalues --- 0.02053 0.02057 0.02057 0.02057 0.02057

Eigenvalues --- 0.02067 0.02067 0.02067 0.02067 0.02070

Eigenvalues --- 0.02070 0.02070 0.02070 0.02083 0.02083

Eigenvalues --- 0.02083 0.02083 0.02178 0.02260 0.02260

Eigenvalues --- 0.02260 0.02260 0.02260 0.02260 0.02260

Eigenvalues --- 0.02260 0.02347 0.02349 0.02349 0.02404

Eigenvalues --- 0.10007 0.10007 0.10007 0.10007 0.10007

Eigenvalues --- 0.10007 0.10007 0.10007 0.10656 0.10656

Eigenvalues --- 0.10656 0.10656 0.10656 0.10656 0.10656

Eigenvalues --- 0.10656 0.13510 0.13510 0.15549 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.17553 0.21871 0.21871 0.22478

Eigenvalues --- 0.22478 0.22478 0.22478 0.24508 0.24509

Eigenvalues --- 0.24509 0.24510 0.24648 0.24744 0.24810

Eigenvalues --- 0.24810 0.24923 0.24924 0.24924 0.24924

Eigenvalues --- 0.24948 0.24992 0.24993 0.24993 0.24995

Eigenvalues --- 0.24997 0.24997 0.24997 0.24997 0.24999

Eigenvalues --- 0.24999 0.24999 0.24999 0.24999 0.24999

Eigenvalues --- 0.24999 0.24999 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.33645 0.33645 0.33698 0.33723 0.34063

Eigenvalues --- 0.34063 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34063 0.34081 0.34081 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34081

Eigenvalues --- 0.34481 0.34598 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34686 0.34686 0.34686

Eigenvalues --- 0.34962 0.34962 0.35632 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35632 0.35632

Eigenvalues --- 0.36790 0.37037 0.37141 0.37141 0.41215

Eigenvalues --- 0.41215 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41215 0.41215 0.41418 0.41418 0.41419

Eigenvalues --- 0.41420 0.41553 0.42492 0.42492 0.42736

Eigenvalues --- 0.44050 0.44570 0.44570 0.44619 0.44661

Eigenvalues --- 0.44934 0.44934 0.45000 0.45000 0.45003

Eigenvalues --- 0.45003 0.45356 0.45362 0.45367 0.45367

Eigenvalues --- 0.47420 0.48191 0.49359 0.49359 0.49879

Eigenvalues --- 0.49981 0.53554 0.53554 0.53554 0.53554

Eigenvalues --- 0.53554 0.53554 0.53554 0.53554 0.55000

Eigenvalues --- 0.55000 0.56096 0.57338 0.57456 0.57456

Eigenvalues --- 0.57598

RFO step: Lambda=-6.47802071D-03 EMin= 1.31568111D-02

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.01397106 RMS(Int)= 0.00004006

Iteration 2 RMS(Cart)= 0.00011225 RMS(Int)= 0.00001753

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00001753

ITry= 1 IFail=0 DXMaxC= 4.46D-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 2.58330 -0.00098 0.00000 -0.00078 -0.00085 2.58246

R2 2.77530 -0.00830 0.00000 -0.02300 -0.02300 2.75231

R3 2.52539 0.01358 0.00000 0.02254 0.02252 2.54791

R4 2.58330 -0.00098 0.00000 -0.00078 -0.00085 2.58246

R5 3.86121 -0.00141 0.00000 -0.00066 -0.00072 3.86049

R6 2.77530 -0.00830 0.00000 -0.02300 -0.02300 2.75231

R7 2.52539 0.01358 0.00000 0.02254 0.02252 2.54792

R8 2.68440 0.00239 0.00000 0.00509 0.00512 2.68952

R9 2.66009 -0.00071 0.00000 -0.00137 -0.00137 2.65873

R10 2.66009 -0.00071 0.00000 -0.00137 -0.00137 2.65873

R11 2.52539 -0.01620 0.00000 -0.02877 -0.02875 2.49665

R12 2.58330 0.00317 0.00000 0.00623 0.00629 2.58959

R13 2.77530 0.00321 0.00000 0.00828 0.00827 2.78357

R14 2.58330 0.00317 0.00000 0.00623 0.00629 2.58959

R15 3.86121 -0.00159 0.00000 -0.00964 -0.00958 3.85163

R16 2.77530 0.00321 0.00000 0.00828 0.00827 2.78357

R17 2.52539 -0.01620 0.00000 -0.02877 -0.02875 2.49665

R18 2.68440 -0.00486 0.00000 -0.01320 -0.01321 2.67119

R19 2.66009 -0.00581 0.00000 -0.01309 -0.01309 2.64700

R20 2.66009 -0.00581 0.00000 -0.01309 -0.01309 2.64700

R21 2.52539 -0.01620 0.00000 -0.02877 -0.02875 2.49665

R22 2.68440 -0.00486 0.00000 -0.01320 -0.01321 2.67119

R23 2.77530 0.00321 0.00000 0.00828 0.00827 2.78357

R24 2.66009 -0.00581 0.00000 -0.01309 -0.01309 2.64700

R25 2.77530 0.00321 0.00000 0.00828 0.00827 2.78357

R26 2.66009 -0.00581 0.00000 -0.01309 -0.01309 2.64700

R27 2.58330 0.00317 0.00000 0.00623 0.00629 2.58959

R28 2.52539 -0.01620 0.00000 -0.02877 -0.02875 2.49665

R29 2.58330 0.00317 0.00000 0.00623 0.00629 2.58959

R30 3.86121 -0.00159 0.00000 -0.00964 -0.00958 3.85163

R31 2.52539 0.01358 0.00000 0.02254 0.02252 2.54791

R32 2.58330 -0.00098 0.00000 -0.00078 -0.00085 2.58246

R33 2.58330 -0.00098 0.00000 -0.00078 -0.00085 2.58246

R34 3.86121 -0.00141 0.00000 -0.00066 -0.00072 3.86049

R35 2.77530 -0.00830 0.00000 -0.02300 -0.02300 2.75231

R36 2.68440 0.00239 0.00000 0.00509 0.00512 2.68952

R37 2.66009 -0.00071 0.00000 -0.00137 -0.00137 2.65873

R38 2.77530 -0.00830 0.00000 -0.02300 -0.02300 2.75231

R39 2.66009 -0.00071 0.00000 -0.00137 -0.00137 2.65873

R40 2.52539 0.01358 0.00000 0.02254 0.02252 2.54791

R41 2.64727 0.00155 0.00000 0.00355 0.00355 2.65082

R42 2.56440 -0.00634 0.00000 -0.01169 -0.01169 2.55271

R43 2.65215 -0.00938 0.00000 -0.02015 -0.02015 2.63200

R44 2.04661 -0.00105 0.00000 -0.00290 -0.00290 2.04371

R45 2.64727 0.00155 0.00000 0.00355 0.00355 2.65082

R46 2.04661 -0.00105 0.00000 -0.00290 -0.00290 2.04371

R47 2.56440 -0.00634 0.00000 -0.01169 -0.01169 2.55271

R48 2.64727 -0.00215 0.00000 -0.00487 -0.00487 2.64240

R49 2.56440 -0.00456 0.00000 -0.00842 -0.00842 2.55599

R50 2.65215 -0.00154 0.00000 -0.00379 -0.00378 2.64837

R51 2.04661 -0.00091 0.00000 -0.00251 -0.00251 2.04410

R52 2.64727 -0.00215 0.00000 -0.00487 -0.00487 2.64240

R53 2.04661 -0.00091 0.00000 -0.00251 -0.00251 2.04410

R54 2.56440 -0.00456 0.00000 -0.00842 -0.00842 2.55599

R55 2.64727 0.00155 0.00000 0.00355 0.00355 2.65082

R56 2.56440 -0.00634 0.00000 -0.01169 -0.01169 2.55271

R57 2.65215 -0.00938 0.00000 -0.02015 -0.02015 2.63200

R58 2.04661 -0.00105 0.00000 -0.00290 -0.00290 2.04371

R59 2.64727 0.00155 0.00000 0.00355 0.00355 2.65082

R60 2.04661 -0.00105 0.00000 -0.00290 -0.00290 2.04371

R61 2.56440 -0.00634 0.00000 -0.01169 -0.01169 2.55271

R62 2.64727 -0.00215 0.00000 -0.00487 -0.00487 2.64240

R63 2.56440 -0.00456 0.00000 -0.00842 -0.00842 2.55599

R64 2.65215 -0.00154 0.00000 -0.00379 -0.00378 2.64837

R65 2.04661 -0.00091 0.00000 -0.00251 -0.00251 2.04410

R66 2.64727 -0.00215 0.00000 -0.00487 -0.00487 2.64240

R67 2.04661 -0.00091 0.00000 -0.00251 -0.00251 2.04410

R68 2.56440 -0.00456 0.00000 -0.00842 -0.00842 2.55599

R69 2.69935 -0.00175 0.00000 -0.00419 -0.00419 2.69516

R70 2.69935 -0.00175 0.00000 -0.00419 -0.00419 2.69516

R71 2.69935 -0.00083 0.00000 -0.00197 -0.00197 2.69737

R72 2.69935 -0.00083 0.00000 -0.00197 -0.00197 2.69737

R73 2.69935 -0.00175 0.00000 -0.00419 -0.00419 2.69516

R74 2.69935 -0.00175 0.00000 -0.00419 -0.00419 2.69516

R75 2.69935 -0.00083 0.00000 -0.00197 -0.00197 2.69737

R76 2.69935 -0.00083 0.00000 -0.00197 -0.00197 2.69737

R77 2.07193 -0.00159 0.00000 -0.00457 -0.00457 2.06737

R78 2.07224 -0.00159 0.00000 -0.00458 -0.00458 2.06765

R79 2.06187 -0.00177 0.00000 -0.00501 -0.00501 2.05686

R80 2.07193 -0.00172 0.00000 -0.00496 -0.00496 2.06697

R81 2.07224 -0.00172 0.00000 -0.00494 -0.00494 2.06730

R82 2.06187 -0.00189 0.00000 -0.00534 -0.00534 2.05654

R83 2.07224 -0.00172 0.00000 -0.00494 -0.00494 2.06730

R84 2.07193 -0.00172 0.00000 -0.00496 -0.00496 2.06697

R85 2.06187 -0.00189 0.00000 -0.00534 -0.00534 2.05654

R86 2.07224 -0.00159 0.00000 -0.00458 -0.00458 2.06765

R87 2.07193 -0.00159 0.00000 -0.00457 -0.00457 2.06737

R88 2.06187 -0.00177 0.00000 -0.00501 -0.00501 2.05686

R89 2.07224 -0.00172 0.00000 -0.00494 -0.00494 2.06730

R90 2.07193 -0.00172 0.00000 -0.00496 -0.00496 2.06697

R91 2.06187 -0.00189 0.00000 -0.00534 -0.00534 2.05654

R92 2.07193 -0.00172 0.00000 -0.00496 -0.00496 2.06697

R93 2.07224 -0.00172 0.00000 -0.00494 -0.00494 2.06730

R94 2.06187 -0.00189 0.00000 -0.00534 -0.00534 2.05654

R95 2.07193 -0.00159 0.00000 -0.00457 -0.00457 2.06737

R96 2.07224 -0.00159 0.00000 -0.00458 -0.00458 2.06765

R97 2.06187 -0.00177 0.00000 -0.00501 -0.00501 2.05686

R98 2.07224 -0.00159 0.00000 -0.00458 -0.00458 2.06765

R99 2.07193 -0.00159 0.00000 -0.00457 -0.00457 2.06737

R100 2.06187 -0.00177 0.00000 -0.00501 -0.00501 2.05686

A1 1.88287 -0.00236 0.00000 -0.00763 -0.00763 1.87523

A2 2.21860 0.00084 0.00000 0.00484 0.00478 2.22338

A3 2.18138 0.00152 0.00000 0.00277 0.00283 2.18421

A4 1.94068 0.00287 0.00000 0.00821 0.00823 1.94891

A5 2.16659 -0.00145 0.00000 -0.00458 -0.00460 2.16199

A6 2.16659 -0.00145 0.00000 -0.00458 -0.00460 2.16199

A7 1.88287 -0.00236 0.00000 -0.00763 -0.00763 1.87523

A8 2.21860 0.00084 0.00000 0.00484 0.00478 2.22338

A9 2.18138 0.00152 0.00000 0.00277 0.00283 2.18421

A10 1.85915 0.00092 0.00000 0.00351 0.00351 1.86267

A11 2.31288 -0.00009 0.00000 -0.00115 -0.00115 2.31173

A12 2.11112 -0.00084 0.00000 -0.00234 -0.00235 2.10877

A13 1.85915 0.00092 0.00000 0.00351 0.00351 1.86267

A14 2.31288 -0.00009 0.00000 -0.00115 -0.00115 2.31173

A15 2.11112 -0.00084 0.00000 -0.00234 -0.00235 2.10877

A16 2.20676 -0.00265 0.00000 -0.01127 -0.01129 2.19547

A17 2.21860 0.00290 0.00000 0.00972 0.00974 2.22834

A18 2.18138 -0.00190 0.00000 -0.00759 -0.00764 2.17374

A19 1.88287 -0.00100 0.00000 -0.00195 -0.00195 1.88092

A20 1.94068 -0.00072 0.00000 -0.00200 -0.00204 1.93865

A21 2.16659 0.00034 0.00000 0.00006 0.00003 2.16662

A22 2.16659 0.00034 0.00000 0.00006 0.00003 2.16662

A23 1.88287 -0.00100 0.00000 -0.00195 -0.00195 1.88092

A24 2.21860 0.00290 0.00000 0.00972 0.00974 2.22834

A25 2.18138 -0.00190 0.00000 -0.00759 -0.00764 2.17374

A26 1.85915 0.00136 0.00000 0.00298 0.00298 1.86213

A27 2.31288 -0.00172 0.00000 -0.00444 -0.00445 2.30843

A28 2.11112 0.00037 0.00000 0.00146 0.00147 2.11259

A29 1.85915 0.00136 0.00000 0.00298 0.00298 1.86213

A30 2.31288 -0.00172 0.00000 -0.00444 -0.00445 2.30843

A31 2.11112 0.00037 0.00000 0.00146 0.00147 2.11259

A32 2.20676 -0.00265 0.00000 -0.01127 -0.01130 2.19547

A33 1.85915 0.00136 0.00000 0.00298 0.00298 1.86213

A34 2.11112 0.00037 0.00000 0.00146 0.00147 2.11259

A35 2.31288 -0.00172 0.00000 -0.00444 -0.00445 2.30843

A36 1.85915 0.00136 0.00000 0.00298 0.00298 1.86213

A37 2.11112 0.00037 0.00000 0.00146 0.00147 2.11259

A38 2.31288 -0.00172 0.00000 -0.00444 -0.00445 2.30843

A39 1.88287 -0.00100 0.00000 -0.00195 -0.00194 1.88092

A40 2.18138 -0.00190 0.00000 -0.00759 -0.00764 2.17374

A41 2.21860 0.00290 0.00000 0.00972 0.00974 2.22834

A42 1.94068 -0.00072 0.00000 -0.00200 -0.00204 1.93864

A43 2.16659 0.00034 0.00000 0.00006 0.00004 2.16663

A44 2.16659 0.00034 0.00000 0.00006 0.00003 2.16662

A45 2.18138 -0.00190 0.00000 -0.00759 -0.00764 2.17374

A46 2.21860 0.00290 0.00000 0.00972 0.00974 2.22834

A47 1.88287 -0.00100 0.00000 -0.00195 -0.00194 1.88092

A48 2.20676 -0.00265 0.00000 -0.01127 -0.01130 2.19547

A49 1.94068 0.00287 0.00000 0.00821 0.00823 1.94891

A50 2.16659 -0.00145 0.00000 -0.00458 -0.00460 2.16199

A51 2.16659 -0.00145 0.00000 -0.00458 -0.00460 2.16199

A52 2.21860 0.00084 0.00000 0.00484 0.00478 2.22338

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D3 3.10413 0.00004 0.00000 -0.00179 -0.00179 3.10235

D4 -0.17878 -0.00020 0.00000 -0.00921 -0.00924 -0.18802

D5 0.00611 -0.00003 0.00000 0.00063 0.00062 0.00673

D6 -3.12691 -0.00007 0.00000 -0.00232 -0.00233 -3.12924

D7 -3.10911 -0.00003 0.00000 0.00123 0.00123 -3.10788

D8 0.04105 -0.00007 0.00000 -0.00172 -0.00172 0.03933

D9 0.09963 0.00063 0.00000 0.01779 0.01779 0.11742

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D17 -0.07921 0.00020 0.00000 0.00244 0.00246 -0.07675

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D29 -3.14073 -0.00011 0.00000 -0.00486 -0.00486 3.13760

D30 -0.00578 -0.00010 0.00000 -0.00463 -0.00462 -0.01040

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D157 -3.13994 0.00001 0.00000 0.00032 0.00031 -3.13962

D158 0.00873 -0.00002 0.00000 -0.00050 -0.00050 0.00823

D159 3.09474 -0.00007 0.00000 -0.00256 -0.00256 3.09217

D160 -0.05398 -0.00005 0.00000 -0.00175 -0.00175 -0.05573

D161 -0.00877 -0.00005 0.00000 -0.00156 -0.00157 -0.01034

D162 3.13994 0.00000 0.00000 0.00015 0.00015 3.14009

D163 3.12575 -0.00005 0.00000 -0.00132 -0.00132 3.12442

D164 -0.00873 0.00001 0.00000 0.00039 0.00039 -0.00834

D165 -3.09474 0.00005 0.00000 0.00166 0.00166 -3.09308

D166 0.05398 0.00004 0.00000 0.00140 0.00140 0.05538

D167 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D168 -3.13463 0.00005 0.00000 0.00167 0.00167 -3.13296

D169 3.13463 -0.00005 0.00000 -0.00167 -0.00167 3.13296

D170 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D171 0.00877 0.00005 0.00000 0.00156 0.00157 0.01034

D172 -3.12575 0.00005 0.00000 0.00132 0.00132 -3.12442

D173 -3.13994 0.00000 0.00000 -0.00015 -0.00015 -3.14009

D174 0.00873 -0.00001 0.00000 -0.00039 -0.00039 0.00834

D175 3.09474 -0.00005 0.00000 -0.00166 -0.00166 3.09308

D176 -0.05398 -0.00004 0.00000 -0.00140 -0.00140 -0.05538

D177 0.00877 0.00004 0.00000 0.00164 0.00164 0.01041

D178 -3.13994 0.00001 0.00000 0.00032 0.00031 -3.13962

D179 -3.12575 0.00002 0.00000 0.00083 0.00083 -3.12492

D180 0.00873 -0.00002 0.00000 -0.00050 -0.00050 0.00823

D181 3.09474 -0.00007 0.00000 -0.00256 -0.00256 3.09217

D182 -0.05398 -0.00005 0.00000 -0.00175 -0.00175 -0.05573

D183 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D184 3.13463 -0.00003 0.00000 -0.00129 -0.00128 3.13335

D185 -3.13463 0.00003 0.00000 0.00129 0.00128 -3.13335

D186 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D187 -0.00877 -0.00004 0.00000 -0.00164 -0.00164 -0.01041

D188 3.12575 -0.00002 0.00000 -0.00083 -0.00083 3.12492

D189 3.13994 -0.00001 0.00000 -0.00032 -0.00031 3.13962

D190 -0.00873 0.00002 0.00000 0.00050 0.00050 -0.00823

D191 -3.09474 0.00007 0.00000 0.00256 0.00256 -3.09217

D192 0.05398 0.00005 0.00000 0.00175 0.00175 0.05573

D193 -0.00877 -0.00005 0.00000 -0.00156 -0.00157 -0.01034

D194 3.13994 0.00000 0.00000 0.00015 0.00015 3.14009

D195 3.12575 -0.00005 0.00000 -0.00132 -0.00132 3.12442

D196 -0.00873 0.00001 0.00000 0.00039 0.00039 -0.00834

D197 -3.09474 0.00005 0.00000 0.00166 0.00166 -3.09308

D198 0.05398 0.00004 0.00000 0.00140 0.00140 0.05538

D199 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D200 -3.13463 0.00005 0.00000 0.00167 0.00167 -3.13296

D201 3.13463 -0.00005 0.00000 -0.00167 -0.00167 3.13296

D202 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D203 0.00877 0.00005 0.00000 0.00156 0.00157 0.01034

D204 -3.12575 0.00005 0.00000 0.00132 0.00132 -3.12442

D205 -3.13994 0.00000 0.00000 -0.00015 -0.00015 -3.14009

D206 0.00873 -0.00001 0.00000 -0.00039 -0.00039 0.00834

D207 3.09474 -0.00005 0.00000 -0.00166 -0.00166 3.09308

D208 -0.05398 -0.00004 0.00000 -0.00140 -0.00140 -0.05538

D209 1.09098 0.00014 0.00000 0.00197 0.00197 1.09295

D210 -1.05123 -0.00010 0.00000 -0.00028 -0.00028 -1.05152

D211 -3.12179 0.00001 0.00000 0.00074 0.00074 -3.12105

D212 1.05123 0.00010 0.00000 0.00028 0.00028 1.05152

D213 -1.09098 -0.00014 0.00000 -0.00197 -0.00197 -1.09295

D214 3.12179 -0.00001 0.00000 -0.00074 -0.00074 3.12105

D215 1.09098 0.00023 0.00000 0.00277 0.00277 1.09375

D216 -1.05123 -0.00020 0.00000 -0.00124 -0.00125 -1.05248

D217 -3.12179 0.00001 0.00000 0.00073 0.00073 -3.12106

D218 1.05123 0.00020 0.00000 0.00124 0.00125 1.05248

D219 -1.09098 -0.00023 0.00000 -0.00277 -0.00277 -1.09375

D220 3.12179 -0.00001 0.00000 -0.00073 -0.00073 3.12106

D221 1.05123 0.00010 0.00000 0.00028 0.00028 1.05152

D222 -1.09098 -0.00014 0.00000 -0.00197 -0.00197 -1.09295

D223 3.12179 -0.00001 0.00000 -0.00074 -0.00074 3.12105

D224 1.09098 0.00014 0.00000 0.00197 0.00197 1.09295

D225 -1.05123 -0.00010 0.00000 -0.00028 -0.00028 -1.05152

D226 -3.12179 0.00001 0.00000 0.00074 0.00074 -3.12105

D227 1.09098 0.00023 0.00000 0.00277 0.00277 1.09375

D228 -1.05123 -0.00020 0.00000 -0.00124 -0.00125 -1.05248

D229 -3.12179 0.00001 0.00000 0.00073 0.00073 -3.12106

D230 1.05123 0.00020 0.00000 0.00124 0.00125 1.05248

D231 -1.09098 -0.00023 0.00000 -0.00277 -0.00277 -1.09375

D232 3.12179 -0.00001 0.00000 -0.00073 -0.00073 3.12106

Item Value Threshold Converged?

Maximum Force 0.016200 0.000450 NO

RMS Force 0.002462 0.000300 NO

Maximum Displacement 0.044609 0.001800 NO

RMS Displacement 0.014052 0.001200 NO

Predicted change in Energy=-3.306165D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 5 23:17:10 2019, MaxMem= 1342177280 cpu: 14.7

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

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

Omega: Change in point group or standard orientation.

Old FWG=D02D [O(Zn1),2SGD(N2),X(C40H32N4O8)]

New FWG=C01 [X(C40H32N8O8Zn1)]

RotChk: IX=0 Diff= 1.07D-08

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 -1.130701 2.804700 0.083172

2 7 0 -0.000001 2.042882 -0.010014

3 6 0 1.130699 2.804700 0.083172

4 6 0 0.711614 4.187214 0.268349

5 6 0 -0.711616 4.187214 0.268349

6 7 0 2.409295 2.387118 -0.010250

7 6 0 2.807822 1.129859 -0.087469

8 7 0 2.038152 -0.000001 0.006823

9 6 0 2.807822 -1.129860 -0.087469

10 6 0 4.207105 -0.706766 -0.268399

11 6 0 4.207105 0.706765 -0.268399

12 7 0 -2.409296 2.387118 -0.010250

13 6 0 -4.207104 0.706764 -0.268399

14 6 0 -4.207104 -0.706766 -0.268399

15 6 0 -2.807821 -1.129860 -0.087469

16 7 0 -2.038149 -0.000001 0.006823

17 6 0 -2.807821 1.129858 -0.087469

18 7 0 -2.409295 -2.387118 -0.010250

19 7 0 -0.000001 -2.042879 -0.010014

20 6 0 -1.130701 -2.804699 0.083172

21 6 0 -0.711616 -4.187213 0.268349

22 6 0 0.711614 -4.187213 0.268349

23 6 0 1.130699 -2.804699 0.083172

24 7 0 2.409295 -2.387119 -0.010250

25 30 0 0.000002 0.000002 -0.006612

26 6 0 -5.396138 1.429083 -0.431215

27 6 0 -6.582958 0.696396 -0.580707

28 6 0 -6.582958 -0.696398 -0.580707

29 6 0 -5.396138 -1.429085 -0.431215

30 6 0 1.432530 -5.383934 0.434524

31 6 0 0.700727 -6.565803 0.585805

32 6 0 -0.700729 -6.565803 0.585805

33 6 0 -1.432532 -5.383934 0.434524

34 6 0 5.396139 1.429083 -0.431216

35 6 0 6.582959 0.696396 -0.580708

36 6 0 6.582959 -0.696398 -0.580708

37 6 0 5.396139 -1.429085 -0.431216

38 6 0 -1.432532 5.383935 0.434525

39 6 0 -0.700729 6.565804 0.585806

40 6 0 0.700727 6.565804 0.585806

41 6 0 1.432530 5.383936 0.434525

42 1 0 7.529130 1.204540 -0.707819

43 1 0 7.529130 -1.204542 -0.707819

44 1 0 1.209325 7.511660 0.715187

45 1 0 -1.209327 7.511660 0.715187

46 1 0 -7.529129 1.204539 -0.707819

47 1 0 -7.529129 -1.204542 -0.707819

48 1 0 -1.209327 -7.511658 0.715187

49 1 0 1.209325 -7.511658 0.715187

50 8 0 2.783504 5.319206 0.445600

51 8 0 -2.783506 5.319205 0.445600

52 8 0 5.330639 2.778291 -0.441746

53 8 0 5.330639 -2.778293 -0.441745

54 8 0 2.783504 -5.319204 0.445600

55 8 0 -2.783506 -5.319204 0.445600

56 8 0 -5.330638 -2.778293 -0.441745

57 8 0 -5.330638 2.778291 -0.441745

58 6 0 3.515441 6.538525 0.553395

59 1 0 3.309695 7.049325 1.498696

60 1 0 3.296888 7.210148 -0.282267

61 1 0 4.564598 6.250533 0.521085

62 6 0 6.549405 3.513943 -0.545962

63 1 0 7.062795 3.310862 -1.490195

64 1 0 7.218937 3.297333 0.291634

65 1 0 6.257460 4.561826 -0.513607

66 6 0 6.549404 -3.513945 -0.545962

67 1 0 7.218937 -3.297335 0.291634

68 1 0 7.062795 -3.310864 -1.490195

69 1 0 6.257460 -4.561828 -0.513607

70 6 0 -3.515443 6.538524 0.553395

71 1 0 -3.296890 7.210147 -0.282267

72 1 0 -3.309698 7.049324 1.498696

73 1 0 -4.564600 6.250533 0.521084

74 6 0 -6.549403 3.513943 -0.545961

75 1 0 -7.218935 3.297333 0.291635

76 1 0 -7.062793 3.310862 -1.490195

77 1 0 -6.257459 4.561826 -0.513607

78 6 0 -6.549403 -3.513946 -0.545961

79 1 0 -7.062793 -3.310864 -1.490194

80 1 0 -7.218935 -3.297335 0.291635

81 1 0 -6.257458 -4.561828 -0.513606

82 6 0 -3.515443 -6.538523 0.553394

83 1 0 -3.309698 -7.049323 1.498696

84 1 0 -3.296890 -7.210146 -0.282267

85 1 0 -4.564600 -6.250531 0.521084

86 6 0 3.515441 -6.538523 0.553395

87 1 0 3.296888 -7.210146 -0.282267

88 1 0 3.309696 -7.049324 1.498696

89 1 0 4.564598 -6.250532 0.521084

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

Rotational constants (GHZ): 0.0444043 0.0442009 0.0224212

Leave Link 202 at Fri Jul 5 23:17:13 2019, MaxMem= 1342177280 cpu: 0.1

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

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

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8036.1481062806 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= 89 NActive= 89 NUniq= 89 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= -0.2279751161 Hartrees.

Nuclear repulsion after empirical dispersion term = 8035.9201311645 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6366

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.12D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 344

GePol: Fraction of low-weight points (<1% of avg) = 5.40%

GePol: Cavity surface area = 700.926 Ang\*\*2

GePol: Cavity volume = 799.999 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0089605378 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8035.9111706267 Hartrees.

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

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

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

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44201 LenP2D= 111066.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.47D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 5 23:17:17 2019, MaxMem= 1342177280 cpu: 2.4

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

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0181 S= 1.0060

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2650.02647276156

Leave Link 401 at Fri Jul 5 23:17:34 2019, MaxMem= 1342177280 cpu: 202.7

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 530000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 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= 121577868.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.55D-15 for 508.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.41D-15 for 6347 5977.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.88D-15 for 2102.

Iteration 1 A^-1\*A deviation from orthogonality is 1.39D-08 for 5604 2327.

Iteration 2 A\*A^-1 deviation from unit magnitude is 1.59D-14 for 506.

Iteration 2 A\*A^-1 deviation from orthogonality is 1.02D-14 for 3952 2083.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.33D-15 for 1573.

Iteration 2 A^-1\*A deviation from orthogonality is 4.61D-16 for 5226 1575.

E= -2649.79051588228

DIIS: error= 1.34D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79051588228 IErMin= 1 ErrMin= 1.34D-03

ErrMax= 1.34D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.97D-03 BMatP= 5.97D-03

IDIUse=3 WtCom= 9.87D-01 WtEn= 1.34D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.680 Goal= None Shift= 0.000

Gap= 0.742 Goal= None Shift= 0.000

GapD= 0.680 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=9.15D-05 MaxDP=4.86D-03 OVMax= 2.05D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 9.09D-05 CP: 1.00D+00

E= -2649.79243191161 Delta-E= -0.001916029336 Rises=F Damp=F

DIIS: error= 3.34D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79243191161 IErMin= 2 ErrMin= 3.34D-04

ErrMax= 3.34D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.13D-04 BMatP= 5.97D-03

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.34D-03

Coeff-Com: 0.843D-01 0.916D+00

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

Coeff: 0.840D-01 0.916D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.83D-05 MaxDP=1.08D-03 DE=-1.92D-03 OVMax= 7.64D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.80D-05 CP: 1.00D+00 1.04D+00

E= -2649.79247197407 Delta-E= -0.000040062461 Rises=F Damp=F

DIIS: error= 2.98D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79247197407 IErMin= 3 ErrMin= 2.98D-04

ErrMax= 2.98D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.80D-04 BMatP= 4.13D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.98D-03

Coeff-Com: -0.910D-02 0.446D+00 0.563D+00

Coeff-En: 0.000D+00 0.346D+00 0.654D+00

Coeff: -0.907D-02 0.446D+00 0.563D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.03D-05 MaxDP=5.41D-04 DE=-4.01D-05 OVMax= 5.04D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 7.33D-06 CP: 1.00D+00 1.04D+00 6.03D-01

E= -2649.79253053390 Delta-E= -0.000058559825 Rises=F Damp=F

DIIS: error= 1.78D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79253053390 IErMin= 4 ErrMin= 1.78D-04

ErrMax= 1.78D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.46D-05 BMatP= 2.80D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.78D-03

Coeff-Com: -0.960D-02 0.152D+00 0.325D+00 0.532D+00

Coeff-En: 0.000D+00 0.000D+00 0.617D-01 0.938D+00

Coeff: -0.958D-02 0.152D+00 0.325D+00 0.533D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.48D-06 MaxDP=2.74D-04 DE=-5.86D-05 OVMax= 1.07D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.60D-06 CP: 1.00D+00 1.05D+00 6.69D-01 7.50D-01

E= -2649.79254007842 Delta-E= -0.000009544523 Rises=F Damp=F

DIIS: error= 5.22D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79254007842 IErMin= 5 ErrMin= 5.22D-05

ErrMax= 5.22D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.69D-06 BMatP= 4.46D-05

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

Coeff-Com: -0.434D-02 0.428D-01 0.138D+00 0.304D+00 0.519D+00

Coeff: -0.434D-02 0.428D-01 0.138D+00 0.304D+00 0.519D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.17D-06 MaxDP=7.64D-05 DE=-9.54D-06 OVMax= 6.42D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.10D-07 CP: 1.00D+00 1.05D+00 6.92D-01 8.30D-01 9.34D-01

E= -2649.79254139604 Delta-E= -0.000001317623 Rises=F Damp=F

DIIS: error= 2.18D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79254139604 IErMin= 6 ErrMin= 2.18D-05

ErrMax= 2.18D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.01D-07 BMatP= 4.69D-06

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

Coeff-Com: 0.466D-03-0.217D-01-0.160D-01 0.378D-02 0.211D+00 0.822D+00

Coeff: 0.466D-03-0.217D-01-0.160D-01 0.378D-02 0.211D+00 0.822D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=8.72D-07 MaxDP=4.58D-05 DE=-1.32D-06 OVMax= 9.02D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.08D-07 CP: 1.00D+00 1.05D+00 7.10D-01 8.73D-01 1.13D+00

CP: 9.92D-01

E= -2649.79254175288 Delta-E= -0.000000356840 Rises=F Damp=F

DIIS: error= 1.04D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79254175288 IErMin= 7 ErrMin= 1.04D-05

ErrMax= 1.04D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.36D-07 BMatP= 5.01D-07

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

Coeff-Com: 0.107D-02-0.185D-01-0.336D-01-0.598D-01-0.185D-01 0.395D+00

Coeff-Com: 0.735D+00

Coeff: 0.107D-02-0.185D-01-0.336D-01-0.598D-01-0.185D-01 0.395D+00

Coeff: 0.735D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=4.50D-07 MaxDP=3.36D-05 DE=-3.57D-07 OVMax= 4.42D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.56D-07 CP: 1.00D+00 1.05D+00 7.15D-01 8.98D-01 1.20D+00

CP: 1.24D+00 1.12D+00

E= -2649.79254183769 Delta-E= -0.000000084809 Rises=F Damp=F

DIIS: error= 5.44D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.79254183769 IErMin= 8 ErrMin= 5.44D-06

ErrMax= 5.44D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.24D-08 BMatP= 1.36D-07

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

Coeff-Com: 0.479D-03-0.527D-02-0.151D-01-0.371D-01-0.699D-01 0.273D-01

Coeff-Com: 0.421D+00 0.679D+00

Coeff: 0.479D-03-0.527D-02-0.151D-01-0.371D-01-0.699D-01 0.273D-01

Coeff: 0.421D+00 0.679D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=2.13D-07 MaxDP=1.42D-05 DE=-8.48D-08 OVMax= 1.89D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.09D-07 CP: 1.00D+00 1.05D+00 7.17D-01 9.09D-01 1.24D+00

CP: 1.31D+00 1.32D+00 8.89D-01

E= -2649.79254185791 Delta-E= -0.000000020214 Rises=F Damp=F

DIIS: error= 2.29D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.79254185791 IErMin= 9 ErrMin= 2.29D-06

ErrMax= 2.29D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.11D-09 BMatP= 4.24D-08

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

Coeff-Com: 0.388D-05 0.193D-02 0.648D-03-0.552D-02-0.314D-01-0.655D-01

Coeff-Com: 0.547D-01 0.375D+00 0.670D+00

Coeff: 0.388D-05 0.193D-02 0.648D-03-0.552D-02-0.314D-01-0.655D-01

Coeff: 0.547D-01 0.375D+00 0.670D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=8.01D-08 MaxDP=5.06D-06 DE=-2.02D-08 OVMax= 7.67D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 5.07D-08 CP: 1.00D+00 1.05D+00 7.17D-01 9.10D-01 1.25D+00

CP: 1.34D+00 1.38D+00 1.04D+00 9.73D-01

E= -2649.79254186196 Delta-E= -0.000000004051 Rises=F Damp=F

DIIS: error= 1.00D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -2649.79254186196 IErMin=10 ErrMin= 1.00D-06

ErrMax= 1.00D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.13D-09 BMatP= 9.11D-09

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

Coeff-Com: -0.933D-04 0.218D-02 0.351D-02 0.418D-02-0.378D-02-0.421D-01

Coeff-Com: -0.590D-01 0.759D-01 0.375D+00 0.644D+00

Coeff: -0.933D-04 0.218D-02 0.351D-02 0.418D-02-0.378D-02-0.421D-01

Coeff: -0.590D-01 0.759D-01 0.375D+00 0.644D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=3.46D-08 MaxDP=2.33D-06 DE=-4.05D-09 OVMax= 2.06D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.43D-08 CP: 1.00D+00 1.05D+00 7.17D-01 9.10D-01 1.26D+00

CP: 1.35D+00 1.41D+00 1.06D+00 1.10D+00 1.01D+00

E= -2649.79254186255 Delta-E= -0.000000000595 Rises=F Damp=F

DIIS: error= 5.47D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -2649.79254186255 IErMin=11 ErrMin= 5.47D-07

ErrMax= 5.47D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.39D-10 BMatP= 2.13D-09

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

Coeff-Com: -0.495D-04 0.635D-03 0.160D-02 0.336D-02 0.542D-02-0.590D-02

Coeff-Com: -0.434D-01-0.435D-01 0.436D-01 0.341D+00 0.698D+00

Coeff: -0.495D-04 0.635D-03 0.160D-02 0.336D-02 0.542D-02-0.590D-02

Coeff: -0.434D-01-0.435D-01 0.436D-01 0.341D+00 0.698D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=1.66D-08 MaxDP=1.31D-06 DE=-5.95D-10 OVMax= 7.86D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.16D-08 CP: 1.00D+00 1.05D+00 7.17D-01 9.10D-01 1.26D+00

CP: 1.35D+00 1.42D+00 1.08D+00 1.16D+00 1.15D+00

CP: 9.33D-01

E= -2649.79254186280 Delta-E= -0.000000000249 Rises=F Damp=F

DIIS: error= 2.50D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -2649.79254186280 IErMin=12 ErrMin= 2.50D-07

ErrMax= 2.50D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.34D-10 BMatP= 4.39D-10

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

Coeff-Com: -0.467D-05-0.216D-03-0.305D-04 0.826D-03 0.408D-02 0.771D-02

Coeff-Com: -0.922D-02-0.434D-01-0.748D-01 0.148D-01 0.409D+00 0.692D+00

Coeff: -0.467D-05-0.216D-03-0.305D-04 0.826D-03 0.408D-02 0.771D-02

Coeff: -0.922D-02-0.434D-01-0.748D-01 0.148D-01 0.409D+00 0.692D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=8.85D-09 MaxDP=6.84D-07 DE=-2.49D-10 OVMax= 4.29D-06

Error on total polarization charges = 0.07276

SCF Done: E(UB3LYP) = -2649.79254186 A.U. after 12 cycles

NFock= 12 Conv=0.89D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0174 S= 1.0058

<L.S>= 0.000000000000E+00

KE= 2.690127236331D+03 PE=-2.235045843247D+04 EE= 8.974627483645D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.62

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0174, after 2.0002

Leave Link 502 at Fri Jul 5 23:27:29 2019, MaxMem= 1342177280 cpu: 7031.4

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

Compute integral first derivatives.

... and contract with generalized density number 0.

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

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44201 LenP2D= 111066.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 275

Leave Link 701 at Fri Jul 5 23:27:48 2019, MaxMem= 1342177280 cpu: 217.6

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

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

Leave Link 702 at Fri Jul 5 23:27:48 2019, MaxMem= 1342177280 cpu: 0.2

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

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Fri Jul 5 23:29:19 2019, MaxMem= 1342177280 cpu: 1093.0

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

Dipole = 3.51056699D-06 1.81333142D-06-1.60790574D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.008183985 0.005126689 0.001739486

2 7 0.000000396 -0.002069632 -0.002017829

3 6 -0.008183499 0.005126308 0.001739428

4 6 0.002616802 -0.002662173 0.000015989

5 6 -0.002616751 -0.002662110 0.000016001

6 7 0.006450179 -0.005970934 -0.001818142

7 6 -0.003763463 0.006741881 0.000929279

8 7 -0.000488336 0.000000437 0.001147079

9 6 -0.003763006 -0.006741360 0.000929207

10 6 0.003212452 0.002624066 -0.000639278

11 6 0.003212413 -0.002624024 -0.000639273

12 7 -0.006450447 -0.005970717 -0.001818134

13 6 -0.003212430 -0.002623970 -0.000639279

14 6 -0.003212469 0.002624012 -0.000639283

15 6 0.003762885 -0.006740822 0.000929198

16 7 0.000487650 0.000000437 0.001146990

17 6 0.003763341 0.006741343 0.000929270

18 7 -0.006450541 0.005970303 -0.001818132

19 7 0.000000396 0.002068945 -0.002017742

20 6 0.008184418 -0.005126753 0.001739492

21 6 -0.002616792 0.002662092 0.000016005

22 6 0.002616843 0.002662155 0.000015994

23 6 -0.008183932 -0.005126371 0.001739432

24 7 0.006450273 0.005970520 -0.001818140

25 30 -0.000000344 -0.000000318 -0.000385093

26 6 0.003204054 0.002894445 0.000551553

27 6 -0.001316972 -0.002315121 -0.000188944

28 6 -0.001316971 0.002315125 -0.000188944

29 6 0.003204067 -0.002894429 0.000551555

30 6 0.001403835 -0.000292260 -0.000051923

31 6 -0.000270586 -0.000367389 0.000013164

32 6 0.000270588 -0.000367399 0.000013164

33 6 -0.001403826 -0.000292234 -0.000051927

34 6 -0.003204062 0.002894402 0.000551554

35 6 0.001316984 -0.002315161 -0.000188946

36 6 0.001316983 0.002315164 -0.000188947

37 6 -0.003204074 -0.002894386 0.000551556

38 6 -0.001403783 0.000292232 -0.000051927

39 6 0.000270620 0.000367409 0.000013167

40 6 -0.000270617 0.000367400 0.000013165

41 6 0.001403793 0.000292259 -0.000051923

42 1 -0.000017060 0.000282465 0.000016576

43 1 -0.000017059 -0.000282465 0.000016576

44 1 -0.000058106 0.000029375 0.000003547

45 1 0.000058106 0.000029375 0.000003547

46 1 0.000017061 0.000282467 0.000016576

47 1 0.000017060 -0.000282467 0.000016576

48 1 0.000058104 -0.000029375 0.000003547

49 1 -0.000058104 -0.000029374 0.000003547

50 8 -0.001386099 0.000812088 0.000109994

51 8 0.001386110 0.000812094 0.000109986

52 8 0.001325699 -0.001009654 -0.000170371

53 8 0.001325705 0.001009657 -0.000170363

54 8 -0.001386093 -0.000812128 0.000109991

55 8 0.001386104 -0.000812134 0.000109984

56 8 -0.001325750 0.001009649 -0.000170361

57 8 -0.001325745 -0.001009646 -0.000170369

58 6 0.000305256 -0.000447594 -0.000056610

59 1 0.000016534 -0.000012927 -0.000016528

60 1 -0.000008034 -0.000032150 0.000022244

61 1 0.000090515 0.000150163 0.000005443

62 6 -0.000382452 0.000318944 0.000063497

63 1 -0.000037378 -0.000026706 0.000004780

64 1 -0.000051786 -0.000058983 -0.000002602

65 1 0.000137544 0.000103873 0.000000550

66 6 -0.000382455 -0.000318944 0.000063498

67 1 -0.000051786 0.000058983 -0.000002602

68 1 -0.000037378 0.000026707 0.000004780

69 1 0.000137546 -0.000103873 0.000000550

70 6 -0.000305257 -0.000447594 -0.000056610

71 1 0.000008034 -0.000032150 0.000022244

72 1 -0.000016533 -0.000012927 -0.000016528

73 1 -0.000090514 0.000150165 0.000005444

74 6 0.000382464 0.000318936 0.000063498

75 1 0.000051783 -0.000058983 -0.000002602

76 1 0.000037375 -0.000026707 0.000004779

77 1 -0.000137543 0.000103873 0.000000550

78 6 0.000382467 -0.000318936 0.000063498

79 1 0.000037374 0.000026707 0.000004779

80 1 0.000051783 0.000058984 -0.000002601

81 1 -0.000137545 -0.000103873 0.000000550

82 6 -0.000305250 0.000447605 -0.000056611

83 1 -0.000016533 0.000012924 -0.000016527

84 1 0.000008034 0.000032148 0.000022244

85 1 -0.000090514 -0.000150164 0.000005443

86 6 0.000305249 0.000447604 -0.000056611

87 1 -0.000008034 0.000032147 0.000022244

88 1 0.000016533 0.000012924 -0.000016527

89 1 0.000090514 -0.000150162 0.000005443

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

Cartesian Forces: Max 0.008184418 RMS 0.002149136

Leave Link 716 at Fri Jul 5 23:29:19 2019, MaxMem= 1342177280 cpu: 2.1

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.005405686 RMS 0.000803346

Search for a local minimum.

Step number 2 out of a maximum of 518

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

RMS Force = .80335D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 2

DE= -3.99D-03 DEPred=-3.31D-03 R= 1.21D+00

TightC=F SS= 1.41D+00 RLast= 1.43D-01 DXNew= 5.0454D-01 4.3035D-01

Trust test= 1.21D+00 RLast= 1.43D-01 DXMaxT set to 4.30D-01

ITU= 1 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.01316 0.01316 0.01316 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01543 0.01546

Eigenvalues --- 0.01565 0.01567 0.01580 0.01598 0.01616

Eigenvalues --- 0.01620 0.01707 0.01710 0.01711 0.01715

Eigenvalues --- 0.01723 0.01829 0.01835 0.01861 0.01861

Eigenvalues --- 0.01887 0.01912 0.01921 0.01923 0.01923

Eigenvalues --- 0.01924 0.01991 0.01995 0.02021 0.02021

Eigenvalues --- 0.02021 0.02022 0.02053 0.02053 0.02053

Eigenvalues --- 0.02053 0.02057 0.02057 0.02057 0.02057

Eigenvalues --- 0.02067 0.02067 0.02067 0.02067 0.02070

Eigenvalues --- 0.02070 0.02070 0.02070 0.02083 0.02083

Eigenvalues --- 0.02083 0.02083 0.02172 0.02259 0.02260

Eigenvalues --- 0.02260 0.02260 0.02260 0.02260 0.02260

Eigenvalues --- 0.02260 0.02344 0.02344 0.02351 0.02371

Eigenvalues --- 0.09979 0.09979 0.09979 0.09982 0.09983

Eigenvalues --- 0.09983 0.09983 0.09999 0.10661 0.10661

Eigenvalues --- 0.10661 0.10661 0.10669 0.10669 0.10669

Eigenvalues --- 0.10669 0.13510 0.13512 0.15390 0.15990

Eigenvalues --- 0.15999 0.15999 0.15999 0.15999 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16062 0.17499 0.21808 0.21866 0.22474

Eigenvalues --- 0.22475 0.22477 0.22478 0.23116 0.24507

Eigenvalues --- 0.24512 0.24512 0.24602 0.24605 0.24701

Eigenvalues --- 0.24782 0.24792 0.24910 0.24922 0.24946

Eigenvalues --- 0.24970 0.24993 0.24994 0.24996 0.24996

Eigenvalues --- 0.24997 0.24998 0.24998 0.24998 0.24999

Eigenvalues --- 0.24999 0.24999 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.26123

Eigenvalues --- 0.32320 0.33646 0.33656 0.33704 0.33731

Eigenvalues --- 0.34063 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34063 0.34071 0.34081 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34081

Eigenvalues --- 0.34147 0.34656 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34686 0.34686 0.34911

Eigenvalues --- 0.34958 0.35150 0.35493 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35632 0.35633

Eigenvalues --- 0.36032 0.37089 0.37126 0.37151 0.41209

Eigenvalues --- 0.41215 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41215 0.41241 0.41395 0.41397 0.41403

Eigenvalues --- 0.41409 0.41411 0.42471 0.42488 0.42778

Eigenvalues --- 0.43565 0.44078 0.44564 0.44570 0.44829

Eigenvalues --- 0.44910 0.44930 0.44998 0.45000 0.45001

Eigenvalues --- 0.45003 0.45300 0.45366 0.45367 0.47038

Eigenvalues --- 0.47410 0.48070 0.48764 0.49329 0.49368

Eigenvalues --- 0.49883 0.51496 0.53554 0.53554 0.53554

Eigenvalues --- 0.53554 0.53554 0.53554 0.53617 0.54506

Eigenvalues --- 0.55021 0.55022 0.56106 0.57435 0.57444

Eigenvalues --- 0.57586

RFO step: Lambda=-9.21473358D-04 EMin= 1.31553589D-02

Quartic linear search produced a step of 0.28416.

Iteration 1 RMS(Cart)= 0.01972622 RMS(Int)= 0.00005570

Iteration 2 RMS(Cart)= 0.00019635 RMS(Int)= 0.00001470

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00001470

ITry= 1 IFail=0 DXMaxC= 7.95D-02 DCOld= 1.00D+10 DXMaxT= 4.30D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.58246 -0.00065 -0.00024 -0.00150 -0.00174 2.58071

R2 2.75231 -0.00187 -0.00653 -0.00309 -0.00962 2.74268

R3 2.54791 0.00541 0.00640 0.00871 0.01508 2.56300

R4 2.58246 -0.00065 -0.00024 -0.00150 -0.00174 2.58071

R5 3.86049 0.00055 -0.00021 0.00529 0.00511 3.86560

R6 2.75231 -0.00187 -0.00653 -0.00309 -0.00962 2.74268

R7 2.54792 0.00540 0.00640 0.00871 0.01508 2.56300

R8 2.68952 0.00120 0.00145 0.00323 0.00467 2.69419

R9 2.65873 0.00107 -0.00039 0.00338 0.00300 2.66172

R10 2.65873 0.00107 -0.00039 0.00338 0.00300 2.66172

R11 2.49665 -0.00401 -0.00817 -0.00446 -0.01265 2.48400

R12 2.58959 0.00153 0.00179 0.00301 0.00482 2.59441

R13 2.78357 0.00261 0.00235 0.00794 0.01028 2.79386

R14 2.58959 0.00153 0.00179 0.00301 0.00482 2.59441

R15 3.85163 -0.00026 -0.00272 -0.00241 -0.00507 3.84655

R16 2.78357 0.00261 0.00235 0.00794 0.01028 2.79386

R17 2.49665 -0.00401 -0.00817 -0.00446 -0.01265 2.48400

R18 2.67119 -0.00029 -0.00375 0.00065 -0.00312 2.66807

R19 2.64700 -0.00029 -0.00372 0.00106 -0.00266 2.64435

R20 2.64700 -0.00029 -0.00372 0.00106 -0.00266 2.64435

R21 2.49665 -0.00401 -0.00817 -0.00446 -0.01265 2.48400

R22 2.67119 -0.00029 -0.00375 0.00065 -0.00312 2.66807

R23 2.78357 0.00261 0.00235 0.00794 0.01028 2.79386

R24 2.64700 -0.00029 -0.00372 0.00106 -0.00266 2.64435

R25 2.78357 0.00261 0.00235 0.00794 0.01028 2.79386

R26 2.64700 -0.00029 -0.00372 0.00106 -0.00266 2.64435

R27 2.58959 0.00153 0.00179 0.00301 0.00482 2.59441

R28 2.49665 -0.00401 -0.00817 -0.00446 -0.01264 2.48400

R29 2.58959 0.00153 0.00179 0.00301 0.00482 2.59441

R30 3.85163 -0.00026 -0.00272 -0.00241 -0.00507 3.84656

R31 2.54791 0.00541 0.00640 0.00872 0.01508 2.56300

R32 2.58246 -0.00065 -0.00024 -0.00150 -0.00174 2.58071

R33 2.58246 -0.00065 -0.00024 -0.00150 -0.00174 2.58071

R34 3.86049 0.00055 -0.00020 0.00529 0.00511 3.86561

R35 2.75231 -0.00187 -0.00653 -0.00309 -0.00962 2.74268

R36 2.68952 0.00120 0.00145 0.00323 0.00467 2.69419

R37 2.65873 0.00107 -0.00039 0.00339 0.00300 2.66172

R38 2.75231 -0.00187 -0.00653 -0.00309 -0.00962 2.74268

R39 2.65873 0.00107 -0.00039 0.00339 0.00300 2.66172

R40 2.54791 0.00540 0.00640 0.00871 0.01508 2.56300

R41 2.65082 0.00176 0.00101 0.00449 0.00550 2.65632

R42 2.55271 -0.00072 -0.00332 0.00004 -0.00329 2.54943

R43 2.63200 -0.00081 -0.00573 0.00090 -0.00482 2.62717

R44 2.04371 0.00012 -0.00082 0.00086 0.00004 2.04374

R45 2.65082 0.00176 0.00101 0.00449 0.00550 2.65632

R46 2.04371 0.00012 -0.00082 0.00086 0.00004 2.04374

R47 2.55271 -0.00072 -0.00332 0.00004 -0.00329 2.54943

R48 2.64240 0.00048 -0.00138 0.00198 0.00060 2.64300

R49 2.55599 -0.00100 -0.00239 -0.00113 -0.00353 2.55246

R50 2.64837 -0.00006 -0.00108 0.00021 -0.00086 2.64751

R51 2.04410 0.00000 -0.00071 0.00038 -0.00033 2.04377

R52 2.64240 0.00048 -0.00138 0.00198 0.00060 2.64300

R53 2.04410 0.00000 -0.00071 0.00038 -0.00033 2.04377

R54 2.55599 -0.00100 -0.00239 -0.00113 -0.00353 2.55246

R55 2.65082 0.00176 0.00101 0.00449 0.00550 2.65632

R56 2.55271 -0.00072 -0.00332 0.00004 -0.00329 2.54943

R57 2.63200 -0.00081 -0.00573 0.00090 -0.00482 2.62717

R58 2.04371 0.00012 -0.00082 0.00086 0.00004 2.04374

R59 2.65082 0.00176 0.00101 0.00449 0.00550 2.65632

R60 2.04371 0.00012 -0.00082 0.00086 0.00004 2.04374

R61 2.55271 -0.00072 -0.00332 0.00004 -0.00329 2.54943

R62 2.64240 0.00048 -0.00138 0.00198 0.00060 2.64300

R63 2.55599 -0.00100 -0.00239 -0.00113 -0.00353 2.55246

R64 2.64837 -0.00006 -0.00108 0.00021 -0.00086 2.64751

R65 2.04410 0.00000 -0.00071 0.00038 -0.00033 2.04377

R66 2.64240 0.00048 -0.00138 0.00198 0.00060 2.64300

R67 2.04410 0.00000 -0.00071 0.00038 -0.00033 2.04377

R68 2.55599 -0.00100 -0.00239 -0.00113 -0.00353 2.55246

R69 2.69516 -0.00009 -0.00119 0.00036 -0.00083 2.69433

R70 2.69516 -0.00009 -0.00119 0.00036 -0.00083 2.69433

R71 2.69737 -0.00012 -0.00056 -0.00006 -0.00062 2.69675

R72 2.69737 -0.00012 -0.00056 -0.00006 -0.00062 2.69675

R73 2.69516 -0.00009 -0.00119 0.00036 -0.00083 2.69433

R74 2.69516 -0.00009 -0.00119 0.00036 -0.00083 2.69433

R75 2.69737 -0.00012 -0.00056 -0.00006 -0.00062 2.69675

R76 2.69737 -0.00012 -0.00056 -0.00006 -0.00062 2.69675

R77 2.06737 -0.00002 -0.00130 0.00061 -0.00068 2.06668

R78 2.06765 -0.00004 -0.00130 0.00057 -0.00073 2.06692

R79 2.05686 0.00005 -0.00142 0.00094 -0.00048 2.05639

R80 2.06697 -0.00002 -0.00141 0.00070 -0.00071 2.06626

R81 2.06730 -0.00002 -0.00140 0.00068 -0.00073 2.06657

R82 2.05654 0.00006 -0.00152 0.00105 -0.00046 2.05607

R83 2.06730 -0.00002 -0.00140 0.00068 -0.00073 2.06657

R84 2.06697 -0.00002 -0.00141 0.00070 -0.00071 2.06626

R85 2.05654 0.00006 -0.00152 0.00105 -0.00046 2.05607

R86 2.06765 -0.00004 -0.00130 0.00057 -0.00073 2.06692

R87 2.06737 -0.00002 -0.00130 0.00061 -0.00068 2.06668

R88 2.05686 0.00005 -0.00142 0.00094 -0.00048 2.05639

R89 2.06730 -0.00002 -0.00140 0.00068 -0.00073 2.06657

R90 2.06697 -0.00002 -0.00141 0.00070 -0.00071 2.06626

R91 2.05654 0.00006 -0.00152 0.00105 -0.00046 2.05607

R92 2.06697 -0.00002 -0.00141 0.00070 -0.00071 2.06626

R93 2.06730 -0.00002 -0.00140 0.00068 -0.00073 2.06657

R94 2.05654 0.00006 -0.00152 0.00105 -0.00046 2.05607

R95 2.06737 -0.00002 -0.00130 0.00061 -0.00068 2.06668

R96 2.06765 -0.00004 -0.00130 0.00057 -0.00073 2.06692

R97 2.05686 0.00005 -0.00142 0.00094 -0.00048 2.05639

R98 2.06765 -0.00004 -0.00130 0.00057 -0.00073 2.06692

R99 2.06737 -0.00002 -0.00130 0.00061 -0.00068 2.06668

R100 2.05686 0.00005 -0.00142 0.00094 -0.00048 2.05639

A1 1.87523 0.00147 -0.00217 0.00877 0.00662 1.88185

A2 2.22338 -0.00159 0.00136 -0.00871 -0.00738 2.21600

A3 2.18421 0.00011 0.00081 -0.00019 0.00063 2.18484

A4 1.94891 -0.00161 0.00234 -0.01026 -0.00798 1.94093

A5 2.16199 0.00078 -0.00131 0.00394 0.00258 2.16456

A6 2.16199 0.00078 -0.00131 0.00395 0.00258 2.16456

A7 1.87523 0.00147 -0.00217 0.00877 0.00662 1.88185

A8 2.22338 -0.00159 0.00136 -0.00871 -0.00738 2.21601

A9 2.18421 0.00011 0.00081 -0.00019 0.00063 2.18484

A10 1.86267 -0.00067 0.00100 -0.00357 -0.00259 1.86007

A11 2.31173 0.00091 -0.00033 0.00414 0.00382 2.31556

A12 2.10877 -0.00024 -0.00067 -0.00056 -0.00122 2.10755

A13 1.86267 -0.00067 0.00100 -0.00357 -0.00259 1.86007

A14 2.31173 0.00091 -0.00033 0.00414 0.00382 2.31556

A15 2.10877 -0.00024 -0.00067 -0.00056 -0.00122 2.10755

A16 2.19547 0.00011 -0.00321 0.00279 -0.00047 2.19500

A17 2.22834 0.00092 0.00277 0.00290 0.00566 2.23400

A18 2.17374 -0.00029 -0.00217 -0.00016 -0.00236 2.17138

A19 1.88092 -0.00063 -0.00055 -0.00276 -0.00329 1.87763

A20 1.93865 0.00050 -0.00058 0.00367 0.00302 1.94167

A21 2.16662 -0.00027 0.00001 -0.00270 -0.00273 2.16389

A22 2.16662 -0.00027 0.00001 -0.00270 -0.00273 2.16390

A23 1.88092 -0.00063 -0.00055 -0.00276 -0.00329 1.87763

A24 2.22834 0.00092 0.00277 0.00290 0.00566 2.23400

A25 2.17374 -0.00029 -0.00217 -0.00016 -0.00235 2.17138

A26 1.86213 0.00038 0.00085 0.00096 0.00179 1.86392

A27 2.30843 -0.00096 -0.00126 -0.00342 -0.00469 2.30374

A28 2.11259 0.00057 0.00042 0.00250 0.00292 2.11551

A29 1.86213 0.00038 0.00085 0.00096 0.00179 1.86392

A30 2.30843 -0.00096 -0.00126 -0.00342 -0.00469 2.30374

A31 2.11259 0.00057 0.00042 0.00250 0.00292 2.11551

A32 2.19547 0.00012 -0.00321 0.00279 -0.00047 2.19500

A33 1.86213 0.00038 0.00085 0.00096 0.00179 1.86392

A34 2.11259 0.00057 0.00042 0.00250 0.00292 2.11551

A35 2.30843 -0.00096 -0.00126 -0.00342 -0.00469 2.30374

A36 1.86213 0.00038 0.00085 0.00096 0.00179 1.86392

A37 2.11259 0.00057 0.00042 0.00250 0.00292 2.11551

A38 2.30843 -0.00096 -0.00126 -0.00342 -0.00469 2.30374

A39 1.88092 -0.00063 -0.00055 -0.00276 -0.00329 1.87763

A40 2.17374 -0.00028 -0.00217 -0.00016 -0.00235 2.17138

A41 2.22834 0.00092 0.00277 0.00290 0.00566 2.23400

A42 1.93864 0.00050 -0.00058 0.00367 0.00302 1.94167

A43 2.16663 -0.00027 0.00001 -0.00270 -0.00273 2.16390

A44 2.16662 -0.00027 0.00001 -0.00270 -0.00273 2.16389

A45 2.17374 -0.00028 -0.00217 -0.00016 -0.00235 2.17138

A46 2.22834 0.00092 0.00277 0.00290 0.00566 2.23400

A47 1.88092 -0.00063 -0.00055 -0.00276 -0.00329 1.87763

A48 2.19547 0.00012 -0.00321 0.00279 -0.00046 2.19500

A49 1.94891 -0.00160 0.00234 -0.01026 -0.00798 1.94093

A50 2.16199 0.00078 -0.00131 0.00394 0.00258 2.16456

A51 2.16199 0.00078 -0.00131 0.00395 0.00258 2.16456

A52 2.22338 -0.00159 0.00136 -0.00871 -0.00738 2.21600

A53 2.18421 0.00011 0.00080 -0.00019 0.00063 2.18484

A54 1.87523 0.00147 -0.00217 0.00877 0.00662 1.88185

A55 1.86267 -0.00067 0.00100 -0.00357 -0.00259 1.86007

A56 2.31173 0.00091 -0.00033 0.00414 0.00382 2.31556

A57 2.10877 -0.00024 -0.00067 -0.00056 -0.00122 2.10755

A58 1.86267 -0.00067 0.00100 -0.00357 -0.00259 1.86007

A59 2.10877 -0.00024 -0.00067 -0.00056 -0.00122 2.10755

A60 2.31173 0.00091 -0.00033 0.00414 0.00382 2.31556

A61 1.87523 0.00147 -0.00217 0.00877 0.00662 1.88185

A62 2.22338 -0.00159 0.00136 -0.00871 -0.00738 2.21601

A63 2.18421 0.00011 0.00080 -0.00019 0.00063 2.18484

A64 2.19547 0.00012 -0.00321 0.00279 -0.00047 2.19500

A65 1.57081 0.00000 0.00000 0.00001 0.00002 1.57083

A66 1.57081 0.00000 0.00000 0.00001 0.00002 1.57082

A67 1.57081 0.00000 0.00000 0.00001 0.00002 1.57082

A68 1.57080 0.00000 0.00000 0.00002 0.00002 1.57082

A69 2.05018 -0.00079 -0.00020 -0.00414 -0.00434 2.04584

A70 2.06553 0.00123 0.00034 0.00621 0.00654 2.07207

A71 2.16746 -0.00044 -0.00014 -0.00205 -0.00220 2.16526

A72 2.12037 0.00022 -0.00023 0.00166 0.00143 2.12179

A73 2.10286 -0.00037 0.00056 -0.00319 -0.00262 2.10024

A74 2.05993 0.00015 -0.00034 0.00155 0.00121 2.06114

A75 2.12037 0.00022 -0.00023 0.00166 0.00143 2.12179

A76 2.05993 0.00015 -0.00034 0.00155 0.00121 2.06114

A77 2.10286 -0.00037 0.00056 -0.00319 -0.00262 2.10024

A78 2.05018 -0.00079 -0.00020 -0.00414 -0.00434 2.04584

A79 2.06553 0.00123 0.00034 0.00621 0.00654 2.07207

A80 2.16746 -0.00044 -0.00014 -0.00205 -0.00220 2.16526

A81 2.05279 0.00007 0.00054 0.00015 0.00069 2.05347

A82 2.06242 -0.00002 -0.00055 0.00017 -0.00037 2.06205

A83 2.16796 -0.00005 0.00000 -0.00031 -0.00031 2.16765

A84 2.12158 0.00017 0.00012 0.00041 0.00053 2.12211

A85 2.10127 -0.00002 0.00011 0.00023 0.00034 2.10161

A86 2.06030 -0.00015 -0.00023 -0.00064 -0.00087 2.05943

A87 2.12158 0.00017 0.00012 0.00041 0.00053 2.12211

A88 2.06030 -0.00015 -0.00023 -0.00064 -0.00087 2.05943

A89 2.10127 -0.00002 0.00011 0.00023 0.00034 2.10161

A90 2.05279 0.00007 0.00054 0.00015 0.00069 2.05347

A91 2.06242 -0.00002 -0.00055 0.00017 -0.00037 2.06205

A92 2.16796 -0.00005 0.00000 -0.00031 -0.00031 2.16765

A93 2.05018 -0.00079 -0.00020 -0.00414 -0.00434 2.04584

A94 2.06553 0.00123 0.00034 0.00621 0.00654 2.07207

A95 2.16746 -0.00044 -0.00014 -0.00205 -0.00220 2.16526

A96 2.12037 0.00022 -0.00023 0.00166 0.00143 2.12179

A97 2.10286 -0.00037 0.00056 -0.00319 -0.00262 2.10024

A98 2.05993 0.00015 -0.00034 0.00155 0.00121 2.06114

A99 2.12037 0.00022 -0.00023 0.00166 0.00143 2.12179

A100 2.05993 0.00015 -0.00034 0.00155 0.00121 2.06114

A101 2.10286 -0.00037 0.00056 -0.00319 -0.00262 2.10024

A102 2.05018 -0.00079 -0.00020 -0.00414 -0.00434 2.04584

A103 2.06553 0.00123 0.00034 0.00621 0.00654 2.07207

A104 2.16746 -0.00044 -0.00014 -0.00205 -0.00220 2.16526

A105 2.05279 0.00007 0.00054 0.00015 0.00069 2.05347

A106 2.06242 -0.00002 -0.00055 0.00017 -0.00037 2.06205

A107 2.16796 -0.00005 0.00000 -0.00031 -0.00031 2.16765

A108 2.12158 0.00017 0.00012 0.00041 0.00053 2.12211

A109 2.10127 -0.00002 0.00011 0.00023 0.00034 2.10161

A110 2.06030 -0.00015 -0.00023 -0.00064 -0.00087 2.05943

A111 2.12158 0.00017 0.00012 0.00041 0.00053 2.12211

A112 2.06030 -0.00015 -0.00023 -0.00064 -0.00087 2.05943

A113 2.10127 -0.00002 0.00011 0.00023 0.00034 2.10161

A114 2.05279 0.00007 0.00054 0.00015 0.00069 2.05347

A115 2.06242 -0.00002 -0.00055 0.00017 -0.00037 2.06205

A116 2.16796 -0.00005 0.00000 -0.00031 -0.00031 2.16765

A117 2.06270 0.00106 -0.00009 0.00545 0.00536 2.06805

A118 2.06270 0.00106 -0.00009 0.00545 0.00536 2.06805

A119 2.06454 0.00079 0.00043 0.00378 0.00422 2.06876

A120 2.06454 0.00079 0.00043 0.00378 0.00422 2.06876

A121 2.06270 0.00106 -0.00009 0.00545 0.00536 2.06805

A122 2.06270 0.00106 -0.00009 0.00545 0.00536 2.06805

A123 2.06454 0.00079 0.00043 0.00378 0.00422 2.06876

A124 2.06454 0.00079 0.00043 0.00378 0.00422 2.06876

A125 1.94762 -0.00003 0.00051 -0.00061 -0.00010 1.94752

A126 1.94394 -0.00008 0.00069 -0.00110 -0.00041 1.94353

A127 1.84027 0.00027 -0.00061 0.00269 0.00207 1.84235

A128 1.91322 -0.00001 -0.00017 -0.00027 -0.00044 1.91278

A129 1.90759 -0.00008 -0.00021 -0.00032 -0.00053 1.90707

A130 1.90951 -0.00007 -0.00024 -0.00029 -0.00054 1.90898

A131 1.94777 -0.00009 0.00055 -0.00117 -0.00062 1.94714

A132 1.94402 -0.00015 0.00071 -0.00174 -0.00103 1.94299

A133 1.83903 0.00030 -0.00097 0.00316 0.00220 1.84123

A134 1.91445 0.00002 0.00018 -0.00035 -0.00018 1.91428

A135 1.90748 -0.00004 -0.00024 0.00013 -0.00011 1.90736

A136 1.90930 -0.00003 -0.00030 0.00015 -0.00016 1.90914

A137 1.94402 -0.00015 0.00071 -0.00174 -0.00103 1.94299

A138 1.94777 -0.00009 0.00055 -0.00117 -0.00062 1.94714

A139 1.83903 0.00030 -0.00097 0.00316 0.00220 1.84123

A140 1.91445 0.00002 0.00018 -0.00035 -0.00018 1.91428

A141 1.90930 -0.00003 -0.00030 0.00015 -0.00016 1.90914

A142 1.90748 -0.00004 -0.00024 0.00013 -0.00011 1.90736

A143 1.94394 -0.00008 0.00069 -0.00110 -0.00041 1.94353

A144 1.94762 -0.00003 0.00051 -0.00061 -0.00010 1.94752

A145 1.84027 0.00027 -0.00061 0.00269 0.00207 1.84235

A146 1.91322 -0.00001 -0.00017 -0.00027 -0.00044 1.91278

A147 1.90951 -0.00007 -0.00024 -0.00029 -0.00054 1.90898

A148 1.90759 -0.00008 -0.00021 -0.00032 -0.00053 1.90707

A149 1.94402 -0.00015 0.00071 -0.00174 -0.00103 1.94299

A150 1.94777 -0.00009 0.00055 -0.00117 -0.00062 1.94714

A151 1.83903 0.00030 -0.00097 0.00316 0.00220 1.84123

A152 1.91445 0.00002 0.00018 -0.00035 -0.00018 1.91428

A153 1.90930 -0.00003 -0.00030 0.00015 -0.00016 1.90914

A154 1.90748 -0.00004 -0.00024 0.00013 -0.00011 1.90736

A155 1.94777 -0.00009 0.00055 -0.00117 -0.00062 1.94714

A156 1.94402 -0.00015 0.00071 -0.00174 -0.00103 1.94299

A157 1.83903 0.00030 -0.00097 0.00316 0.00220 1.84123

A158 1.91445 0.00002 0.00018 -0.00035 -0.00018 1.91428

A159 1.90748 -0.00004 -0.00024 0.00013 -0.00011 1.90736

A160 1.90930 -0.00003 -0.00030 0.00015 -0.00016 1.90914

A161 1.94762 -0.00003 0.00051 -0.00061 -0.00010 1.94752

A162 1.94394 -0.00008 0.00069 -0.00110 -0.00041 1.94353

A163 1.84027 0.00027 -0.00061 0.00269 0.00207 1.84235

A164 1.91322 -0.00001 -0.00017 -0.00027 -0.00044 1.91278

A165 1.90759 -0.00008 -0.00021 -0.00032 -0.00053 1.90707

A166 1.90951 -0.00007 -0.00024 -0.00029 -0.00054 1.90898

A167 1.94394 -0.00008 0.00069 -0.00110 -0.00041 1.94353

A168 1.94762 -0.00003 0.00051 -0.00061 -0.00010 1.94752

A169 1.84027 0.00027 -0.00061 0.00269 0.00207 1.84235

A170 1.91322 -0.00001 -0.00017 -0.00027 -0.00044 1.91278

A171 1.90951 -0.00007 -0.00024 -0.00029 -0.00054 1.90898

A172 1.90759 -0.00008 -0.00021 -0.00032 -0.00053 1.90707

A173 3.14161 0.00000 0.00001 0.00003 0.00003 3.14164

A174 3.14161 0.00000 0.00001 0.00003 0.00003 3.14165

A175 3.13826 0.00002 -0.00069 0.00100 0.00035 3.13861

A176 3.12841 -0.00032 -0.00349 -0.01990 -0.02338 3.10503

D1 -0.01148 0.00013 -0.00032 0.01165 0.01131 -0.00017

D2 2.98134 -0.00012 -0.00243 -0.00512 -0.00755 2.97379

D3 3.10235 0.00007 -0.00051 0.00700 0.00647 3.10882

D4 -0.18802 -0.00018 -0.00263 -0.00977 -0.01239 -0.20040

D5 0.00673 -0.00007 0.00018 -0.00679 -0.00663 0.00010

D6 -3.12924 -0.00013 -0.00066 -0.01000 -0.01068 -3.13992

D7 -3.10788 0.00002 0.00035 -0.00210 -0.00174 -3.10963

D8 0.03933 -0.00004 -0.00049 -0.00530 -0.00579 0.03354

D9 0.11742 0.00034 0.00505 0.01537 0.02040 0.13781

D10 -3.05657 0.00029 0.00479 0.01004 0.01482 -3.04175

D11 0.01148 -0.00013 0.00032 -0.01165 -0.01131 0.00017

D12 -3.10235 -0.00007 0.00051 -0.00700 -0.00647 -3.10882

D13 -2.98134 0.00012 0.00243 0.00512 0.00755 -2.97379

D14 0.18802 0.00018 0.00263 0.00977 0.01239 0.20040

D15 -3.05166 0.00040 0.00279 0.01993 0.02274 -3.02891

D16 0.07675 0.00008 -0.00070 0.00003 -0.00064 0.07611

D17 -0.07675 -0.00008 0.00070 -0.00003 0.00064 -0.07611

D18 3.05166 -0.00040 -0.00279 -0.01993 -0.02274 3.02891

D19 -0.00673 0.00007 -0.00018 0.00679 0.00663 -0.00010

D20 3.12924 0.00013 0.00066 0.01000 0.01067 3.13992

D21 3.10788 -0.00002 -0.00035 0.00210 0.00174 3.10962

D22 -0.03933 0.00004 0.00049 0.00530 0.00579 -0.03354

D23 -0.11742 -0.00034 -0.00505 -0.01537 -0.02040 -0.13781

D24 3.05657 -0.00029 -0.00479 -0.01004 -0.01482 3.04175

D25 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D26 3.13677 0.00006 0.00072 0.00277 0.00348 3.14025

D27 -3.13677 -0.00006 -0.00072 -0.00277 -0.00348 -3.14025

D28 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D29 3.13760 -0.00008 -0.00138 -0.00342 -0.00480 3.13280

D30 -0.01040 -0.00006 -0.00131 -0.00231 -0.00362 -0.01402

D31 -0.01026 -0.00001 -0.00044 0.00015 -0.00029 -0.01055

D32 3.12493 0.00001 -0.00037 0.00126 0.00089 3.12582

D33 -3.13760 0.00008 0.00138 0.00342 0.00480 -3.13280

D34 0.01040 0.00006 0.00131 0.00231 0.00362 0.01402

D35 0.01026 0.00001 0.00044 -0.00015 0.00029 0.01055

D36 -3.12493 -0.00001 0.00037 -0.00126 -0.00089 -3.12582

D37 -0.08931 0.00024 0.00293 0.00739 0.01033 -0.07898

D38 3.07567 0.00022 0.00063 0.00881 0.00944 3.08511

D39 -3.11464 -0.00015 -0.00298 -0.00700 -0.01002 -3.12465

D40 0.18240 0.00012 0.00103 0.00496 0.00598 0.18838

D41 0.00673 -0.00014 -0.00103 -0.00821 -0.00926 -0.00253

D42 -2.97942 0.00013 0.00298 0.00375 0.00674 -2.97268

D43 3.11818 0.00011 0.00258 0.00374 0.00631 3.12449

D44 -0.03209 0.00017 0.00255 0.00891 0.01144 -0.02065

D45 -0.00397 0.00008 0.00061 0.00486 0.00547 0.00149

D46 3.12894 0.00014 0.00058 0.01003 0.01060 3.13954

D47 -0.00673 0.00014 0.00103 0.00821 0.00926 0.00253

D48 3.11464 0.00015 0.00298 0.00700 0.01002 3.12465

D49 2.97942 -0.00013 -0.00298 -0.00375 -0.00674 2.97268

D50 -0.18240 -0.00012 -0.00103 -0.00496 -0.00598 -0.18838

D51 -0.08605 -0.00013 -0.00194 -0.00698 -0.00893 -0.09498

D52 3.05221 -0.00011 -0.00263 -0.00598 -0.00858 3.04363

D53 -3.05221 0.00011 0.00263 0.00598 0.00858 -3.04363

D54 0.08605 0.00013 0.00194 0.00698 0.00893 0.09498

D55 0.00397 -0.00008 -0.00061 -0.00486 -0.00547 -0.00149

D56 -3.12894 -0.00014 -0.00058 -0.01003 -0.01060 -3.13954

D57 -3.11818 -0.00011 -0.00258 -0.00374 -0.00631 -3.12449

D58 0.03209 -0.00017 -0.00255 -0.00891 -0.01144 0.02065

D59 0.08931 -0.00024 -0.00293 -0.00739 -0.01033 0.07898

D60 -3.07567 -0.00022 -0.00063 -0.00881 -0.00944 -3.08511

D61 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D62 -3.13410 -0.00004 0.00004 -0.00443 -0.00442 -3.13851

D63 3.13410 0.00004 -0.00004 0.00443 0.00442 3.13851

D64 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D65 -3.14093 0.00005 0.00043 0.00389 0.00432 -3.13661

D66 0.00655 0.00002 0.00022 0.00217 0.00238 0.00893

D67 0.01037 -0.00001 0.00047 -0.00188 -0.00141 0.00895

D68 -3.12534 -0.00004 0.00025 -0.00360 -0.00335 -3.12870

D69 3.14093 -0.00005 -0.00043 -0.00389 -0.00432 3.13661

D70 -0.00655 -0.00002 -0.00022 -0.00217 -0.00238 -0.00893

D71 -0.01037 0.00001 -0.00047 0.00188 0.00141 -0.00895

D72 3.12534 0.00004 -0.00025 0.00360 0.00335 3.12870

D73 -3.07567 -0.00022 -0.00063 -0.00881 -0.00944 -3.08511

D74 0.08931 -0.00024 -0.00293 -0.00739 -0.01033 0.07898

D75 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D76 -3.13410 -0.00004 0.00004 -0.00443 -0.00442 -3.13851

D77 3.13410 0.00004 -0.00004 0.00443 0.00442 3.13851

D78 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D79 -3.11818 -0.00011 -0.00258 -0.00374 -0.00631 -3.12449

D80 0.00397 -0.00008 -0.00061 -0.00486 -0.00547 -0.00149

D81 0.03209 -0.00017 -0.00255 -0.00891 -0.01144 0.02065

D82 -3.12894 -0.00014 -0.00058 -0.01003 -0.01060 -3.13954

D83 0.01037 -0.00001 0.00047 -0.00188 -0.00141 0.00895

D84 -3.12534 -0.00004 0.00025 -0.00360 -0.00335 -3.12870

D85 -3.14093 0.00005 0.00043 0.00389 0.00432 -3.13661

D86 0.00655 0.00002 0.00022 0.00217 0.00238 0.00893

D87 -0.00397 0.00008 0.00061 0.00486 0.00547 0.00149

D88 3.11818 0.00011 0.00258 0.00374 0.00631 3.12449

D89 3.12894 0.00014 0.00058 0.01003 0.01060 3.13954

D90 -0.03209 0.00017 0.00255 0.00891 0.01144 -0.02065

D91 -0.01037 0.00001 -0.00047 0.00188 0.00141 -0.00895

D92 3.12534 0.00004 -0.00025 0.00360 0.00335 3.12870

D93 3.14093 -0.00005 -0.00043 -0.00389 -0.00432 3.13661

D94 -0.00655 -0.00002 -0.00022 -0.00217 -0.00238 -0.00893

D95 0.00673 -0.00014 -0.00103 -0.00821 -0.00926 -0.00253

D96 -2.97942 0.00013 0.00298 0.00375 0.00674 -2.97269

D97 -3.11464 -0.00015 -0.00298 -0.00700 -0.01002 -3.12465

D98 0.18240 0.00012 0.00103 0.00496 0.00598 0.18838

D99 3.07567 0.00022 0.00063 0.00881 0.00944 3.08511

D100 -0.08931 0.00024 0.00293 0.00739 0.01033 -0.07898

D101 3.11464 0.00015 0.00298 0.00700 0.01002 3.12465

D102 -0.00673 0.00014 0.00103 0.00821 0.00926 0.00253

D103 -0.18240 -0.00012 -0.00103 -0.00496 -0.00598 -0.18838

D104 2.97942 -0.00013 -0.00298 -0.00375 -0.00674 2.97269

D105 3.05221 -0.00011 -0.00263 -0.00598 -0.00858 3.04363

D106 -0.08605 -0.00013 -0.00194 -0.00698 -0.00893 -0.09498

D107 0.08605 0.00013 0.00194 0.00698 0.00893 0.09498

D108 -3.05221 0.00011 0.00263 0.00598 0.00858 -3.04363

D109 -0.11742 -0.00034 -0.00505 -0.01537 -0.02039 -0.13781

D110 3.05657 -0.00029 -0.00479 -0.01004 -0.01482 3.04175

D111 -3.10235 -0.00007 0.00051 -0.00700 -0.00647 -3.10882

D112 0.01148 -0.00013 0.00032 -0.01165 -0.01131 0.00017

D113 0.18802 0.00018 0.00263 0.00977 0.01238 0.20040

D114 -2.98134 0.00012 0.00243 0.00512 0.00755 -2.97379

D115 -0.01148 0.00013 -0.00032 0.01165 0.01131 -0.00017

D116 3.10235 0.00007 -0.00051 0.00700 0.00647 3.10882

D117 2.98134 -0.00012 -0.00243 -0.00512 -0.00755 2.97379

D118 -0.18802 -0.00018 -0.00263 -0.00977 -0.01239 -0.20040

D119 3.05166 -0.00040 -0.00279 -0.01993 -0.02274 3.02891

D120 -0.07675 -0.00008 0.00070 -0.00003 0.00064 -0.07611

D121 0.07675 0.00008 -0.00070 0.00003 -0.00064 0.07611

D122 -3.05166 0.00040 0.00279 0.01993 0.02274 -3.02891

D123 3.10788 -0.00002 -0.00035 0.00210 0.00174 3.10963

D124 -0.03933 0.00004 0.00049 0.00530 0.00579 -0.03354

D125 -0.00673 0.00007 -0.00018 0.00679 0.00663 -0.00010

D126 3.12924 0.00013 0.00066 0.01000 0.01068 3.13992

D127 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D128 3.13677 0.00006 0.00072 0.00277 0.00348 3.14025

D129 -3.13677 -0.00006 -0.00072 -0.00277 -0.00348 -3.14025

D130 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D131 3.13760 -0.00008 -0.00138 -0.00342 -0.00480 3.13280

D132 -0.01040 -0.00006 -0.00131 -0.00231 -0.00362 -0.01402

D133 -0.01026 -0.00001 -0.00044 0.00015 -0.00029 -0.01055

D134 3.12493 0.00001 -0.00037 0.00126 0.00089 3.12582

D135 0.00673 -0.00007 0.00018 -0.00679 -0.00663 0.00010

D136 -3.10788 0.00002 0.00035 -0.00210 -0.00174 -3.10962

D137 -3.12924 -0.00013 -0.00066 -0.01000 -0.01067 -3.13992

D138 0.03933 -0.00004 -0.00049 -0.00530 -0.00579 0.03354

D139 0.01026 0.00001 0.00044 -0.00015 0.00029 0.01055

D140 -3.12493 -0.00001 0.00037 -0.00126 -0.00089 -3.12582

D141 -3.13760 0.00008 0.00138 0.00342 0.00480 -3.13280

D142 0.01040 0.00006 0.00131 0.00231 0.00362 0.01402

D143 0.11742 0.00034 0.00505 0.01537 0.02040 0.13781

D144 -3.05657 0.00029 0.00479 0.01004 0.01482 -3.04175

D145 -0.01041 0.00001 -0.00047 0.00190 0.00143 -0.00899

D146 3.13962 -0.00002 -0.00009 -0.00073 -0.00082 3.13880

D147 3.12492 0.00005 -0.00024 0.00376 0.00351 3.12843

D148 -0.00823 0.00002 0.00014 0.00112 0.00126 -0.00697

D149 -3.09217 0.00007 0.00073 0.00330 0.00403 -3.08815

D150 0.05573 0.00004 0.00050 0.00146 0.00195 0.05768

D151 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D152 -3.13335 -0.00003 0.00036 -0.00255 -0.00218 -3.13553

D153 3.13335 0.00003 -0.00036 0.00255 0.00218 3.13553

D154 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D155 0.01041 -0.00001 0.00047 -0.00190 -0.00143 0.00899

D156 -3.12492 -0.00005 0.00024 -0.00376 -0.00351 -3.12843

D157 -3.13962 0.00002 0.00009 0.00073 0.00082 -3.13880

D158 0.00823 -0.00002 -0.00014 -0.00113 -0.00126 0.00697

D159 3.09217 -0.00007 -0.00073 -0.00330 -0.00403 3.08815

D160 -0.05573 -0.00004 -0.00050 -0.00146 -0.00195 -0.05768

D161 -0.01034 -0.00001 -0.00044 0.00014 -0.00030 -0.01064

D162 3.14009 -0.00001 0.00004 -0.00059 -0.00055 3.13954

D163 3.12442 0.00001 -0.00038 0.00134 0.00096 3.12538

D164 -0.00834 0.00001 0.00011 0.00060 0.00071 -0.00763

D165 -3.09308 0.00004 0.00047 0.00182 0.00229 -3.09079

D166 0.05538 0.00002 0.00040 0.00062 0.00102 0.05640

D167 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D168 -3.13296 0.00000 0.00048 -0.00073 -0.00025 -3.13321

D169 3.13296 0.00000 -0.00048 0.00073 0.00025 3.13321

D170 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D171 0.01034 0.00001 0.00044 -0.00014 0.00030 0.01064

D172 -3.12442 -0.00001 0.00038 -0.00134 -0.00096 -3.12538

D173 -3.14009 0.00001 -0.00004 0.00059 0.00055 -3.13954

D174 0.00834 -0.00001 -0.00011 -0.00060 -0.00071 0.00763

D175 3.09308 -0.00004 -0.00047 -0.00182 -0.00229 3.09079

D176 -0.05538 -0.00002 -0.00040 -0.00062 -0.00102 -0.05640

D177 0.01041 -0.00001 0.00047 -0.00190 -0.00143 0.00899

D178 -3.13962 0.00002 0.00009 0.00073 0.00082 -3.13880

D179 -3.12492 -0.00005 0.00024 -0.00376 -0.00351 -3.12843

D180 0.00823 -0.00002 -0.00014 -0.00112 -0.00126 0.00697

D181 3.09217 -0.00007 -0.00073 -0.00330 -0.00403 3.08815

D182 -0.05573 -0.00004 -0.00050 -0.00146 -0.00195 -0.05768

D183 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D184 3.13335 0.00003 -0.00036 0.00255 0.00218 3.13553

D185 -3.13335 -0.00003 0.00036 -0.00255 -0.00218 -3.13553

D186 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D187 -0.01041 0.00001 -0.00047 0.00190 0.00143 -0.00899

D188 3.12492 0.00005 -0.00024 0.00376 0.00351 3.12843

D189 3.13962 -0.00002 -0.00009 -0.00073 -0.00082 3.13880

D190 -0.00823 0.00002 0.00014 0.00112 0.00126 -0.00697

D191 -3.09217 0.00007 0.00073 0.00330 0.00403 -3.08815

D192 0.05573 0.00004 0.00050 0.00146 0.00195 0.05768

D193 -0.01034 -0.00001 -0.00044 0.00014 -0.00030 -0.01064

D194 3.14009 -0.00001 0.00004 -0.00059 -0.00055 3.13954

D195 3.12442 0.00001 -0.00038 0.00134 0.00096 3.12538

D196 -0.00834 0.00001 0.00011 0.00060 0.00071 -0.00763

D197 -3.09308 0.00004 0.00047 0.00182 0.00229 -3.09079

D198 0.05538 0.00002 0.00040 0.00062 0.00102 0.05640

D199 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D200 -3.13296 0.00000 0.00048 -0.00073 -0.00025 -3.13321

D201 3.13296 0.00000 -0.00048 0.00073 0.00025 3.13321

D202 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D203 0.01034 0.00001 0.00044 -0.00014 0.00030 0.01064

D204 -3.12442 -0.00001 0.00038 -0.00134 -0.00096 -3.12538

D205 -3.14009 0.00001 -0.00004 0.00059 0.00055 -3.13954

D206 0.00834 -0.00001 -0.00011 -0.00060 -0.00071 0.00763

D207 3.09308 -0.00004 -0.00047 -0.00182 -0.00229 3.09079

D208 -0.05538 -0.00002 -0.00040 -0.00062 -0.00102 -0.05640

D209 1.09295 -0.00003 0.00056 0.00028 0.00084 1.09379

D210 -1.05152 0.00006 -0.00008 0.00186 0.00178 -1.04974

D211 -3.12105 0.00002 0.00021 0.00119 0.00140 -3.11965

D212 1.05152 -0.00006 0.00008 -0.00186 -0.00178 1.04974

D213 -1.09295 0.00003 -0.00056 -0.00028 -0.00084 -1.09379

D214 3.12105 -0.00002 -0.00021 -0.00119 -0.00140 3.11965

D215 1.09375 -0.00006 0.00079 0.00031 0.00110 1.09485

D216 -1.05248 0.00009 -0.00035 0.00288 0.00253 -1.04995

D217 -3.12106 0.00003 0.00021 0.00174 0.00195 -3.11911

D218 1.05248 -0.00009 0.00035 -0.00288 -0.00253 1.04995

D219 -1.09375 0.00006 -0.00079 -0.00031 -0.00110 -1.09485

D220 3.12106 -0.00003 -0.00021 -0.00174 -0.00195 3.11911

D221 1.05152 -0.00006 0.00008 -0.00186 -0.00178 1.04974

D222 -1.09295 0.00003 -0.00056 -0.00028 -0.00084 -1.09379

D223 3.12105 -0.00002 -0.00021 -0.00119 -0.00140 3.11965

D224 1.09295 -0.00003 0.00056 0.00028 0.00084 1.09379

D225 -1.05152 0.00006 -0.00008 0.00186 0.00178 -1.04974

D226 -3.12105 0.00002 0.00021 0.00119 0.00140 -3.11965

D227 1.09375 -0.00006 0.00079 0.00031 0.00110 1.09485

D228 -1.05248 0.00009 -0.00035 0.00288 0.00253 -1.04995

D229 -3.12106 0.00003 0.00021 0.00174 0.00195 -3.11911

D230 1.05248 -0.00009 0.00035 -0.00288 -0.00253 1.04995

D231 -1.09375 0.00006 -0.00079 -0.00031 -0.00110 -1.09485

D232 3.12106 -0.00003 -0.00021 -0.00174 -0.00195 3.11911

Item Value Threshold Converged?

Maximum Force 0.005406 0.000450 NO

RMS Force 0.000803 0.000300 NO

Maximum Displacement 0.079489 0.001800 NO

RMS Displacement 0.019671 0.001200 NO

Predicted change in Energy=-6.904560D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 5 23:29:21 2019, MaxMem= 1342177280 cpu: 14.1

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

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=3 Diff= 6.45D-08

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 -1.126869 2.809812 0.067761

2 7 0 -0.000001 2.045588 -0.037787

3 6 0 1.126868 2.809811 0.067761

4 6 0 0.712852 4.187759 0.258313

5 6 0 -0.712852 4.187760 0.258312

6 7 0 2.411707 2.385817 -0.026640

7 6 0 2.804406 1.133133 -0.093131

8 7 0 2.035170 -0.000001 0.002480

9 6 0 2.804406 -1.133135 -0.093130

10 6 0 4.209416 -0.705940 -0.264165

11 6 0 4.209415 0.705940 -0.264165

12 7 0 -2.411708 2.385817 -0.026640

13 6 0 -4.209415 0.705940 -0.264165

14 6 0 -4.209416 -0.705940 -0.264164

15 6 0 -2.804407 -1.133134 -0.093130

16 7 0 -2.035170 -0.000001 0.002480

17 6 0 -2.804406 1.133134 -0.093130

18 7 0 -2.411708 -2.385818 -0.026640

19 7 0 -0.000001 -2.045587 -0.037786

20 6 0 -1.126869 -2.809812 0.067761

21 6 0 -0.712852 -4.187760 0.258312

22 6 0 0.712852 -4.187759 0.258312

23 6 0 1.126868 -2.809812 0.067761

24 7 0 2.411707 -2.385818 -0.026640

25 30 0 0.000001 0.000001 -0.034734

26 6 0 -5.397004 1.431037 -0.412445

27 6 0 -6.586740 0.695121 -0.549717

28 6 0 -6.586741 -0.695120 -0.549716

29 6 0 -5.397005 -1.431036 -0.412444

30 6 0 1.433103 -5.386570 0.425735

31 6 0 0.700500 -6.568249 0.577571

32 6 0 -0.700500 -6.568249 0.577571

33 6 0 -1.433103 -5.386571 0.425734

34 6 0 5.397004 1.431037 -0.412446

35 6 0 6.586740 0.695121 -0.549718

36 6 0 6.586740 -0.695120 -0.549718

37 6 0 5.397004 -1.431037 -0.412445

38 6 0 -1.433103 5.386571 0.425735

39 6 0 -0.700499 6.568249 0.577572

40 6 0 0.700501 6.568248 0.577573

41 6 0 1.433104 5.386570 0.425736

42 1 0 7.533844 1.204429 -0.664817

43 1 0 7.533845 -1.204428 -0.664816

44 1 0 1.208190 7.514356 0.707214

45 1 0 -1.208187 7.514357 0.707213

46 1 0 -7.533844 1.204430 -0.664816

47 1 0 -7.533845 -1.204427 -0.664814

48 1 0 -1.208188 -7.514357 0.707211

49 1 0 1.208189 -7.514357 0.707213

50 8 0 2.782281 5.323191 0.435853

51 8 0 -2.782281 5.323193 0.435851

52 8 0 5.337028 2.778780 -0.420335

53 8 0 5.337030 -2.778780 -0.420332

54 8 0 2.782281 -5.323192 0.435852

55 8 0 -2.782281 -5.323194 0.435849

56 8 0 -5.337031 -2.778779 -0.420331

57 8 0 -5.337029 2.778780 -0.420334

58 6 0 3.519490 6.538998 0.541561

59 1 0 3.317761 7.050946 1.486689

60 1 0 3.301352 7.210964 -0.293428

61 1 0 4.567682 6.248713 0.507037

62 6 0 6.556657 3.514863 -0.505076

63 1 0 7.082236 3.315146 -1.442865

64 1 0 7.214360 3.293416 0.340091

65 1 0 6.266497 4.562962 -0.471955

66 6 0 6.556660 -3.514862 -0.505072

67 1 0 7.214362 -3.293413 0.340095

68 1 0 7.082239 -3.315146 -1.442861

69 1 0 6.266500 -4.562962 -0.471950

70 6 0 -3.519489 6.539001 0.541557

71 1 0 -3.301349 7.210967 -0.293432

72 1 0 -3.317759 7.050949 1.486685

73 1 0 -4.567681 6.248717 0.507032

74 6 0 -6.556658 3.514863 -0.505075

75 1 0 -7.214361 3.293416 0.340092

76 1 0 -7.082237 3.315146 -1.442864

77 1 0 -6.266498 4.562963 -0.471954

78 6 0 -6.556661 -3.514861 -0.505071

79 1 0 -7.082240 -3.315145 -1.442859

80 1 0 -7.214363 -3.293412 0.340097

81 1 0 -6.266502 -4.562961 -0.471948

82 6 0 -3.519489 -6.539002 0.541556

83 1 0 -3.317760 -7.050950 1.486683

84 1 0 -3.301349 -7.210968 -0.293433

85 1 0 -4.567681 -6.248718 0.507031

86 6 0 3.519490 -6.538999 0.541560

87 1 0 3.301351 -7.210965 -0.293429

88 1 0 3.317760 -7.050947 1.486687

89 1 0 4.567681 -6.248714 0.507036

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

Rotational constants (GHZ): 0.0444055 0.0441787 0.0223979

Leave Link 202 at Fri Jul 5 23:29:22 2019, MaxMem= 1342177280 cpu: 0.3

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

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

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8034.7053369873 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= 89 NActive= 89 NUniq= 89 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= -0.2279482870 Hartrees.

Nuclear repulsion after empirical dispersion term = 8034.4773887003 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6386

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.18D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 362

GePol: Fraction of low-weight points (<1% of avg) = 5.67%

GePol: Cavity surface area = 701.197 Ang\*\*2

GePol: Cavity volume = 799.960 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0089026126 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8034.4684860877 Hartrees.

Leave Link 301 at Fri Jul 5 23:29:22 2019, MaxMem= 1342177280 cpu: 1.2

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

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

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

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44193 LenP2D= 111048.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.52D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Fri Jul 5 23:29:26 2019, MaxMem= 1342177280 cpu: 41.4

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 5 23:29:27 2019, MaxMem= 1342177280 cpu: 2.4

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

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0174 S= 1.0058

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2650.02717546493

Leave Link 401 at Fri Jul 5 23:29:44 2019, MaxMem= 1342177280 cpu: 203.8

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 122342988.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.31D-14 for 6380.

Iteration 1 A\*A^-1 deviation from orthogonality is 6.09D-15 for 4678 1553.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.31D-14 for 6380.

Iteration 1 A^-1\*A deviation from orthogonality is 7.83D-11 for 5898 5845.

E= -2649.79147998916

DIIS: error= 1.00D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79147998916 IErMin= 1 ErrMin= 1.00D-03

ErrMax= 1.00D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.33D-03 BMatP= 4.33D-03

IDIUse=3 WtCom= 9.90D-01 WtEn= 1.00D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.682 Goal= None Shift= 0.000

Gap= 0.742 Goal= None Shift= 0.000

RMSDP=6.50D-05 MaxDP=2.60D-03 OVMax= 1.17D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.48D-05 CP: 9.99D-01

E= -2649.79323701178 Delta-E= -0.001757022614 Rises=F Damp=F

DIIS: error= 1.73D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79323701178 IErMin= 2 ErrMin= 1.73D-04

ErrMax= 1.73D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.62D-04 BMatP= 4.33D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.73D-03

Coeff-Com: 0.178D-05 0.100D+01

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

Coeff: 0.178D-05 0.100D+01

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.21D-05 MaxDP=7.30D-04 DE=-1.76D-03 OVMax= 3.69D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.16D-05 CP: 9.99D-01 1.05D+00

E= -2649.79324141823 Delta-E= -0.000004406458 Rises=F Damp=F

DIIS: error= 3.22D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79324141823 IErMin= 2 ErrMin= 1.73D-04

ErrMax= 3.22D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.15D-04 BMatP= 1.62D-04

IDIUse=3 WtCom= 3.58D-01 WtEn= 6.42D-01

Coeff-Com: -0.284D-01 0.558D+00 0.470D+00

Coeff-En: 0.000D+00 0.466D+00 0.534D+00

Coeff: -0.102D-01 0.499D+00 0.511D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=9.04D-06 MaxDP=7.35D-04 DE=-4.41D-06 OVMax= 3.81D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 5.07D-06 CP: 9.99D-01 1.06D+00 3.67D-01

E= -2649.79327664435 Delta-E= -0.000035226112 Rises=F Damp=F

DIIS: error= 1.45D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79327664435 IErMin= 4 ErrMin= 1.45D-04

ErrMax= 1.45D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.95D-05 BMatP= 1.62D-04

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.45D-03

Coeff-Com: -0.125D-01 0.151D+00 0.321D+00 0.541D+00

Coeff-En: 0.000D+00 0.000D+00 0.164D+00 0.836D+00

Coeff: -0.125D-01 0.151D+00 0.320D+00 0.541D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=2.97D-06 MaxDP=2.21D-04 DE=-3.52D-05 OVMax= 6.11D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.70D-06 CP: 9.99D-01 1.06D+00 5.39D-01 7.38D-01

E= -2649.79328440388 Delta-E= -0.000007759538 Rises=F Damp=F

DIIS: error= 4.29D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79328440388 IErMin= 5 ErrMin= 4.29D-05

ErrMax= 4.29D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.56D-06 BMatP= 3.95D-05

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

Coeff-Com: -0.444D-02 0.388D-01 0.140D+00 0.285D+00 0.540D+00

Coeff: -0.444D-02 0.388D-01 0.140D+00 0.285D+00 0.540D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=8.08D-07 MaxDP=6.03D-05 DE=-7.76D-06 OVMax= 4.02D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.03D-07 CP: 9.99D-01 1.06D+00 5.63D-01 8.04D-01 8.46D-01

E= -2649.79328484456 Delta-E= -0.000000440674 Rises=F Damp=F

DIIS: error= 1.57D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79328484456 IErMin= 6 ErrMin= 1.57D-05

ErrMax= 1.57D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.17D-07 BMatP= 1.56D-06

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

Coeff-Com: 0.645D-03-0.189D-01 0.222D-02 0.275D-01 0.307D+00 0.682D+00

Coeff: 0.645D-03-0.189D-01 0.222D-02 0.275D-01 0.307D+00 0.682D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=4.43D-07 MaxDP=2.39D-05 DE=-4.41D-07 OVMax= 3.68D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.96D-07 CP: 9.99D-01 1.06D+00 5.70D-01 8.42D-01 9.88D-01

CP: 9.13D-01

E= -2649.79328497643 Delta-E= -0.000000131868 Rises=F Damp=F

DIIS: error= 5.33D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79328497643 IErMin= 7 ErrMin= 5.33D-06

ErrMax= 5.33D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.73D-08 BMatP= 3.17D-07

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

Coeff-Com: 0.103D-02-0.167D-01-0.195D-01-0.303D-01 0.840D-01 0.376D+00

Coeff-Com: 0.605D+00

Coeff: 0.103D-02-0.167D-01-0.195D-01-0.303D-01 0.840D-01 0.376D+00

Coeff: 0.605D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=2.23D-07 MaxDP=1.11D-05 DE=-1.32D-07 OVMax= 2.41D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.45D-07 CP: 9.99D-01 1.07D+00 5.76D-01 8.57D-01 1.03D+00

CP: 1.10D+00 1.07D+00

E= -2649.79328500761 Delta-E= -0.000000031183 Rises=F Damp=F

DIIS: error= 3.02D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.79328500761 IErMin= 8 ErrMin= 3.02D-06

ErrMax= 3.02D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.49D-08 BMatP= 6.73D-08

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

Coeff-Com: 0.195D-03 0.665D-04-0.750D-02-0.229D-01-0.787D-01-0.936D-01

Coeff-Com: 0.291D+00 0.912D+00

Coeff: 0.195D-03 0.665D-04-0.750D-02-0.229D-01-0.787D-01-0.936D-01

Coeff: 0.291D+00 0.912D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.68D-07 MaxDP=9.10D-06 DE=-3.12D-08 OVMax= 1.75D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 5.68D-08 CP: 9.99D-01 1.07D+00 5.78D-01 8.70D-01 1.07D+00

CP: 1.21D+00 1.41D+00 1.07D+00

E= -2649.79328501834 Delta-E= -0.000000010727 Rises=F Damp=F

DIIS: error= 1.13D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.79328501834 IErMin= 9 ErrMin= 1.13D-06

ErrMax= 1.13D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.19D-09 BMatP= 1.49D-08

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

Coeff-Com: -0.755D-04 0.276D-02 0.458D-04-0.581D-02-0.493D-01-0.996D-01

Coeff-Com: 0.491D-01 0.407D+00 0.696D+00

Coeff: -0.755D-04 0.276D-02 0.458D-04-0.581D-02-0.493D-01-0.996D-01

Coeff: 0.491D-01 0.407D+00 0.696D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=5.11D-08 MaxDP=2.52D-06 DE=-1.07D-08 OVMax= 4.57D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.79D-08 CP: 9.99D-01 1.07D+00 5.79D-01 8.72D-01 1.08D+00

CP: 1.24D+00 1.49D+00 1.20D+00 1.11D+00

E= -2649.79328501946 Delta-E= -0.000000001126 Rises=F Damp=F

DIIS: error= 7.71D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -2649.79328501946 IErMin=10 ErrMin= 7.71D-07

ErrMax= 7.71D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.62D-10 BMatP= 2.19D-09

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

Coeff-Com: -0.863D-04 0.163D-02 0.186D-02 0.183D-02-0.108D-01-0.361D-01

Coeff-Com: -0.337D-01 0.320D-01 0.430D+00 0.613D+00

Coeff: -0.863D-04 0.163D-02 0.186D-02 0.183D-02-0.108D-01-0.361D-01

Coeff: -0.337D-01 0.320D-01 0.430D+00 0.613D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=2.22D-08 MaxDP=1.34D-06 DE=-1.13D-09 OVMax= 1.68D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.47D-08 CP: 9.99D-01 1.07D+00 5.80D-01 8.72D-01 1.08D+00

CP: 1.25D+00 1.52D+00 1.24D+00 1.26D+00 7.92D-01

E= -2649.79328501982 Delta-E= -0.000000000357 Rises=F Damp=F

DIIS: error= 3.27D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -2649.79328501982 IErMin=11 ErrMin= 3.27D-07

ErrMax= 3.27D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.21D-10 BMatP= 8.62D-10

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

Coeff-Com: -0.273D-04 0.227D-03 0.870D-03 0.197D-02 0.483D-02 0.242D-02

Coeff-Com: -0.258D-01-0.665D-01 0.740D-01 0.298D+00 0.710D+00

Coeff: -0.273D-04 0.227D-03 0.870D-03 0.197D-02 0.483D-02 0.242D-02

Coeff: -0.258D-01-0.665D-01 0.740D-01 0.298D+00 0.710D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=9.52D-09 MaxDP=6.71D-07 DE=-3.57D-10 OVMax= 4.43D-06

Error on total polarization charges = 0.07274

SCF Done: E(UB3LYP) = -2649.79328502 A.U. after 11 cycles

NFock= 11 Conv=0.95D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0171 S= 1.0057

<L.S>= 0.000000000000E+00

KE= 2.690122664267D+03 PE=-2.234762491022D+04 EE= 8.973240474844D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.59

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0171, after 2.0002

Leave Link 502 at Fri Jul 5 23:38:39 2019, MaxMem= 1342177280 cpu: 6323.0

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

Compute integral first derivatives.

... and contract with generalized density number 0.

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

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44193 LenP2D= 111048.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 280

Leave Link 701 at Fri Jul 5 23:38:58 2019, MaxMem= 1342177280 cpu: 218.2

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

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

Leave Link 702 at Fri Jul 5 23:38:58 2019, MaxMem= 1342177280 cpu: 0.2

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

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Fri Jul 5 23:40:29 2019, MaxMem= 1342177280 cpu: 1091.9

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

Dipole = 7.00327897D-06 8.81512445D-06-7.28716954D-02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000889150 0.000735529 0.000072518

2 7 0.000000351 -0.000065830 -0.000478102

3 6 -0.000889087 0.000735484 0.000072514

4 6 0.001144799 -0.000212269 0.000374021

5 6 -0.001144863 -0.000212269 0.000374046

6 7 0.000107488 0.000572161 -0.000526486

7 6 -0.000361852 -0.000575537 0.000484704

8 7 0.000337150 0.000000282 0.000845871

9 6 -0.000361888 0.000575534 0.000484700

10 6 0.000231676 0.000761119 -0.000420632

11 6 0.000231689 -0.000761178 -0.000420619

12 7 -0.000107690 0.000572189 -0.000526486

13 6 -0.000231700 -0.000761092 -0.000420615

14 6 -0.000231687 0.000761033 -0.000420628

15 6 0.000362056 0.000575722 0.000484703

16 7 -0.000337389 0.000000283 0.000845805

17 6 0.000362021 -0.000575725 0.000484705

18 7 -0.000107816 -0.000572263 -0.000526501

19 7 0.000000351 0.000065652 -0.000478048

20 6 0.000889368 -0.000735385 0.000072499

21 6 -0.001144939 0.000212248 0.000374047

22 6 0.001144875 0.000212247 0.000374021

23 6 -0.000889305 -0.000735341 0.000072494

24 7 0.000107615 -0.000572234 -0.000526499

25 30 -0.000000440 -0.000000393 -0.001209191

26 6 0.000003713 0.000378982 0.000238594

27 6 -0.000102662 0.000301582 0.000000251

28 6 -0.000102665 -0.000301583 0.000000250

29 6 0.000003704 -0.000378983 0.000238593

30 6 0.000453779 0.000119393 -0.000074201

31 6 -0.000197745 -0.000021919 -0.000005898

32 6 0.000197748 -0.000021918 -0.000005896

33 6 -0.000453776 0.000119392 -0.000074198

34 6 -0.000003692 0.000379013 0.000238594

35 6 0.000102645 0.000301613 0.000000251

36 6 0.000102647 -0.000301614 0.000000250

37 6 -0.000003683 -0.000379015 0.000238593

38 6 -0.000453810 -0.000119378 -0.000074198

39 6 0.000197724 0.000021901 -0.000005898

40 6 -0.000197720 0.000021901 -0.000005898

41 6 0.000453813 -0.000119378 -0.000074200

42 1 0.000085903 0.000199793 -0.000035832

43 1 0.000085900 -0.000199794 -0.000035831

44 1 0.000173953 0.000087344 0.000008507

45 1 -0.000173952 0.000087340 0.000008505

46 1 -0.000085903 0.000199786 -0.000035832

47 1 -0.000085899 -0.000199786 -0.000035832

48 1 -0.000173946 -0.000087341 0.000008506

49 1 0.000173946 -0.000087343 0.000008507

50 8 -0.000137716 -0.000237670 0.000159488

51 8 0.000137697 -0.000237692 0.000159498

52 8 -0.000037629 0.000451721 -0.000160403

53 8 -0.000037648 -0.000451738 -0.000160402

54 8 -0.000137714 0.000237716 0.000159496

55 8 0.000137695 0.000237739 0.000159507

56 8 0.000037697 -0.000451735 -0.000160404

57 8 0.000037679 0.000451717 -0.000160405

58 6 -0.000111453 0.000028041 -0.000042750

59 1 -0.000074756 0.000089747 0.000204006

60 1 -0.000082773 0.000127972 -0.000179156

61 1 0.000144520 -0.000140591 -0.000026841

62 6 -0.000292341 -0.000295466 0.000067250

63 1 0.000166865 -0.000026239 -0.000195887

64 1 0.000232133 -0.000032090 0.000153732

65 1 -0.000148058 0.000170079 0.000023421

66 6 -0.000292343 0.000295465 0.000067246

67 1 0.000232135 0.000032086 0.000153731

68 1 0.000166865 0.000026237 -0.000195887

69 1 -0.000148061 -0.000170081 0.000023420

70 6 0.000111452 0.000028040 -0.000042747

71 1 0.000082770 0.000127973 -0.000179155

72 1 0.000074753 0.000089747 0.000204005

73 1 -0.000144522 -0.000140595 -0.000026840

74 6 0.000292339 -0.000295458 0.000067249

75 1 -0.000232131 -0.000032088 0.000153732

76 1 -0.000166863 -0.000026238 -0.000195885

77 1 0.000148058 0.000170081 0.000023422

78 6 0.000292341 0.000295458 0.000067244

79 1 -0.000166863 0.000026235 -0.000195884

80 1 -0.000232133 0.000032083 0.000153731

81 1 0.000148061 -0.000170083 0.000023421

82 6 0.000111446 -0.000028039 -0.000042747

83 1 0.000074752 -0.000089746 0.000204003

84 1 0.000082768 -0.000127972 -0.000179155

85 1 -0.000144525 0.000140595 -0.000026841

86 6 -0.000111448 -0.000028040 -0.000042749

87 1 -0.000082771 -0.000127971 -0.000179155

88 1 -0.000074755 -0.000089746 0.000204004

89 1 0.000144523 0.000140592 -0.000026842

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

Cartesian Forces: Max 0.001209191 RMS 0.000332500

Leave Link 716 at Fri Jul 5 23:40:30 2019, MaxMem= 1342177280 cpu: 1.1

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.000799721 RMS 0.000179553

Search for a local minimum.

Step number 3 out of a maximum of 518

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

RMS Force = .17955D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3

DE= -7.43D-04 DEPred=-6.90D-04 R= 1.08D+00

TightC=F SS= 1.41D+00 RLast= 1.28D-01 DXNew= 7.2376D-01 3.8408D-01

Trust test= 1.08D+00 RLast= 1.28D-01 DXMaxT set to 4.30D-01

ITU= 1 1 0

Eigenvalues --- 0.01313 0.01316 0.01316 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01481 0.01551

Eigenvalues --- 0.01566 0.01568 0.01579 0.01598 0.01616

Eigenvalues --- 0.01620 0.01659 0.01707 0.01709 0.01711

Eigenvalues --- 0.01715 0.01830 0.01834 0.01864 0.01867

Eigenvalues --- 0.01896 0.01914 0.01922 0.01925 0.01927

Eigenvalues --- 0.01931 0.01995 0.02000 0.02016 0.02021

Eigenvalues --- 0.02022 0.02024 0.02053 0.02053 0.02053

Eigenvalues --- 0.02053 0.02057 0.02057 0.02057 0.02057

Eigenvalues --- 0.02063 0.02067 0.02067 0.02067 0.02068

Eigenvalues --- 0.02070 0.02070 0.02070 0.02070 0.02083

Eigenvalues --- 0.02083 0.02083 0.02094 0.02259 0.02260

Eigenvalues --- 0.02260 0.02260 0.02260 0.02260 0.02260

Eigenvalues --- 0.02262 0.02342 0.02345 0.02354 0.02360

Eigenvalues --- 0.09986 0.09986 0.09986 0.09986 0.09989

Eigenvalues --- 0.09989 0.09989 0.10010 0.10650 0.10650

Eigenvalues --- 0.10650 0.10650 0.10659 0.10659 0.10659

Eigenvalues --- 0.10660 0.13503 0.13508 0.15205 0.15970

Eigenvalues --- 0.15999 0.15999 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16015

Eigenvalues --- 0.16117 0.17540 0.21752 0.21843 0.22473

Eigenvalues --- 0.22473 0.22476 0.22477 0.22892 0.24506

Eigenvalues --- 0.24514 0.24520 0.24537 0.24626 0.24641

Eigenvalues --- 0.24746 0.24763 0.24891 0.24914 0.24937

Eigenvalues --- 0.24991 0.24994 0.24995 0.24998 0.24999

Eigenvalues --- 0.24999 0.24999 0.24999 0.24999 0.24999

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25172 0.26212

Eigenvalues --- 0.31842 0.33644 0.33656 0.33700 0.33732

Eigenvalues --- 0.34063 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34063 0.34072 0.34081 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34081

Eigenvalues --- 0.34238 0.34680 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34686 0.34687 0.34914

Eigenvalues --- 0.34934 0.34958 0.35491 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35632 0.35634

Eigenvalues --- 0.36107 0.37093 0.37117 0.37158 0.41189

Eigenvalues --- 0.41215 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41215 0.41245 0.41406 0.41408 0.41410

Eigenvalues --- 0.41410 0.41413 0.42471 0.42483 0.42682

Eigenvalues --- 0.43969 0.44562 0.44571 0.44676 0.44902

Eigenvalues --- 0.44926 0.44998 0.45000 0.45001 0.45002

Eigenvalues --- 0.45004 0.45298 0.45366 0.45367 0.46945

Eigenvalues --- 0.47385 0.48257 0.49056 0.49317 0.49347

Eigenvalues --- 0.49872 0.53023 0.53554 0.53554 0.53554

Eigenvalues --- 0.53554 0.53554 0.53554 0.54318 0.55017

Eigenvalues --- 0.55018 0.55652 0.56101 0.57427 0.57444

Eigenvalues --- 0.57584

En-DIIS/RFO-DIIS IScMMF= 0 using points: 3 2

RFO step: Lambda=-5.11600936D-05.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 7.43D-04 SmlDif= 1.00D-05

RMS Error= 0.7308136151D-03 NUsed= 2 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.12505 -0.12505

Iteration 1 RMS(Cart)= 0.04359227 RMS(Int)= 0.00015253

Iteration 2 RMS(Cart)= 0.00066196 RMS(Int)= 0.00002542

Iteration 3 RMS(Cart)= 0.00000003 RMS(Int)= 0.00002542

ITry= 1 IFail=0 DXMaxC= 1.75D-01 DCOld= 1.00D+10 DXMaxT= 4.30D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.58071 -0.00004 -0.00022 -0.00039 -0.00058 2.58013

R2 2.74268 -0.00040 -0.00120 -0.00247 -0.00369 2.73899

R3 2.56300 0.00025 0.00189 0.00219 0.00402 2.56702

R4 2.58071 -0.00004 -0.00022 -0.00040 -0.00059 2.58012

R5 3.86560 0.00053 0.00064 0.00282 0.00359 3.86919

R6 2.74268 -0.00040 -0.00120 -0.00247 -0.00369 2.73899

R7 2.56300 0.00025 0.00189 0.00219 0.00400 2.56699

R8 2.69419 0.00069 0.00058 0.00251 0.00305 2.69724

R9 2.66172 -0.00014 0.00037 -0.00031 0.00006 2.66179

R10 2.66172 -0.00014 0.00037 -0.00031 0.00006 2.66179

R11 2.48400 0.00064 -0.00158 -0.00024 -0.00192 2.48208

R12 2.59441 -0.00013 0.00060 0.00016 0.00077 2.59517

R13 2.79386 0.00040 0.00129 0.00201 0.00329 2.79714

R14 2.59441 -0.00013 0.00060 0.00016 0.00078 2.59519

R15 3.84655 0.00009 -0.00063 -0.00116 -0.00167 3.84488

R16 2.79386 0.00040 0.00129 0.00201 0.00329 2.79714

R17 2.48400 0.00064 -0.00158 -0.00024 -0.00189 2.48211

R18 2.66807 -0.00026 -0.00039 -0.00130 -0.00172 2.66634

R19 2.64435 0.00026 -0.00033 -0.00007 -0.00040 2.64394

R20 2.64435 0.00026 -0.00033 -0.00007 -0.00040 2.64394

R21 2.48400 0.00064 -0.00158 -0.00024 -0.00190 2.48210

R22 2.66807 -0.00026 -0.00039 -0.00130 -0.00171 2.66636

R23 2.79386 0.00040 0.00129 0.00201 0.00329 2.79715

R24 2.64435 0.00026 -0.00033 -0.00007 -0.00040 2.64394

R25 2.79386 0.00040 0.00129 0.00201 0.00329 2.79715

R26 2.64435 0.00026 -0.00033 -0.00007 -0.00040 2.64394

R27 2.59441 -0.00013 0.00060 0.00016 0.00077 2.59517

R28 2.48400 0.00064 -0.00158 -0.00024 -0.00187 2.48213

R29 2.59441 -0.00013 0.00060 0.00016 0.00075 2.59516

R30 3.84656 0.00009 -0.00063 -0.00116 -0.00173 3.84483

R31 2.56300 0.00025 0.00189 0.00220 0.00404 2.56704

R32 2.58071 -0.00005 -0.00022 -0.00040 -0.00060 2.58012

R33 2.58071 -0.00005 -0.00022 -0.00040 -0.00061 2.58010

R34 3.86561 0.00053 0.00064 0.00280 0.00353 3.86913

R35 2.74268 -0.00040 -0.00120 -0.00247 -0.00368 2.73900

R36 2.69419 0.00069 0.00058 0.00251 0.00307 2.69726

R37 2.66172 -0.00014 0.00037 -0.00031 0.00006 2.66179

R38 2.74268 -0.00040 -0.00120 -0.00247 -0.00368 2.73900

R39 2.66172 -0.00014 0.00037 -0.00031 0.00006 2.66179

R40 2.56300 0.00025 0.00189 0.00220 0.00402 2.56701

R41 2.65632 0.00032 0.00069 0.00116 0.00185 2.65817

R42 2.54943 0.00027 -0.00041 -0.00007 -0.00049 2.54894

R43 2.62717 0.00080 -0.00060 0.00098 0.00038 2.62755

R44 2.04374 0.00017 0.00000 0.00041 0.00041 2.04416

R45 2.65632 0.00032 0.00069 0.00116 0.00185 2.65817

R46 2.04374 0.00017 0.00000 0.00041 0.00041 2.04416

R47 2.54943 0.00027 -0.00041 -0.00007 -0.00048 2.54894

R48 2.64300 0.00022 0.00008 0.00033 0.00041 2.64341

R49 2.55246 -0.00025 -0.00044 -0.00102 -0.00146 2.55099

R50 2.64751 0.00022 -0.00011 0.00033 0.00022 2.64773

R51 2.04377 0.00016 -0.00004 0.00037 0.00033 2.04410

R52 2.64300 0.00022 0.00008 0.00033 0.00041 2.64341

R53 2.04377 0.00016 -0.00004 0.00037 0.00033 2.04410

R54 2.55246 -0.00025 -0.00044 -0.00102 -0.00146 2.55099

R55 2.65632 0.00032 0.00069 0.00116 0.00185 2.65817

R56 2.54943 0.00027 -0.00041 -0.00007 -0.00049 2.54894

R57 2.62717 0.00080 -0.00060 0.00098 0.00038 2.62755

R58 2.04374 0.00017 0.00000 0.00041 0.00041 2.04416

R59 2.65632 0.00032 0.00069 0.00116 0.00185 2.65817

R60 2.04374 0.00017 0.00000 0.00041 0.00041 2.04416

R61 2.54943 0.00027 -0.00041 -0.00007 -0.00048 2.54894

R62 2.64300 0.00022 0.00008 0.00033 0.00041 2.64341

R63 2.55246 -0.00025 -0.00044 -0.00102 -0.00146 2.55099

R64 2.64751 0.00022 -0.00011 0.00033 0.00022 2.64773

R65 2.04377 0.00016 -0.00004 0.00037 0.00033 2.04410

R66 2.64300 0.00022 0.00008 0.00033 0.00041 2.64341

R67 2.04377 0.00016 -0.00004 0.00037 0.00033 2.04410

R68 2.55246 -0.00025 -0.00044 -0.00102 -0.00146 2.55099

R69 2.69433 0.00002 -0.00010 -0.00016 -0.00026 2.69407

R70 2.69433 0.00002 -0.00010 -0.00016 -0.00026 2.69407

R71 2.69675 -0.00013 -0.00008 -0.00047 -0.00054 2.69620

R72 2.69675 -0.00013 -0.00008 -0.00047 -0.00054 2.69620

R73 2.69433 0.00002 -0.00010 -0.00016 -0.00026 2.69407

R74 2.69433 0.00002 -0.00010 -0.00016 -0.00026 2.69407

R75 2.69675 -0.00013 -0.00008 -0.00047 -0.00054 2.69620

R76 2.69675 -0.00013 -0.00008 -0.00047 -0.00054 2.69620

R77 2.06668 0.00023 -0.00009 0.00053 0.00044 2.06712

R78 2.06692 0.00023 -0.00009 0.00052 0.00043 2.06736

R79 2.05639 0.00018 -0.00006 0.00033 0.00027 2.05665

R80 2.06626 0.00025 -0.00009 0.00058 0.00049 2.06675

R81 2.06657 0.00026 -0.00009 0.00062 0.00052 2.06709

R82 2.05607 0.00020 -0.00006 0.00040 0.00034 2.05641

R83 2.06657 0.00026 -0.00009 0.00062 0.00052 2.06709

R84 2.06626 0.00025 -0.00009 0.00058 0.00049 2.06675

R85 2.05607 0.00020 -0.00006 0.00040 0.00034 2.05641

R86 2.06692 0.00023 -0.00009 0.00052 0.00043 2.06736

R87 2.06668 0.00023 -0.00009 0.00053 0.00044 2.06712

R88 2.05639 0.00018 -0.00006 0.00033 0.00027 2.05665

R89 2.06657 0.00026 -0.00009 0.00062 0.00052 2.06709

R90 2.06626 0.00025 -0.00009 0.00058 0.00049 2.06675

R91 2.05607 0.00020 -0.00006 0.00040 0.00034 2.05641

R92 2.06626 0.00025 -0.00009 0.00058 0.00049 2.06675

R93 2.06657 0.00026 -0.00009 0.00062 0.00052 2.06709

R94 2.05607 0.00020 -0.00006 0.00040 0.00034 2.05641

R95 2.06668 0.00023 -0.00009 0.00053 0.00044 2.06712

R96 2.06692 0.00023 -0.00009 0.00052 0.00043 2.06736

R97 2.05639 0.00018 -0.00006 0.00033 0.00027 2.05665

R98 2.06692 0.00023 -0.00009 0.00052 0.00043 2.06736

R99 2.06668 0.00023 -0.00009 0.00053 0.00044 2.06712

R100 2.05639 0.00018 -0.00006 0.00033 0.00027 2.05665

A1 1.88185 0.00034 0.00083 0.00115 0.00201 1.88386

A2 2.21600 -0.00022 -0.00092 -0.00136 -0.00229 2.21371

A3 2.18484 -0.00012 0.00008 0.00046 0.00048 2.18532

A4 1.94093 -0.00031 -0.00100 -0.00105 -0.00214 1.93879

A5 2.16456 0.00014 0.00032 -0.00009 0.00022 2.16478

A6 2.16456 0.00014 0.00032 -0.00009 0.00027 2.16483

A7 1.88185 0.00034 0.00083 0.00115 0.00202 1.88387

A8 2.21601 -0.00022 -0.00092 -0.00136 -0.00230 2.21371

A9 2.18484 -0.00012 0.00008 0.00046 0.00049 2.18532

A10 1.86007 -0.00019 -0.00032 -0.00062 -0.00096 1.85912

A11 2.31556 0.00014 0.00048 0.00061 0.00109 2.31665

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D103 -0.18838 -0.00027 -0.00075 -0.01552 -0.01627 -0.20465

D104 2.97269 -0.00034 -0.00084 -0.01873 -0.01958 2.95310

D105 3.04363 0.00008 -0.00107 0.00439 0.00332 3.04694

D106 -0.09498 -0.00028 -0.00112 -0.01655 -0.01766 -0.11264

D107 0.09498 0.00028 0.00112 0.01655 0.01766 0.11264

D108 -3.04363 -0.00008 0.00107 -0.00439 -0.00331 -3.04694

D109 -0.13781 -0.00030 -0.00255 -0.01595 -0.01849 -0.15630

D110 3.04175 -0.00048 -0.00185 -0.02556 -0.02740 3.01436

D111 -3.10882 0.00004 -0.00081 -0.00020 -0.00099 -3.10981

D112 0.00017 0.00018 -0.00141 0.00805 0.00665 0.00682

D113 0.20040 0.00018 0.00155 0.00761 0.00915 0.20956

D114 -2.97379 0.00032 0.00094 0.01586 0.01679 -2.95699

D115 -0.00017 -0.00018 0.00141 -0.00805 -0.00665 -0.00682

D116 3.10882 -0.00004 0.00081 0.00020 0.00100 3.10982

D117 2.97379 -0.00032 -0.00094 -0.01586 -0.01680 2.95699

D118 -0.20040 -0.00018 -0.00155 -0.00761 -0.00916 -0.20956

D119 3.02891 -0.00026 -0.00284 -0.01523 -0.01808 3.01083

D120 -0.07611 0.00006 0.00008 0.00635 0.00643 -0.06968

D121 0.07611 -0.00006 -0.00008 -0.00635 -0.00643 0.06969

D122 -3.02891 0.00026 0.00284 0.01523 0.01809 -3.01083

D123 3.10963 0.00003 0.00022 0.00327 0.00349 3.11312

D124 -0.03354 0.00003 0.00072 0.00246 0.00318 -0.03035

D125 -0.00010 -0.00011 0.00083 -0.00475 -0.00392 -0.00403

D126 3.13992 -0.00011 0.00133 -0.00556 -0.00423 3.13568

D127 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D128 3.14025 0.00000 0.00044 -0.00070 -0.00026 3.13998

D129 -3.14025 0.00000 -0.00044 0.00070 0.00026 -3.13998

D130 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D131 3.13280 -0.00003 -0.00060 -0.00127 -0.00187 3.13092

D132 -0.01402 -0.00005 -0.00045 -0.00216 -0.00261 -0.01663

D133 -0.01055 -0.00003 -0.00004 -0.00218 -0.00222 -0.01277

D134 3.12582 -0.00005 0.00011 -0.00307 -0.00296 3.12286

D135 0.00010 0.00011 -0.00083 0.00474 0.00392 0.00402

D136 -3.10962 -0.00003 -0.00022 -0.00328 -0.00350 -3.11312

D137 -3.13992 0.00011 -0.00133 0.00556 0.00423 -3.13569

D138 0.03354 -0.00003 -0.00072 -0.00246 -0.00319 0.03035

D139 0.01055 0.00003 0.00004 0.00218 0.00222 0.01277

D140 -3.12582 0.00005 -0.00011 0.00307 0.00296 -3.12286

D141 -3.13280 0.00003 0.00060 0.00127 0.00187 -3.13093

D142 0.01402 0.00005 0.00045 0.00216 0.00261 0.01663

D143 0.13781 0.00030 0.00255 0.01595 0.01849 0.15630

D144 -3.04175 0.00048 0.00185 0.02556 0.02740 -3.01436

D145 -0.00899 0.00002 0.00018 0.00107 0.00125 -0.00774

D146 3.13880 0.00004 -0.00010 0.00198 0.00188 3.14068

D147 3.12843 -0.00003 0.00044 -0.00143 -0.00099 3.12744

D148 -0.00697 -0.00001 0.00016 -0.00051 -0.00036 -0.00732

D149 -3.08815 -0.00001 0.00050 -0.00045 0.00005 -3.08809

D150 0.05768 0.00004 0.00024 0.00209 0.00233 0.06001

D151 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D152 -3.13553 0.00002 -0.00027 0.00090 0.00063 -3.13490

D153 3.13553 -0.00002 0.00027 -0.00090 -0.00063 3.13490

D154 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D155 0.00899 -0.00002 -0.00018 -0.00107 -0.00125 0.00774

D156 -3.12843 0.00003 -0.00044 0.00143 0.00099 -3.12744

D157 -3.13880 -0.00004 0.00010 -0.00198 -0.00188 -3.14068

D158 0.00697 0.00001 -0.00016 0.00052 0.00036 0.00732

D159 3.08815 0.00001 -0.00050 0.00045 -0.00005 3.08809

D160 -0.05768 -0.00004 -0.00024 -0.00209 -0.00233 -0.06001

D161 -0.01064 -0.00003 -0.00004 -0.00221 -0.00224 -0.01288

D162 3.13954 -0.00001 -0.00007 -0.00049 -0.00056 3.13898

D163 3.12538 -0.00005 0.00012 -0.00315 -0.00303 3.12235

D164 -0.00763 -0.00003 0.00009 -0.00143 -0.00134 -0.00897

D165 -3.09079 0.00004 0.00029 0.00228 0.00256 -3.08823

D166 0.05640 0.00006 0.00013 0.00323 0.00336 0.05975

D167 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D168 -3.13321 0.00003 -0.00003 0.00169 0.00166 -3.13155

D169 3.13321 -0.00003 0.00003 -0.00169 -0.00166 3.13155

D170 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D171 0.01064 0.00003 0.00004 0.00221 0.00224 0.01288

D172 -3.12538 0.00005 -0.00012 0.00315 0.00303 -3.12235

D173 -3.13954 0.00001 0.00007 0.00049 0.00056 -3.13898

D174 0.00763 0.00003 -0.00009 0.00143 0.00134 0.00897

D175 3.09079 -0.00004 -0.00029 -0.00228 -0.00256 3.08823

D176 -0.05640 -0.00006 -0.00013 -0.00323 -0.00336 -0.05975

D177 0.00899 -0.00002 -0.00018 -0.00107 -0.00125 0.00774

D178 -3.13880 -0.00004 0.00010 -0.00198 -0.00188 -3.14068

D179 -3.12843 0.00003 -0.00044 0.00143 0.00099 -3.12744

D180 0.00697 0.00001 -0.00016 0.00051 0.00036 0.00732

D181 3.08815 0.00001 -0.00050 0.00045 -0.00005 3.08809

D182 -0.05768 -0.00004 -0.00024 -0.00209 -0.00233 -0.06001

D183 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D184 3.13553 -0.00002 0.00027 -0.00090 -0.00063 3.13490

D185 -3.13553 0.00002 -0.00027 0.00090 0.00063 -3.13490

D186 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D187 -0.00899 0.00002 0.00018 0.00107 0.00125 -0.00774

D188 3.12843 -0.00003 0.00044 -0.00143 -0.00099 3.12744

D189 3.13880 0.00004 -0.00010 0.00198 0.00188 3.14068

D190 -0.00697 -0.00001 0.00016 -0.00052 -0.00036 -0.00732

D191 -3.08815 -0.00001 0.00050 -0.00045 0.00005 -3.08809

D192 0.05768 0.00004 0.00024 0.00209 0.00233 0.06001

D193 -0.01064 -0.00003 -0.00004 -0.00221 -0.00224 -0.01288

D194 3.13954 -0.00001 -0.00007 -0.00049 -0.00055 3.13898

D195 3.12538 -0.00005 0.00012 -0.00315 -0.00303 3.12235

D196 -0.00763 -0.00003 0.00009 -0.00143 -0.00134 -0.00897

D197 -3.09079 0.00004 0.00029 0.00228 0.00256 -3.08823

D198 0.05640 0.00006 0.00013 0.00323 0.00336 0.05975

D199 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D200 -3.13321 0.00003 -0.00003 0.00169 0.00166 -3.13155

D201 3.13321 -0.00003 0.00003 -0.00169 -0.00166 3.13155

D202 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D203 0.01064 0.00003 0.00004 0.00221 0.00224 0.01288

D204 -3.12538 0.00005 -0.00012 0.00315 0.00303 -3.12235

D205 -3.13954 0.00001 0.00007 0.00049 0.00055 -3.13898

D206 0.00763 0.00003 -0.00009 0.00143 0.00134 0.00897

D207 3.09079 -0.00004 -0.00029 -0.00228 -0.00256 3.08823

D208 -0.05640 -0.00006 -0.00013 -0.00323 -0.00336 -0.05975

D209 1.09379 0.00001 0.00011 0.00121 0.00131 1.09511

D210 -1.04974 0.00001 0.00022 0.00105 0.00128 -1.04846

D211 -3.11965 0.00002 0.00018 0.00119 0.00137 -3.11828

D212 1.04974 -0.00001 -0.00022 -0.00105 -0.00128 1.04846

D213 -1.09379 -0.00001 -0.00011 -0.00121 -0.00131 -1.09511

D214 3.11965 -0.00002 -0.00018 -0.00119 -0.00137 3.11828

D215 1.09485 0.00005 0.00014 0.00235 0.00249 1.09734

D216 -1.04995 0.00000 0.00032 0.00167 0.00199 -1.04796

D217 -3.11911 0.00001 0.00024 0.00189 0.00213 -3.11698

D218 1.04995 0.00000 -0.00032 -0.00167 -0.00199 1.04796

D219 -1.09485 -0.00005 -0.00014 -0.00235 -0.00249 -1.09734

D220 3.11911 -0.00001 -0.00024 -0.00189 -0.00213 3.11698

D221 1.04974 -0.00001 -0.00022 -0.00105 -0.00128 1.04846

D222 -1.09379 -0.00001 -0.00011 -0.00121 -0.00131 -1.09511

D223 3.11965 -0.00002 -0.00018 -0.00119 -0.00137 3.11828

D224 1.09379 0.00001 0.00011 0.00121 0.00131 1.09511

D225 -1.04974 0.00001 0.00022 0.00105 0.00128 -1.04846

D226 -3.11965 0.00002 0.00018 0.00119 0.00137 -3.11828

D227 1.09485 0.00005 0.00014 0.00235 0.00249 1.09734

D228 -1.04995 0.00000 0.00032 0.00167 0.00199 -1.04796

D229 -3.11911 0.00001 0.00024 0.00189 0.00213 -3.11698

D230 1.04995 0.00000 -0.00032 -0.00167 -0.00199 1.04796

D231 -1.09485 -0.00005 -0.00014 -0.00235 -0.00249 -1.09734

D232 3.11911 -0.00001 -0.00024 -0.00189 -0.00213 3.11698

Item Value Threshold Converged?

Maximum Force 0.000800 0.000450 NO

RMS Force 0.000180 0.000300 YES

Maximum Displacement 0.174738 0.001800 NO

RMS Displacement 0.043637 0.001200 NO

Predicted change in Energy=-1.358819D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 5 23:40:31 2019, MaxMem= 1342177280 cpu: 15.9

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

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=3 Diff= 4.40D-08

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 -1.125774 2.810488 0.053888

2 7 0 0.000017 2.047368 -0.066194

3 6 0 1.125801 2.810485 0.053887

4 6 0 0.713676 4.181686 0.279183

5 6 0 -0.713645 4.181687 0.279185

6 7 0 2.412127 2.385938 -0.047893

7 6 0 2.802765 1.133814 -0.116980

8 7 0 2.033641 0.000019 -0.022486

9 6 0 2.802768 -1.133783 -0.116980

10 6 0 4.208338 -0.705467 -0.295486

11 6 0 4.208336 0.705501 -0.295485

12 7 0 -2.412116 2.385943 -0.047893

13 6 0 -4.208358 0.705505 -0.295489

14 6 0 -4.208360 -0.705470 -0.295490

15 6 0 -2.802789 -1.133788 -0.116983

16 7 0 -2.033683 0.000019 -0.022489

17 6 0 -2.802786 1.133819 -0.116983

18 7 0 -2.412120 -2.385929 -0.047893

19 7 0 0.000017 -2.047413 -0.066194

20 6 0 -1.125779 -2.810510 0.053889

21 6 0 -0.713648 -4.181711 0.279186

22 6 0 0.713679 -4.181710 0.279185

23 6 0 1.125806 -2.810507 0.053888

24 7 0 2.412132 -2.385924 -0.047893

25 30 0 -0.000034 -0.000038 -0.084616

26 6 0 -5.394563 1.432011 -0.445923

27 6 0 -6.584470 0.695240 -0.587094

28 6 0 -6.584471 -0.695201 -0.587095

29 6 0 -5.394566 -1.431975 -0.445925

30 6 0 1.433788 -5.375944 0.477378

31 6 0 0.700577 -6.553628 0.656789

32 6 0 -0.700540 -6.553630 0.656791

33 6 0 -1.433754 -5.375947 0.477381

34 6 0 5.394540 1.432009 -0.445917

35 6 0 6.584448 0.695240 -0.587086

36 6 0 6.584449 -0.695200 -0.587087

37 6 0 5.394543 -1.431973 -0.445918

38 6 0 -1.433752 5.375923 0.477377

39 6 0 -0.700540 6.553606 0.656785

40 6 0 0.700577 6.553605 0.656783

41 6 0 1.433786 5.375920 0.477374

42 1 0 7.530770 1.205641 -0.705781

43 1 0 7.530772 -1.205599 -0.705782

44 1 0 1.208786 7.496091 0.810061

45 1 0 -1.208747 7.496094 0.810063

46 1 0 -7.530792 1.205640 -0.705790

47 1 0 -7.530795 -1.205599 -0.705791

48 1 0 -1.208747 -7.496117 0.810071

49 1 0 1.208786 -7.496115 0.810068

50 8 0 2.782150 5.312061 0.489375

51 8 0 -2.782116 5.312067 0.489380

52 8 0 5.334516 2.779488 -0.454719

53 8 0 5.334522 -2.779451 -0.454721

54 8 0 2.782152 -5.312087 0.489380

55 8 0 -2.782118 -5.312093 0.489386

56 8 0 -5.334546 -2.779453 -0.454727

57 8 0 -5.334541 2.779490 -0.454725

58 6 0 3.518546 6.525432 0.623151

59 1 0 3.315200 7.016135 1.579406

60 1 0 3.301106 7.215790 -0.197187

61 1 0 4.566862 6.235730 0.583445

62 6 0 6.553428 3.515941 -0.541685

63 1 0 7.077084 3.318036 -1.481232

64 1 0 7.214123 3.294483 0.301502

65 1 0 6.261777 4.563749 -0.506577

66 6 0 6.553434 -3.515903 -0.541688

67 1 0 7.214130 -3.294444 0.301499

68 1 0 7.077091 -3.317996 -1.481235

69 1 0 6.261786 -4.563710 -0.506581

70 6 0 -3.518510 6.525439 0.623159

71 1 0 -3.301070 7.215797 -0.197180

72 1 0 -3.315160 7.016142 1.579413

73 1 0 -4.566826 6.235739 0.583455

74 6 0 -6.553452 3.515942 -0.541693

75 1 0 -7.214149 3.294483 0.301493

76 1 0 -7.077108 3.318036 -1.481241

77 1 0 -6.261803 4.563750 -0.506585

78 6 0 -6.553460 -3.515903 -0.541697

79 1 0 -7.077115 -3.317996 -1.481244

80 1 0 -7.214156 -3.294444 0.301490

81 1 0 -6.261812 -4.563711 -0.506590

82 6 0 -3.518511 -6.525465 0.623167

83 1 0 -3.315160 -7.016166 1.579421

84 1 0 -3.301071 -7.215825 -0.197171

85 1 0 -4.566827 -6.235767 0.583463

86 6 0 3.518547 -6.525458 0.623159

87 1 0 3.301107 -7.215818 -0.197178

88 1 0 3.315199 -7.016160 1.579414

89 1 0 4.566863 -6.235758 0.583453

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

Rotational constants (GHZ): 0.0444396 0.0441091 0.0224415

Leave Link 202 at Fri Jul 5 23:40:33 2019, MaxMem= 1342177280 cpu: 0.3

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

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

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8034.7360837848 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= 89 NActive= 89 NUniq= 89 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= -0.2278656573 Hartrees.

Nuclear repulsion after empirical dispersion term = 8034.5082181275 Hartrees.

No density basis found on file 724.

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Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6382

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.21D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 334

GePol: Fraction of low-weight points (<1% of avg) = 5.23%

GePol: Cavity surface area = 700.297 Ang\*\*2

GePol: Cavity volume = 799.527 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0089748375 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8034.4992432900 Hartrees.

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

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

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

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44221 LenP2D= 111092.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.63D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 5 23:40:38 2019, MaxMem= 1342177280 cpu: 2.5

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

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0171 S= 1.0057

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2650.02620341658

Leave Link 401 at Fri Jul 5 23:40:55 2019, MaxMem= 1342177280 cpu: 203.6

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 530000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 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= 122189772.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.33D-15 for 6374.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.78D-15 for 4975 4301.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.33D-15 for 6374.

Iteration 1 A^-1\*A deviation from orthogonality is 9.84D-08 for 6257 6205.

Iteration 2 A\*A^-1 deviation from unit magnitude is 4.22D-15 for 397.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.26D-15 for 5663 80.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.22D-15 for 735.

Iteration 2 A^-1\*A deviation from orthogonality is 4.77D-16 for 2826 2546.

E= -2649.78902264442

DIIS: error= 1.35D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.78902264442 IErMin= 1 ErrMin= 1.35D-03

ErrMax= 1.35D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.65D-03 BMatP= 9.65D-03

IDIUse=3 WtCom= 9.86D-01 WtEn= 1.35D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.684 Goal= None Shift= 0.000

Gap= 0.743 Goal= None Shift= 0.000

GapD= 0.684 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=8.48D-05 MaxDP=3.66D-03 OVMax= 9.32D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 8.47D-05 CP: 1.00D+00

E= -2649.79334444904 Delta-E= -0.004321804621 Rises=F Damp=F

DIIS: error= 2.04D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79334444904 IErMin= 2 ErrMin= 2.04D-04

ErrMax= 2.04D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D-04 BMatP= 9.65D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.04D-03

Coeff-Com: -0.592D-01 0.106D+01

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

Coeff: -0.591D-01 0.106D+01

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.01D-05 MaxDP=4.69D-04 DE=-4.32D-03 OVMax= 1.82D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 8.99D-06 CP: 1.00D+00 1.05D+00

E= -2649.79339491644 Delta-E= -0.000050467401 Rises=F Damp=F

DIIS: error= 1.52D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79339491644 IErMin= 3 ErrMin= 1.52D-04

ErrMax= 1.52D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.64D-05 BMatP= 1.13D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.52D-03

Coeff-Com: -0.311D-01 0.468D+00 0.563D+00

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

Coeff: -0.311D-01 0.467D+00 0.564D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=5.33D-06 MaxDP=3.51D-04 DE=-5.05D-05 OVMax= 1.15D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.41D-06 CP: 1.00D+00 1.06D+00 6.79D-01

E= -2649.79340320676 Delta-E= -0.000008290313 Rises=F Damp=F

DIIS: error= 9.23D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79340320676 IErMin= 4 ErrMin= 9.23D-05

ErrMax= 9.23D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.73D-05 BMatP= 5.64D-05

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

Coeff-Com: -0.671D-02 0.738D-01 0.355D+00 0.578D+00

Coeff: -0.671D-02 0.738D-01 0.355D+00 0.578D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=2.10D-06 MaxDP=1.47D-04 DE=-8.29D-06 OVMax= 2.92D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.10D-06 CP: 1.00D+00 1.06D+00 8.15D-01 7.06D-01

E= -2649.79340658700 Delta-E= -0.000003380243 Rises=F Damp=F

DIIS: error= 7.78D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79340658700 IErMin= 5 ErrMin= 7.78D-06

ErrMax= 7.78D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.81D-07 BMatP= 1.73D-05

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

Coeff-Com: 0.353D-03-0.171D-01 0.623D-01 0.166D+00 0.789D+00

Coeff: 0.353D-03-0.171D-01 0.623D-01 0.166D+00 0.789D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=4.35D-07 MaxDP=1.75D-05 DE=-3.38D-06 OVMax= 1.71D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.40D-07 CP: 1.00D+00 1.06D+00 8.31D-01 7.47D-01 8.83D-01

E= -2649.79340665467 Delta-E= -0.000000067666 Rises=F Damp=F

DIIS: error= 5.75D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79340665467 IErMin= 6 ErrMin= 5.75D-06

ErrMax= 5.75D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.01D-07 BMatP= 2.81D-07

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

Coeff-Com: 0.617D-03-0.146D-01 0.134D-01 0.571D-01 0.451D+00 0.492D+00

Coeff: 0.617D-03-0.146D-01 0.134D-01 0.571D-01 0.451D+00 0.492D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.80D-07 MaxDP=1.10D-05 DE=-6.77D-08 OVMax= 6.71D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.48D-07 CP: 1.00D+00 1.06D+00 8.34D-01 7.54D-01 9.36D-01

CP: 7.79D-01

E= -2649.79340668105 Delta-E= -0.000000026384 Rises=F Damp=F

DIIS: error= 1.63D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79340668105 IErMin= 7 ErrMin= 1.63D-06

ErrMax= 1.63D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.82D-09 BMatP= 1.01D-07

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

Coeff-Com: 0.189D-03-0.290D-02-0.502D-02-0.616D-02 0.468D-01 0.205D+00

Coeff-Com: 0.762D+00

Coeff: 0.189D-03-0.290D-02-0.502D-02-0.616D-02 0.468D-01 0.205D+00

Coeff: 0.762D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=8.65D-08 MaxDP=4.23D-06 DE=-2.64D-08 OVMax= 7.41D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 5.68D-08 CP: 1.00D+00 1.06D+00 8.36D-01 7.56D-01 9.58D-01

CP: 9.35D-01 1.11D+00

E= -2649.79340668506 Delta-E= -0.000000004009 Rises=F Damp=F

DIIS: error= 1.17D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.79340668506 IErMin= 8 ErrMin= 1.17D-06

ErrMax= 1.17D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.51D-09 BMatP= 7.82D-09

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

Coeff-Com: -0.303D-04 0.162D-02-0.543D-02-0.160D-01-0.726D-01 0.655D-02

Coeff-Com: 0.410D+00 0.676D+00

Coeff: -0.303D-04 0.162D-02-0.543D-02-0.160D-01-0.726D-01 0.655D-02

Coeff: 0.410D+00 0.676D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=5.00D-08 MaxDP=2.55D-06 DE=-4.01D-09 OVMax= 3.76D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.66D-08 CP: 1.00D+00 1.06D+00 8.37D-01 7.58D-01 9.73D-01

CP: 1.01D+00 1.30D+00 9.63D-01

E= -2649.79340668654 Delta-E= -0.000000001482 Rises=F Damp=F

DIIS: error= 6.42D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.79340668654 IErMin= 9 ErrMin= 6.42D-07

ErrMax= 6.42D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.05D-10 BMatP= 2.51D-09

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

Coeff-Com: -0.681D-04 0.170D-02-0.147D-02-0.715D-02-0.522D-01-0.501D-01

Coeff-Com: 0.251D-01 0.375D+00 0.710D+00

Coeff: -0.681D-04 0.170D-02-0.147D-02-0.715D-02-0.522D-01-0.501D-01

Coeff: 0.251D-01 0.375D+00 0.710D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=2.72D-08 MaxDP=1.54D-06 DE=-1.48D-09 OVMax= 2.53D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.44D-08 CP: 1.00D+00 1.06D+00 8.37D-01 7.59D-01 9.78D-01

CP: 1.04D+00 1.40D+00 1.15D+00 9.61D-01

E= -2649.79340668697 Delta-E= -0.000000000426 Rises=F Damp=F

DIIS: error= 3.86D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -2649.79340668697 IErMin=10 ErrMin= 3.86D-07

ErrMax= 3.86D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.36D-10 BMatP= 6.05D-10

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

Coeff-Com: -0.294D-04 0.557D-03 0.353D-03-0.563D-03-0.129D-01-0.268D-01

Coeff-Com: -0.668D-01 0.692D-01 0.377D+00 0.660D+00

Coeff: -0.294D-04 0.557D-03 0.353D-03-0.563D-03-0.129D-01-0.268D-01

Coeff: -0.668D-01 0.692D-01 0.377D+00 0.660D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.13D-08 MaxDP=8.93D-07 DE=-4.26D-10 OVMax= 1.03D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 6.46D-09 CP: 1.00D+00 1.06D+00 8.37D-01 7.59D-01 9.80D-01

CP: 1.06D+00 1.42D+00 1.21D+00 1.17D+00 9.94D-01

E= -2649.79340668679 Delta-E= 0.000000000178 Rises=F Damp=F

DIIS: error= 2.01D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=10 EnMin= -2649.79340668697 IErMin=11 ErrMin= 2.01D-07

ErrMax= 2.01D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.25D-11 BMatP= 1.36D-10

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

Coeff-Com: 0.487D-05-0.226D-03 0.651D-03 0.191D-02 0.898D-02 0.600D-03

Coeff-Com: -0.466D-01-0.756D-01-0.650D-02 0.358D+00 0.759D+00

Coeff: 0.487D-05-0.226D-03 0.651D-03 0.191D-02 0.898D-02 0.600D-03

Coeff: -0.466D-01-0.756D-01-0.650D-02 0.358D+00 0.759D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=6.26D-09 MaxDP=4.98D-07 DE= 1.78D-10 OVMax= 5.15D-06

Error on total polarization charges = 0.07275

SCF Done: E(UB3LYP) = -2649.79340669 A.U. after 11 cycles

NFock= 11 Conv=0.63D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0170 S= 1.0057

<L.S>= 0.000000000000E+00

KE= 2.690103841594D+03 PE=-2.234766963042D+04 EE= 8.973273138846D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0170, after 2.0002

Leave Link 502 at Fri Jul 5 23:49:56 2019, MaxMem= 1342177280 cpu: 6384.0

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

Compute integral first derivatives.

... and contract with generalized density number 0.

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

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44221 LenP2D= 111092.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 275

Leave Link 701 at Fri Jul 5 23:50:15 2019, MaxMem= 1342177280 cpu: 218.3

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

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

Leave Link 702 at Fri Jul 5 23:50:15 2019, MaxMem= 1342177280 cpu: 0.2

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

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Fri Jul 5 23:51:47 2019, MaxMem= 1342177280 cpu: 1100.5

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

Dipole =-5.52580821D-05-4.49160721D-05-1.66609389D-02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.001116464 -0.000751650 0.000767898

2 7 -0.000006376 0.000186746 -0.001197976

3 6 0.001108930 -0.000745391 0.000768849

4 6 0.000006223 0.000470761 0.000018066

5 6 -0.000007037 0.000469664 0.000017768

6 7 -0.001446478 0.001234255 0.000048667

7 6 0.000564502 -0.001689655 -0.000466693

8 7 0.000105108 -0.000007986 0.002109984

9 6 0.000555979 0.001679507 -0.000465445

10 6 -0.000626523 -0.000147226 0.000046735

11 6 -0.000625810 0.000146437 0.000046633

12 7 0.001450308 0.001229792 0.000048547

13 6 0.000626026 0.000145491 0.000046720

14 6 0.000626739 -0.000146280 0.000046823

15 6 -0.000553787 0.001669913 -0.000465237

16 7 -0.000093744 -0.000007987 0.002111874

17 6 -0.000562310 -0.001680060 -0.000466481

18 7 0.001451362 -0.001221691 0.000048531

19 7 -0.000006376 -0.000173900 -0.001199946

20 6 -0.001123621 0.000752818 0.000767944

21 6 -0.000006416 -0.000469314 0.000017702

22 6 0.000005603 -0.000470411 0.000018001

23 6 0.001116087 0.000746559 0.000768895

24 7 -0.001447534 -0.001226155 0.000048650

25 30 0.000005270 0.000005977 -0.002812172

26 6 -0.000777574 -0.000573931 -0.000078834

27 6 0.000315043 0.000709614 0.000064436

28 6 0.000315012 -0.000709699 0.000064446

29 6 -0.000777811 0.000573627 -0.000078877

30 6 -0.000249257 0.000229883 -0.000065486

31 6 -0.000189825 -0.000063016 0.000041384

32 6 0.000189764 -0.000062848 0.000041352

33 6 0.000249074 0.000229420 -0.000065412

34 6 0.000777727 -0.000573239 -0.000078856

35 6 -0.000315254 0.000710317 0.000064478

36 6 -0.000315223 -0.000710402 0.000064488

37 6 0.000777965 0.000572936 -0.000078897

38 6 0.000248297 -0.000229378 -0.000065400

39 6 0.000189170 0.000062648 0.000041296

40 6 -0.000189232 0.000062817 0.000041329

41 6 -0.000248481 -0.000229842 -0.000065476

42 1 0.000040915 0.000013219 -0.000010892

43 1 0.000040906 -0.000013225 -0.000010893

44 1 0.000012466 0.000022995 -0.000019699

45 1 -0.000012473 0.000022997 -0.000019695

46 1 -0.000040935 0.000013186 -0.000010891

47 1 -0.000040927 -0.000013192 -0.000010892

48 1 -0.000012441 -0.000023019 -0.000019698

49 1 0.000012434 -0.000023017 -0.000019701

50 8 0.000131475 0.000164547 -0.000261738

51 8 -0.000131721 0.000164423 -0.000261657

52 8 0.000020508 0.000214001 0.000107921

53 8 0.000020381 -0.000214121 0.000107765

54 8 0.000131446 -0.000163842 -0.000261672

55 8 -0.000131692 -0.000163719 -0.000261590

56 8 -0.000019552 -0.000214012 0.000107738

57 8 -0.000019679 0.000213892 0.000107893

58 6 0.000091567 0.000274608 -0.000013088

59 1 -0.000019526 -0.000037874 0.000090695

60 1 -0.000028432 -0.000034426 -0.000061940

61 1 0.000083465 -0.000007902 0.000007676

62 6 -0.000081493 -0.000053775 0.000054152

63 1 0.000046807 -0.000030813 -0.000086186

64 1 0.000051099 -0.000041164 0.000064046

65 1 0.000004485 0.000105082 -0.000001011

66 6 -0.000081431 0.000053785 0.000054142

67 1 0.000051092 0.000041170 0.000064044

68 1 0.000046800 0.000030814 -0.000086184

69 1 0.000004452 -0.000105092 -0.000000993

70 6 -0.000091530 0.000274618 -0.000013079

71 1 0.000028438 -0.000034424 -0.000061940

72 1 0.000019530 -0.000037875 0.000090695

73 1 -0.000083477 -0.000007926 0.000007656

74 6 0.000081289 -0.000053650 0.000054140

75 1 -0.000051051 -0.000041166 0.000064038

76 1 -0.000046756 -0.000030814 -0.000086170

77 1 -0.000004498 0.000105099 -0.000001001

78 6 0.000081227 0.000053659 0.000054130

79 1 -0.000046749 0.000030814 -0.000086167

80 1 -0.000051043 0.000041172 0.000064036

81 1 -0.000004466 -0.000105109 -0.000000983

82 6 -0.000091667 -0.000274830 -0.000013058

83 1 0.000019533 0.000037931 0.000090675

84 1 0.000028440 0.000034475 -0.000061930

85 1 -0.000083497 0.000007908 0.000007650

86 6 0.000091704 -0.000274820 -0.000013067

87 1 -0.000028434 0.000034477 -0.000061930

88 1 -0.000019530 0.000037930 0.000090674

89 1 0.000083484 0.000007884 0.000007669

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

Cartesian Forces: Max 0.002812172 RMS 0.000504248

Leave Link 716 at Fri Jul 5 23:51:47 2019, MaxMem= 1342177280 cpu: 0.5

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.001182928 RMS 0.000243206

Search for a local minimum.

Step number 4 out of a maximum of 518

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

RMS Force = .24321D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4

DE= -1.22D-04 DEPred=-1.36D-04 R= 8.95D-01

TightC=F SS= 1.41D+00 RLast= 1.18D-01 DXNew= 7.2376D-01 3.5516D-01

Trust test= 8.95D-01 RLast= 1.18D-01 DXMaxT set to 4.30D-01

ITU= 1 1 1 0

Eigenvalues --- 0.00464 0.01316 0.01316 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01318 0.01555

Eigenvalues --- 0.01568 0.01569 0.01580 0.01599 0.01616

Eigenvalues --- 0.01620 0.01645 0.01707 0.01709 0.01712

Eigenvalues --- 0.01715 0.01830 0.01831 0.01867 0.01873

Eigenvalues --- 0.01904 0.01916 0.01927 0.01931 0.01932

Eigenvalues --- 0.01941 0.01999 0.02006 0.02021 0.02022

Eigenvalues --- 0.02022 0.02028 0.02053 0.02053 0.02053

Eigenvalues --- 0.02053 0.02057 0.02057 0.02057 0.02057

Eigenvalues --- 0.02067 0.02067 0.02067 0.02067 0.02070

Eigenvalues --- 0.02070 0.02070 0.02070 0.02081 0.02083

Eigenvalues --- 0.02083 0.02085 0.02258 0.02260 0.02260

Eigenvalues --- 0.02260 0.02260 0.02260 0.02260 0.02260

Eigenvalues --- 0.02338 0.02342 0.02346 0.02358 0.05544

Eigenvalues --- 0.09981 0.09981 0.09981 0.09987 0.09987

Eigenvalues --- 0.09987 0.09989 0.10017 0.10654 0.10654

Eigenvalues --- 0.10654 0.10654 0.10663 0.10663 0.10663

Eigenvalues --- 0.10663 0.13496 0.13508 0.15223 0.15986

Eigenvalues --- 0.15999 0.15999 0.15999 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16003 0.16035

Eigenvalues --- 0.16213 0.17522 0.21675 0.21804 0.22473

Eigenvalues --- 0.22473 0.22476 0.22476 0.24051 0.24467

Eigenvalues --- 0.24506 0.24515 0.24527 0.24565 0.24624

Eigenvalues --- 0.24681 0.24735 0.24876 0.24900 0.24931

Eigenvalues --- 0.24989 0.24995 0.24996 0.24999 0.24999

Eigenvalues --- 0.24999 0.24999 0.24999 0.24999 0.24999

Eigenvalues --- 0.24999 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25072 0.25917 0.27271

Eigenvalues --- 0.33639 0.33655 0.33695 0.33731 0.33736

Eigenvalues --- 0.34063 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34069 0.34078 0.34081 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34098

Eigenvalues --- 0.34206 0.34686 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34686 0.34734 0.34835

Eigenvalues --- 0.34913 0.34958 0.35626 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35632 0.35656

Eigenvalues --- 0.36518 0.37105 0.37111 0.37159 0.41181

Eigenvalues --- 0.41215 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41215 0.41327 0.41384 0.41411 0.41413

Eigenvalues --- 0.41413 0.41416 0.42468 0.42481 0.43574

Eigenvalues --- 0.43959 0.44560 0.44571 0.44665 0.44891

Eigenvalues --- 0.44923 0.44998 0.45000 0.45001 0.45004

Eigenvalues --- 0.45204 0.45366 0.45367 0.45816 0.46746

Eigenvalues --- 0.47379 0.48226 0.49295 0.49331 0.49776

Eigenvalues --- 0.49867 0.53554 0.53554 0.53554 0.53554

Eigenvalues --- 0.53554 0.53554 0.53586 0.54181 0.54999

Eigenvalues --- 0.55013 0.56093 0.57252 0.57417 0.57443

Eigenvalues --- 0.57581

En-DIIS/RFO-DIIS IScMMF= 0 using points: 4 3 2

RFO step: Lambda=-7.88468733D-05.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=F DC= 7.43D-04 SmlDif= 1.00D-05

RMS Error= 0.9810823708D-03 NUsed= 3 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.69851 0.62008 -0.31859

Iteration 1 RMS(Cart)= 0.02149070 RMS(Int)= 0.00011593

Iteration 2 RMS(Cart)= 0.00042533 RMS(Int)= 0.00006392

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00006392

ITry= 1 IFail=0 DXMaxC= 1.50D-01 DCOld= 1.00D+10 DXMaxT= 4.30D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.58013 0.00025 -0.00038 0.00007 -0.00024 2.57989

R2 2.73899 0.00062 -0.00195 -0.00200 -0.00399 2.73501

R3 2.56702 -0.00094 0.00359 0.00094 0.00436 2.57138

R4 2.58012 0.00025 -0.00038 0.00006 -0.00028 2.57984

R5 3.86919 0.00036 0.00055 0.00599 0.00687 3.87606

R6 2.73899 0.00062 -0.00195 -0.00200 -0.00398 2.73501

R7 2.56699 -0.00093 0.00360 0.00093 0.00430 2.57129

R8 2.69724 0.00021 0.00057 0.00264 0.00310 2.70034

R9 2.66179 0.00022 0.00094 -0.00036 0.00058 2.66236

R10 2.66179 0.00022 0.00094 -0.00036 0.00058 2.66236

R11 2.48208 0.00118 -0.00345 0.00066 -0.00302 2.47906

R12 2.59517 -0.00030 0.00130 -0.00017 0.00120 2.59638

R13 2.79714 -0.00016 0.00229 0.00146 0.00370 2.80085

R14 2.59519 -0.00030 0.00130 -0.00016 0.00123 2.59642

R15 3.84488 0.00002 -0.00111 0.00046 -0.00029 3.84459

R16 2.79714 -0.00016 0.00229 0.00145 0.00370 2.80084

R17 2.48211 0.00117 -0.00346 0.00066 -0.00297 2.47915

R18 2.66634 -0.00005 -0.00047 -0.00194 -0.00253 2.66381

R19 2.64394 0.00047 -0.00073 0.00031 -0.00041 2.64354

R20 2.64394 0.00047 -0.00073 0.00031 -0.00041 2.64354

R21 2.48210 0.00117 -0.00346 0.00066 -0.00298 2.47912

R22 2.66636 -0.00005 -0.00048 -0.00194 -0.00251 2.66385

R23 2.79715 -0.00016 0.00228 0.00146 0.00371 2.80086

R24 2.64394 0.00046 -0.00072 0.00031 -0.00041 2.64353

R25 2.79715 -0.00016 0.00228 0.00145 0.00371 2.80086

R26 2.64394 0.00046 -0.00072 0.00031 -0.00041 2.64353

R27 2.59517 -0.00030 0.00130 -0.00017 0.00120 2.59637

R28 2.48213 0.00116 -0.00347 0.00066 -0.00293 2.47921

R29 2.59516 -0.00029 0.00131 -0.00017 0.00116 2.59632

R30 3.84483 0.00002 -0.00110 0.00041 -0.00044 3.84440

R31 2.56704 -0.00095 0.00359 0.00095 0.00440 2.57144

R32 2.58012 0.00025 -0.00038 0.00006 -0.00028 2.57984

R33 2.58010 0.00025 -0.00037 0.00006 -0.00031 2.57979

R34 3.86913 0.00035 0.00057 0.00592 0.00671 3.87585

R35 2.73900 0.00062 -0.00196 -0.00200 -0.00398 2.73502

R36 2.69726 0.00020 0.00056 0.00265 0.00313 2.70038

R37 2.66179 0.00022 0.00094 -0.00036 0.00057 2.66236

R38 2.73900 0.00062 -0.00196 -0.00200 -0.00397 2.73502

R39 2.66179 0.00022 0.00094 -0.00036 0.00057 2.66236

R40 2.56701 -0.00094 0.00359 0.00094 0.00434 2.57135

R41 2.65817 -0.00045 0.00119 0.00053 0.00172 2.65989

R42 2.54894 0.00019 -0.00090 0.00004 -0.00086 2.54809

R43 2.62755 0.00031 -0.00165 0.00131 -0.00034 2.62721

R44 2.04416 0.00004 -0.00011 0.00046 0.00035 2.04450

R45 2.65817 -0.00045 0.00119 0.00053 0.00172 2.65989

R46 2.04416 0.00004 -0.00011 0.00046 0.00035 2.04450

R47 2.54894 0.00019 -0.00090 0.00004 -0.00086 2.54809

R48 2.64341 0.00000 0.00007 0.00020 0.00027 2.64368

R49 2.55099 0.00024 -0.00068 -0.00092 -0.00160 2.54939

R50 2.64773 -0.00032 -0.00034 -0.00003 -0.00037 2.64736

R51 2.04410 0.00002 -0.00021 0.00042 0.00022 2.04432

R52 2.64341 0.00000 0.00007 0.00020 0.00027 2.64368

R53 2.04410 0.00002 -0.00021 0.00042 0.00022 2.04432

R54 2.55099 0.00024 -0.00068 -0.00092 -0.00160 2.54939

R55 2.65817 -0.00045 0.00119 0.00053 0.00172 2.65989

R56 2.54894 0.00019 -0.00090 0.00004 -0.00086 2.54809

R57 2.62755 0.00031 -0.00165 0.00131 -0.00035 2.62720

R58 2.04416 0.00004 -0.00011 0.00046 0.00035 2.04450

R59 2.65817 -0.00045 0.00119 0.00053 0.00172 2.65989

R60 2.04416 0.00004 -0.00011 0.00046 0.00035 2.04450

R61 2.54894 0.00019 -0.00090 0.00004 -0.00086 2.54809

R62 2.64341 0.00000 0.00007 0.00020 0.00027 2.64367

R63 2.55099 0.00024 -0.00068 -0.00092 -0.00160 2.54939

R64 2.64773 -0.00032 -0.00034 -0.00003 -0.00037 2.64736

R65 2.04410 0.00002 -0.00021 0.00042 0.00022 2.04432

R66 2.64341 0.00000 0.00007 0.00020 0.00027 2.64367

R67 2.04410 0.00002 -0.00021 0.00042 0.00022 2.04432

R68 2.55099 0.00024 -0.00068 -0.00092 -0.00160 2.54939

R69 2.69407 0.00023 -0.00019 0.00005 -0.00014 2.69393

R70 2.69407 0.00023 -0.00019 0.00005 -0.00014 2.69393

R71 2.69620 0.00001 -0.00003 -0.00054 -0.00057 2.69563

R72 2.69620 0.00001 -0.00003 -0.00054 -0.00057 2.69563

R73 2.69407 0.00023 -0.00019 0.00005 -0.00013 2.69393

R74 2.69407 0.00023 -0.00019 0.00005 -0.00013 2.69393

R75 2.69620 0.00001 -0.00003 -0.00054 -0.00057 2.69563

R76 2.69620 0.00001 -0.00003 -0.00054 -0.00057 2.69563

R77 2.06712 0.00007 -0.00035 0.00064 0.00029 2.06742

R78 2.06736 0.00003 -0.00036 0.00059 0.00023 2.06758

R79 2.05665 0.00008 -0.00023 0.00040 0.00017 2.05682

R80 2.06675 0.00010 -0.00037 0.00074 0.00037 2.06712

R81 2.06709 0.00009 -0.00039 0.00077 0.00038 2.06748

R82 2.05641 0.00010 -0.00025 0.00050 0.00025 2.05666

R83 2.06709 0.00009 -0.00039 0.00077 0.00038 2.06748

R84 2.06675 0.00010 -0.00037 0.00074 0.00037 2.06712

R85 2.05641 0.00010 -0.00025 0.00050 0.00025 2.05666

R86 2.06736 0.00003 -0.00036 0.00059 0.00023 2.06758

R87 2.06712 0.00007 -0.00035 0.00064 0.00029 2.06742

R88 2.05665 0.00008 -0.00023 0.00040 0.00017 2.05682

R89 2.06709 0.00009 -0.00039 0.00077 0.00038 2.06748

R90 2.06675 0.00010 -0.00037 0.00074 0.00037 2.06712

R91 2.05641 0.00010 -0.00025 0.00050 0.00025 2.05666

R92 2.06675 0.00010 -0.00037 0.00074 0.00037 2.06712

R93 2.06709 0.00009 -0.00039 0.00077 0.00038 2.06748

R94 2.05641 0.00010 -0.00025 0.00050 0.00025 2.05666

R95 2.06712 0.00007 -0.00035 0.00064 0.00029 2.06742

R96 2.06736 0.00003 -0.00036 0.00059 0.00023 2.06758

R97 2.05665 0.00008 -0.00023 0.00040 0.00017 2.05682

R98 2.06736 0.00003 -0.00036 0.00059 0.00023 2.06758

R99 2.06712 0.00007 -0.00035 0.00064 0.00029 2.06742

R100 2.05665 0.00008 -0.00023 0.00040 0.00017 2.05682

A1 1.88386 0.00010 0.00150 0.00132 0.00295 1.88681

A2 2.21371 -0.00005 -0.00166 -0.00075 -0.00241 2.21131

A3 2.18532 -0.00006 0.00005 -0.00044 -0.00050 2.18482

A4 1.93879 -0.00009 -0.00190 -0.00132 -0.00347 1.93532

A5 2.16478 0.00003 0.00076 -0.00049 0.00023 2.16501

A6 2.16483 0.00003 0.00074 -0.00045 0.00036 2.16519

A7 1.88387 0.00010 0.00150 0.00132 0.00295 1.88682

A8 2.21371 -0.00005 -0.00166 -0.00076 -0.00243 2.21128

A9 2.18532 -0.00006 0.00005 -0.00043 -0.00049 2.18483

A10 1.85912 -0.00005 -0.00054 -0.00063 -0.00121 1.85791

A11 2.31665 0.00016 0.00089 0.00069 0.00159 2.31824

A12 2.10742 -0.00011 -0.00035 -0.00005 -0.00038 2.10704

A13 1.85911 -0.00005 -0.00054 -0.00063 -0.00121 1.85791

A14 2.31665 0.00016 0.00089 0.00068 0.00159 2.31824

A15 2.10742 -0.00011 -0.00035 -0.00005 -0.00038 2.10704

A16 2.19384 0.00018 0.00020 -0.00076 -0.00073 2.19312

A17 2.23554 -0.00018 0.00134 0.00066 0.00200 2.23753

A18 2.17076 0.00001 -0.00056 -0.00109 -0.00182 2.16894

A19 1.87677 0.00016 -0.00079 0.00046 -0.00016 1.87661

A20 1.94251 -0.00013 0.00071 -0.00080 -0.00036 1.94215

A21 2.16243 0.00003 -0.00043 -0.00146 -0.00186 2.16057

A22 2.16237 0.00003 -0.00041 -0.00150 -0.00199 2.16038

A23 1.87677 0.00016 -0.00079 0.00046 -0.00017 1.87660

A24 2.23554 -0.00017 0.00134 0.00067 0.00202 2.23756

A25 2.17076 0.00001 -0.00056 -0.00110 -0.00183 2.16893

A26 1.86436 -0.00010 0.00044 -0.00006 0.00035 1.86471

A27 2.30204 0.00028 -0.00098 -0.00054 -0.00153 2.30051

A28 2.11678 -0.00018 0.00055 0.00061 0.00117 2.11795

A29 1.86436 -0.00010 0.00044 -0.00006 0.00035 1.86471

A30 2.30204 0.00028 -0.00098 -0.00054 -0.00153 2.30051

A31 2.11678 -0.00018 0.00055 0.00060 0.00116 2.11795

A32 2.19386 0.00018 0.00020 -0.00076 -0.00069 2.19317

A33 1.86436 -0.00010 0.00044 -0.00006 0.00035 1.86471

A34 2.11678 -0.00018 0.00055 0.00060 0.00116 2.11794

A35 2.30204 0.00028 -0.00098 -0.00054 -0.00153 2.30052

A36 1.86436 -0.00010 0.00044 -0.00006 0.00035 1.86471

A37 2.11678 -0.00018 0.00055 0.00060 0.00116 2.11795

A38 2.30204 0.00027 -0.00098 -0.00054 -0.00153 2.30051

A39 1.87675 0.00017 -0.00078 0.00046 -0.00020 1.87655

A40 2.17078 0.00000 -0.00057 -0.00109 -0.00177 2.16901

A41 2.23553 -0.00017 0.00134 0.00067 0.00200 2.23753

A42 1.94254 -0.00013 0.00070 -0.00079 -0.00029 1.94225

A43 2.16235 0.00004 -0.00040 -0.00151 -0.00203 2.16033

A44 2.16241 0.00003 -0.00042 -0.00147 -0.00189 2.16052

A45 2.17078 0.00001 -0.00057 -0.00108 -0.00176 2.16902

A46 2.23553 -0.00017 0.00134 0.00066 0.00198 2.23750

A47 1.87675 0.00016 -0.00079 0.00046 -0.00019 1.87656

A48 2.19388 0.00018 0.00019 -0.00075 -0.00065 2.19324

A49 1.93882 -0.00010 -0.00191 -0.00131 -0.00341 1.93542

A50 2.16476 0.00003 0.00076 -0.00050 0.00019 2.16496

A51 2.16482 0.00003 0.00074 -0.00046 0.00032 2.16514

A52 2.21370 -0.00005 -0.00166 -0.00076 -0.00243 2.21128

A53 2.18535 -0.00006 0.00005 -0.00043 -0.00045 2.18490

A54 1.88385 0.00011 0.00151 0.00131 0.00291 1.88676

A55 1.85912 -0.00005 -0.00054 -0.00063 -0.00121 1.85791

A56 2.31665 0.00016 0.00089 0.00069 0.00160 2.31824

A57 2.10742 -0.00011 -0.00035 -0.00005 -0.00039 2.10703

A58 1.85912 -0.00005 -0.00054 -0.00063 -0.00121 1.85791

A59 2.10742 -0.00011 -0.00035 -0.00005 -0.00039 2.10703

A60 2.31665 0.00016 0.00089 0.00069 0.00160 2.31824

A61 1.88385 0.00011 0.00150 0.00131 0.00292 1.88677

A62 2.21370 -0.00005 -0.00165 -0.00076 -0.00244 2.21125

A63 2.18535 -0.00006 0.00005 -0.00042 -0.00044 2.18491

A64 2.19387 0.00018 0.00019 -0.00076 -0.00069 2.19318

A65 1.57047 0.00000 0.00011 -0.00069 -0.00096 1.56950

A66 1.57052 -0.00001 0.00010 -0.00066 -0.00084 1.56968

A67 1.57053 -0.00001 0.00010 -0.00065 -0.00084 1.56969

A68 1.57057 -0.00001 0.00008 -0.00063 -0.00071 1.56986

A69 2.04430 0.00022 -0.00092 -0.00043 -0.00134 2.04296

A70 2.07340 0.00002 0.00168 0.00017 0.00186 2.07526

A71 2.16547 -0.00024 -0.00076 0.00025 -0.00052 2.16495

A72 2.12208 -0.00005 0.00037 -0.00017 0.00019 2.12227

A73 2.09891 0.00003 -0.00044 -0.00080 -0.00123 2.09768

A74 2.06217 0.00001 0.00007 0.00097 0.00105 2.06322

A75 2.12208 -0.00005 0.00037 -0.00017 0.00019 2.12227

A76 2.06217 0.00001 0.00007 0.00097 0.00105 2.06322

A77 2.09891 0.00003 -0.00044 -0.00080 -0.00123 2.09768

A78 2.04430 0.00022 -0.00092 -0.00043 -0.00134 2.04295

A79 2.07340 0.00002 0.00168 0.00017 0.00186 2.07526

A80 2.16547 -0.00024 -0.00076 0.00025 -0.00052 2.16495

A81 2.05317 0.00005 0.00031 -0.00037 -0.00006 2.05310

A82 2.06212 0.00044 -0.00014 0.00098 0.00084 2.06296

A83 2.16789 -0.00049 -0.00017 -0.00060 -0.00077 2.16712

A84 2.12253 0.00006 0.00004 0.00041 0.00045 2.12298

A85 2.10072 -0.00003 0.00038 -0.00111 -0.00073 2.09999

A86 2.05989 -0.00003 -0.00041 0.00070 0.00029 2.06018

A87 2.12253 0.00006 0.00004 0.00041 0.00045 2.12298

A88 2.05989 -0.00003 -0.00041 0.00070 0.00029 2.06018

A89 2.10072 -0.00003 0.00038 -0.00111 -0.00073 2.09999

A90 2.05317 0.00005 0.00031 -0.00037 -0.00006 2.05310

A91 2.06212 0.00044 -0.00014 0.00098 0.00084 2.06296

A92 2.16789 -0.00049 -0.00017 -0.00060 -0.00077 2.16712

A93 2.04430 0.00022 -0.00092 -0.00043 -0.00134 2.04296

A94 2.07340 0.00002 0.00168 0.00018 0.00186 2.07526

A95 2.16547 -0.00024 -0.00076 0.00024 -0.00052 2.16495

A96 2.12208 -0.00004 0.00037 -0.00017 0.00019 2.12227

A97 2.09891 0.00003 -0.00044 -0.00080 -0.00123 2.09768

A98 2.06217 0.00001 0.00007 0.00097 0.00105 2.06322

A99 2.12208 -0.00004 0.00037 -0.00017 0.00019 2.12227

A100 2.06217 0.00001 0.00007 0.00097 0.00105 2.06322

A101 2.09891 0.00003 -0.00044 -0.00080 -0.00123 2.09768

A102 2.04430 0.00022 -0.00092 -0.00043 -0.00134 2.04295

A103 2.07340 0.00002 0.00168 0.00018 0.00186 2.07526

A104 2.16547 -0.00024 -0.00076 0.00024 -0.00052 2.16495

A105 2.05317 0.00005 0.00031 -0.00037 -0.00006 2.05310

A106 2.06212 0.00044 -0.00014 0.00098 0.00084 2.06296

A107 2.16789 -0.00049 -0.00017 -0.00060 -0.00077 2.16712

A108 2.12252 0.00006 0.00004 0.00041 0.00045 2.12297

A109 2.10072 -0.00003 0.00037 -0.00111 -0.00073 2.09999

A110 2.05989 -0.00003 -0.00041 0.00070 0.00029 2.06019

A111 2.12252 0.00006 0.00004 0.00041 0.00045 2.12297

A112 2.05989 -0.00003 -0.00041 0.00070 0.00029 2.06019

A113 2.10072 -0.00003 0.00037 -0.00111 -0.00073 2.09999

A114 2.05317 0.00005 0.00031 -0.00037 -0.00006 2.05310

A115 2.06212 0.00044 -0.00014 0.00098 0.00084 2.06296

A116 2.16789 -0.00049 -0.00017 -0.00060 -0.00077 2.16712

A117 2.06748 -0.00009 0.00188 -0.00204 -0.00016 2.06732

A118 2.06748 -0.00009 0.00188 -0.00203 -0.00016 2.06732

A119 2.06920 -0.00018 0.00121 -0.00073 0.00048 2.06968

A120 2.06920 -0.00018 0.00121 -0.00073 0.00048 2.06968

A121 2.06748 -0.00009 0.00188 -0.00203 -0.00016 2.06732

A122 2.06748 -0.00009 0.00188 -0.00203 -0.00015 2.06732

A123 2.06920 -0.00018 0.00121 -0.00073 0.00048 2.06968

A124 2.06920 -0.00018 0.00121 -0.00073 0.00048 2.06968

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A130 1.90929 0.00002 -0.00027 0.00053 0.00026 1.90955

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A132 1.94392 -0.00003 -0.00061 0.00126 0.00065 1.94457

A133 1.84011 0.00007 0.00104 -0.00163 -0.00060 1.83952

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A176 3.08051 -0.00095 -0.00006 -0.04990 -0.04996 3.03055

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D2 2.95699 0.00049 0.00266 -0.00644 -0.00377 2.95322

D3 3.10981 0.00047 0.00177 0.01266 0.01437 3.12418

D4 -0.20956 0.00029 -0.00119 -0.00086 -0.00205 -0.21160

D5 0.00403 -0.00039 -0.00330 -0.00418 -0.00747 -0.00344

D6 -3.13568 -0.00044 -0.00468 -0.00587 -0.01055 3.13695

D7 -3.11311 -0.00020 0.00050 -0.00963 -0.00912 -3.12224

D8 0.03036 -0.00025 -0.00088 -0.01133 -0.01221 0.01815

D9 0.15630 0.00007 0.00092 0.01942 0.02032 0.17661

D10 -3.01436 -0.00016 -0.00354 0.02593 0.02236 -2.99200

D11 0.00683 -0.00067 -0.00561 -0.00709 -0.01265 -0.00582

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D13 -2.95699 -0.00049 -0.00266 0.00644 0.00378 -2.95320

D14 0.20956 -0.00029 0.00118 0.00086 0.00206 0.21162

D15 -3.01083 0.00058 0.00179 0.03262 0.03443 -2.97640

D16 0.06968 -0.00037 0.00173 -0.01728 -0.01552 0.05416

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D25 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D30 -0.01663 0.00012 -0.00037 -0.00075 -0.00112 -0.01775

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D32 3.12286 0.00018 0.00118 0.00114 0.00232 3.12518

D33 -3.13092 0.00000 0.00096 0.00255 0.00352 -3.12740

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D37 -0.07461 0.00022 0.00197 0.00782 0.00982 -0.06479

D38 3.08565 0.00029 0.00285 0.00528 0.00814 3.09379

D39 -3.12134 -0.00030 -0.00419 -0.00189 -0.00608 -3.12742

D40 0.20466 0.00004 -0.00300 0.01985 0.01686 0.22151

D41 0.00409 -0.00037 -0.00495 0.00030 -0.00464 -0.00055

D42 -2.95310 -0.00003 -0.00376 0.02204 0.01829 -2.93480

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D44 -0.01762 0.00019 0.00273 0.00718 0.00990 -0.00772

D45 -0.00241 0.00022 0.00292 -0.00018 0.00274 0.00033

D46 3.13938 0.00026 0.00343 0.00508 0.00849 -3.13531

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D48 3.12134 0.00030 0.00419 0.00189 0.00607 3.12741

D49 2.95311 0.00003 0.00376 -0.02203 -0.01828 2.93483

D50 -0.20465 -0.00004 0.00300 -0.01985 -0.01684 -0.22149

D51 -0.11264 -0.00027 0.00248 -0.02634 -0.02382 -0.13646

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D53 -3.04694 0.00012 0.00373 -0.00197 0.00177 -3.04517

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D85 -3.13365 0.00003 0.00049 0.00406 0.00455 -3.12910

D86 0.01400 -0.00006 -0.00077 0.00495 0.00418 0.01819

D87 -0.00241 0.00022 0.00292 -0.00018 0.00273 0.00032

D88 3.12377 0.00015 0.00223 0.00193 0.00414 3.12791

D89 3.13939 0.00026 0.00343 0.00507 0.00849 -3.13531

D90 -0.01762 0.00019 0.00273 0.00718 0.00990 -0.00772

D91 -0.00771 0.00001 0.00008 0.00181 0.00189 -0.00582

D92 3.12782 0.00010 0.00133 0.00092 0.00226 3.13007

D93 3.13365 -0.00003 -0.00049 -0.00407 -0.00456 3.12910

D94 -0.01400 0.00006 0.00077 -0.00496 -0.00419 -0.01819

D95 0.00409 -0.00037 -0.00495 0.00030 -0.00464 -0.00055

D96 -2.95311 -0.00003 -0.00376 0.02204 0.01828 -2.93483

D97 -3.12134 -0.00030 -0.00419 -0.00189 -0.00608 -3.12742

D98 0.20465 0.00004 -0.00300 0.01985 0.01685 0.22149

D99 3.08565 0.00029 0.00285 0.00527 0.00813 3.09379

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D103 -0.20465 -0.00004 0.00300 -0.01985 -0.01686 -0.22151

D104 2.95310 0.00003 0.00376 -0.02204 -0.01830 2.93480

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D107 0.11264 0.00027 -0.00248 0.02634 0.02383 0.13647

D108 -3.04694 0.00012 0.00373 -0.00197 0.00177 -3.04517

D109 -0.15630 -0.00007 -0.00092 -0.01942 -0.02032 -0.17662

D110 3.01436 0.00016 0.00354 -0.02594 -0.02237 2.99199

D111 -3.10981 -0.00047 -0.00176 -0.01267 -0.01438 -3.12420

D112 0.00682 -0.00067 -0.00561 -0.00709 -0.01266 -0.00584

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D115 -0.00682 0.00067 0.00561 0.00710 0.01266 0.00584

D116 3.10982 0.00047 0.00176 0.01267 0.01439 3.12421

D117 2.95699 0.00049 0.00266 -0.00645 -0.00379 2.95320

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D121 0.06969 -0.00037 0.00173 -0.01727 -0.01551 0.05417

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D215 1.09734 -0.00002 -0.00040 0.00279 0.00239 1.09973

D216 -1.04796 0.00003 0.00021 0.00201 0.00222 -1.04574

D217 -3.11698 0.00000 -0.00002 0.00224 0.00222 -3.11476

D218 1.04796 -0.00003 -0.00021 -0.00201 -0.00222 1.04574

D219 -1.09734 0.00002 0.00040 -0.00279 -0.00239 -1.09973

D220 3.11698 0.00000 0.00002 -0.00224 -0.00222 3.11476

D221 1.04846 -0.00001 -0.00018 -0.00127 -0.00145 1.04701

D222 -1.09511 -0.00001 0.00013 -0.00161 -0.00148 -1.09659

D223 3.11828 0.00000 -0.00003 -0.00145 -0.00148 3.11680

D224 1.09511 0.00001 -0.00013 0.00161 0.00148 1.09659

D225 -1.04846 0.00001 0.00018 0.00127 0.00145 -1.04701

D226 -3.11828 0.00000 0.00003 0.00145 0.00148 -3.11680

D227 1.09734 -0.00002 -0.00040 0.00279 0.00239 1.09973

D228 -1.04796 0.00003 0.00021 0.00202 0.00222 -1.04574

D229 -3.11698 0.00000 -0.00002 0.00224 0.00222 -3.11476

D230 1.04796 -0.00003 -0.00021 -0.00201 -0.00222 1.04574

D231 -1.09734 0.00002 0.00040 -0.00279 -0.00239 -1.09973

D232 3.11698 0.00000 0.00002 -0.00224 -0.00222 3.11476

Item Value Threshold Converged?

Maximum Force 0.001183 0.000450 NO

RMS Force 0.000243 0.000300 YES

Maximum Displacement 0.150365 0.001800 NO

RMS Displacement 0.021465 0.001200 NO

Predicted change in Energy=-2.017493D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Fri Jul 5 23:51:48 2019, MaxMem= 1342177280 cpu: 15.4

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

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=3 Diff= 9.65D-08

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 -1.124282 2.812376 0.028170

2 7 0 0.000061 2.050587 -0.110952

3 6 0 1.124378 2.812371 0.028164

4 6 0 0.714529 4.179266 0.269648

5 6 0 -0.714430 4.179268 0.269655

6 7 0 2.412776 2.385760 -0.069052

7 6 0 2.801444 1.134240 -0.129214

8 7 0 2.031216 0.000064 -0.039160

9 6 0 2.801448 -1.134140 -0.129221

10 6 0 4.210523 -0.704762 -0.293198

11 6 0 4.210522 0.704865 -0.293190

12 7 0 -2.412733 2.385773 -0.069049

13 6 0 -4.210588 0.704875 -0.293200

14 6 0 -4.210589 -0.704774 -0.293208

15 6 0 -2.801509 -1.134154 -0.129224

16 7 0 -2.031348 0.000064 -0.039161

17 6 0 -2.801505 1.134254 -0.129217

18 7 0 -2.412744 -2.385724 -0.069056

19 7 0 0.000061 -2.050722 -0.110957

20 6 0 -1.124297 -2.812438 0.028168

21 6 0 -0.714441 -4.179335 0.269661

22 6 0 0.714541 -4.179333 0.269655

23 6 0 1.124393 -2.812433 0.028162

24 7 0 2.412788 -2.385710 -0.069059

25 30 0 -0.000118 -0.000124 -0.152074

26 6 0 -5.397956 1.432658 -0.425125

27 6 0 -6.590295 0.695181 -0.550272

28 6 0 -6.590296 -0.695077 -0.550282

29 6 0 -5.397957 -1.432556 -0.425143

30 6 0 1.434336 -5.372185 0.479142

31 6 0 0.700515 -6.547944 0.669465

32 6 0 -0.700409 -6.547945 0.669472

33 6 0 -1.434233 -5.372188 0.479155

34 6 0 5.397890 1.432653 -0.425106

35 6 0 6.590231 0.695181 -0.550246

36 6 0 6.590232 -0.695076 -0.550256

37 6 0 5.397890 -1.432549 -0.425124

38 6 0 -1.434228 5.372121 0.479135

39 6 0 -0.700409 6.547882 0.669443

40 6 0 0.700513 6.547882 0.669436

41 6 0 1.434330 5.372119 0.479122

42 1 0 7.537778 1.206669 -0.655387

43 1 0 7.537778 -1.206562 -0.655404

44 1 0 1.209057 7.489048 0.830347

45 1 0 -1.208950 7.489049 0.830359

46 1 0 -7.537842 1.206667 -0.655420

47 1 0 -7.537843 -1.206562 -0.655437

48 1 0 -1.208948 -7.489112 0.830397

49 1 0 1.209056 -7.489110 0.830385

50 8 0 2.781963 5.310277 0.488070

51 8 0 -2.781862 5.310279 0.488097

52 8 0 5.339243 2.779747 -0.432257

53 8 0 5.339243 -2.779643 -0.432293

54 8 0 2.781970 -5.310345 0.488094

55 8 0 -2.781867 -5.310348 0.488121

56 8 0 -5.339311 -2.779650 -0.432315

57 8 0 -5.339312 2.779752 -0.432279

58 6 0 3.516557 6.523895 0.628581

59 1 0 3.315172 7.006908 1.589333

60 1 0 3.295040 7.219820 -0.186106

61 1 0 4.565258 6.236065 0.583325

62 6 0 6.559483 3.515667 -0.497403

63 1 0 7.097861 3.321437 -1.429597

64 1 0 7.207491 3.290963 0.354984

65 1 0 6.267206 4.563452 -0.462721

66 6 0 6.559481 -3.515564 -0.497452

67 1 0 7.207492 -3.290873 0.354937

68 1 0 7.097859 -3.321321 -1.429643

69 1 0 6.267203 -4.563349 -0.462783

70 6 0 -3.516454 6.523897 0.628617

71 1 0 -3.294946 7.219823 -0.186072

72 1 0 -3.315060 7.006909 1.589367

73 1 0 -4.565156 6.236066 0.583370

74 6 0 -6.559552 3.515671 -0.497433

75 1 0 -7.207565 3.290968 0.354950

76 1 0 -7.097925 3.321438 -1.429630

77 1 0 -6.267276 4.563457 -0.462751

78 6 0 -6.559550 -3.515569 -0.497482

79 1 0 -7.097921 -3.321325 -1.429677

80 1 0 -7.207565 -3.290879 0.354903

81 1 0 -6.267272 -4.563355 -0.462814

82 6 0 -3.516458 -6.523966 0.628653

83 1 0 -3.315060 -7.006969 1.589407

84 1 0 -3.294951 -7.219898 -0.186030

85 1 0 -4.565159 -6.236137 0.583408

86 6 0 3.516562 -6.523963 0.628618

87 1 0 3.295047 -7.219895 -0.186064

88 1 0 3.315173 -7.006967 1.589373

89 1 0 4.565263 -6.236134 0.583363

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

Rotational constants (GHZ): 0.0444913 0.0440758 0.0224365

Leave Link 202 at Fri Jul 5 23:51:50 2019, MaxMem= 1342177280 cpu: 0.1

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

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

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8034.9156196339 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= 89 NActive= 89 NUniq= 89 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= -0.2278908286 Hartrees.

Nuclear repulsion after empirical dispersion term = 8034.6877288054 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6450

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.24D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 412

GePol: Fraction of low-weight points (<1% of avg) = 6.39%

GePol: Cavity surface area = 700.585 Ang\*\*2

GePol: Cavity volume = 799.685 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0089190943 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8034.6788097111 Hartrees.

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

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

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

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44225 LenP2D= 111100.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.75D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Fri Jul 5 23:51:53 2019, MaxMem= 1342177280 cpu: 41.8

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

DipDrv: MaxL=1.

Leave Link 303 at Fri Jul 5 23:51:54 2019, MaxMem= 1342177280 cpu: 2.5

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

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0170 S= 1.0057

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2650.02540046556

Leave Link 401 at Fri Jul 5 23:52:11 2019, MaxMem= 1342177280 cpu: 203.4

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 124807500.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.11D-15 for 5639.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.06D-15 for 4035 922.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.88D-15 for 6443.

Iteration 1 A^-1\*A deviation from orthogonality is 3.63D-09 for 5963 5909.

Iteration 2 A\*A^-1 deviation from unit magnitude is 5.77D-15 for 1447.

Iteration 2 A\*A^-1 deviation from orthogonality is 4.89D-15 for 4233 251.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.44D-15 for 400.

Iteration 2 A^-1\*A deviation from orthogonality is 4.24D-16 for 4777 1384.

E= -2649.79107975906

DIIS: error= 1.09D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79107975906 IErMin= 1 ErrMin= 1.09D-03

ErrMax= 1.09D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.04D-03 BMatP= 6.04D-03

IDIUse=3 WtCom= 9.89D-01 WtEn= 1.09D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.685 Goal= None Shift= 0.000

Gap= 0.743 Goal= None Shift= 0.000

GapD= 0.685 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=8.06D-05 MaxDP=5.25D-03 OVMax= 7.60D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 8.06D-05 CP: 1.00D+00

E= -2649.79370911885 Delta-E= -0.002629359786 Rises=F Damp=F

DIIS: error= 1.49D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79370911885 IErMin= 2 ErrMin= 1.49D-04

ErrMax= 1.49D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.41D-05 BMatP= 6.04D-03

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.49D-03

Coeff-Com: -0.544D-01 0.105D+01

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

Coeff: -0.543D-01 0.105D+01

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=8.83D-06 MaxDP=3.23D-04 DE=-2.63D-03 OVMax= 1.82D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 8.01D-06 CP: 1.00D+00 1.05D+00

E= -2649.79374059250 Delta-E= -0.000031473657 Rises=F Damp=F

DIIS: error= 1.19D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79374059250 IErMin= 3 ErrMin= 1.19D-04

ErrMax= 1.19D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.35D-05 BMatP= 8.41D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.19D-03

Coeff-Com: -0.300D-01 0.459D+00 0.571D+00

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

Coeff: -0.300D-01 0.458D+00 0.572D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.39D-06 MaxDP=2.70D-04 DE=-3.15D-05 OVMax= 1.05D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.71D-06 CP: 1.00D+00 1.05D+00 7.13D-01

E= -2649.79374664287 Delta-E= -0.000006050363 Rises=F Damp=F

DIIS: error= 7.29D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79374664287 IErMin= 4 ErrMin= 7.29D-05

ErrMax= 7.29D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.18D-05 BMatP= 4.35D-05

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

Coeff-Com: -0.836D-02 0.103D+00 0.347D+00 0.558D+00

Coeff: -0.836D-02 0.103D+00 0.347D+00 0.558D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.80D-06 MaxDP=1.23D-04 DE=-6.05D-06 OVMax= 2.53D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.11D-06 CP: 1.00D+00 1.05D+00 8.12D-01 6.86D-01

E= -2649.79374887910 Delta-E= -0.000002236229 Rises=F Damp=F

DIIS: error= 1.38D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79374887910 IErMin= 5 ErrMin= 1.38D-05

ErrMax= 1.38D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.85D-07 BMatP= 1.18D-05

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

Coeff-Com: -0.542D-03-0.500D-02 0.833D-01 0.210D+00 0.712D+00

Coeff: -0.542D-03-0.500D-02 0.833D-01 0.210D+00 0.712D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.39D-07 MaxDP=2.33D-05 DE=-2.24D-06 OVMax= 1.67D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.37D-07 CP: 1.00D+00 1.05D+00 8.28D-01 7.47D-01 9.19D-01

E= -2649.79374896176 Delta-E= -0.000000082666 Rises=F Damp=F

DIIS: error= 1.03D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79374896176 IErMin= 6 ErrMin= 1.03D-05

ErrMax= 1.03D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.30D-07 BMatP= 3.85D-07

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

Coeff-Com: 0.706D-03-0.164D-01 0.646D-02 0.539D-01 0.419D+00 0.537D+00

Coeff: 0.706D-03-0.164D-01 0.646D-02 0.539D-01 0.419D+00 0.537D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.96D-07 MaxDP=1.76D-05 DE=-8.27D-08 OVMax= 1.29D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.60D-07 CP: 1.00D+00 1.05D+00 8.37D-01 7.56D-01 9.85D-01

CP: 8.56D-01

E= -2649.79374898958 Delta-E= -0.000000027820 Rises=F Damp=F

DIIS: error= 2.42D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79374898958 IErMin= 7 ErrMin= 2.42D-06

ErrMax= 2.42D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-08 BMatP= 1.30D-07

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

Coeff-Com: 0.372D-03-0.660D-02-0.622D-02-0.130D-02 0.990D-01 0.243D+00

Coeff-Com: 0.672D+00

Coeff: 0.372D-03-0.660D-02-0.622D-02-0.130D-02 0.990D-01 0.243D+00

Coeff: 0.672D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=9.32D-08 MaxDP=7.19D-06 DE=-2.78D-08 OVMax= 6.47D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.94D-08 CP: 1.00D+00 1.05D+00 8.39D-01 7.60D-01 1.01D+00

CP: 9.93D-01 1.07D+00

E= -2649.79374899435 Delta-E= -0.000000004766 Rises=F Damp=F

DIIS: error= 1.74D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.79374899435 IErMin= 8 ErrMin= 1.74D-06

ErrMax= 1.74D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.05D-09 BMatP= 1.10D-08

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

Coeff-Com: 0.273D-05 0.141D-02-0.608D-02-0.203D-01-0.805D-01-0.167D-01

Coeff-Com: 0.460D+00 0.662D+00

Coeff: 0.273D-05 0.141D-02-0.608D-02-0.203D-01-0.805D-01-0.167D-01

Coeff: 0.460D+00 0.662D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=6.97D-08 MaxDP=3.81D-06 DE=-4.77D-09 OVMax= 6.16D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.38D-08 CP: 1.00D+00 1.05D+00 8.41D-01 7.64D-01 1.03D+00

CP: 1.08D+00 1.32D+00 8.95D-01

E= -2649.79374899701 Delta-E= -0.000000002667 Rises=F Damp=F

DIIS: error= 7.82D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.79374899701 IErMin= 9 ErrMin= 7.82D-07

ErrMax= 7.82D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.24D-10 BMatP= 5.05D-09

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

Coeff-Com: -0.798D-04 0.206D-02-0.881D-03-0.820D-02-0.547D-01-0.561D-01

Coeff-Com: 0.309D-01 0.287D+00 0.800D+00

Coeff: -0.798D-04 0.206D-02-0.881D-03-0.820D-02-0.547D-01-0.561D-01

Coeff: 0.309D-01 0.287D+00 0.800D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=3.29D-08 MaxDP=1.69D-06 DE=-2.67D-09 OVMax= 2.95D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.69D-08 CP: 1.00D+00 1.05D+00 8.41D-01 7.65D-01 1.04D+00

CP: 1.13D+00 1.43D+00 1.08D+00 9.97D-01

E= -2649.79374899721 Delta-E= -0.000000000198 Rises=F Damp=F

DIIS: error= 4.09D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -2649.79374899721 IErMin=10 ErrMin= 4.09D-07

ErrMax= 4.09D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.08D-10 BMatP= 6.24D-10

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

Coeff-Com: -0.462D-04 0.933D-03 0.589D-03-0.119D-02-0.172D-01-0.277D-01

Coeff-Com: -0.642D-01 0.609D-01 0.467D+00 0.581D+00

Coeff: -0.462D-04 0.933D-03 0.589D-03-0.119D-02-0.172D-01-0.277D-01

Coeff: -0.642D-01 0.609D-01 0.467D+00 0.581D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.18D-08 MaxDP=8.40D-07 DE=-1.98D-10 OVMax= 9.89D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 7.64D-09 CP: 1.00D+00 1.05D+00 8.41D-01 7.65D-01 1.05D+00

CP: 1.14D+00 1.45D+00 1.12D+00 1.17D+00 9.10D-01

E= -2649.79374899748 Delta-E= -0.000000000264 Rises=F Damp=F

DIIS: error= 1.66D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -2649.79374899748 IErMin=11 ErrMin= 1.66D-07

ErrMax= 1.66D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.73D-11 BMatP= 2.08D-10

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

Coeff-Com: 0.812D-05-0.328D-03 0.520D-03 0.221D-02 0.113D-01 0.817D-02

Coeff-Com: -0.397D-01-0.660D-01-0.770D-01 0.233D+00 0.928D+00

Coeff: 0.812D-05-0.328D-03 0.520D-03 0.221D-02 0.113D-01 0.817D-02

Coeff: -0.397D-01-0.660D-01-0.770D-01 0.233D+00 0.928D+00

Gap= 0.047 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=6.97D-09 MaxDP=5.09D-07 DE=-2.64D-10 OVMax= 5.84D-06

Error on total polarization charges = 0.07278

SCF Done: E(UB3LYP) = -2649.79374900 A.U. after 11 cycles

NFock= 11 Conv=0.70D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0169 S= 1.0056

<L.S>= 0.000000000000E+00

KE= 2.690095209125D+03 PE=-2.234801142534D+04 EE= 8.973443657509D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.60

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0169, after 2.0002

Leave Link 502 at Sat Jul 6 00:01:16 2019, MaxMem= 1342177280 cpu: 6436.0

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

Compute integral first derivatives.

... and contract with generalized density number 0.

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

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44225 LenP2D= 111100.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 279

Leave Link 701 at Sat Jul 6 00:01:35 2019, MaxMem= 1342177280 cpu: 221.7

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

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

Leave Link 702 at Sat Jul 6 00:01:35 2019, MaxMem= 1342177280 cpu: 0.3

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

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 00:03:06 2019, MaxMem= 1342177280 cpu: 1087.2

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

Dipole =-2.42479414D-04-2.20885965D-04 3.63039242D-02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.003270992 -0.002269904 -0.000124521

2 7 -0.000022703 -0.000166885 0.000469255

3 6 0.003248420 -0.002251012 -0.000121509

4 6 -0.001133220 0.001296115 0.000155543

5 6 0.001131142 0.001292914 0.000154661

6 7 -0.003078393 0.002628890 0.000583639

7 6 0.001620237 -0.003150286 -0.000841710

8 7 -0.001153101 -0.000026198 0.003340529

9 6 0.001595757 0.003120659 -0.000837990

10 6 -0.001592688 -0.001177149 0.000180285

11 6 -0.001590753 0.001175295 0.000179952

12 7 0.003090507 0.002615065 0.000583319

13 6 0.001591488 0.001171730 0.000180153

14 6 0.001593422 -0.001173583 0.000180485

15 6 -0.001590356 0.003090850 -0.000837545

16 7 0.001188655 -0.000026200 0.003349009

17 6 -0.001614838 -0.003120464 -0.000841259

18 7 0.003094317 -0.002590744 0.000583423

19 7 -0.000022704 0.000206382 0.000464231

20 6 -0.003293234 0.002272211 -0.000123821

21 6 0.001133425 -0.001291580 0.000154510

22 6 -0.001135503 -0.001294781 0.000155393

23 6 0.003270674 0.002253321 -0.000120807

24 7 -0.003082212 -0.002604566 0.000583739

25 30 0.000022008 0.000020916 -0.006652189

26 6 -0.001685977 -0.001494280 -0.000206770

27 6 0.000741280 0.001290101 0.000104894

28 6 0.000741212 -0.001290317 0.000104904

29 6 -0.001686602 0.001493425 -0.000206835

30 6 -0.000849677 0.000332179 -0.000111773

31 6 -0.000144306 -0.000089517 0.000064123

32 6 0.000144131 -0.000089030 0.000064021

33 6 0.000849144 0.000330763 -0.000111518

34 6 0.001686343 -0.001492353 -0.000206798

35 6 -0.000741853 0.001291990 0.000105012

36 6 -0.000741785 -0.001292206 0.000105022

37 6 0.001686968 0.001491497 -0.000206862

38 6 0.000847195 -0.000330758 -0.000111489

39 6 0.000142571 0.000088585 0.000063866

40 6 -0.000142746 0.000089073 0.000063967

41 6 -0.000847728 -0.000332175 -0.000111746

42 1 -0.000005158 -0.000142306 -0.000007554

43 1 -0.000005167 0.000142304 -0.000007560

44 1 -0.000098913 -0.000037708 -0.000026086

45 1 0.000098896 -0.000037689 -0.000026073

46 1 0.000005097 -0.000142368 -0.000007543

47 1 0.000005104 0.000142366 -0.000007548

48 1 0.000098950 0.000037637 -0.000026088

49 1 -0.000098966 0.000037654 -0.000026101

50 8 0.000678338 -0.000045230 -0.000215523

51 8 -0.000678711 -0.000045381 -0.000215315

52 8 -0.000274875 0.000458114 0.000153097

53 8 -0.000274947 -0.000458015 0.000152678

54 8 0.000677962 0.000046514 -0.000215419

55 8 -0.000678335 0.000046662 -0.000215212

56 8 0.000276885 -0.000457604 0.000152681

57 8 0.000276811 0.000457706 0.000153100

58 6 0.000217230 0.000350072 0.000031133

59 1 0.000034501 -0.000072203 -0.000010793

60 1 0.000019410 -0.000086985 0.000027202

61 1 0.000025230 0.000056977 0.000034702

62 6 -0.000013957 0.000117940 -0.000002912

63 1 -0.000003824 -0.000026826 0.000011993

64 1 -0.000013396 -0.000020490 -0.000031476

65 1 0.000097468 0.000042329 -0.000013491

66 6 -0.000013786 -0.000117934 -0.000002876

67 1 -0.000013428 0.000020540 -0.000031480

68 1 -0.000003834 0.000026825 0.000011996

69 1 0.000097398 -0.000042316 -0.000013466

70 6 -0.000217126 0.000350086 0.000031132

71 1 -0.000019394 -0.000086974 0.000027202

72 1 -0.000034483 -0.000072203 -0.000010787

73 1 -0.000025242 0.000056925 0.000034678

74 6 0.000013349 0.000118302 -0.000002905

75 1 0.000013533 -0.000020510 -0.000031492

76 1 0.000003963 -0.000026836 0.000012025

77 1 -0.000097510 0.000042350 -0.000013499

78 6 0.000013178 -0.000118299 -0.000002868

79 1 0.000003973 0.000026836 0.000012028

80 1 0.000013566 0.000020562 -0.000031496

81 1 -0.000097442 -0.000042337 -0.000013473

82 6 -0.000217496 -0.000350695 0.000031186

83 1 -0.000034463 0.000072356 -0.000010833

84 1 -0.000019380 0.000087115 0.000027235

85 1 -0.000025271 -0.000056994 0.000034701

86 6 0.000217601 -0.000350680 0.000031185

87 1 0.000019396 0.000087127 0.000027235

88 1 0.000034480 0.000072356 -0.000010838

89 1 0.000025259 -0.000057047 0.000034725

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

Cartesian Forces: Max 0.006652189 RMS 0.001089363

Leave Link 716 at Sat Jul 6 00:03:06 2019, MaxMem= 1342177280 cpu: 0.5

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.002668423 RMS 0.000428542

Search for a local minimum.

Step number 5 out of a maximum of 518

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

RMS Force = .42854D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

DE= -3.42D-04 DEPred=-2.02D-04 R= 1.70D+00

TightC=F SS= 1.41D+00 RLast= 1.52D-01 DXNew= 7.2376D-01 4.5684D-01

Trust test= 1.70D+00 RLast= 1.52D-01 DXMaxT set to 4.57D-01

ITU= 1 1 1 1 0

Eigenvalues --- -0.04569 0.00010 0.01311 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01316 0.01316

Eigenvalues --- 0.01542 0.01569 0.01570 0.01580 0.01599

Eigenvalues --- 0.01616 0.01621 0.01646 0.01707 0.01709

Eigenvalues --- 0.01712 0.01716 0.01810 0.01832 0.01871

Eigenvalues --- 0.01881 0.01913 0.01917 0.01919 0.01929

Eigenvalues --- 0.01937 0.01952 0.02008 0.02016 0.02022

Eigenvalues --- 0.02022 0.02023 0.02025 0.02053 0.02053

Eigenvalues --- 0.02053 0.02053 0.02057 0.02057 0.02057

Eigenvalues --- 0.02057 0.02067 0.02067 0.02067 0.02067

Eigenvalues --- 0.02070 0.02070 0.02070 0.02070 0.02072

Eigenvalues --- 0.02083 0.02083 0.02085 0.02245 0.02260

Eigenvalues --- 0.02260 0.02260 0.02260 0.02260 0.02260

Eigenvalues --- 0.02260 0.02342 0.02344 0.02348 0.02362

Eigenvalues --- 0.09977 0.09977 0.09977 0.09979 0.09990

Eigenvalues --- 0.09990 0.09990 0.10005 0.10656 0.10657

Eigenvalues --- 0.10657 0.10657 0.10663 0.10664 0.10664

Eigenvalues --- 0.10664 0.13476 0.13505 0.15130 0.15382

Eigenvalues --- 0.15979 0.15997 0.15999 0.15999 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16088 0.16270 0.21587 0.21760 0.22473

Eigenvalues --- 0.22473 0.22475 0.22476 0.23087 0.24330

Eigenvalues --- 0.24368 0.24474 0.24504 0.24510 0.24515

Eigenvalues --- 0.24594 0.24653 0.24716 0.24767 0.24861

Eigenvalues --- 0.24876 0.24921 0.24992 0.24997 0.24998

Eigenvalues --- 0.24998 0.24998 0.24998 0.24999 0.24999

Eigenvalues --- 0.24999 0.24999 0.24999 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.26952

Eigenvalues --- 0.32778 0.33637 0.33653 0.33692 0.33729

Eigenvalues --- 0.33894 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34063 0.34064 0.34073 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34081

Eigenvalues --- 0.34081 0.34572 0.34640 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34686 0.34686 0.34687

Eigenvalues --- 0.34912 0.34959 0.35548 0.35627 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35632 0.35632

Eigenvalues --- 0.35997 0.37106 0.37120 0.37161 0.41182

Eigenvalues --- 0.41215 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41215 0.41250 0.41348 0.41414 0.41416

Eigenvalues --- 0.41416 0.41418 0.42168 0.42466 0.42480

Eigenvalues --- 0.43802 0.44341 0.44556 0.44571 0.44877

Eigenvalues --- 0.44921 0.44979 0.44998 0.45000 0.45001

Eigenvalues --- 0.45004 0.45279 0.45365 0.45367 0.46525

Eigenvalues --- 0.47349 0.48095 0.48998 0.49269 0.49314

Eigenvalues --- 0.49856 0.52111 0.53406 0.53554 0.53554

Eigenvalues --- 0.53554 0.53554 0.53554 0.53554 0.54709

Eigenvalues --- 0.54979 0.55020 0.56083 0.57404 0.57442

Eigenvalues --- 0.57576

Eigenvalue 1 is -4.57D-02 should be greater than 0.000000 Eigenvector:

A175 A176 D107 D106 D51

1 0.28145 -0.21221 0.17704 -0.17698 -0.17681

D54 D110 D10 D144 D24

1 0.17675 -0.16792 0.16790 0.16786 -0.16785

Eigenvalue 2 is 9.61D-05 Eigenvector:

A176 D122 D18 D119 D15

1 0.29898 -0.20259 0.20254 0.20250 -0.20246

D115 D112 D11 D1 D20

1 -0.17201 0.17200 0.17195 -0.17194 -0.13605

Use linear search instead of GDIIS.

RFO step: Lambda=-4.58597701D-02 EMin=-4.56935298D-02

I= 1 Eig= -4.57D-02 Dot1= 1.65D-03

I= 1 Stepn= 6.00D-01 RXN= 6.00D-01 EDone=F

Mixed 1 eigenvectors in step. Raw Step.Grad= 1.65D-03.

RFO eigenvector is Hessian eigenvector with negative curvature.

Taking step of 6.00D-01 in eigenvector direction(s). Step.Grad= -4.75D-05.

Skip linear search -- no minimum in search direction.

Iteration 1 RMS(Cart)= 0.25156745 RMS(Int)= 0.00477466

Iteration 2 RMS(Cart)= 0.02216983 RMS(Int)= 0.00094740

Iteration 3 RMS(Cart)= 0.00007915 RMS(Int)= 0.00094727

Iteration 4 RMS(Cart)= 0.00000008 RMS(Int)= 0.00094727

ITry= 1 IFail=0 DXMaxC= 9.67D-01 DCOld= 1.00D+10 DXMaxT= 4.57D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.57989 0.00031 0.00000 -0.00112 0.00024 2.58013

R2 2.73501 0.00126 0.00000 0.00003 -0.00033 2.73468

R3 2.57138 -0.00264 0.00000 -0.01570 -0.01727 2.55411

R4 2.57984 0.00031 0.00000 -0.00111 -0.00035 2.57950

R5 3.87606 -0.00042 0.00000 -0.02560 -0.02078 3.85528

R6 2.73501 0.00126 0.00000 0.00007 -0.00027 2.73474

R7 2.57129 -0.00261 0.00000 -0.01547 -0.01823 2.55306

R8 2.70034 -0.00055 0.00000 -0.01165 -0.01281 2.68753

R9 2.66236 -0.00002 0.00000 -0.00635 -0.00631 2.65605

R10 2.66236 -0.00001 0.00000 -0.00633 -0.00630 2.65607

R11 2.47906 0.00185 0.00000 -0.00330 -0.00646 2.47260

R12 2.59638 -0.00052 0.00000 0.00073 0.00058 2.59695

R13 2.80085 -0.00103 0.00000 -0.01181 -0.01212 2.78873

R14 2.59642 -0.00053 0.00000 0.00072 0.00116 2.59758

R15 3.84459 -0.00086 0.00000 -0.04253 -0.03883 3.80576

R16 2.80084 -0.00103 0.00000 -0.01183 -0.01215 2.78869

R17 2.47915 0.00181 0.00000 -0.00356 -0.00556 2.47359

R18 2.66381 0.00026 0.00000 -0.00033 -0.00144 2.66237

R19 2.64354 0.00049 0.00000 -0.00257 -0.00258 2.64096

R20 2.64354 0.00049 0.00000 -0.00258 -0.00259 2.64095

R21 2.47912 0.00181 0.00000 -0.00358 -0.00594 2.47318

R22 2.66385 0.00025 0.00000 -0.00045 -0.00099 2.66286

R23 2.80086 -0.00104 0.00000 -0.01186 -0.01199 2.78887

R24 2.64353 0.00049 0.00000 -0.00261 -0.00264 2.64090

R25 2.80086 -0.00104 0.00000 -0.01187 -0.01202 2.78883

R26 2.64353 0.00049 0.00000 -0.00260 -0.00262 2.64091

R27 2.59637 -0.00052 0.00000 0.00077 0.00052 2.59689

R28 2.47921 0.00177 0.00000 -0.00384 -0.00504 2.47416

R29 2.59632 -0.00051 0.00000 0.00079 -0.00006 2.59626

R30 3.84440 -0.00088 0.00000 -0.04291 -0.04135 3.80304

R31 2.57144 -0.00267 0.00000 -0.01585 -0.01664 2.55480

R32 2.57984 0.00031 0.00000 -0.00110 -0.00039 2.57945

R33 2.57979 0.00032 0.00000 -0.00109 -0.00097 2.57882

R34 3.87585 -0.00044 0.00000 -0.02654 -0.02384 3.85201

R35 2.73502 0.00126 0.00000 0.00001 -0.00019 2.73483

R36 2.70038 -0.00056 0.00000 -0.01169 -0.01231 2.68808

R37 2.66236 -0.00001 0.00000 -0.00634 -0.00632 2.65604

R38 2.73502 0.00126 0.00000 0.00005 -0.00013 2.73490

R39 2.66236 -0.00002 0.00000 -0.00636 -0.00634 2.65602

R40 2.57135 -0.00263 0.00000 -0.01562 -0.01760 2.55376

R41 2.65989 -0.00100 0.00000 -0.00362 -0.00359 2.65630

R42 2.54809 0.00058 0.00000 0.00498 0.00498 2.55306

R43 2.62721 0.00047 0.00000 0.00294 0.00299 2.63020

R44 2.04450 -0.00007 0.00000 -0.00196 -0.00196 2.04255

R45 2.65989 -0.00100 0.00000 -0.00362 -0.00359 2.65630

R46 2.04450 -0.00007 0.00000 -0.00196 -0.00196 2.04255

R47 2.54809 0.00058 0.00000 0.00497 0.00497 2.55306

R48 2.64368 0.00003 0.00000 0.00275 0.00273 2.64641

R49 2.54939 0.00096 0.00000 0.00769 0.00769 2.55709

R50 2.64736 -0.00028 0.00000 0.00395 0.00392 2.65128

R51 2.04432 -0.00008 0.00000 -0.00196 -0.00196 2.04235

R52 2.64368 0.00003 0.00000 0.00274 0.00272 2.64640

R53 2.04432 -0.00008 0.00000 -0.00196 -0.00196 2.04235

R54 2.54939 0.00096 0.00000 0.00769 0.00769 2.55709

R55 2.65989 -0.00100 0.00000 -0.00362 -0.00362 2.65627

R56 2.54809 0.00058 0.00000 0.00498 0.00498 2.55306

R57 2.62720 0.00047 0.00000 0.00296 0.00297 2.63018

R58 2.04450 -0.00007 0.00000 -0.00196 -0.00196 2.04255

R59 2.65989 -0.00100 0.00000 -0.00363 -0.00362 2.65627

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R61 2.54809 0.00058 0.00000 0.00497 0.00497 2.55306

R62 2.64367 0.00003 0.00000 0.00274 0.00270 2.64637

R63 2.54939 0.00096 0.00000 0.00770 0.00770 2.55709

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R65 2.04432 -0.00008 0.00000 -0.00196 -0.00196 2.04235

R66 2.64367 0.00003 0.00000 0.00274 0.00271 2.64638

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R68 2.54939 0.00096 0.00000 0.00770 0.00770 2.55709

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R72 2.69563 0.00012 0.00000 0.00073 0.00073 2.69636

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R74 2.69393 0.00037 0.00000 0.00145 0.00145 2.69538

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R76 2.69563 0.00012 0.00000 0.00073 0.00073 2.69637

R77 2.06742 -0.00005 0.00000 -0.00216 -0.00216 2.06526

R78 2.06758 -0.00008 0.00000 -0.00190 -0.00190 2.06568

R79 2.05682 0.00001 0.00000 -0.00165 -0.00165 2.05518

R80 2.06712 -0.00001 0.00000 -0.00206 -0.00206 2.06506

R81 2.06748 -0.00003 0.00000 -0.00208 -0.00208 2.06540

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A11 2.31824 -0.00016 0.00000 -0.00650 -0.00657 2.31167

A12 2.10704 0.00007 0.00000 0.00577 0.00590 2.11293

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A69 2.04296 0.00035 0.00000 -0.00234 -0.00246 2.04050

A70 2.07526 -0.00037 0.00000 -0.00996 -0.00995 2.06531

A71 2.16495 0.00002 0.00000 0.01222 0.01223 2.17718

A72 2.12227 -0.00002 0.00000 0.00091 0.00090 2.12317

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A74 2.06322 -0.00011 0.00000 -0.00308 -0.00308 2.06014

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A81 2.05310 -0.00007 0.00000 -0.00618 -0.00623 2.04688

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A83 2.16712 -0.00015 0.00000 0.01719 0.01712 2.18424

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A85 2.09999 0.00007 0.00000 0.00171 0.00170 2.10170

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A94 2.07526 -0.00036 0.00000 -0.00992 -0.00991 2.06535

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D63 -3.13639 0.00001 0.00000 -0.00170 -0.00157 -3.13796

D64 0.00000 0.00000 0.00000 -0.00001 0.00000 0.00000

D65 -3.12909 0.00000 0.00000 -0.00320 -0.00304 -3.13214

D66 0.01820 -0.00003 0.00000 0.01165 0.01169 0.02989

D67 0.00582 -0.00002 0.00000 -0.00105 -0.00109 0.00473

D68 -3.13008 -0.00005 0.00000 0.01380 0.01364 -3.11643

D69 3.12910 0.00000 0.00000 0.00322 0.00309 3.13219

D70 -0.01819 0.00003 0.00000 -0.01163 -0.01163 -0.02983

D71 -0.00582 0.00002 0.00000 0.00106 0.00109 -0.00473

D72 3.13008 0.00005 0.00000 -0.01378 -0.01364 3.11644

D73 -3.09378 -0.00034 0.00000 -0.00325 -0.00331 -3.09709

D74 0.06480 -0.00023 0.00000 -0.00379 -0.00408 0.06072

D75 0.00000 0.00000 0.00000 0.00002 0.00004 0.00004

D76 3.13640 -0.00001 0.00000 0.00176 0.00165 3.13805

D77 -3.13639 0.00001 0.00000 -0.00173 -0.00161 -3.13800

D78 0.00000 0.00000 0.00000 0.00001 0.00000 0.00000

D79 -3.12792 0.00000 0.00000 0.03117 0.03129 -3.09663

D80 -0.00033 -0.00010 0.00000 0.03157 0.03188 0.03155

D81 0.00772 -0.00002 0.00000 0.03317 0.03318 0.04090

D82 3.13531 -0.00012 0.00000 0.03357 0.03377 -3.11411

D83 0.00582 -0.00002 0.00000 -0.00106 -0.00107 0.00475

D84 -3.13008 -0.00005 0.00000 0.01383 0.01369 -3.11639

D85 -3.12910 0.00000 0.00000 -0.00329 -0.00318 -3.13228

D86 0.01819 -0.00003 0.00000 0.01159 0.01158 0.02977

D87 0.00032 0.00010 0.00000 -0.03160 -0.03193 -0.03161

D88 3.12791 0.00000 0.00000 -0.03121 -0.03143 3.09648

D89 -3.13531 0.00012 0.00000 -0.03360 -0.03378 3.11409

D90 -0.00772 0.00002 0.00000 -0.03320 -0.03328 -0.04100

D91 -0.00582 0.00002 0.00000 0.00104 0.00107 -0.00475

D92 3.13007 0.00005 0.00000 -0.01385 -0.01370 3.11638

D93 3.12910 0.00000 0.00000 0.00326 0.00313 3.13223

D94 -0.01819 0.00003 0.00000 -0.01162 -0.01164 -0.02983

D95 -0.00055 -0.00017 0.00000 0.05358 0.05362 0.05307

D96 -2.93483 0.00033 0.00000 0.09075 0.09043 -2.84440

D97 -3.12742 -0.00007 0.00000 0.05324 0.05316 -3.07426

D98 0.22149 0.00043 0.00000 0.09041 0.08996 0.31146

D99 3.09379 0.00034 0.00000 0.00325 0.00337 3.09715

D100 -0.06480 0.00023 0.00000 0.00377 0.00403 -0.06077

D101 3.12743 0.00007 0.00000 -0.05322 -0.05304 3.07439

D102 0.00056 0.00017 0.00000 -0.05357 -0.05360 -0.05304

D103 -0.22151 -0.00043 0.00000 -0.09043 -0.09027 -0.31178

D104 2.93480 -0.00033 0.00000 -0.09078 -0.09082 2.84398

D105 3.04518 0.00017 0.00000 0.06268 0.06178 3.10696

D106 -0.13646 -0.00079 0.00000 -0.10619 -0.10562 -0.24207

D107 0.13647 0.00079 0.00000 0.10622 0.10572 0.24219

D108 -3.04517 -0.00016 0.00000 -0.06264 -0.06167 -3.10684

D109 -0.17662 -0.00016 0.00000 -0.04111 -0.04052 -0.21715

D110 2.99199 -0.00016 0.00000 -0.10075 -0.10008 2.89191

D111 -3.12420 -0.00052 0.00000 0.00398 0.00417 -3.12003

D112 -0.00584 -0.00052 0.00000 0.05515 0.05554 0.04971

D113 0.21160 -0.00051 0.00000 -0.01934 -0.01922 0.19238

D114 -2.95322 -0.00050 0.00000 0.03182 0.03215 -2.92107

D115 0.00584 0.00052 0.00000 -0.05516 -0.05554 -0.04971

D116 3.12421 0.00052 0.00000 -0.00395 -0.00406 3.12014

D117 2.95320 0.00051 0.00000 -0.03183 -0.03241 2.92078

D118 -0.21162 0.00051 0.00000 0.01938 0.01907 -0.19255

D119 2.97639 -0.00086 0.00000 -0.05089 -0.05072 2.92567

D120 -0.05416 0.00086 0.00000 0.07644 0.07620 0.02204

D121 0.05417 -0.00085 0.00000 -0.07636 -0.07598 -0.02181

D122 -2.97638 0.00086 0.00000 0.05096 0.05094 -2.92544

D123 3.12225 0.00032 0.00000 0.01781 0.01716 3.13941

D124 -0.01814 0.00026 0.00000 -0.00370 -0.00403 -0.02218

D125 0.00345 0.00031 0.00000 -0.03260 -0.03297 -0.02952

D126 -3.13695 0.00025 0.00000 -0.05411 -0.05416 3.09208

D127 0.00000 0.00000 0.00000 -0.00001 0.00000 0.00001

D128 -3.14057 -0.00005 0.00000 -0.01835 -0.01826 3.12435

D129 3.14058 0.00005 0.00000 0.01833 0.01825 -3.12436

D130 0.00000 0.00000 0.00000 -0.00001 -0.00002 -0.00002

D131 3.12741 0.00009 0.00000 0.01417 0.01393 3.14134

D132 -0.01775 0.00013 0.00000 -0.00546 -0.00549 -0.02325

D133 -0.01285 0.00003 0.00000 -0.00983 -0.00979 -0.02264

D134 3.12517 0.00006 0.00000 -0.02945 -0.02921 3.09596

D135 -0.00345 -0.00031 0.00000 0.03261 0.03297 0.02952

D136 -3.12226 -0.00032 0.00000 -0.01783 -0.01728 -3.13954

D137 3.13694 -0.00025 0.00000 0.05412 0.05419 -3.09205

D138 0.01814 -0.00026 0.00000 0.00368 0.00394 0.02208

D139 0.01285 -0.00003 0.00000 0.00983 0.00981 0.02266

D140 -3.12517 -0.00006 0.00000 0.02946 0.02923 -3.09594

D141 -3.12741 -0.00009 0.00000 -0.01415 -0.01393 -3.14134

D142 0.01775 -0.00013 0.00000 0.00548 0.00549 0.02324

D143 0.17662 0.00016 0.00000 0.04103 0.04040 0.21702

D144 -2.99199 0.00016 0.00000 0.10072 0.10008 -2.89190

D145 -0.00584 0.00002 0.00000 0.00105 0.00107 -0.00476

D146 -3.14136 0.00000 0.00000 0.00679 0.00683 -3.13453

D147 3.12974 0.00004 0.00000 -0.01475 -0.01482 3.11491

D148 -0.00579 0.00003 0.00000 -0.00902 -0.00907 -0.01486

D149 -3.08575 -0.00003 0.00000 -0.02055 -0.02057 -3.10631

D150 0.06197 -0.00006 0.00000 -0.00450 -0.00448 0.05748

D151 0.00000 0.00000 0.00000 0.00001 0.00000 0.00000

D152 -3.13565 -0.00002 0.00000 0.00561 0.00561 -3.13003

D153 3.13565 0.00002 0.00000 -0.00560 -0.00561 3.13004

D154 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D155 0.00583 -0.00002 0.00000 -0.00105 -0.00108 0.00475

D156 -3.12974 -0.00004 0.00000 0.01476 0.01483 -3.11491

D157 3.14136 0.00000 0.00000 -0.00678 -0.00683 3.13453

D158 0.00579 -0.00003 0.00000 0.00903 0.00907 0.01487

D159 3.08575 0.00003 0.00000 0.02055 0.02057 3.10632

D160 -0.06197 0.00006 0.00000 0.00449 0.00448 -0.05749

D161 -0.01297 0.00003 0.00000 -0.00988 -0.00982 -0.02279

D162 3.13768 -0.00002 0.00000 0.00470 0.00477 -3.14073

D163 3.12482 0.00007 0.00000 -0.03086 -0.03094 3.09387

D164 -0.00771 0.00002 0.00000 -0.01628 -0.01635 -0.02406

D165 -3.08440 -0.00005 0.00000 -0.01565 -0.01569 -3.10010

D166 0.06101 -0.00009 0.00000 0.00543 0.00547 0.06649

D167 0.00000 0.00000 0.00000 0.00000 -0.00001 -0.00001

D168 -3.13273 -0.00004 0.00000 0.01424 0.01422 -3.11850

D169 3.13273 0.00004 0.00000 -0.01424 -0.01423 3.11850

D170 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D171 0.01297 -0.00003 0.00000 0.00988 0.00982 0.02279

D172 -3.12482 -0.00007 0.00000 0.03086 0.03094 -3.09387

D173 -3.13768 0.00002 0.00000 -0.00470 -0.00478 3.14072

D174 0.00771 -0.00002 0.00000 0.01628 0.01634 0.02406

D175 3.08440 0.00005 0.00000 0.01563 0.01567 3.10008

D176 -0.06101 0.00009 0.00000 -0.00545 -0.00549 -0.06650

D177 0.00583 -0.00002 0.00000 -0.00106 -0.00109 0.00474

D178 3.14136 0.00000 0.00000 -0.00677 -0.00682 3.13455

D179 -3.12974 -0.00005 0.00000 0.01470 0.01477 -3.11497

D180 0.00579 -0.00003 0.00000 0.00899 0.00904 0.01483

D181 3.08575 0.00003 0.00000 0.02050 0.02051 3.10626

D182 -0.06197 0.00006 0.00000 0.00449 0.00447 -0.05750

D183 0.00000 0.00000 0.00000 -0.00001 0.00000 0.00000

D184 3.13565 0.00002 0.00000 -0.00559 -0.00558 3.13006

D185 -3.13565 -0.00002 0.00000 0.00558 0.00558 -3.13007

D186 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D187 -0.00583 0.00002 0.00000 0.00106 0.00110 -0.00474

D188 3.12974 0.00005 0.00000 -0.01471 -0.01477 3.11497

D189 -3.14136 0.00000 0.00000 0.00677 0.00682 -3.13454

D190 -0.00579 0.00003 0.00000 -0.00900 -0.00904 -0.01484

D191 -3.08575 -0.00003 0.00000 -0.02050 -0.02051 -3.10626

D192 0.06197 -0.00006 0.00000 -0.00448 -0.00446 0.05750

D193 -0.01297 0.00003 0.00000 -0.00988 -0.00978 -0.02275

D194 3.13769 -0.00002 0.00000 0.00471 0.00480 -3.14070

D195 3.12482 0.00007 0.00000 -0.03086 -0.03091 3.09391

D196 -0.00771 0.00002 0.00000 -0.01628 -0.01633 -0.02404

D197 -3.08441 -0.00005 0.00000 -0.01564 -0.01569 -3.10009

D198 0.06101 -0.00009 0.00000 0.00544 0.00548 0.06649

D199 0.00000 0.00000 0.00000 0.00000 0.00001 0.00001

D200 -3.13273 -0.00004 0.00000 0.01424 0.01421 -3.11852

D201 3.13273 0.00004 0.00000 -0.01424 -0.01420 3.11853

D202 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D203 0.01297 -0.00003 0.00000 0.00987 0.00978 0.02275

D204 -3.12482 -0.00007 0.00000 0.03086 0.03091 -3.09391

D205 -3.13769 0.00002 0.00000 -0.00470 -0.00479 3.14071

D206 0.00771 -0.00002 0.00000 0.01628 0.01634 0.02404

D207 3.08440 0.00005 0.00000 0.01566 0.01571 3.10011

D208 -0.06101 0.00009 0.00000 -0.00542 -0.00547 -0.06648

D209 1.09658 0.00001 0.00000 0.00034 0.00034 1.09692

D210 -1.04701 0.00000 0.00000 -0.00051 -0.00051 -1.04752

D211 -3.11680 -0.00002 0.00000 -0.00085 -0.00085 -3.11765

D212 1.04701 0.00000 0.00000 0.00050 0.00051 1.04752

D213 -1.09658 -0.00001 0.00000 -0.00034 -0.00034 -1.09692

D214 3.11680 0.00002 0.00000 0.00085 0.00085 3.11765

D215 1.09973 -0.00005 0.00000 -0.00080 -0.00080 1.09893

D216 -1.04574 0.00005 0.00000 0.00179 0.00180 -1.04395

D217 -3.11476 -0.00001 0.00000 -0.00016 -0.00016 -3.11493

D218 1.04574 -0.00005 0.00000 -0.00179 -0.00180 1.04395

D219 -1.09973 0.00005 0.00000 0.00079 0.00079 -1.09893

D220 3.11476 0.00001 0.00000 0.00016 0.00016 3.11492

D221 1.04701 0.00000 0.00000 0.00051 0.00051 1.04752

D222 -1.09659 -0.00001 0.00000 -0.00033 -0.00033 -1.09692

D223 3.11680 0.00002 0.00000 0.00085 0.00085 3.11765

D224 1.09659 0.00001 0.00000 0.00033 0.00034 1.09692

D225 -1.04701 0.00000 0.00000 -0.00050 -0.00051 -1.04752

D226 -3.11680 -0.00002 0.00000 -0.00085 -0.00085 -3.11765

D227 1.09973 -0.00005 0.00000 -0.00079 -0.00079 1.09893

D228 -1.04574 0.00005 0.00000 0.00180 0.00180 -1.04394

D229 -3.11476 -0.00001 0.00000 -0.00016 -0.00016 -3.11493

D230 1.04574 -0.00005 0.00000 -0.00179 -0.00180 1.04395

D231 -1.09973 0.00005 0.00000 0.00079 0.00080 -1.09893

D232 3.11476 0.00001 0.00000 0.00016 0.00017 3.11493

Item Value Threshold Converged?

Maximum Force 0.002668 0.000450 NO

RMS Force 0.000429 0.000300 NO

Maximum Displacement 0.967299 0.001800 NO

RMS Displacement 0.260066 0.001200 NO

Predicted change in Energy=-9.688593D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 00:03:08 2019, MaxMem= 1342177280 cpu: 15.1

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

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=3 Diff= 5.78D-06

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 -1.121015 2.782381 -0.028786

2 7 0 0.000791 2.027356 -0.217611

3 6 0 1.122190 2.782411 -0.028901

4 6 0 0.711652 4.110371 0.373922

5 6 0 -0.710530 4.110332 0.373994

6 7 0 2.405450 2.378890 -0.154075

7 6 0 2.779889 1.129195 -0.254518

8 7 0 1.998076 0.000847 -0.190055

9 6 0 2.779884 -1.127906 -0.254625

10 6 0 4.180470 -0.703804 -0.444931

11 6 0 4.180489 0.705063 -0.444828

12 7 0 -2.404894 2.378963 -0.153925

13 6 0 -4.181223 0.705158 -0.444812

14 6 0 -4.181192 -0.703966 -0.444914

15 6 0 -2.780545 -1.128080 -0.254501

16 7 0 -1.999612 0.000832 -0.189915

17 6 0 -2.780569 1.129325 -0.254395

18 7 0 -2.404998 -2.378303 -0.154030

19 7 0 0.000809 -2.028990 -0.217625

20 6 0 -1.121174 -2.783094 -0.028760

21 6 0 -0.710639 -4.111086 0.374128

22 6 0 0.711830 -4.111114 0.374055

23 6 0 1.122396 -2.783106 -0.028876

24 7 0 2.405594 -2.378191 -0.154181

25 30 0 -0.001499 -0.001686 -0.429979

26 6 0 -5.363285 1.434062 -0.601158

27 6 0 -6.550302 0.696486 -0.752271

28 6 0 -6.550274 -0.695354 -0.752377

29 6 0 -5.363227 -1.432902 -0.601371

30 6 0 1.436943 -5.257084 0.743389

31 6 0 0.702077 -6.400038 1.082203

32 6 0 -0.700919 -6.400014 1.082263

33 6 0 -1.435772 -5.257036 0.743519

34 6 0 5.362555 1.434051 -0.600987

35 6 0 6.549611 0.696535 -0.751941

36 6 0 6.549594 -0.695296 -0.752048

37 6 0 5.362521 -1.432805 -0.601202

38 6 0 -1.435759 5.256299 0.743203

39 6 0 -0.700970 6.399339 1.081829

40 6 0 0.702020 6.399374 1.081770

41 6 0 1.436842 5.256371 0.743074

42 1 0 7.494562 1.204611 -0.883109

43 1 0 7.494533 -1.203376 -0.883294

44 1 0 1.208042 7.308519 1.374089

45 1 0 -1.207014 7.308458 1.374190

46 1 0 -7.495247 1.204536 -0.883597

47 1 0 -7.495198 -1.203423 -0.883782

48 1 0 -1.206935 -7.309111 1.374746

49 1 0 1.208086 -7.309152 1.374643

50 8 0 2.786406 5.161605 0.769932

51 8 0 -2.785316 5.161460 0.770175

52 8 0 5.286288 2.782772 -0.620972

53 8 0 5.286229 -2.781517 -0.621396

54 8 0 2.786507 -5.162345 0.770291

55 8 0 -2.785330 -5.162246 0.770536

56 8 0 -5.286918 -2.781613 -0.621622

57 8 0 -5.287023 2.782781 -0.621200

58 6 0 3.555392 6.319358 1.090371

59 1 0 3.350246 6.672543 2.104065

60 1 0 3.375397 7.128842 0.378169

61 1 0 4.594764 6.006058 1.024655

62 6 0 6.489914 3.540389 -0.735872

63 1 0 6.999172 3.344999 -1.682792

64 1 0 7.172489 3.337514 0.093283

65 1 0 6.183110 4.583064 -0.702677

66 6 0 6.489846 -3.539132 -0.736415

67 1 0 7.172423 -3.336390 0.092770

68 1 0 6.999105 -3.343600 -1.683306

69 1 0 6.183028 -4.581807 -0.703382

70 6 0 -3.554336 6.319180 1.090651

71 1 0 -3.374441 7.128656 0.378415

72 1 0 -3.349126 6.672399 2.104320

73 1 0 -4.593696 6.005821 1.025026

74 6 0 -6.490638 3.540386 -0.736358

75 1 0 -7.173360 3.337547 0.092683

76 1 0 -6.999717 3.344937 -1.683362

77 1 0 -6.183852 4.583066 -0.703167

78 6 0 -6.490511 -3.539234 -0.736898

79 1 0 -6.999595 -3.343654 -1.683873

80 1 0 -7.173238 -3.336539 0.092173

81 1 0 -6.183693 -4.581909 -0.703867

82 6 0 -3.554289 -6.319964 1.091180

83 1 0 -3.349016 -6.673052 2.104881

84 1 0 -3.374388 -7.129512 0.379030

85 1 0 -4.593667 -6.006663 1.025566

86 6 0 3.555452 -6.320083 1.090898

87 1 0 3.375463 -7.129642 0.378781

88 1 0 3.350250 -6.673141 2.104624

89 1 0 4.594837 -6.006823 1.025193

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

Rotational constants (GHZ): 0.0454773 0.0438373 0.0230430

Leave Link 202 at Sat Jul 6 00:03:09 2019, MaxMem= 1342177280 cpu: 0.1

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

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

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8071.3576677370 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= 89 NActive= 89 NUniq= 89 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= -0.2280900986 Hartrees.

Nuclear repulsion after empirical dispersion term = 8071.1295776384 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6335

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.11D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 349

GePol: Fraction of low-weight points (<1% of avg) = 5.51%

GePol: Cavity surface area = 701.210 Ang\*\*2

GePol: Cavity volume = 798.370 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0089714419 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8071.1206061965 Hartrees.

Leave Link 301 at Sat Jul 6 00:03:09 2019, MaxMem= 1342177280 cpu: 1.4

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

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

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

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44667 LenP2D= 112062.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 6.05D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 00:03:13 2019, MaxMem= 1342177280 cpu: 41.7

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

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 00:03:13 2019, MaxMem= 1342177280 cpu: 2.4

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

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000003 0.000001 -0.000002 Ang= 0.00 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>= 2.0170 S= 1.0056

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2650.03106647178

Leave Link 401 at Sat Jul 6 00:03:31 2019, MaxMem= 1342177280 cpu: 204.5

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 120396675.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.55D-15 for 6331.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.75D-15 for 6334 5972.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.55D-15 for 6331.

Iteration 1 A^-1\*A deviation from orthogonality is 7.55D-13 for 4649 4570.

E= -2649.65455569212

DIIS: error= 9.49D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.65455569212 IErMin= 1 ErrMin= 9.49D-03

ErrMax= 9.49D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.03D-01 BMatP= 3.03D-01

IDIUse=3 WtCom= 9.05D-01 WtEn= 9.49D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.686 Goal= None Shift= 0.000

Gap= 0.745 Goal= None Shift= 0.000

GapD= 0.686 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=4.34D-04 MaxDP=2.03D-02 OVMax= 5.37D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.34D-04 CP: 9.98D-01

E= -2649.79021599726 Delta-E= -0.135660305134 Rises=F Damp=F

DIIS: error= 1.20D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79021599726 IErMin= 2 ErrMin= 1.20D-03

ErrMax= 1.20D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.71D-03 BMatP= 3.03D-01

IDIUse=3 WtCom= 9.88D-01 WtEn= 1.20D-02

Coeff-Com: -0.584D-01 0.106D+01

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

Coeff: -0.576D-01 0.106D+01

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.068 Goal= None Shift= 0.000

RMSDP=5.57D-05 MaxDP=2.13D-03 DE=-1.36D-01 OVMax= 8.22D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 5.04D-05 CP: 9.97D-01 1.05D+00

E= -2649.79159641367 Delta-E= -0.001380416412 Rises=F Damp=F

DIIS: error= 9.85D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79159641367 IErMin= 3 ErrMin= 9.85D-04

ErrMax= 9.85D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.61D-03 BMatP= 3.71D-03

IDIUse=3 WtCom= 9.90D-01 WtEn= 9.85D-03

Coeff-Com: -0.348D-01 0.522D+00 0.513D+00

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

Coeff: -0.344D-01 0.517D+00 0.518D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=3.10D-05 MaxDP=2.04D-03 DE=-1.38D-03 OVMax= 5.07D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.53D-05 CP: 9.98D-01 1.06D+00 6.67D-01

E= -2649.79198936921 Delta-E= -0.000392955539 Rises=F Damp=F

DIIS: error= 4.84D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79198936921 IErMin= 4 ErrMin= 4.84D-04

ErrMax= 4.84D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.52D-04 BMatP= 2.61D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.84D-03

Coeff-Com: -0.773D-02 0.881D-01 0.317D+00 0.603D+00

Coeff-En: 0.000D+00 0.000D+00 0.195D+00 0.805D+00

Coeff: -0.770D-02 0.876D-01 0.316D+00 0.604D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=1.22D-05 MaxDP=7.33D-04 DE=-3.93D-04 OVMax= 2.10D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 6.38D-06 CP: 9.97D-01 1.06D+00 7.82D-01 6.70D-01

E= -2649.79209425031 Delta-E= -0.000104881103 Rises=F Damp=F

DIIS: error= 8.59D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79209425031 IErMin= 5 ErrMin= 8.59D-05

ErrMax= 8.59D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.25D-05 BMatP= 5.52D-04

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

Coeff-Com: -0.111D-02 0.220D-02 0.102D+00 0.266D+00 0.630D+00

Coeff: -0.111D-02 0.220D-02 0.102D+00 0.266D+00 0.630D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=2.81D-06 MaxDP=1.94D-04 DE=-1.05D-04 OVMax= 1.07D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.17D-06 CP: 9.97D-01 1.06D+00 7.89D-01 7.12D-01 7.82D-01

E= -2649.79209761555 Delta-E= -0.000003365243 Rises=F Damp=F

DIIS: error= 5.24D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79209761555 IErMin= 6 ErrMin= 5.24D-05

ErrMax= 5.24D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.72D-06 BMatP= 2.25D-05

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

Coeff-Com: 0.418D-03-0.123D-01 0.184D-01 0.825D-01 0.406D+00 0.505D+00

Coeff: 0.418D-03-0.123D-01 0.184D-01 0.825D-01 0.406D+00 0.505D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=1.30D-06 MaxDP=1.04D-04 DE=-3.37D-06 OVMax= 2.97D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 7.12D-07 CP: 9.97D-01 1.06D+00 7.94D-01 7.21D-01 8.29D-01

CP: 5.42D-01

E= -2649.79209926218 Delta-E= -0.000001646626 Rises=F Damp=F

DIIS: error= 1.49D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79209926218 IErMin= 7 ErrMin= 1.49D-05

ErrMax= 1.49D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.70D-07 BMatP= 7.72D-06

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

Coeff-Com: 0.321D-03-0.708D-02 0.234D-02 0.260D-01 0.176D+00 0.275D+00

Coeff-Com: 0.528D+00

Coeff: 0.321D-03-0.708D-02 0.234D-02 0.260D-01 0.176D+00 0.275D+00

Coeff: 0.528D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=3.96D-07 MaxDP=2.63D-05 DE=-1.65D-06 OVMax= 1.92D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 3.26D-07 CP: 9.97D-01 1.06D+00 7.94D-01 7.21D-01 8.30D-01

CP: 6.13D-01 7.74D-01

E= -2649.79209937343 Delta-E= -0.000000111257 Rises=F Damp=F

DIIS: error= 4.58D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.79209937343 IErMin= 8 ErrMin= 4.58D-06

ErrMax= 4.58D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.21D-08 BMatP= 4.70D-07

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

Coeff-Com: 0.544D-04-0.570D-03-0.301D-02-0.532D-02-0.488D-02 0.140D-01

Coeff-Com: 0.265D+00 0.735D+00

Coeff: 0.544D-04-0.570D-03-0.301D-02-0.532D-02-0.488D-02 0.140D-01

Coeff: 0.265D+00 0.735D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=1.74D-07 MaxDP=8.82D-06 DE=-1.11D-07 OVMax= 1.12D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.20D-07 CP: 9.97D-01 1.06D+00 7.95D-01 7.22D-01 8.37D-01

CP: 6.17D-01 9.28D-01 9.98D-01

E= -2649.79209939380 Delta-E= -0.000000020364 Rises=F Damp=F

DIIS: error= 1.54D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.79209939380 IErMin= 9 ErrMin= 1.54D-06

ErrMax= 1.54D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.98D-09 BMatP= 6.21D-08

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

Coeff-Com: -0.218D-04 0.744D-03-0.146D-02-0.499D-02-0.245D-01-0.330D-01

Coeff-Com: 0.367D-01 0.259D+00 0.767D+00

Coeff: -0.218D-04 0.744D-03-0.146D-02-0.499D-02-0.245D-01-0.330D-01

Coeff: 0.367D-01 0.259D+00 0.767D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=7.73D-08 MaxDP=4.67D-06 DE=-2.04D-08 OVMax= 5.85D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 5.16D-08 CP: 9.97D-01 1.06D+00 7.95D-01 7.23D-01 8.37D-01

CP: 6.24D-01 9.88D-01 1.10D+00 1.08D+00

E= -2649.79209939705 Delta-E= -0.000000003249 Rises=F Damp=F

DIIS: error= 1.30D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -2649.79209939705 IErMin=10 ErrMin= 1.30D-06

ErrMax= 1.30D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.74D-09 BMatP= 5.98D-09

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

Coeff-Com: -0.248D-04 0.563D-03-0.212D-03-0.167D-02-0.133D-01-0.232D-01

Coeff-Com: -0.342D-01-0.123D-01 0.455D+00 0.629D+00

Coeff: -0.248D-04 0.563D-03-0.212D-03-0.167D-02-0.133D-01-0.232D-01

Coeff: -0.342D-01-0.123D-01 0.455D+00 0.629D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=4.46D-08 MaxDP=2.97D-06 DE=-3.25D-09 OVMax= 3.58D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.85D-08 CP: 9.97D-01 1.06D+00 7.95D-01 7.23D-01 8.38D-01

CP: 6.25D-01 1.01D+00 1.16D+00 1.24D+00 9.12D-01

E= -2649.79209939802 Delta-E= -0.000000000971 Rises=F Damp=F

DIIS: error= 6.04D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -2649.79209939802 IErMin=11 ErrMin= 6.04D-07

ErrMax= 6.04D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.22D-10 BMatP= 2.74D-09

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

Coeff-Com: -0.589D-05 0.632D-04 0.286D-03 0.588D-03 0.360D-03-0.273D-02

Coeff-Com: -0.258D-01-0.821D-01 0.169D-01 0.325D+00 0.768D+00

Coeff: -0.589D-05 0.632D-04 0.286D-03 0.588D-03 0.360D-03-0.273D-02

Coeff: -0.258D-01-0.821D-01 0.169D-01 0.325D+00 0.768D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=2.38D-08 MaxDP=1.76D-06 DE=-9.71D-10 OVMax= 1.69D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.31D-08 CP: 9.97D-01 1.06D+00 7.95D-01 7.23D-01 8.38D-01

CP: 6.27D-01 1.02D+00 1.18D+00 1.33D+00 1.12D+00

CP: 8.70D-01

E= -2649.79209939832 Delta-E= -0.000000000306 Rises=F Damp=F

DIIS: error= 2.56D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -2649.79209939832 IErMin=12 ErrMin= 2.56D-07

ErrMax= 2.56D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.32D-10 BMatP= 5.22D-10

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

Coeff-Com: 0.190D-05-0.835D-04 0.200D-03 0.689D-03 0.298D-02 0.321D-02

Coeff-Com: -0.632D-02-0.436D-01-0.827D-01 0.596D-01 0.433D+00 0.633D+00

Coeff: 0.190D-05-0.835D-04 0.200D-03 0.689D-03 0.298D-02 0.321D-02

Coeff: -0.632D-02-0.436D-01-0.827D-01 0.596D-01 0.433D+00 0.633D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=8.79D-09 MaxDP=7.71D-07 DE=-3.06D-10 OVMax= 6.05D-06

Error on total polarization charges = 0.07326

SCF Done: E(UB3LYP) = -2649.79209940 A.U. after 12 cycles

NFock= 12 Conv=0.88D-08 -V/T= 1.9849

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0168 S= 1.0056

<L.S>= 0.000000000000E+00

KE= 2.690367915922D+03 PE=-2.242121843044D+04 EE= 9.009937808919D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0168, after 2.0002

Leave Link 502 at Sat Jul 6 00:13:28 2019, MaxMem= 1342177280 cpu: 7069.2

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

Compute integral first derivatives.

... and contract with generalized density number 0.

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

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44667 LenP2D= 112062.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 273

Leave Link 701 at Sat Jul 6 00:13:47 2019, MaxMem= 1342177280 cpu: 218.2

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

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

Leave Link 702 at Sat Jul 6 00:13:47 2019, MaxMem= 1342177280 cpu: 0.2

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

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 00:15:20 2019, MaxMem= 1342177280 cpu: 1109.4

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

Dipole =-3.37272142D-03-3.79532062D-03 1.52930496D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.001880443 0.000921141 0.006065622

2 7 -0.000282867 0.001863771 -0.006416692

3 6 -0.002162211 0.001142878 0.006120127

4 6 0.000597141 0.000429035 -0.001948952

5 6 -0.000615274 0.000396103 -0.001956932

6 7 -0.000843288 0.000521377 -0.000133575

7 6 0.002832719 -0.002854147 -0.003774975

8 7 0.004522362 -0.000341343 0.003855345

9 6 0.002556605 0.002522165 -0.003712365

10 6 -0.000103099 0.001604710 0.001258280

11 6 -0.000086875 -0.001621040 0.001255532

12 7 0.001027486 0.000396673 -0.000144922

13 6 0.000098096 -0.001666920 0.001265698

14 6 0.000114362 0.001650642 0.001268500

15 6 -0.002521017 0.002181607 -0.003698017

16 7 -0.004130626 -0.000341887 0.003931584

17 6 -0.002797399 -0.002512060 -0.003760516

18 7 0.001102215 -0.000116037 -0.000130707

19 7 -0.000283211 -0.001435583 -0.006497815

20 6 0.001597541 -0.000911064 0.006069967

21 6 -0.000577436 -0.000377430 -0.001958827

22 6 0.000559320 -0.000410419 -0.001950844

23 6 -0.001877752 -0.001132840 0.006124496

24 7 -0.000918834 -0.000240280 -0.000119241

25 30 0.000295020 0.000326800 -0.001359798

26 6 -0.000287296 0.001091136 -0.001114447

27 6 0.000066147 0.001286355 0.000162056

28 6 0.000065363 -0.001287500 0.000162190

29 6 -0.000292115 -0.001097275 -0.001115541

30 6 0.001125579 -0.000828269 0.001208423

31 6 0.001326800 0.001041215 -0.000113379

32 6 -0.001327659 0.001046288 -0.000114684

33 6 -0.001129760 -0.000840999 0.001212854

34 6 0.000288553 0.001109443 -0.001112154

35 6 -0.000069887 0.001302756 0.000163094

36 6 -0.000069092 -0.001303871 0.000163232

37 6 0.000293365 -0.001115550 -0.001113249

38 6 -0.001148439 0.000841096 0.001214107

39 6 -0.001343797 -0.001050719 -0.000117373

40 6 0.001342928 -0.001045650 -0.000116089

41 6 0.001144256 0.000828390 0.001209697

42 1 0.000747317 0.000612349 -0.000061462

43 1 0.000746807 -0.000612124 -0.000061576

44 1 0.000837336 0.000928609 0.000101784

45 1 -0.000837182 0.000928625 0.000101767

46 1 -0.000747422 0.000611733 -0.000061186

47 1 -0.000746956 -0.000611504 -0.000061304

48 1 -0.000836520 -0.000928459 0.000101473

49 1 0.000836648 -0.000928449 0.000101502

50 8 -0.001739091 0.002578280 -0.000569686

51 8 0.001746521 0.002580242 -0.000568469

52 8 0.001416664 -0.000739340 0.000317797

53 8 0.001420239 0.000741750 0.000318599

54 8 -0.001745120 -0.002562996 -0.000579518

55 8 0.001752427 -0.002564787 -0.000578356

56 8 -0.001408817 0.000747943 0.000326935

57 8 -0.001405477 -0.000745613 0.000326015

58 6 -0.001701988 -0.000170706 -0.000259911

59 1 -0.000706880 0.000094657 0.000761058

60 1 -0.000283426 0.000568266 -0.000338972

61 1 0.000467692 -0.000253050 -0.000107892

62 6 0.000351798 -0.001456879 0.000087750

63 1 0.000217167 -0.000318094 -0.000823544

64 1 0.000115138 -0.000341045 0.000801121

65 1 -0.000339278 0.000457255 0.000034096

66 6 0.000354179 0.001457789 0.000086893

67 1 0.000115219 0.000340651 0.000800881

68 1 0.000216868 0.000317971 -0.000823280

69 1 -0.000339838 -0.000457193 0.000035288

70 6 0.001702242 -0.000170374 -0.000260194

71 1 0.000283228 0.000568290 -0.000339036

72 1 0.000706866 0.000094855 0.000761284

73 1 -0.000467773 -0.000252758 -0.000108460

74 6 -0.000357791 -0.001453889 0.000086177

75 1 -0.000113777 -0.000340791 0.000801259

76 1 -0.000215446 -0.000318440 -0.000823036

77 1 0.000339365 0.000456811 0.000035094

78 6 -0.000360121 0.001454766 0.000085378

79 1 -0.000215161 0.000318332 -0.000822775

80 1 -0.000113865 0.000340398 0.000801009

81 1 0.000339892 -0.000456747 0.000036314

82 6 0.001696072 0.000164308 -0.000259066

83 1 0.000707216 -0.000093190 0.000760607

84 1 0.000283578 -0.000566844 -0.000338912

85 1 -0.000466978 0.000250810 -0.000108248

86 6 -0.001695825 0.000164655 -0.000258746

87 1 -0.000283752 -0.000566815 -0.000338870

88 1 -0.000707219 -0.000093015 0.000760377

89 1 0.000466852 0.000251058 -0.000107668

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

Cartesian Forces: Max 0.006497815 RMS 0.001517161

Leave Link 716 at Sat Jul 6 00:15:20 2019, MaxMem= 1342177280 cpu: 0.6

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.007445773 RMS 0.001760969

Search for a local minimum.

Step number 6 out of a maximum of 518

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

RMS Force = .17610D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 2 3 4 6

5

ITU= 0 1 1 1 1 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.65162.

Iteration 1 RMS(Cart)= 0.16817419 RMS(Int)= 0.00206350

Iteration 2 RMS(Cart)= 0.00885308 RMS(Int)= 0.00021450

Iteration 3 RMS(Cart)= 0.00001102 RMS(Int)= 0.00021449

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00021449

ITry= 1 IFail=0 DXMaxC= 6.29D-01 DCOld= 1.00D+10 DXMaxT= 4.57D-01 DXLimC= 3.00D+00 Rises=T

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

(Linear) (Quad) (Total)

R1 2.58013 0.00214 -0.00015 0.00000 -0.00046 2.57967

R2 2.73468 0.00329 0.00021 0.00000 0.00030 2.73497

R3 2.55411 0.00364 0.01126 0.00000 0.01162 2.56573

R4 2.57950 0.00223 0.00023 0.00000 0.00006 2.57955

R5 3.85528 0.00550 0.01354 0.00000 0.01245 3.86773

R6 2.73474 0.00328 0.00017 0.00000 0.00025 2.73500

R7 2.55306 0.00409 0.01188 0.00000 0.01251 2.56557

R8 2.68753 0.00190 0.00835 0.00000 0.00861 2.69615

R9 2.65605 0.00369 0.00411 0.00000 0.00410 2.66015

R10 2.65607 0.00371 0.00410 0.00000 0.00409 2.66016

R11 2.47260 0.00486 0.00421 0.00000 0.00492 2.47753

R12 2.59695 0.00117 -0.00038 0.00000 -0.00034 2.59661

R13 2.78873 0.00259 0.00790 0.00000 0.00796 2.79669

R14 2.59758 0.00103 -0.00076 0.00000 -0.00086 2.59672

R15 3.80576 0.00745 0.02531 0.00000 0.02446 3.83021

R16 2.78869 0.00261 0.00792 0.00000 0.00799 2.79668

R17 2.47359 0.00431 0.00362 0.00000 0.00407 2.47766

R18 2.66237 0.00031 0.00094 0.00000 0.00119 2.66356

R19 2.64096 0.00306 0.00168 0.00000 0.00168 2.64264

R20 2.64095 0.00304 0.00169 0.00000 0.00169 2.64264

R21 2.47318 0.00448 0.00387 0.00000 0.00441 2.47758

R22 2.66286 0.00020 0.00065 0.00000 0.00077 2.66363

R23 2.78887 0.00256 0.00781 0.00000 0.00784 2.79671

R24 2.64090 0.00303 0.00172 0.00000 0.00172 2.64262

R25 2.78883 0.00257 0.00784 0.00000 0.00787 2.79670

R26 2.64091 0.00305 0.00171 0.00000 0.00172 2.64263

R27 2.59689 0.00118 -0.00034 0.00000 -0.00029 2.59660

R28 2.47416 0.00393 0.00329 0.00000 0.00355 2.47772

R29 2.59626 0.00132 0.00004 0.00000 0.00023 2.59649

R30 3.80304 0.00740 0.02695 0.00000 0.02658 3.82963

R31 2.55480 0.00327 0.01084 0.00000 0.01103 2.56583

R32 2.57945 0.00227 0.00025 0.00000 0.00009 2.57954

R33 2.57882 0.00236 0.00063 0.00000 0.00061 2.57943

R34 3.85201 0.00544 0.01553 0.00000 0.01493 3.86694

R35 2.73483 0.00324 0.00012 0.00000 0.00017 2.73500

R36 2.68808 0.00178 0.00802 0.00000 0.00816 2.69624

R37 2.65604 0.00369 0.00412 0.00000 0.00412 2.66015

R38 2.73490 0.00323 0.00008 0.00000 0.00012 2.73502

R39 2.65602 0.00368 0.00413 0.00000 0.00413 2.66015

R40 2.55376 0.00372 0.01147 0.00000 0.01192 2.56568

R41 2.65630 -0.00079 0.00234 0.00000 0.00233 2.65863

R42 2.55306 -0.00250 -0.00324 0.00000 -0.00324 2.54982

R43 2.63020 -0.00069 -0.00195 0.00000 -0.00196 2.62824

R44 2.04255 0.00095 0.00127 0.00000 0.00127 2.04382

R45 2.65630 -0.00079 0.00234 0.00000 0.00233 2.65863

R46 2.04255 0.00095 0.00127 0.00000 0.00127 2.04382

R47 2.55306 -0.00251 -0.00324 0.00000 -0.00324 2.54982

R48 2.64641 -0.00223 -0.00178 0.00000 -0.00177 2.64463

R49 2.55709 -0.00416 -0.00501 0.00000 -0.00501 2.55207

R50 2.65128 -0.00191 -0.00255 0.00000 -0.00254 2.64873

R51 2.04235 0.00120 0.00128 0.00000 0.00128 2.04363

R52 2.64640 -0.00223 -0.00177 0.00000 -0.00177 2.64463

R53 2.04235 0.00120 0.00128 0.00000 0.00128 2.04363

R54 2.55709 -0.00417 -0.00501 0.00000 -0.00501 2.55207

R55 2.65627 -0.00079 0.00236 0.00000 0.00236 2.65863

R56 2.55306 -0.00250 -0.00324 0.00000 -0.00324 2.54982

R57 2.63018 -0.00066 -0.00194 0.00000 -0.00194 2.62824

R58 2.04255 0.00095 0.00127 0.00000 0.00127 2.04382

R59 2.65627 -0.00079 0.00236 0.00000 0.00236 2.65863

R60 2.04255 0.00095 0.00127 0.00000 0.00127 2.04382

R61 2.55306 -0.00250 -0.00324 0.00000 -0.00324 2.54982

R62 2.64637 -0.00223 -0.00176 0.00000 -0.00175 2.64462

R63 2.55709 -0.00417 -0.00501 0.00000 -0.00501 2.55208

R64 2.65127 -0.00188 -0.00255 0.00000 -0.00253 2.64874

R65 2.04235 0.00120 0.00128 0.00000 0.00128 2.04363

R66 2.64638 -0.00223 -0.00176 0.00000 -0.00176 2.64463

R67 2.04235 0.00120 0.00128 0.00000 0.00128 2.04363

R68 2.55709 -0.00416 -0.00501 0.00000 -0.00501 2.55208

R69 2.69537 -0.00099 -0.00094 0.00000 -0.00094 2.69443

R70 2.69537 -0.00099 -0.00094 0.00000 -0.00094 2.69443

R71 2.69636 -0.00060 -0.00047 0.00000 -0.00047 2.69588

R72 2.69636 -0.00060 -0.00047 0.00000 -0.00047 2.69588

R73 2.69538 -0.00099 -0.00094 0.00000 -0.00094 2.69444

R74 2.69538 -0.00099 -0.00094 0.00000 -0.00094 2.69443

R75 2.69637 -0.00059 -0.00048 0.00000 -0.00048 2.69589

R76 2.69637 -0.00059 -0.00048 0.00000 -0.00048 2.69589

R77 2.06526 0.00087 0.00141 0.00000 0.00141 2.06666

R78 2.06568 0.00069 0.00124 0.00000 0.00124 2.06692

R79 2.05518 0.00053 0.00107 0.00000 0.00107 2.05625

R80 2.06506 0.00087 0.00134 0.00000 0.00134 2.06641

R81 2.06540 0.00074 0.00135 0.00000 0.00135 2.06675

R82 2.05485 0.00054 0.00118 0.00000 0.00118 2.05603

R83 2.06540 0.00074 0.00135 0.00000 0.00135 2.06675

R84 2.06506 0.00087 0.00134 0.00000 0.00134 2.06641

R85 2.05485 0.00054 0.00118 0.00000 0.00118 2.05603

R86 2.06568 0.00069 0.00124 0.00000 0.00124 2.06692

R87 2.06526 0.00087 0.00141 0.00000 0.00141 2.06666

R88 2.05518 0.00053 0.00107 0.00000 0.00107 2.05625

R89 2.06540 0.00074 0.00136 0.00000 0.00136 2.06675

R90 2.06506 0.00087 0.00134 0.00000 0.00134 2.06641

R91 2.05485 0.00053 0.00118 0.00000 0.00118 2.05603

R92 2.06506 0.00087 0.00134 0.00000 0.00134 2.06641

R93 2.06539 0.00074 0.00136 0.00000 0.00136 2.06675

R94 2.05485 0.00053 0.00118 0.00000 0.00118 2.05603

R95 2.06525 0.00087 0.00141 0.00000 0.00141 2.06666

R96 2.06568 0.00069 0.00124 0.00000 0.00124 2.06692

R97 2.05518 0.00053 0.00107 0.00000 0.00107 2.05625

R98 2.06568 0.00069 0.00124 0.00000 0.00124 2.06692

R99 2.06525 0.00087 0.00141 0.00000 0.00141 2.06666

R100 2.05518 0.00052 0.00107 0.00000 0.00107 2.05625

A1 1.88903 0.00090 -0.00144 0.00000 -0.00163 1.88740

A2 2.21757 -0.00193 -0.00408 0.00000 -0.00413 2.21344

A3 2.17623 0.00107 0.00560 0.00000 0.00611 2.18233

A4 1.92835 -0.00103 0.00454 0.00000 0.00523 1.93358

A5 2.16937 0.00055 -0.00284 0.00000 -0.00290 2.16646

A6 2.17178 0.00037 -0.00430 0.00000 -0.00486 2.16692

A7 1.88916 0.00089 -0.00153 0.00000 -0.00174 1.88742

A8 2.21718 -0.00197 -0.00384 0.00000 -0.00383 2.21335

A9 2.17648 0.00112 0.00544 0.00000 0.00593 2.18241

A10 1.85842 -0.00033 -0.00033 0.00000 -0.00028 1.85814

A11 2.31167 0.00252 0.00428 0.00000 0.00429 2.31596

A12 2.11293 -0.00218 -0.00384 0.00000 -0.00387 2.10906

A13 1.85841 -0.00031 -0.00033 0.00000 -0.00027 1.85814

A14 2.31167 0.00252 0.00428 0.00000 0.00429 2.31596

A15 2.11294 -0.00220 -0.00385 0.00000 -0.00388 2.10906

A16 2.17026 0.00315 0.01489 0.00000 0.01545 2.18570

A17 2.23673 -0.00207 0.00052 0.00000 0.00060 2.23733

A18 2.16036 0.00164 0.00559 0.00000 0.00579 2.16615

A19 1.88600 0.00042 -0.00612 0.00000 -0.00639 1.87961

A20 1.92672 -0.00051 0.01006 0.00000 0.01070 1.93742

A21 2.16554 0.00009 -0.00324 0.00000 -0.00373 2.16181

A22 2.16287 0.00031 -0.00162 0.00000 -0.00162 2.16125

A23 1.88585 0.00044 -0.00603 0.00000 -0.00627 1.87958

A24 2.23713 -0.00202 0.00028 0.00000 0.00030 2.23743

A25 2.16011 0.00157 0.00575 0.00000 0.00597 2.16608

A26 1.86230 -0.00013 0.00157 0.00000 0.00169 1.86399

A27 2.30132 0.00147 -0.00053 0.00000 -0.00061 2.30072

A28 2.11956 -0.00134 -0.00105 0.00000 -0.00109 2.11847

A29 1.86231 -0.00015 0.00156 0.00000 0.00168 1.86399

A30 2.30131 0.00148 -0.00052 0.00000 -0.00060 2.30072

A31 2.11956 -0.00133 -0.00105 0.00000 -0.00109 2.11847

A32 2.17096 0.00306 0.01447 0.00000 0.01485 2.18581

A33 1.86231 -0.00013 0.00156 0.00000 0.00168 1.86399

A34 2.11951 -0.00133 -0.00102 0.00000 -0.00105 2.11846

A35 2.30136 0.00145 -0.00055 0.00000 -0.00064 2.30073

A36 1.86230 -0.00011 0.00157 0.00000 0.00169 1.86399

A37 2.11951 -0.00134 -0.00102 0.00000 -0.00105 2.11846

A38 2.30137 0.00145 -0.00056 0.00000 -0.00065 2.30073

A39 1.88528 0.00050 -0.00569 0.00000 -0.00578 1.87949

A40 2.16103 0.00144 0.00520 0.00000 0.00519 2.16622

A41 2.23679 -0.00195 0.00048 0.00000 0.00059 2.23738

A42 1.92787 -0.00068 0.00937 0.00000 0.00973 1.93760

A43 2.16227 0.00039 -0.00126 0.00000 -0.00112 2.16115

A44 2.16494 0.00018 -0.00288 0.00000 -0.00324 2.16171

A45 2.16129 0.00151 0.00504 0.00000 0.00501 2.16629

A46 2.23639 -0.00200 0.00073 0.00000 0.00089 2.23728

A47 1.88542 0.00048 -0.00578 0.00000 -0.00590 1.87952

A48 2.17172 0.00297 0.01402 0.00000 0.01423 2.18595

A49 1.92958 -0.00123 0.00380 0.00000 0.00422 1.93380

A50 2.16874 0.00065 -0.00246 0.00000 -0.00239 2.16635

A51 2.17116 0.00047 -0.00392 0.00000 -0.00435 2.16681

A52 2.21720 -0.00188 -0.00386 0.00000 -0.00383 2.21337

A53 2.17721 0.00094 0.00501 0.00000 0.00531 2.18252

A54 1.88841 0.00098 -0.00108 0.00000 -0.00113 1.88728

A55 1.85842 -0.00030 -0.00034 0.00000 -0.00028 1.85814

A56 2.31172 0.00250 0.00425 0.00000 0.00425 2.31597

A57 2.11288 -0.00220 -0.00381 0.00000 -0.00382 2.10905

A58 1.85843 -0.00032 -0.00034 0.00000 -0.00029 1.85814

A59 2.11287 -0.00218 -0.00380 0.00000 -0.00382 2.10905

A60 2.31172 0.00249 0.00425 0.00000 0.00425 2.31598

A61 1.88854 0.00097 -0.00116 0.00000 -0.00124 1.88730

A62 2.21681 -0.00192 -0.00362 0.00000 -0.00353 2.21328

A63 2.17746 0.00100 0.00486 0.00000 0.00513 2.18259

A64 2.17102 0.00306 0.01444 0.00000 0.01482 2.18584

A65 1.55603 0.00036 0.00878 0.00000 0.01048 1.56651

A66 1.55825 0.00008 0.00745 0.00000 0.00866 1.56691

A67 1.55851 0.00004 0.00728 0.00000 0.00850 1.56701

A68 1.56074 -0.00024 0.00595 0.00000 0.00668 1.56741

A69 2.04050 0.00158 0.00160 0.00000 0.00163 2.04213

A70 2.06531 0.00344 0.00649 0.00000 0.00648 2.07179

A71 2.17718 -0.00501 -0.00797 0.00000 -0.00797 2.16921

A72 2.12317 -0.00025 -0.00059 0.00000 -0.00059 2.12259

A73 2.09981 -0.00007 -0.00139 0.00000 -0.00139 2.09842

A74 2.06014 0.00032 0.00201 0.00000 0.00201 2.06215

A75 2.12317 -0.00024 -0.00059 0.00000 -0.00058 2.12259

A76 2.06014 0.00032 0.00201 0.00000 0.00201 2.06215

A77 2.09982 -0.00007 -0.00139 0.00000 -0.00139 2.09842

A78 2.04050 0.00158 0.00160 0.00000 0.00163 2.04213

A79 2.06532 0.00345 0.00648 0.00000 0.00648 2.07179

A80 2.17717 -0.00502 -0.00796 0.00000 -0.00796 2.16921

A81 2.04688 0.00221 0.00406 0.00000 0.00407 2.05094

A82 2.05181 0.00481 0.00726 0.00000 0.00728 2.05909

A83 2.18424 -0.00701 -0.01116 0.00000 -0.01114 2.17310

A84 2.12321 -0.00003 -0.00015 0.00000 -0.00014 2.12307

A85 2.10170 -0.00030 -0.00111 0.00000 -0.00111 2.10059

A86 2.05805 0.00034 0.00139 0.00000 0.00139 2.05944

A87 2.12321 -0.00002 -0.00015 0.00000 -0.00014 2.12307

A88 2.05805 0.00033 0.00139 0.00000 0.00139 2.05944

A89 2.10170 -0.00030 -0.00111 0.00000 -0.00111 2.10059

A90 2.04687 0.00222 0.00406 0.00000 0.00407 2.05094

A91 2.05182 0.00481 0.00726 0.00000 0.00728 2.05909

A92 2.18424 -0.00701 -0.01116 0.00000 -0.01114 2.17310

A93 2.04048 0.00156 0.00161 0.00000 0.00164 2.04212

A94 2.06535 0.00346 0.00646 0.00000 0.00646 2.07181

A95 2.17715 -0.00501 -0.00795 0.00000 -0.00795 2.16920

A96 2.12314 -0.00023 -0.00057 0.00000 -0.00055 2.12259

A97 2.09983 -0.00008 -0.00140 0.00000 -0.00141 2.09842

A98 2.06016 0.00031 0.00200 0.00000 0.00199 2.06215

A99 2.12314 -0.00023 -0.00057 0.00000 -0.00055 2.12258

A100 2.06016 0.00031 0.00200 0.00000 0.00199 2.06215

A101 2.09983 -0.00008 -0.00140 0.00000 -0.00141 2.09842

A102 2.04048 0.00156 0.00161 0.00000 0.00164 2.04212

A103 2.06536 0.00347 0.00645 0.00000 0.00645 2.07181

A104 2.17714 -0.00502 -0.00794 0.00000 -0.00795 2.16920

A105 2.04685 0.00220 0.00408 0.00000 0.00409 2.05093

A106 2.05184 0.00483 0.00725 0.00000 0.00726 2.05910

A107 2.18425 -0.00702 -0.01116 0.00000 -0.01115 2.17310

A108 2.12317 0.00000 -0.00013 0.00000 -0.00010 2.12307

A109 2.10171 -0.00031 -0.00112 0.00000 -0.00112 2.10059

A110 2.05807 0.00033 0.00138 0.00000 0.00138 2.05944

A111 2.12317 -0.00001 -0.00013 0.00000 -0.00010 2.12307

A112 2.05807 0.00033 0.00138 0.00000 0.00138 2.05944

A113 2.10171 -0.00031 -0.00112 0.00000 -0.00112 2.10059

A114 2.04685 0.00220 0.00407 0.00000 0.00408 2.05094

A115 2.05184 0.00483 0.00725 0.00000 0.00727 2.05910

A116 2.18424 -0.00702 -0.01116 0.00000 -0.01115 2.17310

A117 2.07753 -0.00598 -0.00665 0.00000 -0.00665 2.07088

A118 2.07752 -0.00598 -0.00665 0.00000 -0.00665 2.07088

A119 2.07560 -0.00450 -0.00386 0.00000 -0.00386 2.07174

A120 2.07560 -0.00450 -0.00386 0.00000 -0.00386 2.07174

A121 2.07752 -0.00598 -0.00665 0.00000 -0.00665 2.07088

A122 2.07752 -0.00598 -0.00664 0.00000 -0.00664 2.07088

A123 2.07560 -0.00450 -0.00385 0.00000 -0.00385 2.07174

A124 2.07560 -0.00450 -0.00386 0.00000 -0.00386 2.07174

A125 1.94926 -0.00080 -0.00135 0.00000 -0.00135 1.94791

A126 1.94544 0.00007 -0.00152 0.00000 -0.00152 1.94392

A127 1.84195 0.00008 -0.00039 0.00000 -0.00039 1.84156

A128 1.91145 0.00003 0.00118 0.00000 0.00118 1.91263

A129 1.90555 0.00044 0.00144 0.00000 0.00144 1.90699

A130 1.90851 0.00022 0.00068 0.00000 0.00068 1.90919

A131 1.94760 -0.00018 0.00027 0.00000 0.00027 1.94787

A132 1.94676 -0.00059 -0.00143 0.00000 -0.00143 1.94533

A133 1.84281 -0.00015 -0.00215 0.00000 -0.00215 1.84067

A134 1.91043 0.00043 0.00195 0.00000 0.00195 1.91238

A135 1.90645 0.00025 0.00061 0.00000 0.00061 1.90707

A136 1.90820 0.00025 0.00064 0.00000 0.00064 1.90884

A137 1.94675 -0.00059 -0.00143 0.00000 -0.00143 1.94533

A138 1.94760 -0.00018 0.00027 0.00000 0.00027 1.94787

A139 1.84281 -0.00016 -0.00215 0.00000 -0.00215 1.84066

A140 1.91043 0.00043 0.00195 0.00000 0.00195 1.91238

A141 1.90820 0.00025 0.00064 0.00000 0.00064 1.90884

A142 1.90645 0.00025 0.00061 0.00000 0.00061 1.90707

A143 1.94544 0.00007 -0.00152 0.00000 -0.00152 1.94392

A144 1.94926 -0.00080 -0.00136 0.00000 -0.00136 1.94791

A145 1.84195 0.00008 -0.00039 0.00000 -0.00039 1.84156

A146 1.91145 0.00003 0.00118 0.00000 0.00118 1.91263

A147 1.90851 0.00021 0.00068 0.00000 0.00068 1.90919

A148 1.90555 0.00044 0.00144 0.00000 0.00144 1.90699

A149 1.94676 -0.00059 -0.00143 0.00000 -0.00143 1.94533

A150 1.94759 -0.00018 0.00027 0.00000 0.00027 1.94787

A151 1.84282 -0.00015 -0.00215 0.00000 -0.00215 1.84067

A152 1.91044 0.00043 0.00195 0.00000 0.00195 1.91238

A153 1.90820 0.00025 0.00064 0.00000 0.00064 1.90884

A154 1.90645 0.00025 0.00062 0.00000 0.00062 1.90707

A155 1.94759 -0.00018 0.00027 0.00000 0.00027 1.94787

A156 1.94675 -0.00059 -0.00143 0.00000 -0.00142 1.94533

A157 1.84281 -0.00016 -0.00215 0.00000 -0.00215 1.84067

A158 1.91044 0.00043 0.00195 0.00000 0.00195 1.91238

A159 1.90645 0.00025 0.00061 0.00000 0.00061 1.90707

A160 1.90821 0.00025 0.00064 0.00000 0.00064 1.90884

A161 1.94926 -0.00080 -0.00135 0.00000 -0.00135 1.94791

A162 1.94543 0.00007 -0.00151 0.00000 -0.00151 1.94392

A163 1.84195 0.00008 -0.00039 0.00000 -0.00039 1.84156

A164 1.91145 0.00003 0.00118 0.00000 0.00118 1.91263

A165 1.90555 0.00044 0.00144 0.00000 0.00144 1.90699

A166 1.90851 0.00021 0.00068 0.00000 0.00068 1.90919

A167 1.94543 0.00007 -0.00151 0.00000 -0.00151 1.94392

A168 1.94926 -0.00080 -0.00135 0.00000 -0.00135 1.94790

A169 1.84196 0.00008 -0.00040 0.00000 -0.00040 1.84156

A170 1.91145 0.00003 0.00118 0.00000 0.00118 1.91263

A171 1.90851 0.00021 0.00068 0.00000 0.00068 1.90919

A172 1.90555 0.00044 0.00144 0.00000 0.00144 1.90699

A173 3.11899 -0.00016 0.01339 0.00000 0.01534 3.13432

A174 3.11925 -0.00019 0.01323 0.00000 0.01518 3.13443

A175 3.34903 -0.00061 -0.10908 0.00000 -0.10884 3.24019

A176 2.90363 0.00052 0.08270 0.00000 0.08273 2.98636

D1 -0.05000 0.00193 0.03637 0.00000 0.03649 -0.01350

D2 2.92102 0.00127 0.02099 0.00000 0.02106 2.94208

D3 3.11969 0.00031 0.00292 0.00000 0.00299 3.12268

D4 -0.19248 -0.00036 -0.01246 0.00000 -0.01243 -0.20492

D5 0.02971 -0.00113 -0.02160 0.00000 -0.02172 0.00800

D6 -3.09198 -0.00124 -0.03535 0.00000 -0.03538 -3.12736

D7 -3.13914 0.00039 0.01101 0.00000 0.01083 -3.12831

D8 0.02235 0.00027 -0.00273 0.00000 -0.00283 0.01952

D9 0.21697 0.00014 -0.02630 0.00000 -0.02615 0.19082

D10 -2.89218 -0.00172 -0.06505 0.00000 -0.06487 -2.95705

D11 0.04999 -0.00193 -0.03637 0.00000 -0.03649 0.01350

D12 -3.11980 -0.00030 -0.00285 0.00000 -0.00291 -3.12271

D13 -2.92074 -0.00129 -0.02116 0.00000 -0.02129 -2.94203

D14 0.19265 0.00034 0.01236 0.00000 0.01229 0.20494

D15 -2.92598 0.00021 -0.03285 0.00000 -0.03281 -2.95879

D16 -0.02183 0.00066 0.04952 0.00000 0.04946 0.02763

D17 0.02160 -0.00067 -0.04938 0.00000 -0.04928 -0.02768

D18 2.92575 -0.00022 0.03300 0.00000 0.03298 2.95873

D19 -0.02971 0.00113 0.02161 0.00000 0.02172 -0.00800

D20 3.09196 0.00124 0.03537 0.00000 0.03540 3.12736

D21 3.13927 -0.00039 -0.01109 0.00000 -0.01093 3.12834

D22 -0.02225 -0.00028 0.00267 0.00000 0.00276 -0.01949

D23 -0.21684 -0.00014 0.02622 0.00000 0.02606 -0.19078

D24 2.89217 0.00173 0.06505 0.00000 0.06488 2.95705

D25 -0.00001 0.00000 0.00000 0.00000 0.00000 0.00000

D26 3.12445 0.00016 0.01184 0.00000 0.01181 3.13625

D27 -3.12444 -0.00016 -0.01185 0.00000 -0.01181 -3.13625

D28 0.00002 0.00000 -0.00001 0.00000 -0.00001 0.00000

D29 3.14127 0.00005 -0.00903 0.00000 -0.00897 3.13230

D30 -0.02331 0.00040 0.00362 0.00000 0.00364 -0.01968

D31 -0.02262 0.00020 0.00637 0.00000 0.00636 -0.01626

D32 3.09598 0.00056 0.01903 0.00000 0.01897 3.11495

D33 -3.14127 -0.00005 0.00903 0.00000 0.00897 -3.13230

D34 0.02332 -0.00040 -0.00363 0.00000 -0.00364 0.01968

D35 0.02260 -0.00020 -0.00636 0.00000 -0.00634 0.01626

D36 -3.09600 -0.00056 -0.01901 0.00000 -0.01895 -3.11495

D37 -0.06064 -0.00009 -0.00270 0.00000 -0.00281 -0.06345

D38 3.09727 0.00074 -0.00227 0.00000 -0.00233 3.09494

D39 -3.07424 -0.00039 -0.03465 0.00000 -0.03465 -3.10888

D40 0.31171 0.00000 -0.05877 0.00000 -0.05878 0.25293

D41 0.05309 -0.00111 -0.03495 0.00000 -0.03499 0.01811

D42 -2.84415 -0.00071 -0.05907 0.00000 -0.05912 -2.90327

D43 3.09649 -0.00007 0.02048 0.00000 0.02053 3.11703

D44 -0.04093 -0.00001 0.02164 0.00000 0.02167 -0.01927

D45 -0.03160 0.00065 0.02081 0.00000 0.02090 -0.01070

D46 3.11415 0.00071 0.02197 0.00000 0.02203 3.13618

D47 -0.05312 0.00111 0.03497 0.00000 0.03500 -0.01811

D48 3.07411 0.00040 0.03473 0.00000 0.03475 3.10886

D49 2.84457 0.00068 0.05881 0.00000 0.05877 2.90334

D50 -0.31138 -0.00003 0.05857 0.00000 0.05851 -0.25287

D51 -0.24191 -0.00003 0.06871 0.00000 0.06861 -0.17330

D52 3.10659 -0.00057 -0.04003 0.00000 -0.03976 3.06683

D53 -3.10670 0.00054 0.04010 0.00000 0.03983 -3.06687

D54 0.24180 0.00000 -0.06865 0.00000 -0.06853 0.17326

D55 0.03167 -0.00065 -0.02084 0.00000 -0.02094 0.01072

D56 -3.11413 -0.00071 -0.02198 0.00000 -0.02204 -3.13617

D57 -3.09635 0.00005 -0.02057 0.00000 -0.02065 -3.11699

D58 0.04104 0.00000 -0.02171 0.00000 -0.02174 0.01929

D59 0.06069 0.00011 0.00268 0.00000 0.00278 0.06347

D60 -3.09733 -0.00072 0.00230 0.00000 0.00239 -3.09494

D61 -0.00004 0.00000 0.00003 0.00000 0.00003 -0.00001

D62 3.13791 -0.00004 -0.00099 0.00000 -0.00096 3.13696

D63 -3.13796 0.00004 0.00102 0.00000 0.00099 -3.13698

D64 0.00000 0.00000 0.00000 0.00000 0.00000 -0.00001

D65 -3.13214 0.00017 0.00198 0.00000 0.00194 -3.13019

D66 0.02989 -0.00025 -0.00762 0.00000 -0.00763 0.02226

D67 0.00473 0.00011 0.00071 0.00000 0.00072 0.00545

D68 -3.11643 -0.00031 -0.00889 0.00000 -0.00885 -3.12528

D69 3.13219 -0.00017 -0.00201 0.00000 -0.00198 3.13021

D70 -0.02983 0.00025 0.00758 0.00000 0.00759 -0.02224

D71 -0.00473 -0.00011 -0.00071 0.00000 -0.00072 -0.00544

D72 3.11644 0.00031 0.00889 0.00000 0.00885 3.12529

D73 -3.09709 -0.00077 0.00216 0.00000 0.00220 -3.09489

D74 0.06072 0.00007 0.00266 0.00000 0.00275 0.06347

D75 0.00004 0.00000 -0.00003 0.00000 -0.00003 0.00001

D76 3.13805 -0.00005 -0.00107 0.00000 -0.00105 3.13700

D77 -3.13800 0.00004 0.00105 0.00000 0.00102 -3.13698

D78 0.00000 0.00000 0.00000 0.00000 0.00000 0.00001

D79 -3.09663 0.00008 -0.02039 0.00000 -0.02043 -3.11706

D80 0.03155 -0.00064 -0.02077 0.00000 -0.02085 0.01070

D81 0.04090 0.00001 -0.02162 0.00000 -0.02163 0.01926

D82 -3.11411 -0.00071 -0.02200 0.00000 -0.02205 -3.13616

D83 0.00475 0.00011 0.00070 0.00000 0.00070 0.00545

D84 -3.11639 -0.00031 -0.00892 0.00000 -0.00889 -3.12527

D85 -3.13228 0.00018 0.00207 0.00000 0.00205 -3.13024

D86 0.02977 -0.00025 -0.00755 0.00000 -0.00755 0.02222

D87 -0.03161 0.00065 0.02081 0.00000 0.02089 -0.01072

D88 3.09648 -0.00006 0.02048 0.00000 0.02055 3.11703

D89 3.11409 0.00071 0.02201 0.00000 0.02206 3.13615

D90 -0.04100 -0.00001 0.02168 0.00000 0.02171 -0.01929

D91 -0.00475 -0.00011 -0.00070 0.00000 -0.00071 -0.00546

D92 3.11638 0.00031 0.00893 0.00000 0.00889 3.12527

D93 3.13223 -0.00017 -0.00204 0.00000 -0.00201 3.13022

D94 -0.02983 0.00025 0.00758 0.00000 0.00759 -0.02224

D95 0.05307 -0.00111 -0.03494 0.00000 -0.03496 0.01810

D96 -2.84440 -0.00068 -0.05892 0.00000 -0.05887 -2.90327

D97 -3.07426 -0.00039 -0.03464 0.00000 -0.03464 -3.10890

D98 0.31146 0.00004 -0.05862 0.00000 -0.05855 0.25290

D99 3.09715 0.00075 -0.00219 0.00000 -0.00226 3.09489

D100 -0.06077 -0.00009 -0.00263 0.00000 -0.00272 -0.06349

D101 3.07439 0.00038 0.03456 0.00000 0.03454 3.10893

D102 -0.05304 0.00111 0.03492 0.00000 0.03494 -0.01810

D103 -0.31178 -0.00002 0.05882 0.00000 0.05882 -0.25296

D104 2.84398 0.00071 0.05918 0.00000 0.05922 2.90320

D105 3.10696 -0.00059 -0.04026 0.00000 -0.04009 3.06687

D106 -0.24207 0.00002 0.06882 0.00000 0.06875 -0.17332

D107 0.24219 0.00001 -0.06889 0.00000 -0.06883 0.17336

D108 -3.10684 0.00062 0.04019 0.00000 0.04001 -3.06683

D109 -0.21715 -0.00012 0.02641 0.00000 0.02630 -0.19085

D110 2.89191 0.00176 0.06521 0.00000 0.06510 2.95701

D111 -3.12003 -0.00028 -0.00272 0.00000 -0.00272 -3.12275

D112 0.04971 -0.00191 -0.03619 0.00000 -0.03626 0.01345

D113 0.19238 0.00038 0.01252 0.00000 0.01254 0.20492

D114 -2.92107 -0.00125 -0.02095 0.00000 -0.02100 -2.94207

D115 -0.04971 0.00191 0.03619 0.00000 0.03626 -0.01345

D116 3.12014 0.00027 0.00265 0.00000 0.00264 3.12278

D117 2.92078 0.00127 0.02112 0.00000 0.02123 2.94201

D118 -0.19255 -0.00037 -0.01242 0.00000 -0.01240 -0.20495

D119 2.92567 -0.00019 0.03305 0.00000 0.03307 2.95874

D120 0.02204 -0.00071 -0.04965 0.00000 -0.04966 -0.02762

D121 -0.02181 0.00072 0.04951 0.00000 0.04949 0.02768

D122 -2.92544 0.00020 -0.03319 0.00000 -0.03325 -2.95869

D123 3.13941 -0.00042 -0.01118 0.00000 -0.01106 3.12835

D124 -0.02218 -0.00029 0.00263 0.00000 0.00268 -0.01949

D125 -0.02952 0.00111 0.02148 0.00000 0.02156 -0.00796

D126 3.09208 0.00124 0.03529 0.00000 0.03530 3.12738

D127 0.00001 0.00000 0.00000 0.00000 0.00000 0.00000

D128 3.12435 0.00017 0.01190 0.00000 0.01189 3.13624

D129 -3.12436 -0.00018 -0.01189 0.00000 -0.01188 -3.13624

D130 -0.00002 0.00000 0.00001 0.00000 0.00001 0.00000

D131 3.14134 0.00004 -0.00908 0.00000 -0.00903 3.13231

D132 -0.02325 0.00039 0.00358 0.00000 0.00358 -0.01967

D133 -0.02264 0.00021 0.00638 0.00000 0.00638 -0.01627

D134 3.09596 0.00056 0.01903 0.00000 0.01898 3.11494

D135 0.02952 -0.00111 -0.02149 0.00000 -0.02156 0.00796

D136 -3.13954 0.00043 0.01126 0.00000 0.01116 -3.12838

D137 -3.09205 -0.00124 -0.03531 0.00000 -0.03532 -3.12738

D138 0.02208 0.00029 -0.00257 0.00000 -0.00261 0.01947

D139 0.02266 -0.00021 -0.00639 0.00000 -0.00639 0.01627

D140 -3.09594 -0.00056 -0.01905 0.00000 -0.01900 -3.11494

D141 -3.14134 -0.00004 0.00908 0.00000 0.00903 -3.13231

D142 0.02324 -0.00039 -0.00358 0.00000 -0.00357 0.01966

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D144 -2.89190 -0.00177 -0.06522 0.00000 -0.06511 -2.95701

D145 -0.00476 -0.00011 -0.00070 0.00000 -0.00071 -0.00547

D146 -3.13453 -0.00026 -0.00445 0.00000 -0.00446 -3.13900

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D148 -0.01486 0.00031 0.00591 0.00000 0.00592 -0.00894

D149 -3.10631 0.00061 0.01340 0.00000 0.01340 -3.09291

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D158 0.01487 -0.00031 -0.00591 0.00000 -0.00592 0.00894

D159 3.10632 -0.00061 -0.01340 0.00000 -0.01340 3.09291

D160 -0.05749 -0.00006 -0.00292 0.00000 -0.00291 -0.06041

D161 -0.02279 0.00018 0.00640 0.00000 0.00639 -0.01641

D162 -3.14073 -0.00025 -0.00311 0.00000 -0.00313 3.13933

D163 3.09387 0.00075 0.02016 0.00000 0.02019 3.11406

D164 -0.02406 0.00032 0.01065 0.00000 0.01067 -0.01339

D165 -3.10010 -0.00015 0.01023 0.00000 0.01024 -3.08986

D166 0.06649 -0.00069 -0.00357 0.00000 -0.00358 0.06291

D167 -0.00001 0.00000 0.00000 0.00000 0.00000 0.00000

D168 -3.11850 -0.00041 -0.00927 0.00000 -0.00927 -3.12777

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D170 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D171 0.02279 -0.00018 -0.00640 0.00000 -0.00639 0.01641

D172 -3.09387 -0.00075 -0.02016 0.00000 -0.02019 -3.11406

D173 3.14072 0.00025 0.00311 0.00000 0.00313 -3.13933

D174 0.02406 -0.00032 -0.01065 0.00000 -0.01067 0.01339

D175 3.10008 0.00015 -0.01021 0.00000 -0.01022 3.08985

D176 -0.06650 0.00068 0.00358 0.00000 0.00359 -0.06291

D177 0.00474 0.00012 0.00071 0.00000 0.00072 0.00546

D178 3.13455 0.00026 0.00444 0.00000 0.00445 3.13900

D179 -3.11497 -0.00045 -0.00962 0.00000 -0.00963 -3.12461

D180 0.01483 -0.00031 -0.00589 0.00000 -0.00590 0.00893

D181 3.10626 -0.00061 -0.01337 0.00000 -0.01337 3.09289

D182 -0.05750 -0.00006 -0.00291 0.00000 -0.00291 -0.06041

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D185 -3.13007 -0.00013 -0.00364 0.00000 -0.00363 -3.13370

D186 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D187 -0.00474 -0.00012 -0.00072 0.00000 -0.00073 -0.00546

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D189 -3.13454 -0.00026 -0.00444 0.00000 -0.00446 -3.13900

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D191 -3.10626 0.00061 0.01337 0.00000 0.01337 -3.09289

D192 0.05750 0.00006 0.00291 0.00000 0.00291 0.06041

D193 -0.02275 0.00018 0.00637 0.00000 0.00635 -0.01640

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D195 3.09391 0.00074 0.02014 0.00000 0.02016 3.11407

D196 -0.02404 0.00031 0.01064 0.00000 0.01066 -0.01339

D197 -3.10009 -0.00015 0.01022 0.00000 0.01023 -3.08986

D198 0.06649 -0.00068 -0.00357 0.00000 -0.00358 0.06291

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D201 3.11853 0.00041 0.00926 0.00000 0.00925 3.12777

D202 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D203 0.02275 -0.00018 -0.00637 0.00000 -0.00635 0.01640

D204 -3.09391 -0.00074 -0.02014 0.00000 -0.02016 -3.11407

D205 3.14071 0.00025 0.00312 0.00000 0.00314 -3.13934

D206 0.02404 -0.00031 -0.01065 0.00000 -0.01066 0.01339

D207 3.10011 0.00015 -0.01024 0.00000 -0.01025 3.08987

D208 -0.06648 0.00068 0.00356 0.00000 0.00357 -0.06290

D209 1.09692 -0.00024 -0.00022 0.00000 -0.00022 1.09670

D210 -1.04752 0.00025 0.00033 0.00000 0.00033 -1.04719

D211 -3.11765 -0.00009 0.00055 0.00000 0.00055 -3.11710

D212 1.04752 -0.00025 -0.00033 0.00000 -0.00033 1.04719

D213 -1.09692 0.00024 0.00022 0.00000 0.00022 -1.09670

D214 3.11765 0.00009 -0.00055 0.00000 -0.00055 3.11710

D215 1.09893 -0.00011 0.00052 0.00000 0.00052 1.09945

D216 -1.04395 -0.00011 -0.00117 0.00000 -0.00117 -1.04512

D217 -3.11493 0.00000 0.00011 0.00000 0.00011 -3.11482

D218 1.04395 0.00011 0.00117 0.00000 0.00117 1.04512

D219 -1.09893 0.00011 -0.00052 0.00000 -0.00052 -1.09945

D220 3.11492 0.00000 -0.00010 0.00000 -0.00010 3.11482

D221 1.04752 -0.00025 -0.00033 0.00000 -0.00033 1.04719

D222 -1.09692 0.00024 0.00022 0.00000 0.00022 -1.09670

D223 3.11765 0.00009 -0.00055 0.00000 -0.00055 3.11710

D224 1.09692 -0.00024 -0.00022 0.00000 -0.00022 1.09670

D225 -1.04752 0.00025 0.00033 0.00000 0.00033 -1.04719

D226 -3.11765 -0.00009 0.00055 0.00000 0.00055 -3.11710

D227 1.09893 -0.00011 0.00052 0.00000 0.00052 1.09945

D228 -1.04394 -0.00011 -0.00117 0.00000 -0.00117 -1.04512

D229 -3.11493 0.00000 0.00011 0.00000 0.00011 -3.11482

D230 1.04395 0.00011 0.00117 0.00000 0.00117 1.04512

D231 -1.09893 0.00011 -0.00052 0.00000 -0.00052 -1.09945

D232 3.11493 0.00000 -0.00011 0.00000 -0.00011 3.11482

Item Value Threshold Converged?

Maximum Force 0.007446 0.000450 NO

RMS Force 0.001761 0.000300 NO

Maximum Displacement 0.628981 0.001800 NO

RMS Displacement 0.169786 0.001200 NO

Predicted change in Energy=-1.106313D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 00:15:21 2019, MaxMem= 1342177280 cpu: 12.8

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

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=3 Diff= 2.86D-06

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 -1.123444 2.803207 0.008126

2 7 0 0.000148 2.043878 -0.148286

3 6 0 1.123645 2.803244 0.008094

4 6 0 0.713444 4.158791 0.306250

5 6 0 -0.713296 4.158761 0.306270

6 7 0 2.410449 2.383947 -0.099236

7 6 0 2.794472 1.132601 -0.173491

8 7 0 2.020486 0.000177 -0.092142

9 6 0 2.794447 -1.132337 -0.173499

10 6 0 4.200577 -0.704635 -0.346976

11 6 0 4.200597 0.704860 -0.346960

12 7 0 -2.410340 2.383928 -0.099190

13 6 0 -4.200677 0.704860 -0.346938

14 6 0 -4.200650 -0.704670 -0.346954

15 6 0 -2.794513 -1.132367 -0.173443

16 7 0 -2.020698 0.000169 -0.092075

17 6 0 -2.794548 1.132608 -0.173435

18 7 0 -2.410335 -2.383771 -0.099191

19 7 0 0.000157 -2.044134 -0.148297

20 6 0 -1.123463 -2.803297 0.008138

21 6 0 -0.713303 -4.158855 0.306310

22 6 0 0.713487 -4.158880 0.306291

23 6 0 1.123688 -2.803324 0.008106

24 7 0 2.410465 -2.383771 -0.099238

25 30 0 -0.000263 -0.000338 -0.249417

26 6 0 -5.386254 1.432984 -0.487684

27 6 0 -6.576759 0.695454 -0.622155

28 6 0 -6.576733 -0.695349 -0.622175

29 6 0 -5.386201 -1.432837 -0.487722

30 6 0 1.435103 -5.337914 0.572253

31 6 0 0.700881 -6.504393 0.814710

32 6 0 -0.700768 -6.504370 0.814727

33 6 0 -1.434956 -5.337867 0.572290

34 6 0 5.386178 1.433003 -0.487648

35 6 0 6.576690 0.695482 -0.622067

36 6 0 6.576671 -0.695321 -0.622087

37 6 0 5.386138 -1.432810 -0.487686

38 6 0 -1.434972 5.337772 0.572209

39 6 0 -0.700797 6.504286 0.814618

40 6 0 0.700854 6.504315 0.814601

41 6 0 1.435073 5.337831 0.572172

42 1 0 7.523397 1.205764 -0.736515

43 1 0 7.523363 -1.205627 -0.736550

44 1 0 1.208501 7.436456 1.021785

45 1 0 -1.208478 7.436406 1.021815

46 1 0 -7.523463 1.205730 -0.736653

47 1 0 -7.523418 -1.205657 -0.736688

48 1 0 -1.208443 -7.436488 1.021950

49 1 0 1.208529 -7.436529 1.021921

50 8 0 2.783527 5.265288 0.588357

51 8 0 -2.783422 5.265171 0.588428

52 8 0 5.321512 2.780708 -0.499381

53 8 0 5.321436 -2.780512 -0.499460

54 8 0 2.783555 -5.265369 0.588446

55 8 0 -2.783405 -5.265274 0.588516

56 8 0 -5.321477 -2.780537 -0.499513

57 8 0 -5.321578 2.780688 -0.499435

58 6 0 3.530212 6.462678 0.792603

59 1 0 3.327457 6.901311 1.773684

60 1 0 3.323136 7.199818 0.011531

61 1 0 4.575833 6.165963 0.741204

62 6 0 6.536222 3.524219 -0.582198

63 1 0 7.064302 3.329575 -1.519735

64 1 0 7.196586 3.307102 0.262143

65 1 0 6.238939 4.570267 -0.548092

66 6 0 6.536127 -3.524051 -0.582302

67 1 0 7.196498 -3.306975 0.262044

68 1 0 7.064210 -3.329391 -1.519835

69 1 0 6.238817 -4.570092 -0.548227

70 6 0 -3.530153 6.462530 0.792684

71 1 0 -3.323128 7.199673 0.011602

72 1 0 -3.327393 6.901178 1.773757

73 1 0 -4.575763 6.165769 0.741312

74 6 0 -6.536279 3.524207 -0.582334

75 1 0 -7.196693 3.307107 0.261972

76 1 0 -7.064304 3.329550 -1.519899

77 1 0 -6.238992 4.570254 -0.548228

78 6 0 -6.536154 -3.524095 -0.582438

79 1 0 -7.064183 -3.329427 -1.519999

80 1 0 -7.196576 -3.307041 0.261873

81 1 0 -6.238831 -4.570133 -0.548363

82 6 0 -3.530126 -6.462636 0.792806

83 1 0 -3.327354 -6.901258 1.773889

84 1 0 -3.323100 -7.199794 0.011740

85 1 0 -4.575740 -6.165886 0.741436

86 6 0 3.530240 -6.462755 0.792725

87 1 0 3.323169 -7.199912 0.011669

88 1 0 3.327476 -6.901364 1.773815

89 1 0 4.575863 -6.166043 0.741328

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

Rotational constants (GHZ): 0.0447839 0.0440232 0.0226200

Leave Link 202 at Sat Jul 6 00:15:22 2019, MaxMem= 1342177280 cpu: 0.5

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

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

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8046.5068548788 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= 89 NActive= 89 NUniq= 89 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= -0.2279813064 Hartrees.

Nuclear repulsion after empirical dispersion term = 8046.2788735724 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6466

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.34D-10

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 373

GePol: Fraction of low-weight points (<1% of avg) = 5.77%

GePol: Cavity surface area = 700.047 Ang\*\*2

GePol: Cavity volume = 799.316 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0088753100 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8046.2699982623 Hartrees.

Leave Link 301 at Sat Jul 6 00:15:22 2019, MaxMem= 1342177280 cpu: 1.6

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

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

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

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44328 LenP2D= 111359.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.84D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 00:15:26 2019, MaxMem= 1342177280 cpu: 41.6

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

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 00:15:27 2019, MaxMem= 1342177280 cpu: 2.5

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

Lowest energy guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000002 0.000001 -0.000001 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000001 0.000001 0.000001 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 3.48D-01

Max alpha theta= 4.939 degrees.

Max beta theta= 4.925 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0169 S= 1.0056

Leave Link 401 at Sat Jul 6 00:15:37 2019, MaxMem= 1342177280 cpu: 123.6

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 125427468.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.18D-14 for 6446.

Iteration 1 A\*A^-1 deviation from orthogonality is 8.13D-15 for 2857 1078.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.18D-14 for 6446.

Iteration 1 A^-1\*A deviation from orthogonality is 1.14D-10 for 6447 6409.

Iteration 2 A\*A^-1 deviation from unit magnitude is 1.54D-14 for 494.

Iteration 2 A\*A^-1 deviation from orthogonality is 1.24D-14 for 2575 482.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.55D-15 for 1024.

Iteration 2 A^-1\*A deviation from orthogonality is 6.77D-16 for 6433 2108.

E= -2649.79389096029

DIIS: error= 2.62D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79389096029 IErMin= 1 ErrMin= 2.62D-04

ErrMax= 2.62D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.57D-04 BMatP= 1.57D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.62D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 17.533 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 1036280 IAlg= 4 N= 1128 NDim= 1128 NE2= 1186103 trying DSYEV.

Gap= 17.530 Goal= None Shift= 0.000

RMSDP=1.91D-05 MaxDP=9.57D-04 OVMax= 1.25D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.88D-05 CP: 1.00D+00

E= -2649.79393289712 Delta-E= -0.000041936828 Rises=F Damp=F

DIIS: error= 1.56D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79393289712 IErMin= 2 ErrMin= 1.56D-04

ErrMax= 1.56D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.89D-05 BMatP= 1.57D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.56D-03

Coeff-Com: 0.252D+00 0.748D+00

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

Coeff: 0.251D+00 0.749D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=5.09D-06 MaxDP=2.76D-04 DE=-4.19D-05 OVMax= 1.16D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.80D-06 CP: 1.00D+00 9.23D-01

E= -2649.79393428491 Delta-E= -0.000001387798 Rises=F Damp=F

DIIS: error= 1.31D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79393428491 IErMin= 3 ErrMin= 1.31D-04

ErrMax= 1.31D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.99D-05 BMatP= 3.89D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.31D-03

Coeff-Com: -0.603D-02 0.467D+00 0.539D+00

Coeff-En: 0.000D+00 0.445D+00 0.555D+00

Coeff: -0.603D-02 0.467D+00 0.539D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.54D-06 MaxDP=1.99D-04 DE=-1.39D-06 OVMax= 7.51D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.22D-06 CP: 1.00D+00 9.61D-01 5.66D-01

E= -2649.79393882901 Delta-E= -0.000004544094 Rises=F Damp=F

DIIS: error= 2.14D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79393882901 IErMin= 4 ErrMin= 2.14D-05

ErrMax= 2.14D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-06 BMatP= 2.99D-05

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

Coeff-Com: -0.967D-02 0.229D+00 0.292D+00 0.489D+00

Coeff: -0.967D-02 0.229D+00 0.292D+00 0.489D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=5.68D-07 MaxDP=4.58D-05 DE=-4.54D-06 OVMax= 1.47D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.12D-07 CP: 1.00D+00 9.62D-01 6.01D-01 6.37D-01

E= -2649.79393902066 Delta-E= -0.000000191654 Rises=F Damp=F

DIIS: error= 5.09D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79393902066 IErMin= 5 ErrMin= 5.09D-06

ErrMax= 5.09D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.29D-08 BMatP= 1.04D-06

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

Coeff-Com: -0.392D-02 0.604D-01 0.805D-01 0.247D+00 0.616D+00

Coeff: -0.392D-02 0.604D-01 0.805D-01 0.247D+00 0.616D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.35D-07 MaxDP=7.52D-06 DE=-1.92D-07 OVMax= 3.63D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.42D-08 CP: 1.00D+00 9.62D-01 5.94D-01 6.81D-01 7.72D-01

E= -2649.79393903430 Delta-E= -0.000000013639 Rises=F Damp=F

DIIS: error= 1.32D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79393903430 IErMin= 6 ErrMin= 1.32D-06

ErrMax= 1.32D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.70D-09 BMatP= 7.29D-08

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

Coeff-Com: -0.135D-02 0.183D-01 0.240D-01 0.963D-01 0.306D+00 0.557D+00

Coeff: -0.135D-02 0.183D-01 0.240D-01 0.963D-01 0.306D+00 0.557D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.55D-08 MaxDP=4.25D-06 DE=-1.36D-08 OVMax= 1.65D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.82D-08 CP: 1.00D+00 9.63D-01 5.93D-01 6.88D-01 8.04D-01

CP: 7.88D-01

E= -2649.79393903530 Delta-E= -0.000000001000 Rises=F Damp=F

DIIS: error= 7.34D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79393903530 IErMin= 7 ErrMin= 7.34D-07

ErrMax= 7.34D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.25D-09 BMatP= 4.70D-09

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

Coeff-Com: 0.224D-04-0.254D-02-0.385D-02 0.372D-02 0.548D-01 0.352D+00

Coeff-Com: 0.596D+00

Coeff: 0.224D-04-0.254D-02-0.385D-02 0.372D-02 0.548D-01 0.352D+00

Coeff: 0.596D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.04D-08 MaxDP=1.71D-06 DE=-1.00D-09 OVMax= 7.64D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.71D-08 CP: 1.00D+00 9.62D-01 5.93D-01 6.91D-01 8.16D-01

CP: 8.62D-01 8.37D-01

E= -2649.79393903548 Delta-E= -0.000000000178 Rises=F Damp=F

DIIS: error= 2.69D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.79393903548 IErMin= 8 ErrMin= 2.69D-07

ErrMax= 2.69D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.49D-10 BMatP= 1.25D-09

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

Coeff-Com: 0.163D-03-0.371D-02-0.510D-02-0.107D-01-0.121D-01 0.102D+00

Coeff-Com: 0.303D+00 0.626D+00

Coeff: 0.163D-03-0.371D-02-0.510D-02-0.107D-01-0.121D-01 0.102D+00

Coeff: 0.303D+00 0.626D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=9.61D-09 MaxDP=7.01D-07 DE=-1.78D-10 OVMax= 7.46D-06

Error on total polarization charges = 0.07292

SCF Done: E(UB3LYP) = -2649.79393904 A.U. after 8 cycles

NFock= 8 Conv=0.96D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0168 S= 1.0056

<L.S>= 0.000000000000E+00

KE= 2.690180776849D+03 PE=-2.237130005305D+04 EE= 8.985055338908D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.57

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0168, after 2.0002

Leave Link 502 at Sat Jul 6 00:22:37 2019, MaxMem= 1342177280 cpu: 4929.1

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

Compute integral first derivatives.

... and contract with generalized density number 0.

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

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44328 LenP2D= 111359.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 287

Leave Link 701 at Sat Jul 6 00:22:56 2019, MaxMem= 1342177280 cpu: 220.9

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

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

Leave Link 702 at Sat Jul 6 00:22:56 2019, MaxMem= 1342177280 cpu: 0.2

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

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 00:24:27 2019, MaxMem= 1342177280 cpu: 1098.4

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

Dipole =-7.77640472D-04-1.17720766D-03 7.79520034D-02

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.001661799 -0.001029564 0.002123485

2 7 -0.000056034 -0.000389362 -0.001298351

3 6 0.001627796 -0.001002715 0.002129732

4 6 -0.000543056 0.000800516 -0.000669612

5 6 0.000543485 0.000796928 -0.000670167

6 7 -0.002557997 0.001949512 0.000165460

7 6 0.001919776 -0.002851798 -0.001842707

8 7 0.000163755 -0.000066362 0.004972382

9 6 0.001886352 0.002812664 -0.001836188

10 6 -0.001127315 -0.000200276 0.000578896

11 6 -0.001126670 0.000200373 0.000578522

12 7 0.002588867 0.001940282 0.000164539

13 6 0.001127630 0.000191352 0.000579855

14 6 0.001128285 -0.000191263 0.000580230

15 6 -0.001891474 0.002767955 -0.001838819

16 7 -0.000105150 -0.000066530 0.004993418

17 6 -0.001925078 -0.002807249 -0.001845297

18 7 0.002603979 -0.001907376 0.000167039

19 7 -0.000056190 0.000459378 -0.001295651

20 6 -0.001705915 0.001022987 0.002125667

21 6 0.000550748 -0.000793328 -0.000670097

22 6 -0.000550352 -0.000796934 -0.000669529

23 6 0.001671804 0.000996054 0.002131924

24 7 -0.002573003 -0.001916778 0.000167918

25 30 0.000066779 0.000080093 -0.009156016

26 6 -0.001192991 -0.000545102 -0.000527228

27 6 0.000495416 0.001273767 0.000127624

28 6 0.000495405 -0.001273620 0.000127665

29 6 -0.001193029 0.000544695 -0.000527281

30 6 -0.000126553 -0.000154394 0.000305798

31 6 0.000378831 0.000319207 -0.000005735

32 6 -0.000378855 0.000319818 -0.000005827

33 6 0.000125958 -0.000155764 0.000306105

34 6 0.001192021 -0.000544413 -0.000526206

35 6 -0.000494950 0.001274039 0.000127581

36 6 -0.000494927 -0.001273879 0.000127630

37 6 0.001192054 0.000544012 -0.000526259

38 6 0.000124817 0.000155394 0.000306241

39 6 -0.000380354 -0.000320075 -0.000006045

40 6 0.000380319 -0.000319463 -0.000005954

41 6 -0.000125421 0.000154027 0.000305933

42 1 0.000255746 0.000129266 -0.000019554

43 1 0.000255719 -0.000129181 -0.000019554

44 1 0.000221452 0.000295156 -0.000003349

45 1 -0.000221363 0.000295225 -0.000003322

46 1 -0.000255673 0.000129415 -0.000019423

47 1 -0.000255668 -0.000129335 -0.000019421

48 1 -0.000221391 -0.000295008 -0.000003401

49 1 0.000221471 -0.000294952 -0.000003422

50 8 -0.000369783 0.000995234 -0.000138930

51 8 0.000370967 0.000995462 -0.000138011

52 8 0.000625606 -0.000342613 0.000128098

53 8 0.000626353 0.000343565 0.000126956

54 8 -0.000369979 -0.000994372 -0.000139061

55 8 0.000371164 -0.000994567 -0.000138159

56 8 -0.000626030 0.000342831 0.000127406

57 8 -0.000625265 -0.000341885 0.000128577

58 6 -0.000561124 0.000156296 -0.000007944

59 1 -0.000222123 -0.000025966 0.000281038

60 1 -0.000060857 0.000096194 -0.000075945

61 1 0.000186216 -0.000047173 -0.000073686

62 6 0.000123923 -0.000416264 0.000037203

63 1 0.000080956 -0.000127636 -0.000277202

64 1 0.000017534 -0.000152738 0.000267396

65 1 -0.000064038 0.000203172 0.000064810

66 6 0.000124110 0.000416149 0.000037284

67 1 0.000017539 0.000152739 0.000267386

68 1 0.000080929 0.000127607 -0.000277165

69 1 -0.000063974 -0.000203149 0.000064851

70 6 0.000561385 0.000156096 -0.000008040

71 1 0.000060670 0.000096309 -0.000075917

72 1 0.000222107 -0.000025882 0.000281113

73 1 -0.000186032 -0.000047125 -0.000073655

74 6 -0.000124492 -0.000416202 0.000037021

75 1 -0.000017313 -0.000152793 0.000267633

76 1 -0.000080822 -0.000127737 -0.000277179

77 1 0.000063875 0.000203044 0.000064832

78 6 -0.000124677 0.000416071 0.000037133

79 1 -0.000080800 0.000127716 -0.000277144

80 1 -0.000017312 0.000152816 0.000267623

81 1 0.000063790 -0.000203017 0.000064879

82 6 0.000560628 -0.000156812 -0.000007895

83 1 0.000222121 0.000026089 0.000281030

84 1 0.000060660 -0.000096168 -0.000075807

85 1 -0.000185838 0.000047083 -0.000073519

86 6 -0.000560390 -0.000156987 -0.000007808

87 1 -0.000060822 -0.000096068 -0.000075835

88 1 -0.000222138 0.000026165 0.000280963

89 1 0.000186017 0.000047121 -0.000073559

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

Cartesian Forces: Max 0.009156016 RMS 0.001081823

Leave Link 716 at Sat Jul 6 00:24:27 2019, MaxMem= 1342177280 cpu: 0.6

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.002860270 RMS 0.000749105

Search for a local minimum.

Step number 7 out of a maximum of 518

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

RMS Force = .74911D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 2 3 4 6

5 7

ITU= 0 0 1 1 1 1 0

Use linear search instead of GDIIS.

Eigenvalues --- -0.52908 0.00008 0.00685 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01316 0.01316

Eigenvalues --- 0.01318 0.01549 0.01570 0.01571 0.01581

Eigenvalues --- 0.01600 0.01617 0.01621 0.01643 0.01707

Eigenvalues --- 0.01710 0.01713 0.01716 0.01832 0.01834

Eigenvalues --- 0.01873 0.01887 0.01919 0.01923 0.01930

Eigenvalues --- 0.01943 0.01968 0.02009 0.02015 0.02020

Eigenvalues --- 0.02022 0.02028 0.02040 0.02049 0.02053

Eigenvalues --- 0.02053 0.02053 0.02053 0.02057 0.02057

Eigenvalues --- 0.02057 0.02057 0.02067 0.02067 0.02067

Eigenvalues --- 0.02068 0.02071 0.02071 0.02071 0.02071

Eigenvalues --- 0.02084 0.02084 0.02107 0.02152 0.02260

Eigenvalues --- 0.02260 0.02260 0.02260 0.02260 0.02260

Eigenvalues --- 0.02260 0.02306 0.02343 0.02350 0.02365

Eigenvalues --- 0.02583 0.09974 0.09974 0.09974 0.09982

Eigenvalues --- 0.09982 0.09982 0.09985 0.09989 0.10651

Eigenvalues --- 0.10653 0.10653 0.10653 0.10655 0.10655

Eigenvalues --- 0.10655 0.10657 0.13467 0.13512 0.15166

Eigenvalues --- 0.15748 0.15994 0.15998 0.15998 0.15998

Eigenvalues --- 0.15999 0.15999 0.15999 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16003

Eigenvalues --- 0.16022 0.16057 0.19085 0.21477 0.21697

Eigenvalues --- 0.22178 0.22473 0.22473 0.22474 0.22475

Eigenvalues --- 0.24113 0.24286 0.24415 0.24469 0.24509

Eigenvalues --- 0.24515 0.24552 0.24680 0.24710 0.24847

Eigenvalues --- 0.24856 0.24914 0.24995 0.24997 0.24997

Eigenvalues --- 0.24997 0.24997 0.24998 0.24998 0.24998

Eigenvalues --- 0.24998 0.24998 0.24998 0.24999 0.24999

Eigenvalues --- 0.24999 0.24999 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25031 0.25673

Eigenvalues --- 0.31776 0.33088 0.33633 0.33639 0.33682

Eigenvalues --- 0.33720 0.34052 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34063 0.34063 0.34067 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34081

Eigenvalues --- 0.34081 0.34155 0.34621 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34686 0.34686 0.34686

Eigenvalues --- 0.34911 0.34958 0.35405 0.35525 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35632 0.35632

Eigenvalues --- 0.35657 0.37100 0.37133 0.37163 0.40808

Eigenvalues --- 0.41133 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41215 0.41215 0.41234 0.41416 0.41416

Eigenvalues --- 0.41418 0.41420 0.41422 0.41708 0.42457

Eigenvalues --- 0.42482 0.43812 0.44548 0.44570 0.44784

Eigenvalues --- 0.44843 0.44909 0.44998 0.44999 0.45000

Eigenvalues --- 0.45002 0.45167 0.45365 0.45366 0.46405

Eigenvalues --- 0.47319 0.47404 0.47740 0.48659 0.49244

Eigenvalues --- 0.49306 0.49849 0.53338 0.53554 0.53554

Eigenvalues --- 0.53554 0.53554 0.53554 0.53554 0.54681

Eigenvalues --- 0.54974 0.55134 0.56073 0.57380 0.57431

Eigenvalues --- 0.57564

Eigenvalue 1 is -5.29D-01 should be greater than 0.000000 Eigenvector:

R30 R15 R11 R34 R5

1 -0.23245 -0.22561 -0.19734 -0.19566 -0.18806

R21 R17 R28 A117 A118

1 -0.18484 -0.17841 -0.16589 0.15288 0.15287

RFO step: Lambda=-5.29496913D-01 EMin=-5.29081166D-01

I= 1 Eig= -5.29D-01 Dot1= -8.90D-03

I= 1 Stepn= -6.00D-01 RXN= 6.00D-01 EDone=F

Mixed 1 eigenvectors in step. Raw Step.Grad= 8.90D-03.

RFO eigenvector is Hessian eigenvector with negative curvature.

Taking step of 6.00D-01 in eigenvector direction(s). Step.Grad= 4.12D-04.

Skip linear search -- no minimum in search direction.

Maximum step size ( 0.457) exceeded in Quadratic search.

-- Step size not scaled.

Iteration 1 RMS(Cart)= 0.20591049 RMS(Int)= 0.00560085

Iteration 2 RMS(Cart)= 0.01518042 RMS(Int)= 0.00022784

Iteration 3 RMS(Cart)= 0.00012666 RMS(Int)= 0.00022514

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00022514

ITry= 1 IFail=0 DXMaxC= 9.35D-01 DCOld= 1.00D+10 DXMaxT= 4.57D-01 DXLimC= 3.00D+00 Rises=F

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

(Linear) (Quad) (Total)

R1 2.57967 0.00110 0.00000 0.01683 0.01671 2.59638

R2 2.73497 0.00193 0.00000 0.03657 0.03651 2.77149

R3 2.56573 -0.00073 0.00000 0.01596 0.01534 2.58107

R4 2.57955 0.00111 0.00000 0.02200 0.02179 2.60135

R5 3.86773 0.00118 0.00000 0.11283 0.11348 3.98121

R6 2.73500 0.00193 0.00000 0.03605 0.03601 2.77100

R7 2.56557 -0.00068 0.00000 0.02741 0.02663 2.59220

R8 2.69615 0.00014 0.00000 0.05209 0.05203 2.74818

R9 2.66015 0.00142 0.00000 0.02724 0.02730 2.68746

R10 2.66016 0.00142 0.00000 0.02726 0.02732 2.68748

R11 2.47753 0.00272 0.00000 0.11841 0.11784 2.59537

R12 2.59661 0.00025 0.00000 -0.01169 -0.01132 2.58529

R13 2.79669 0.00047 0.00000 0.03088 0.03080 2.82749

R14 2.59672 0.00024 0.00000 -0.01708 -0.01670 2.58002

R15 3.83021 0.00200 0.00000 0.13536 0.13662 3.96683

R16 2.79668 0.00048 0.00000 0.03139 0.03130 2.82798

R17 2.47766 0.00266 0.00000 0.10704 0.10662 2.58428

R18 2.66356 0.00028 0.00000 -0.00064 -0.00082 2.66274

R19 2.64264 0.00164 0.00000 0.04617 0.04624 2.68888

R20 2.64264 0.00164 0.00000 0.04614 0.04621 2.68884

R21 2.47758 0.00269 0.00000 0.11090 0.11046 2.58804

R22 2.66363 0.00027 0.00000 -0.00421 -0.00430 2.65932

R23 2.79671 0.00047 0.00000 0.02992 0.02986 2.82657

R24 2.64262 0.00164 0.00000 0.04643 0.04649 2.68911

R25 2.79670 0.00048 0.00000 0.03043 0.03036 2.82706

R26 2.64263 0.00165 0.00000 0.04646 0.04652 2.68915

R27 2.59660 0.00026 0.00000 -0.01127 -0.01099 2.58561

R28 2.47772 0.00263 0.00000 0.09953 0.09922 2.57694

R29 2.59649 0.00028 0.00000 -0.00587 -0.00559 2.59089

R30 3.82963 0.00198 0.00000 0.13947 0.14042 3.97004

R31 2.56583 -0.00077 0.00000 0.00813 0.00765 2.57348

R32 2.57954 0.00112 0.00000 0.02226 0.02210 2.60164

R33 2.57943 0.00113 0.00000 0.02744 0.02719 2.60662

R34 3.86694 0.00116 0.00000 0.11739 0.11783 3.98477

R35 2.73500 0.00193 0.00000 0.03555 0.03551 2.77051

R36 2.69624 0.00013 0.00000 0.04846 0.04848 2.74472

R37 2.66015 0.00142 0.00000 0.02746 0.02752 2.68767

R38 2.73502 0.00193 0.00000 0.03504 0.03501 2.77003

R39 2.66015 0.00142 0.00000 0.02744 0.02750 2.68765

R40 2.56568 -0.00072 0.00000 0.01959 0.01896 2.58463

R41 2.65863 -0.00109 0.00000 -0.00860 -0.00866 2.64997

R42 2.54982 -0.00087 0.00000 -0.01416 -0.01416 2.53566

R43 2.62824 -0.00027 0.00000 0.02411 0.02399 2.65223

R44 2.04382 0.00029 0.00000 0.01671 0.01671 2.06053

R45 2.65863 -0.00109 0.00000 -0.00856 -0.00862 2.65001

R46 2.04382 0.00029 0.00000 0.01671 0.01671 2.06053

R47 2.54982 -0.00088 0.00000 -0.01416 -0.01416 2.53566

R48 2.64463 -0.00091 0.00000 -0.01876 -0.01882 2.62581

R49 2.55207 -0.00109 0.00000 -0.04372 -0.04372 2.50835

R50 2.64873 -0.00109 0.00000 -0.01856 -0.01868 2.63006

R51 2.04363 0.00036 0.00000 0.01880 0.01880 2.06243

R52 2.64463 -0.00091 0.00000 -0.01871 -0.01877 2.62585

R53 2.04363 0.00036 0.00000 0.01880 0.01880 2.06243

R54 2.55207 -0.00109 0.00000 -0.04375 -0.04375 2.50833

R55 2.65863 -0.00109 0.00000 -0.00833 -0.00840 2.65023

R56 2.54982 -0.00087 0.00000 -0.01417 -0.01417 2.53565

R57 2.62824 -0.00027 0.00000 0.02456 0.02443 2.65267

R58 2.04382 0.00029 0.00000 0.01671 0.01671 2.06053

R59 2.65863 -0.00109 0.00000 -0.00829 -0.00836 2.65027

R60 2.04382 0.00029 0.00000 0.01671 0.01671 2.06053

R61 2.54982 -0.00088 0.00000 -0.01416 -0.01416 2.53565

R62 2.64462 -0.00091 0.00000 -0.01849 -0.01856 2.62607

R63 2.55208 -0.00109 0.00000 -0.04376 -0.04376 2.50831

R64 2.64874 -0.00108 0.00000 -0.01815 -0.01828 2.63046

R65 2.04363 0.00036 0.00000 0.01880 0.01880 2.06244

R66 2.64463 -0.00091 0.00000 -0.01853 -0.01860 2.62603

R67 2.04363 0.00036 0.00000 0.01881 0.01881 2.06244

R68 2.55208 -0.00109 0.00000 -0.04373 -0.04373 2.50834

R69 2.69443 -0.00018 0.00000 -0.00625 -0.00625 2.68819

R70 2.69443 -0.00018 0.00000 -0.00624 -0.00624 2.68819

R71 2.69588 -0.00013 0.00000 -0.00862 -0.00862 2.68727

R72 2.69588 -0.00013 0.00000 -0.00861 -0.00861 2.68727

R73 2.69444 -0.00018 0.00000 -0.00624 -0.00624 2.68819

R74 2.69443 -0.00018 0.00000 -0.00624 -0.00624 2.68819

R75 2.69589 -0.00013 0.00000 -0.00862 -0.00862 2.68726

R76 2.69589 -0.00013 0.00000 -0.00863 -0.00863 2.68726

R77 2.06666 0.00028 0.00000 0.02093 0.02093 2.08759

R78 2.06692 0.00013 0.00000 0.01799 0.01799 2.08491

R79 2.05625 0.00020 0.00000 0.01481 0.01481 2.07106

R80 2.06641 0.00030 0.00000 0.02172 0.02172 2.08812

R81 2.06675 0.00025 0.00000 0.02132 0.02132 2.08807

R82 2.05603 0.00021 0.00000 0.01641 0.01641 2.07244

R83 2.06675 0.00025 0.00000 0.02132 0.02132 2.08807

R84 2.06641 0.00030 0.00000 0.02172 0.02172 2.08812

R85 2.05603 0.00021 0.00000 0.01641 0.01641 2.07244

R86 2.06692 0.00013 0.00000 0.01799 0.01799 2.08491

R87 2.06666 0.00028 0.00000 0.02093 0.02093 2.08760

R88 2.05625 0.00020 0.00000 0.01480 0.01480 2.07105

R89 2.06675 0.00025 0.00000 0.02132 0.02132 2.08807

R90 2.06641 0.00030 0.00000 0.02172 0.02172 2.08812

R91 2.05603 0.00021 0.00000 0.01641 0.01641 2.07244

R92 2.06641 0.00030 0.00000 0.02172 0.02172 2.08812

R93 2.06675 0.00025 0.00000 0.02132 0.02132 2.08807

R94 2.05603 0.00021 0.00000 0.01641 0.01641 2.07244

R95 2.06666 0.00028 0.00000 0.02093 0.02093 2.08759

R96 2.06692 0.00013 0.00000 0.01799 0.01799 2.08491

R97 2.05625 0.00019 0.00000 0.01480 0.01480 2.07105

R98 2.06692 0.00013 0.00000 0.01799 0.01799 2.08491

R99 2.06666 0.00028 0.00000 0.02093 0.02093 2.08759

R100 2.05625 0.00020 0.00000 0.01480 0.01480 2.07105

A1 1.88740 0.00029 0.00000 0.00806 0.00841 1.89580

A2 2.21344 -0.00032 0.00000 -0.01854 -0.01874 2.19470

A3 2.18233 0.00004 0.00000 0.01048 0.01033 2.19267

A4 1.93358 -0.00050 0.00000 0.00031 -0.00030 1.93328

A5 2.16646 0.00023 0.00000 0.00463 0.00471 2.17118

A6 2.16692 0.00021 0.00000 -0.00677 -0.00629 2.16064

A7 1.88742 0.00029 0.00000 0.00716 0.00753 1.89494

A8 2.21335 -0.00033 0.00000 -0.01739 -0.01760 2.19575

A9 2.18241 0.00004 0.00000 0.01023 0.01008 2.19248

A10 1.85814 -0.00003 0.00000 -0.00787 -0.00796 1.85019

A11 2.31596 0.00087 0.00000 0.03247 0.03235 2.34831

A12 2.10906 -0.00084 0.00000 -0.02464 -0.02445 2.08461

A13 1.85814 -0.00003 0.00000 -0.00748 -0.00758 1.85056

A14 2.31596 0.00087 0.00000 0.03232 0.03221 2.34817

A15 2.10906 -0.00084 0.00000 -0.02488 -0.02469 2.08438

A16 2.18570 0.00089 0.00000 0.04792 0.04738 2.23309

A17 2.23733 -0.00103 0.00000 -0.02990 -0.02969 2.20764

A18 2.16615 0.00059 0.00000 0.02636 0.02570 2.19185

A19 1.87961 0.00043 0.00000 0.00339 0.00378 1.88338

A20 1.93742 -0.00052 0.00000 0.00489 0.00409 1.94151

A21 2.16181 0.00019 0.00000 -0.01061 -0.01012 2.15169

A22 2.16125 0.00021 0.00000 0.00108 0.00111 2.16236

A23 1.87958 0.00043 0.00000 0.00435 0.00475 1.88433

A24 2.23743 -0.00103 0.00000 -0.03114 -0.03097 2.20646

A25 2.16608 0.00059 0.00000 0.02664 0.02602 2.19210

A26 1.86399 -0.00017 0.00000 -0.00614 -0.00614 1.85785

A27 2.30072 0.00105 0.00000 0.02161 0.02145 2.32216

A28 2.11847 -0.00088 0.00000 -0.01549 -0.01534 2.10313

A29 1.86399 -0.00017 0.00000 -0.00651 -0.00650 1.85749

A30 2.30072 0.00105 0.00000 0.02177 0.02160 2.32231

A31 2.11847 -0.00088 0.00000 -0.01528 -0.01513 2.10334

A32 2.18581 0.00088 0.00000 0.04407 0.04359 2.22940

A33 1.86399 -0.00017 0.00000 -0.00583 -0.00582 1.85817

A34 2.11846 -0.00088 0.00000 -0.01507 -0.01493 2.10353

A35 2.30073 0.00105 0.00000 0.02089 0.02072 2.32145

A36 1.86399 -0.00016 0.00000 -0.00546 -0.00546 1.85853

A37 2.11846 -0.00088 0.00000 -0.01529 -0.01514 2.10331

A38 2.30073 0.00105 0.00000 0.02073 0.02057 2.32129

A39 1.87949 0.00043 0.00000 0.00710 0.00740 1.88690

A40 2.16622 0.00058 0.00000 0.02197 0.02151 2.18773

A41 2.23738 -0.00102 0.00000 -0.02921 -0.02911 2.20826

A42 1.93760 -0.00053 0.00000 -0.00196 -0.00258 1.93502

A43 2.16115 0.00021 0.00000 0.00447 0.00440 2.16555

A44 2.16171 0.00020 0.00000 -0.00723 -0.00683 2.15487

A45 2.16629 0.00059 0.00000 0.02169 0.02119 2.18749

A46 2.23728 -0.00103 0.00000 -0.02797 -0.02783 2.20945

A47 1.87952 0.00044 0.00000 0.00613 0.00642 1.88594

A48 2.18595 0.00087 0.00000 0.04052 0.04015 2.22610

A49 1.93380 -0.00052 0.00000 -0.00651 -0.00692 1.92688

A50 2.16635 0.00024 0.00000 0.00802 0.00801 2.17436

A51 2.16681 0.00022 0.00000 -0.00338 -0.00300 2.16381

A52 2.21337 -0.00032 0.00000 -0.01686 -0.01710 2.19628

A53 2.18252 0.00003 0.00000 0.00599 0.00597 2.18849

A54 1.88728 0.00029 0.00000 0.01087 0.01113 1.89841

A55 1.85814 -0.00002 0.00000 -0.00688 -0.00698 1.85116

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D158 0.00894 -0.00019 0.00000 -0.00365 -0.00359 0.00535

D159 3.09291 -0.00033 0.00000 -0.00707 -0.00703 3.08588

D160 -0.06041 -0.00004 0.00000 -0.00310 -0.00313 -0.06354

D161 -0.01641 -0.00001 0.00000 -0.00231 -0.00234 -0.01874

D162 3.13933 -0.00007 0.00000 -0.00272 -0.00270 3.13663

D163 3.11406 0.00006 0.00000 -0.00066 -0.00075 3.11331

D164 -0.01339 0.00001 0.00000 -0.00107 -0.00111 -0.01450

D165 -3.08986 -0.00027 0.00000 -0.00418 -0.00420 -3.09406

D166 0.06291 -0.00034 0.00000 -0.00558 -0.00556 0.05735

D167 0.00000 0.00000 0.00000 0.00001 0.00002 0.00002

D168 -3.12777 -0.00006 0.00000 -0.00022 -0.00018 -3.12795

D169 3.12777 0.00006 0.00000 0.00024 0.00021 3.12797

D170 0.00000 0.00000 0.00000 0.00001 0.00001 0.00001

D171 0.01641 0.00001 0.00000 0.00233 0.00236 0.01876

D172 -3.11406 -0.00006 0.00000 0.00067 0.00075 -3.11331

D173 -3.13933 0.00007 0.00000 0.00274 0.00273 -3.13660

D174 0.01339 -0.00001 0.00000 0.00108 0.00113 0.01452

D175 3.08985 0.00027 0.00000 0.00416 0.00419 3.09404

D176 -0.06291 0.00034 0.00000 0.00558 0.00556 -0.05736

D177 0.00546 -0.00001 0.00000 -0.00035 -0.00037 0.00509

D178 3.13900 0.00010 0.00000 0.00032 0.00028 3.13928

D179 -3.12461 -0.00030 0.00000 -0.00433 -0.00426 -3.12887

D180 0.00893 -0.00019 0.00000 -0.00366 -0.00360 0.00533

D181 3.09289 -0.00033 0.00000 -0.00708 -0.00705 3.08584

D182 -0.06041 -0.00004 0.00000 -0.00312 -0.00316 -0.06356

D183 0.00000 0.00000 0.00000 -0.00002 -0.00002 -0.00002

D184 3.13370 0.00011 0.00000 0.00059 0.00057 3.13427

D185 -3.13370 -0.00011 0.00000 -0.00062 -0.00060 -3.13431

D186 0.00000 0.00000 0.00000 -0.00001 -0.00001 -0.00001

D187 -0.00546 0.00001 0.00000 0.00033 0.00035 -0.00511

D188 3.12461 0.00030 0.00000 0.00432 0.00424 3.12885

D189 -3.13900 -0.00010 0.00000 -0.00035 -0.00032 -3.13932

D190 -0.00893 0.00019 0.00000 0.00363 0.00358 -0.00536

D191 -3.09289 0.00033 0.00000 0.00708 0.00704 -3.08585

D192 0.06041 0.00004 0.00000 0.00311 0.00314 0.06355

D193 -0.01640 -0.00001 0.00000 -0.00242 -0.00246 -0.01886

D194 3.13934 -0.00007 0.00000 -0.00276 -0.00275 3.13658

D195 3.11407 0.00006 0.00000 -0.00079 -0.00088 3.11319

D196 -0.01339 0.00001 0.00000 -0.00113 -0.00117 -0.01456

D197 -3.08986 -0.00027 0.00000 -0.00420 -0.00422 -3.09408

D198 0.06291 -0.00034 0.00000 -0.00558 -0.00556 0.05735

D199 0.00000 0.00000 0.00000 -0.00001 -0.00002 -0.00002

D200 -3.12777 -0.00005 0.00000 -0.00016 -0.00012 -3.12790

D201 3.12777 0.00005 0.00000 0.00014 0.00010 3.12787

D202 0.00000 0.00000 0.00000 -0.00001 -0.00001 -0.00001

D203 0.01640 0.00001 0.00000 0.00240 0.00244 0.01884

D204 -3.11407 -0.00006 0.00000 0.00078 0.00087 -3.11319

D205 -3.13934 0.00007 0.00000 0.00274 0.00273 -3.13661

D206 0.01339 -0.00001 0.00000 0.00111 0.00116 0.01455

D207 3.08987 0.00027 0.00000 0.00421 0.00424 3.09410

D208 -0.06290 0.00034 0.00000 0.00559 0.00556 -0.05734

D209 1.09670 -0.00001 0.00000 -0.00015 -0.00016 1.09654

D210 -1.04719 0.00011 0.00000 0.00272 0.00271 -1.04448

D211 -3.11710 0.00002 0.00000 0.00143 0.00145 -3.11565

D212 1.04719 -0.00011 0.00000 -0.00272 -0.00271 1.04448

D213 -1.09670 0.00001 0.00000 0.00015 0.00016 -1.09654

D214 3.11710 -0.00002 0.00000 -0.00143 -0.00145 3.11564

D215 1.09945 -0.00005 0.00000 0.00349 0.00349 1.10294

D216 -1.04512 0.00003 0.00000 -0.00203 -0.00201 -1.04713

D217 -3.11482 0.00007 0.00000 0.00231 0.00229 -3.11253

D218 1.04512 -0.00003 0.00000 0.00203 0.00201 1.04713

D219 -1.09945 0.00005 0.00000 -0.00349 -0.00349 -1.10294

D220 3.11482 -0.00007 0.00000 -0.00231 -0.00229 3.11253

D221 1.04719 -0.00011 0.00000 -0.00272 -0.00271 1.04448

D222 -1.09670 0.00002 0.00000 0.00015 0.00017 -1.09653

D223 3.11710 -0.00002 0.00000 -0.00143 -0.00145 3.11565

D224 1.09670 -0.00001 0.00000 -0.00015 -0.00016 1.09654

D225 -1.04719 0.00011 0.00000 0.00272 0.00271 -1.04448

D226 -3.11710 0.00002 0.00000 0.00143 0.00145 -3.11564

D227 1.09945 -0.00005 0.00000 0.00349 0.00349 1.10294

D228 -1.04512 0.00003 0.00000 -0.00203 -0.00201 -1.04713

D229 -3.11482 0.00007 0.00000 0.00232 0.00230 -3.11252

D230 1.04512 -0.00003 0.00000 0.00203 0.00201 1.04713

D231 -1.09945 0.00005 0.00000 -0.00348 -0.00349 -1.10293

D232 3.11482 -0.00007 0.00000 -0.00231 -0.00229 3.11253

Item Value Threshold Converged?

Maximum Force 0.002860 0.000450 NO

RMS Force 0.000749 0.000300 NO

Maximum Displacement 0.935366 0.001800 NO

RMS Displacement 0.213501 0.001200 NO

Predicted change in Energy=-1.035647D-01

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 00:24:29 2019, MaxMem= 1342177280 cpu: 15.2

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

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=0 Diff= 6.13D-04

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 -1.135905 2.863696 -0.024368

2 7 0 -0.004865 2.106671 -0.212470

3 6 0 1.127718 2.865849 -0.023102

4 6 0 0.721910 4.232713 0.319228

5 6 0 -0.732361 4.231403 0.318370

6 7 0 2.420325 2.422037 -0.140822

7 6 0 2.862983 1.125108 -0.231857

8 7 0 2.093986 -0.004016 -0.158664

9 6 0 2.861634 -1.130768 -0.230459

10 6 0 4.287944 -0.707955 -0.392921

11 6 0 4.288720 0.701104 -0.393866

12 7 0 -2.422114 2.419541 -0.142360

13 6 0 -4.281244 0.698435 -0.394904

14 6 0 -4.279893 -0.708817 -0.393953

15 6 0 -2.854189 -1.131884 -0.231320

16 7 0 -2.081689 -0.004885 -0.159063

17 6 0 -2.856460 1.123857 -0.232728

18 7 0 -2.419289 -2.421136 -0.140510

19 7 0 -0.004004 -2.094658 -0.212576

20 6 0 -1.134507 -2.857301 -0.023573

21 6 0 -0.729691 -4.224073 0.319189

22 6 0 0.722751 -4.224775 0.320042

23 6 0 1.128684 -2.858507 -0.022312

24 7 0 2.419501 -2.421631 -0.138986

25 30 0 0.007024 0.006956 -0.384314

26 6 0 -5.501067 1.419909 -0.523290

27 6 0 -6.695158 0.694296 -0.641987

28 6 0 -6.693878 -0.709203 -0.641130

29 6 0 -5.498482 -1.432554 -0.521521

30 6 0 1.421307 -5.423078 0.634467

31 6 0 0.691170 -6.572183 0.912356

32 6 0 -0.700595 -6.571570 0.911613

33 6 0 -1.429491 -5.421842 0.632932

34 6 0 5.508279 1.422776 -0.522084

35 6 0 6.702552 0.697165 -0.640577

36 6 0 6.701846 -0.706565 -0.639728

37 6 0 5.506859 -1.430892 -0.520330

38 6 0 -1.432331 5.428925 0.632222

39 6 0 -0.703437 6.578805 0.910846

40 6 0 0.688541 6.579998 0.911591

41 6 0 1.419636 5.431350 0.633763

42 1 0 7.652620 1.222459 -0.742471

43 1 0 7.651395 -1.232914 -0.740999

44 1 0 1.210385 7.508420 1.150032

45 1 0 -1.227101 7.506341 1.148738

46 1 0 -7.645332 1.219369 -0.744015

47 1 0 -7.643103 -1.236109 -0.742531

48 1 0 -1.224044 -7.499245 1.149427

49 1 0 1.213573 -7.500307 1.150717

50 8 0 2.745440 5.476889 0.679021

51 8 0 -2.758239 5.472310 0.676098

52 8 0 5.511570 2.764488 -0.537872

53 8 0 5.508926 -2.772626 -0.534530

54 8 0 2.747158 -5.467663 0.679483

55 8 0 -2.755407 -5.465377 0.676571

56 8 0 -5.499680 -2.774291 -0.535665

57 8 0 -5.504586 2.761623 -0.539036

58 6 0 3.257108 6.776284 0.949853

59 1 0 2.935040 7.127607 1.946459

60 1 0 2.942839 7.498503 0.177275

61 1 0 4.346821 6.661364 0.928929

62 6 0 6.797296 3.368919 -0.599268

63 1 0 7.326342 3.113884 -1.535251

64 1 0 7.418511 3.085303 0.269402

65 1 0 6.596068 4.446656 -0.572454

66 6 0 6.794098 -3.378307 -0.595270

67 1 0 7.415620 -3.094233 0.273030

68 1 0 7.323329 -3.124867 -1.531582

69 1 0 6.591886 -4.455826 -0.567166

70 6 0 -3.272304 6.770868 0.946410

71 1 0 -2.958409 7.493610 0.174169

72 1 0 -2.951853 7.122705 1.943356

73 1 0 -4.361805 6.654175 0.924345

74 6 0 -6.790411 3.365813 -0.600630

75 1 0 -7.411714 3.082051 0.267932

76 1 0 -7.319251 3.110705 -1.536709

77 1 0 -6.589391 4.443585 -0.573746

78 6 0 -6.784458 -3.380780 -0.596594

79 1 0 -7.313690 -3.127709 -1.533004

80 1 0 -7.406297 -3.097057 0.271595

81 1 0 -6.581575 -4.458169 -0.568409

82 6 0 -3.269391 -6.764005 0.946720

83 1 0 -2.949080 -7.115865 1.943701

84 1 0 -2.955283 -7.486669 0.174491

85 1 0 -4.358897 -6.647426 0.924466

86 6 0 3.259826 -6.766701 0.950150

87 1 0 2.945944 -7.489104 0.177586

88 1 0 2.938195 -7.118315 1.946793

89 1 0 4.349449 -6.650988 0.929034

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

Rotational constants (GHZ): 0.0427791 0.0422754 0.0217477

Leave Link 202 at Sat Jul 6 00:24:30 2019, MaxMem= 1342177280 cpu: 0.5

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

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

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 7919.9808937057 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= 89 NActive= 89 NUniq= 89 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= -0.2249561376 Hartrees.

Nuclear repulsion after empirical dispersion term = 7919.7559375681 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6457

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.49D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 343

GePol: Fraction of low-weight points (<1% of avg) = 5.31%

GePol: Cavity surface area = 714.526 Ang\*\*2

GePol: Cavity volume = 813.180 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0098804370 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 7919.7460571311 Hartrees.

Leave Link 301 at Sat Jul 6 00:24:30 2019, MaxMem= 1342177280 cpu: 1.3

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

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

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

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 43372 LenP2D= 108705.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 6.73D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 00:24:34 2019, MaxMem= 1342177280 cpu: 41.6

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

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 00:24:35 2019, MaxMem= 1342177280 cpu: 2.4

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

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000122 0.000151 -0.000102 Ang= 0.03 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>= 2.0172 S= 1.0057

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2649.91299486653

Leave Link 401 at Sat Jul 6 00:24:52 2019, MaxMem= 1342177280 cpu: 198.9

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 530000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 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= 125078547.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.24D-14 for 1595.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.93D-15 for 5175 1559.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.40D-14 for 1583.

Iteration 1 A^-1\*A deviation from orthogonality is 8.58D-13 for 6445 6339.

E= -2649.60148749290

DIIS: error= 9.17D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.60148749290 IErMin= 1 ErrMin= 9.17D-03

ErrMax= 9.17D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.41D-01 BMatP= 3.41D-01

IDIUse=3 WtCom= 9.08D-01 WtEn= 9.17D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.571 Goal= None Shift= 0.000

Gap= 0.637 Goal= None Shift= 0.000

GapD= 0.571 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=5.34D-04 MaxDP=2.13D-02 OVMax= 5.05D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.32D-04 CP: 9.94D-01

E= -2649.72906624957 Delta-E= -0.127578756672 Rises=F Damp=F

DIIS: error= 1.46D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.72906624957 IErMin= 2 ErrMin= 1.46D-03

ErrMax= 1.46D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.94D-03 BMatP= 3.41D-01

IDIUse=3 WtCom= 9.85D-01 WtEn= 1.46D-02

Coeff-Com: -0.806D-02 0.101D+01

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

Coeff: -0.794D-02 0.101D+01

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.062 Goal= None Shift= 0.000

RMSDP=1.08D-04 MaxDP=6.66D-03 DE=-1.28D-01 OVMax= 2.76D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.08D-04 CP: 9.92D-01 9.93D-01

E= -2649.72933740774 Delta-E= -0.000271158164 Rises=F Damp=F

DIIS: error= 2.11D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.72933740774 IErMin= 2 ErrMin= 1.46D-03

ErrMax= 2.11D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.17D-02 BMatP= 9.94D-03

IDIUse=3 WtCom= 1.79D-01 WtEn= 8.21D-01

Coeff-Com: -0.305D-01 0.542D+00 0.489D+00

Coeff-En: 0.000D+00 0.466D+00 0.534D+00

Coeff: -0.546D-02 0.479D+00 0.526D+00

Gap= 0.035 Goal= None Shift= 0.000

Gap= 0.064 Goal= None Shift= 0.000

RMSDP=7.04D-05 MaxDP=4.88D-03 DE=-2.71D-04 OVMax= 2.22D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.49D-05 CP: 9.93D-01 1.01D+00 5.07D-01

E= -2649.73133637295 Delta-E= -0.001998965208 Rises=F Damp=F

DIIS: error= 6.37D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.73133637295 IErMin= 4 ErrMin= 6.37D-04

ErrMax= 6.37D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.89D-03 BMatP= 9.94D-03

IDIUse=3 WtCom= 9.94D-01 WtEn= 6.37D-03

Coeff-Com: -0.138D-01 0.181D+00 0.321D+00 0.512D+00

Coeff-En: 0.000D+00 0.000D+00 0.133D+00 0.867D+00

Coeff: -0.137D-01 0.180D+00 0.320D+00 0.514D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=2.34D-05 MaxDP=1.66D-03 DE=-2.00D-03 OVMax= 7.03D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.13D-05 CP: 9.93D-01 1.01D+00 5.87D-01 5.87D-01

E= -2649.73170893188 Delta-E= -0.000372558934 Rises=F Damp=F

DIIS: error= 2.09D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.73170893188 IErMin= 5 ErrMin= 2.09D-04

ErrMax= 2.09D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.54D-05 BMatP= 1.89D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.09D-03

Coeff-Com: -0.553D-02 0.606D-01 0.145D+00 0.288D+00 0.512D+00

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

Coeff: -0.552D-02 0.605D-01 0.145D+00 0.287D+00 0.513D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=5.19D-06 MaxDP=4.92D-04 DE=-3.73D-04 OVMax= 1.56D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.10D-06 CP: 9.93D-01 1.01D+00 5.91D-01 6.25D-01 7.65D-01

E= -2649.73172720957 Delta-E= -0.000018277691 Rises=F Damp=F

DIIS: error= 7.87D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.73172720957 IErMin= 6 ErrMin= 7.87D-05

ErrMax= 7.87D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.31D-05 BMatP= 9.54D-05

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

Coeff-Com: -0.742D-03 0.253D-02 0.277D-01 0.756D-01 0.298D+00 0.597D+00

Coeff: -0.742D-03 0.253D-02 0.277D-01 0.756D-01 0.298D+00 0.597D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=2.01D-06 MaxDP=1.80D-04 DE=-1.83D-05 OVMax= 6.07D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.42D-06 CP: 9.93D-01 1.01D+00 5.95D-01 6.29D-01 8.15D-01

CP: 7.09D-01

E= -2649.73172998550 Delta-E= -0.000002775923 Rises=F Damp=F

DIIS: error= 2.61D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.73172998550 IErMin= 7 ErrMin= 2.61D-05

ErrMax= 2.61D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.01D-06 BMatP= 1.31D-05

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

Coeff-Com: 0.124D-03-0.493D-02 0.145D-02 0.162D-01 0.130D+00 0.367D+00

Coeff-Com: 0.490D+00

Coeff: 0.124D-03-0.493D-02 0.145D-02 0.162D-01 0.130D+00 0.367D+00

Coeff: 0.490D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=7.40D-07 MaxDP=5.17D-05 DE=-2.78D-06 OVMax= 2.86D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 4.68D-07 CP: 9.93D-01 1.01D+00 5.96D-01 6.29D-01 8.23D-01

CP: 7.71D-01 6.54D-01

E= -2649.73173045042 Delta-E= -0.000000464926 Rises=F Damp=F

DIIS: error= 6.52D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.73173045042 IErMin= 8 ErrMin= 6.52D-06

ErrMax= 6.52D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.24D-07 BMatP= 2.01D-06

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

Coeff-Com: 0.147D-03-0.249D-02-0.315D-02-0.263D-02 0.134D-01 0.711D-01

Coeff-Com: 0.212D+00 0.712D+00

Coeff: 0.147D-03-0.249D-02-0.315D-02-0.263D-02 0.134D-01 0.711D-01

Coeff: 0.212D+00 0.712D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=2.44D-07 MaxDP=2.51D-05 DE=-4.65D-07 OVMax= 1.18D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.00D-07 CP: 9.93D-01 1.01D+00 5.96D-01 6.31D-01 8.27D-01

CP: 7.78D-01 7.20D-01 1.04D+00

E= -2649.73173049773 Delta-E= -0.000000047310 Rises=F Damp=F

DIIS: error= 3.54D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.73173049773 IErMin= 9 ErrMin= 3.54D-06

ErrMax= 3.54D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.37D-08 BMatP= 1.24D-07

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

Coeff-Com: 0.292D-04 0.721D-04-0.140D-02-0.393D-02-0.202D-01-0.444D-01

Coeff-Com: -0.127D-01 0.282D+00 0.800D+00

Coeff: 0.292D-04 0.721D-04-0.140D-02-0.393D-02-0.202D-01-0.444D-01

Coeff: -0.127D-01 0.282D+00 0.800D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=1.42D-07 MaxDP=1.29D-05 DE=-4.73D-08 OVMax= 7.31D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.06D-07 CP: 9.93D-01 1.01D+00 5.96D-01 6.31D-01 8.28D-01

CP: 7.86D-01 7.47D-01 1.20D+00 1.05D+00

E= -2649.73173050955 Delta-E= -0.000000011822 Rises=F Damp=F

DIIS: error= 1.52D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -2649.73173050955 IErMin=10 ErrMin= 1.52D-06

ErrMax= 1.52D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.20D-08 BMatP= 2.37D-08

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

Coeff-Com: -0.140D-04 0.637D-03-0.146D-03-0.196D-02-0.163D-01-0.468D-01

Coeff-Com: -0.605D-01 0.465D-02 0.512D+00 0.609D+00

Coeff: -0.140D-04 0.637D-03-0.146D-03-0.196D-02-0.163D-01-0.468D-01

Coeff: -0.605D-01 0.465D-02 0.512D+00 0.609D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=8.27D-08 MaxDP=5.48D-06 DE=-1.18D-08 OVMax= 3.74D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.40D-08 CP: 9.93D-01 1.01D+00 5.96D-01 6.31D-01 8.28D-01

CP: 7.89D-01 7.67D-01 1.27D+00 1.22D+00 8.52D-01

E= -2649.73173051382 Delta-E= -0.000000004262 Rises=F Damp=F

DIIS: error= 6.26D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -2649.73173051382 IErMin=11 ErrMin= 6.26D-07

ErrMax= 6.26D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.46D-09 BMatP= 1.20D-08

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

Coeff-Com: -0.142D-04 0.311D-03 0.264D-03-0.676D-04-0.322D-02-0.129D-01

Coeff-Com: -0.265D-01-0.615D-01 0.690D-01 0.289D+00 0.746D+00

Coeff: -0.142D-04 0.311D-03 0.264D-03-0.676D-04-0.322D-02-0.129D-01

Coeff: -0.265D-01-0.615D-01 0.690D-01 0.289D+00 0.746D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=3.67D-08 MaxDP=3.44D-06 DE=-4.26D-09 OVMax= 2.80D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.37D-08 CP: 9.93D-01 1.01D+00 5.96D-01 6.31D-01 8.28D-01

CP: 7.89D-01 7.69D-01 1.30D+00 1.30D+00 1.02D+00

CP: 1.04D+00

E= -2649.73173051476 Delta-E= -0.000000000940 Rises=F Damp=F

DIIS: error= 3.73D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -2649.73173051476 IErMin=12 ErrMin= 3.73D-07

ErrMax= 3.73D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.35D-10 BMatP= 1.46D-09

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

Coeff-Com: -0.566D-05 0.753D-04 0.164D-03 0.249D-03 0.665D-03-0.230D-03

Coeff-Com: -0.599D-02-0.365D-01-0.387D-01 0.773D-01 0.423D+00 0.580D+00

Coeff: -0.566D-05 0.753D-04 0.164D-03 0.249D-03 0.665D-03-0.230D-03

Coeff: -0.599D-02-0.365D-01-0.387D-01 0.773D-01 0.423D+00 0.580D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=1.92D-08 MaxDP=1.69D-06 DE=-9.40D-10 OVMax= 2.14D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.46D-08 CP: 9.93D-01 1.01D+00 5.96D-01 6.31D-01 8.28D-01

CP: 7.89D-01 7.69D-01 1.30D+00 1.32D+00 1.07D+00

CP: 1.23D+00 1.11D+00

E= -2649.73173051482 Delta-E= -0.000000000064 Rises=F Damp=F

DIIS: error= 2.66D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -2649.73173051482 IErMin=13 ErrMin= 2.66D-07

ErrMax= 2.66D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.06D-10 BMatP= 4.35D-10

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

Coeff-Com: 0.888D-06-0.495D-04 0.683D-05 0.153D-03 0.125D-02 0.369D-02

Coeff-Com: 0.469D-02-0.728D-03-0.412D-01-0.369D-01 0.137D-03 0.313D+00

Coeff-Com: 0.756D+00

Coeff: 0.888D-06-0.495D-04 0.683D-05 0.153D-03 0.125D-02 0.369D-02

Coeff: 0.469D-02-0.728D-03-0.412D-01-0.369D-01 0.137D-03 0.313D+00

Coeff: 0.756D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=1.77D-08 MaxDP=1.81D-06 DE=-6.37D-11 OVMax= 2.34D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 7.71D-09 CP: 9.93D-01 1.01D+00 5.96D-01 6.31D-01 8.28D-01

CP: 7.89D-01 7.70D-01 1.30D+00 1.33D+00 1.11D+00

CP: 1.36D+00 1.60D+00 1.43D+00

E= -2649.73173051497 Delta-E= -0.000000000153 Rises=F Damp=F

DIIS: error= 2.23D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -2649.73173051497 IErMin=14 ErrMin= 2.23D-07

ErrMax= 2.23D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.34D-11 BMatP= 1.06D-10

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

Coeff-Com: 0.211D-05-0.492D-04-0.405D-04 0.272D-04 0.534D-03 0.224D-02

Coeff-Com: 0.432D-02 0.929D-02-0.134D-01-0.387D-01-0.117D+00 0.330D-01

Coeff-Com: 0.370D+00 0.749D+00

Coeff: 0.211D-05-0.492D-04-0.405D-04 0.272D-04 0.534D-03 0.224D-02

Coeff: 0.432D-02 0.929D-02-0.134D-01-0.387D-01-0.117D+00 0.330D-01

Coeff: 0.370D+00 0.749D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=1.67D-08 MaxDP=1.68D-06 DE=-1.53D-10 OVMax= 2.45D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 4.99D-09 CP: 9.93D-01 1.01D+00 5.96D-01 6.31D-01 8.28D-01

CP: 7.89D-01 7.70D-01 1.31D+00 1.34D+00 1.14D+00

CP: 1.48D+00 1.98D+00 2.12D+00 1.60D+00

E= -2649.73173051518 Delta-E= -0.000000000204 Rises=F Damp=F

DIIS: error= 1.92D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -2649.73173051518 IErMin=15 ErrMin= 1.92D-07

ErrMax= 1.92D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.36D-11 BMatP= 3.34D-11

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

Coeff-Com: 0.761D-06-0.514D-05-0.240D-04-0.476D-04-0.260D-03-0.377D-03

Coeff-Com: 0.248D-03 0.519D-02 0.928D-02-0.372D-02-0.670D-01-0.912D-01

Coeff-Com: -0.137D+00 0.522D+00 0.763D+00

Coeff: 0.761D-06-0.514D-05-0.240D-04-0.476D-04-0.260D-03-0.377D-03

Coeff: 0.248D-03 0.519D-02 0.928D-02-0.372D-02-0.670D-01-0.912D-01

Coeff: -0.137D+00 0.522D+00 0.763D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=1.76D-08 MaxDP=1.58D-06 DE=-2.04D-10 OVMax= 2.60D-05

Cycle 16 Pass 1 IDiag 1:

RMSU= 2.79D-09 CP: 9.93D-01 1.01D+00 5.96D-01 6.31D-01 8.28D-01

CP: 7.89D-01 7.70D-01 1.31D+00 1.35D+00 1.17D+00

CP: 1.58D+00 2.38D+00 2.77D+00 2.62D+00 1.67D+00

E= -2649.73173051498 Delta-E= 0.000000000195 Rises=F Damp=F

DIIS: error= 1.88D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=15 EnMin= -2649.73173051518 IErMin=16 ErrMin= 1.88D-07

ErrMax= 1.88D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-11 BMatP= 2.36D-11

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

Coeff-Com: -0.328D-06 0.136D-04 0.242D-05-0.325D-04-0.297D-03-0.909D-03

Coeff-Com: -0.137D-02-0.353D-03 0.842D-02 0.117D-01 0.235D-02-0.403D-01

Coeff-Com: -0.224D+00 0.919D-01 0.183D+00 0.970D+00

Coeff: -0.328D-06 0.136D-04 0.242D-05-0.325D-04-0.297D-03-0.909D-03

Coeff: -0.137D-02-0.353D-03 0.842D-02 0.117D-01 0.235D-02-0.403D-01

Coeff: -0.224D+00 0.919D-01 0.183D+00 0.970D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=1.87D-08 MaxDP=1.67D-06 DE= 1.95D-10 OVMax= 2.85D-05

Cycle 17 Pass 1 IDiag 1:

RMSU= 9.07D-09 CP: 9.93D-01 1.01D+00 5.96D-01 6.31D-01 8.28D-01

CP: 7.89D-01 7.70D-01 1.31D+00 1.35D+00 1.19D+00

CP: 1.69D+00 2.78D+00 3.00D+00 3.00D+00 2.82D+00

CP: 1.78D+00

E= -2649.73173051525 Delta-E= -0.000000000267 Rises=F Damp=F

DIIS: error= 1.68D-07 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -2649.73173051525 IErMin=17 ErrMin= 1.68D-07

ErrMax= 1.68D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.39D-11 BMatP= 1.05D-11

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

Coeff-Com: -0.580D-06 0.102D-04 0.149D-04 0.649D-05-0.177D-04-0.296D-03

Coeff-Com: -0.100D-02-0.290D-02-0.640D-03 0.101D-01 0.349D-01 0.414D-01

Coeff-Com: -0.103D+00-0.150D+00-0.508D+00 0.989D+00 0.690D+00

Coeff: -0.580D-06 0.102D-04 0.149D-04 0.649D-05-0.177D-04-0.296D-03

Coeff: -0.100D-02-0.290D-02-0.640D-03 0.101D-01 0.349D-01 0.414D-01

Coeff: -0.103D+00-0.150D+00-0.508D+00 0.989D+00 0.690D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=1.93D-08 MaxDP=1.60D-06 DE=-2.67D-10 OVMax= 2.92D-05

Cycle 18 Pass 1 IDiag 1:

RMSU= 7.00D-09 CP: 9.93D-01 1.01D+00 5.96D-01 6.31D-01 8.28D-01

CP: 7.89D-01 7.71D-01 1.31D+00 1.36D+00 1.22D+00

CP: 1.80D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

CP: 3.00D+00 2.50D+00

E= -2649.73173051518 Delta-E= 0.000000000073 Rises=F Damp=F

DIIS: error= 1.50D-07 at cycle 18 NSaved= 18.

NSaved=18 IEnMin=17 EnMin= -2649.73173051525 IErMin=18 ErrMin= 1.50D-07

ErrMax= 1.50D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.32D-12 BMatP= 1.05D-11

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

Coeff-Com: -0.146D-06-0.489D-05 0.861D-05 0.357D-04 0.262D-03 0.646D-03

Coeff-Com: 0.530D-03-0.176D-02-0.910D-02-0.193D-02 0.188D-01 0.892D-01

Coeff-Com: 0.986D-01-0.840D-01-0.759D+00 0.156D+00-0.175D+00 0.167D+01

Coeff: -0.146D-06-0.489D-05 0.861D-05 0.357D-04 0.262D-03 0.646D-03

Coeff: 0.530D-03-0.176D-02-0.910D-02-0.193D-02 0.188D-01 0.892D-01

Coeff: 0.986D-01-0.840D-01-0.759D+00 0.156D+00-0.175D+00 0.167D+01

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=3.71D-08 MaxDP=3.04D-06 DE= 7.28D-11 OVMax= 5.63D-05

Cycle 19 Pass 1 IDiag 1:

RMSU= 2.48D-08 CP: 9.93D-01 1.01D+00 5.96D-01 6.31D-01 8.28D-01

CP: 7.89D-01 7.71D-01 1.31D+00 1.38D+00 1.26D+00

CP: 2.00D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

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

E= -2649.73173051511 Delta-E= 0.000000000069 Rises=F Damp=F

DIIS: error= 1.22D-07 at cycle 19 NSaved= 19.

NSaved=19 IEnMin=17 EnMin= -2649.73173051525 IErMin=19 ErrMin= 1.22D-07

ErrMax= 1.22D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.57D-12 BMatP= 8.32D-12

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

Coeff-Com: 0.719D-06-0.178D-04-0.146D-04 0.196D-04 0.210D-03 0.899D-03

Coeff-Com: 0.178D-02 0.259D-02-0.623D-02-0.124D-01-0.389D-01 0.266D-01

Coeff-Com: 0.148D+00 0.267D+00-0.743D-01-0.783D+00-0.178D+01 0.176D+01

Coeff-Com: 0.149D+01

Coeff: 0.719D-06-0.178D-04-0.146D-04 0.196D-04 0.210D-03 0.899D-03

Coeff: 0.178D-02 0.259D-02-0.623D-02-0.124D-01-0.389D-01 0.266D-01

Coeff: 0.148D+00 0.267D+00-0.743D-01-0.783D+00-0.178D+01 0.176D+01

Coeff: 0.149D+01

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=6.35D-08 MaxDP=5.11D-06 DE= 6.91D-11 OVMax= 9.64D-05

Cycle 20 Pass 1 IDiag 1:

RMSU= 2.24D-08 CP: 9.93D-01 1.01D+00 5.96D-01 6.31D-01 8.28D-01

CP: 7.89D-01 7.72D-01 1.32D+00 1.40D+00 1.34D+00

CP: 2.34D+00 3.00D+00 3.00D+00 3.00D+00 3.00D+00

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

E= -2649.73173051555 Delta-E= -0.000000000440 Rises=F Damp=F

DIIS: error= 7.10D-08 at cycle 20 NSaved= 20.

NSaved=20 IEnMin=20 EnMin= -2649.73173051555 IErMin=20 ErrMin= 7.10D-08

ErrMax= 7.10D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.72D-12 BMatP= 7.57D-12

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

Coeff-Com: 0.467D-06-0.588D-05-0.140D-04-0.147D-04-0.797D-04 0.930D-05

Coeff-Com: 0.598D-03 0.270D-02 0.321D-02-0.417D-02-0.356D-01-0.406D-01

Coeff-Com: -0.196D-01 0.246D+00 0.375D+00-0.267D+00-0.996D+00-0.556D-01

Coeff-Com: 0.581D+00 0.121D+01

Coeff: 0.467D-06-0.588D-05-0.140D-04-0.147D-04-0.797D-04 0.930D-05

Coeff: 0.598D-03 0.270D-02 0.321D-02-0.417D-02-0.356D-01-0.406D-01

Coeff: -0.196D-01 0.246D+00 0.375D+00-0.267D+00-0.996D+00-0.556D-01

Coeff: 0.581D+00 0.121D+01

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=4.61D-08 MaxDP=3.70D-06 DE=-4.40D-10 OVMax= 6.99D-05

Cycle 21 Pass 1 IDiag 1:

Restarting incremental Fock formation.

E= -2649.73173051352 Delta-E= 0.000000002028 Rises=F Damp=F

DIIS: error= 4.16D-08 at cycle 21 NSaved= 20.

NSaved=20 IEnMin=19 EnMin= -2649.73173051555 IErMin=20 ErrMin= 4.16D-08

ErrMax= 4.16D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.93D-12 BMatP= 2.72D-12

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

Coeff-Com: 0.501D-05-0.302D-05-0.223D-04-0.179D-03-0.495D-03-0.523D-03

Coeff-Com: 0.620D-03 0.575D-02 0.372D-02-0.657D-02-0.448D-01-0.103D+00

Coeff-Com: 0.641D-01 0.318D+00 0.266D+00 0.603D-01-0.978D+00-0.379D+00

Coeff-Com: 0.109D+01 0.706D+00

Coeff: 0.501D-05-0.302D-05-0.223D-04-0.179D-03-0.495D-03-0.523D-03

Coeff: 0.620D-03 0.575D-02 0.372D-02-0.657D-02-0.448D-01-0.103D+00

Coeff: 0.641D-01 0.318D+00 0.266D+00 0.603D-01-0.978D+00-0.379D+00

Coeff: 0.109D+01 0.706D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=3.30D-08 MaxDP=2.61D-06 DE= 2.03D-09 OVMax= 4.95D-05

Cycle 22 Pass 1 IDiag 1:

RMSU= 3.30D-08 CP: 1.00D+00

E= -2649.73173051335 Delta-E= 0.000000000171 Rises=F Damp=F

DIIS: error= 9.53D-09 at cycle 22 NSaved= 20.

NSaved=20 IEnMin=18 EnMin= -2649.73173051555 IErMin=20 ErrMin= 9.53D-09

ErrMax= 9.53D-09 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.06D-13 BMatP= 1.93D-12

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

Coeff-Com: -0.552D-06-0.452D-05-0.162D-04-0.772D-04-0.144D-03 0.506D-05

Coeff-Com: 0.731D-03 0.730D-03 0.184D-02-0.614D-02-0.225D-01-0.129D-01

Coeff-Com: 0.277D-01 0.154D+00 0.180D+00-0.322D+00-0.265D+00 0.170D+00

Coeff-Com: 0.270D+00 0.823D+00

Coeff: -0.552D-06-0.452D-05-0.162D-04-0.772D-04-0.144D-03 0.506D-05

Coeff: 0.731D-03 0.730D-03 0.184D-02-0.614D-02-0.225D-01-0.129D-01

Coeff: 0.277D-01 0.154D+00 0.180D+00-0.322D+00-0.265D+00 0.170D+00

Coeff: 0.270D+00 0.823D+00

Gap= 0.034 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=7.99D-09 MaxDP=6.14D-07 DE= 1.71D-10 OVMax= 1.15D-05

Error on total polarization charges = 0.07176

SCF Done: E(UB3LYP) = -2649.73173051 A.U. after 22 cycles

NFock= 22 Conv=0.80D-08 -V/T= 1.9854

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0180 S= 1.0060

<L.S>= 0.000000000000E+00

KE= 2.688931504091D+03 PE=-2.211612317390D+04 EE= 8.857713882161D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.20

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0180, after 2.0002

Leave Link 502 at Sat Jul 6 00:40:50 2019, MaxMem= 1342177280 cpu: 11388.5

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

Compute integral first derivatives.

... and contract with generalized density number 0.

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

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 43372 LenP2D= 108705.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 287

Leave Link 701 at Sat Jul 6 00:41:09 2019, MaxMem= 1342177280 cpu: 216.4

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

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

Leave Link 702 at Sat Jul 6 00:41:09 2019, MaxMem= 1342177280 cpu: 0.2

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

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

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

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

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

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

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

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 00:42:38 2019, MaxMem= 1342177280 cpu: 1069.0

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

Dipole =-3.46742909D-03-1.44162457D-02 1.86240705D-01

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

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.003183572 -0.008473204 0.000345187

2 7 0.002105294 0.003291262 0.002564233

3 6 0.005780684 -0.010846749 -0.000191807

4 6 -0.010386001 -0.001973059 -0.000781243

5 6 0.010604296 -0.001538587 -0.000674867

6 7 0.013507036 -0.030435814 -0.001172438

7 6 -0.017040758 0.041368204 0.001645953

8 7 -0.008881151 0.002532725 0.000185097

9 6 -0.014413282 -0.039336973 0.001177448

10 6 0.003106304 -0.012078604 0.000090170

11 6 0.002829820 0.012234135 0.000110206

12 7 -0.015737246 -0.030128452 -0.001238586

13 6 -0.002898303 0.012793148 0.000070551

14 6 -0.003181375 -0.012624015 0.000047246

15 6 0.013868993 -0.036223590 0.001049126

16 7 0.005105417 0.002460550 -0.000181336

17 6 0.016488961 0.038472376 0.001528095

18 7 -0.016552569 0.027735580 -0.001263763

19 7 0.002048815 -0.006813216 0.003183875

20 6 -0.000228312 0.008079988 0.000314445

21 6 0.010407310 0.001372888 -0.000627420

22 6 -0.010176181 0.001813697 -0.000740281

23 6 0.003030753 0.010457247 -0.000224923

24 7 0.014207232 0.028142287 -0.001183381

25 30 -0.000547250 -0.000522757 0.002949906

26 6 0.008768546 -0.010537892 0.000521631

27 6 -0.001312136 -0.014313049 -0.000099853

28 6 -0.001330239 0.014334202 -0.000111181

29 6 0.008847907 0.010622081 0.000528628

30 6 -0.017907268 0.011027784 -0.002525239

31 6 -0.009907766 -0.009058424 0.002044454

32 6 0.009916308 -0.009127478 0.002061663

33 6 0.017962654 0.011170832 -0.002565697

34 6 -0.008765854 -0.010727214 0.000524352

35 6 0.001315853 -0.014510156 -0.000105964

36 6 0.001331283 0.014534165 -0.000115256

37 6 -0.008840603 0.010809637 0.000530087

38 6 0.018166859 -0.011137561 -0.002566674

39 6 0.010097467 0.009123050 0.002069448

40 6 -0.010086214 0.009058573 0.002052342

41 6 -0.018110370 -0.010999345 -0.002528569

42 1 -0.005850728 -0.007339442 0.000770220

43 1 -0.005835478 0.007347041 0.000766146

44 1 -0.011750627 -0.007436165 -0.002158482

45 1 0.011757529 -0.007409354 -0.002149830

46 1 0.005855564 -0.007333433 0.000767189

47 1 0.005839415 0.007338658 0.000763877

48 1 0.011746208 0.007411592 -0.002143836

49 1 -0.011736892 0.007432756 -0.002151726

50 8 0.016301347 -0.001866404 -0.002189751

51 8 -0.016523205 -0.002029666 -0.002271167

52 8 -0.002909301 0.001191503 0.000991100

53 8 -0.003110749 -0.001389330 0.001074254

54 8 0.016501837 0.001996528 -0.002256204

55 8 -0.016707537 0.002168731 -0.002313836

56 8 0.003269823 -0.001616599 0.001133130

57 8 0.003077551 0.001416263 0.001063721

58 6 0.020483747 0.002300591 0.002028922

59 1 0.006102709 -0.001675505 -0.006497534

60 1 0.004473203 -0.004124456 0.004800960

61 1 -0.004364065 0.002206034 0.000651095

62 6 0.003850284 0.013543538 -0.000063869

63 1 -0.003849474 0.003114091 0.006063535

64 1 -0.004031111 0.003170903 -0.005711457

65 1 0.003441435 -0.004678623 -0.000360780

66 6 0.003799502 -0.013536463 -0.000048587

67 1 -0.004031618 -0.003170757 -0.005707944

68 1 -0.003844501 -0.003110211 0.006062494

69 1 0.003444139 0.004671329 -0.000364768

70 6 -0.020493374 0.002265810 0.002013568

71 1 -0.004470196 -0.004131703 0.004799292

72 1 -0.006100731 -0.001685560 -0.006505630

73 1 0.004359442 0.002208229 0.000654365

74 6 -0.003792754 0.013522252 -0.000057428

75 1 0.004019282 0.003170312 -0.005711324

76 1 0.003842108 0.003112929 0.006057968

77 1 -0.003437909 -0.004673371 -0.000357811

78 6 -0.003742986 -0.013517083 -0.000041035

79 1 0.003836411 -0.003110137 0.006057069

80 1 0.004019721 -0.003168230 -0.005707837

81 1 -0.003438250 0.004664627 -0.000361679

82 6 -0.020468806 -0.002215119 0.001997480

83 1 -0.006095937 0.001682252 -0.006500809

84 1 -0.004466532 0.004120648 0.004800029

85 1 0.004352826 -0.002205636 0.000652479

86 6 0.020458673 -0.002247212 0.002011603

87 1 0.004468104 0.004115384 0.004801535

88 1 0.006098466 0.001673268 -0.006493659

89 1 -0.004357907 -0.002203081 0.000649287

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

Cartesian Forces: Max 0.041368204 RMS 0.009348847

Leave Link 716 at Sat Jul 6 00:42:38 2019, MaxMem= 1342177280 cpu: 0.6

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

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

Internal Forces: Max 0.071638695 RMS 0.012322296

Search for a local minimum.

Step number 8 out of a maximum of 518

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

RMS Force = .12322D-01 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 2 3 4 6

5 8 7

ITU= 0 0 0 1 1 1 1 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.93183.

Iteration 1 RMS(Cart)= 0.18871768 RMS(Int)= 0.00504098

Iteration 2 RMS(Cart)= 0.01522538 RMS(Int)= 0.00002528

Iteration 3 RMS(Cart)= 0.00007943 RMS(Int)= 0.00001428

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001428

ITry= 1 IFail=0 DXMaxC= 8.69D-01 DCOld= 1.00D+10 DXMaxT= 4.57D-01 DXLimC= 3.00D+00 Rises=T

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

(Linear) (Quad) (Total)

R1 2.59638 -0.01254 -0.01557 0.00000 -0.01556 2.58082

R2 2.77149 -0.01388 -0.03402 0.00000 -0.03402 2.73747

R3 2.58107 -0.00711 -0.01430 0.00000 -0.01426 2.56681

R4 2.60135 -0.01349 -0.02031 0.00000 -0.02030 2.58105

R5 3.98121 -0.02750 -0.10575 0.00000 -0.10579 3.87543

R6 2.77100 -0.01338 -0.03355 0.00000 -0.03355 2.73745

R7 2.59220 -0.01106 -0.02482 0.00000 -0.02477 2.56744

R8 2.74818 -0.01119 -0.04848 0.00000 -0.04848 2.69970

R9 2.68746 -0.01332 -0.02544 0.00000 -0.02544 2.66201

R10 2.68748 -0.01363 -0.02546 0.00000 -0.02546 2.66202

R11 2.59537 -0.04497 -0.10981 0.00000 -0.10978 2.48560

R12 2.58529 -0.00343 0.01055 0.00000 0.01052 2.59581

R13 2.82749 -0.01338 -0.02870 0.00000 -0.02870 2.79880

R14 2.58002 -0.00197 0.01556 0.00000 0.01554 2.59556

R15 3.96683 -0.02613 -0.12730 0.00000 -0.12738 3.83944

R16 2.82798 -0.01401 -0.02917 0.00000 -0.02916 2.79882

R17 2.58428 -0.04122 -0.09935 0.00000 -0.09932 2.48496

R18 2.66274 0.00357 0.00076 0.00000 0.00078 2.66351

R19 2.68888 -0.01901 -0.04308 0.00000 -0.04309 2.64579

R20 2.68884 -0.01866 -0.04306 0.00000 -0.04306 2.64578

R21 2.58804 -0.04266 -0.10293 0.00000 -0.10290 2.48514

R22 2.65932 0.00409 0.00401 0.00000 0.00402 2.66334

R23 2.82657 -0.01354 -0.02783 0.00000 -0.02782 2.79875

R24 2.68911 -0.01886 -0.04332 0.00000 -0.04332 2.64579

R25 2.82706 -0.01415 -0.02829 0.00000 -0.02829 2.79877

R26 2.68915 -0.01919 -0.04335 0.00000 -0.04335 2.64579

R27 2.58561 -0.00342 0.01024 0.00000 0.01022 2.59583

R28 2.57694 -0.03875 -0.09246 0.00000 -0.09244 2.48450

R29 2.59089 -0.00480 0.00521 0.00000 0.00519 2.59609

R30 3.97004 -0.02442 -0.13084 0.00000 -0.13090 3.83914

R31 2.57348 -0.00451 -0.00713 0.00000 -0.00710 2.56638

R32 2.60164 -0.01371 -0.02059 0.00000 -0.02058 2.58106

R33 2.60662 -0.01460 -0.02534 0.00000 -0.02533 2.58130

R34 3.98477 -0.02573 -0.10980 0.00000 -0.10982 3.87494

R35 2.77051 -0.01388 -0.03309 0.00000 -0.03309 2.73742

R36 2.74472 -0.01087 -0.04517 0.00000 -0.04517 2.69955

R37 2.68767 -0.01380 -0.02564 0.00000 -0.02565 2.66202

R38 2.77003 -0.01341 -0.03262 0.00000 -0.03262 2.73741

R39 2.68765 -0.01349 -0.02563 0.00000 -0.02563 2.66202

R40 2.58463 -0.00863 -0.01767 0.00000 -0.01762 2.56701

R41 2.64997 0.00347 0.00807 0.00000 0.00808 2.65805

R42 2.53566 0.01653 0.01320 0.00000 0.01320 2.54885

R43 2.65223 -0.00747 -0.02236 0.00000 -0.02235 2.62988

R44 2.06053 -0.00871 -0.01557 0.00000 -0.01557 2.04496

R45 2.65001 0.00337 0.00803 0.00000 0.00804 2.65805

R46 2.06053 -0.00870 -0.01557 0.00000 -0.01557 2.04496

R47 2.53566 0.01673 0.01320 0.00000 0.01320 2.54885

R48 2.62581 0.01676 0.01754 0.00000 0.01754 2.64335

R49 2.50835 0.04296 0.04074 0.00000 0.04074 2.54909

R50 2.63006 0.00761 0.01740 0.00000 0.01741 2.64747

R51 2.06243 -0.01241 -0.01752 0.00000 -0.01752 2.04491

R52 2.62585 0.01669 0.01749 0.00000 0.01750 2.64335

R53 2.06243 -0.01240 -0.01752 0.00000 -0.01752 2.04491

R54 2.50833 0.04318 0.04077 0.00000 0.04077 2.54909

R55 2.65023 0.00328 0.00783 0.00000 0.00783 2.65806

R56 2.53565 0.01632 0.01320 0.00000 0.01320 2.54885

R57 2.65267 -0.00807 -0.02276 0.00000 -0.02276 2.62991

R58 2.06053 -0.00870 -0.01557 0.00000 -0.01557 2.04496

R59 2.65027 0.00317 0.00779 0.00000 0.00779 2.65806

R60 2.06053 -0.00870 -0.01557 0.00000 -0.01557 2.04496

R61 2.53565 0.01652 0.01320 0.00000 0.01320 2.54885

R62 2.62607 0.01652 0.01729 0.00000 0.01729 2.64336

R63 2.50831 0.04303 0.04078 0.00000 0.04078 2.54909

R64 2.63046 0.00708 0.01703 0.00000 0.01704 2.64750

R65 2.06244 -0.01241 -0.01752 0.00000 -0.01752 2.04491

R66 2.62603 0.01659 0.01733 0.00000 0.01734 2.64336

R67 2.06244 -0.01242 -0.01752 0.00000 -0.01752 2.04491

R68 2.50834 0.04280 0.04075 0.00000 0.04075 2.54909

R69 2.68819 0.00861 0.00582 0.00000 0.00582 2.69401

R70 2.68819 0.00860 0.00582 0.00000 0.00582 2.69401

R71 2.68727 0.00591 0.00803 0.00000 0.00803 2.69530

R72 2.68727 0.00588 0.00803 0.00000 0.00803 2.69530

R73 2.68819 0.00857 0.00582 0.00000 0.00582 2.69401

R74 2.68819 0.00856 0.00582 0.00000 0.00582 2.69401

R75 2.68726 0.00584 0.00804 0.00000 0.00804 2.69530

R76 2.68726 0.00587 0.00804 0.00000 0.00804 2.69530

R77 2.08759 -0.00817 -0.01950 0.00000 -0.01950 2.06809

R78 2.08491 -0.00734 -0.01676 0.00000 -0.01676 2.06815

R79 2.07106 -0.00458 -0.01380 0.00000 -0.01380 2.05726

R80 2.08812 -0.00770 -0.02024 0.00000 -0.02024 2.06789

R81 2.08807 -0.00757 -0.01986 0.00000 -0.01986 2.06821

R82 2.07244 -0.00524 -0.01529 0.00000 -0.01529 2.05715

R83 2.08807 -0.00757 -0.01986 0.00000 -0.01986 2.06821

R84 2.08812 -0.00769 -0.02024 0.00000 -0.02024 2.06789

R85 2.07244 -0.00523 -0.01529 0.00000 -0.01529 2.05715

R86 2.08491 -0.00734 -0.01676 0.00000 -0.01676 2.06815

R87 2.08760 -0.00818 -0.01951 0.00000 -0.01951 2.06809

R88 2.07105 -0.00458 -0.01380 0.00000 -0.01380 2.05726

R89 2.08807 -0.00756 -0.01987 0.00000 -0.01987 2.06820

R90 2.08812 -0.00769 -0.02024 0.00000 -0.02024 2.06789

R91 2.07244 -0.00523 -0.01529 0.00000 -0.01529 2.05715

R92 2.08812 -0.00768 -0.02024 0.00000 -0.02024 2.06789

R93 2.08807 -0.00756 -0.01987 0.00000 -0.01987 2.06820

R94 2.07244 -0.00523 -0.01529 0.00000 -0.01529 2.05715

R95 2.08759 -0.00817 -0.01950 0.00000 -0.01950 2.06809

R96 2.08491 -0.00733 -0.01676 0.00000 -0.01676 2.06815

R97 2.07105 -0.00458 -0.01379 0.00000 -0.01379 2.05726

R98 2.08491 -0.00733 -0.01676 0.00000 -0.01676 2.06815

R99 2.08759 -0.00817 -0.01950 0.00000 -0.01950 2.06809

R100 2.07105 -0.00458 -0.01379 0.00000 -0.01379 2.05726

A1 1.89580 -0.00566 -0.00784 0.00000 -0.00786 1.88795

A2 2.19470 0.00725 0.01746 0.00000 0.01747 2.21218

A3 2.19267 -0.00160 -0.00963 0.00000 -0.00962 2.18305

A4 1.93328 0.00796 0.00028 0.00000 0.00032 1.93360

A5 2.17118 -0.00454 -0.00439 0.00000 -0.00440 2.16678

A6 2.16064 -0.00348 0.00586 0.00000 0.00583 2.16646

A7 1.89494 -0.00570 -0.00701 0.00000 -0.00704 1.88791

A8 2.19575 0.00751 0.01640 0.00000 0.01642 2.21216

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D111 -3.13454 -0.00131 0.01099 0.00000 0.01099 -3.12355

D112 0.00210 -0.00158 0.01057 0.00000 0.01058 0.01268

D113 0.20422 -0.00077 0.00065 0.00000 0.00067 0.20488

D114 -2.94233 -0.00104 0.00024 0.00000 0.00025 -2.94208

D115 -0.00215 0.00158 -0.01053 0.00000 -0.01053 -0.01268

D116 3.13399 0.00132 -0.01045 0.00000 -0.01045 3.12354

D117 2.94372 0.00089 -0.00159 0.00000 -0.00160 2.94212

D118 -0.20333 0.00063 -0.00151 0.00000 -0.00152 -0.20485

D119 2.92305 -0.00141 0.03326 0.00000 0.03323 2.95628

D120 -0.00500 0.00202 -0.02108 0.00000 -0.02105 -0.02605

D121 0.00471 -0.00210 0.02141 0.00000 0.02138 0.02608

D122 -2.92334 0.00133 -0.03294 0.00000 -0.03290 -2.95624

D123 3.13546 0.00071 -0.00663 0.00000 -0.00663 3.12883

D124 -0.01938 0.00067 -0.00011 0.00000 -0.00011 -0.01948

D125 -0.00121 0.00095 -0.00630 0.00000 -0.00630 -0.00751

D126 3.12714 0.00090 0.00022 0.00000 0.00023 3.12736

D127 -0.00007 0.00000 0.00006 0.00000 0.00006 0.00000

D128 3.13082 -0.00028 0.00505 0.00000 0.00504 3.13586

D129 -3.13081 0.00028 -0.00506 0.00000 -0.00505 -3.13586

D130 0.00008 0.00000 -0.00008 0.00000 -0.00008 0.00000

D131 3.13783 0.00017 -0.00514 0.00000 -0.00514 3.13269

D132 -0.01353 0.00065 -0.00572 0.00000 -0.00573 -0.01925

D133 -0.01838 0.00002 0.00197 0.00000 0.00198 -0.01641

D134 3.11345 0.00050 0.00140 0.00000 0.00139 3.11484

D135 0.00132 -0.00094 0.00619 0.00000 0.00620 0.00751

D136 -3.13486 -0.00072 0.00603 0.00000 0.00604 -3.12882

D137 -3.12721 -0.00088 -0.00016 0.00000 -0.00016 -3.12737

D138 0.01980 -0.00066 -0.00032 0.00000 -0.00032 0.01949

D139 0.01827 -0.00001 -0.00187 0.00000 -0.00187 0.01640

D140 -3.11355 -0.00048 -0.00130 0.00000 -0.00130 -3.11484

D141 -3.13775 -0.00018 0.00506 0.00000 0.00506 -3.13268

D142 0.01362 -0.00065 0.00563 0.00000 0.00563 0.01926

D143 0.21643 0.00047 -0.02387 0.00000 -0.02388 0.19255

D144 -2.93150 0.00016 -0.02377 0.00000 -0.02378 -2.95529

D145 -0.00506 -0.00002 -0.00038 0.00000 -0.00038 -0.00544

D146 -3.13927 -0.00006 0.00026 0.00000 0.00025 -3.13902

D147 3.12888 -0.00009 -0.00400 0.00000 -0.00400 3.12489

D148 -0.00532 -0.00013 -0.00337 0.00000 -0.00337 -0.00869

D149 -3.08587 -0.00037 -0.00656 0.00000 -0.00656 -3.09243

D150 0.06355 -0.00035 -0.00293 0.00000 -0.00293 0.06062

D151 0.00002 -0.00001 -0.00002 0.00000 -0.00002 0.00000

D152 -3.13428 -0.00008 0.00055 0.00000 0.00055 -3.13373

D153 3.13432 0.00006 -0.00058 0.00000 -0.00058 3.13374

D154 0.00001 -0.00001 -0.00001 0.00000 -0.00001 0.00000

D155 0.00508 0.00002 0.00036 0.00000 0.00036 0.00544

D156 -3.12886 0.00007 0.00399 0.00000 0.00398 -3.12488

D157 3.13930 0.00005 -0.00029 0.00000 -0.00028 3.13902

D158 0.00535 0.00011 0.00335 0.00000 0.00334 0.00870

D159 3.08588 0.00036 0.00656 0.00000 0.00655 3.09243

D160 -0.06354 0.00034 0.00292 0.00000 0.00292 -0.06062

D161 -0.01874 0.00012 0.00218 0.00000 0.00218 -0.01656

D162 3.13663 -0.00004 0.00252 0.00000 0.00252 3.13915

D163 3.11331 0.00011 0.00070 0.00000 0.00070 3.11401

D164 -0.01450 -0.00006 0.00104 0.00000 0.00104 -0.01346

D165 -3.09406 -0.00022 0.00392 0.00000 0.00392 -3.09015

D166 0.05735 -0.00033 0.00518 0.00000 0.00518 0.06253

D167 0.00002 0.00000 -0.00002 0.00000 -0.00002 0.00000

D168 -3.12795 -0.00027 0.00017 0.00000 0.00017 -3.12778

D169 3.12797 0.00027 -0.00019 0.00000 -0.00019 3.12778

D170 0.00001 0.00000 -0.00001 0.00000 -0.00001 0.00000

D171 0.01876 -0.00013 -0.00220 0.00000 -0.00220 0.01656

D172 -3.11331 -0.00012 -0.00070 0.00000 -0.00071 -3.11401

D173 -3.13660 0.00004 -0.00255 0.00000 -0.00255 -3.13915

D174 0.01452 0.00005 -0.00105 0.00000 -0.00105 0.01346

D175 3.09404 0.00021 -0.00390 0.00000 -0.00390 3.09014

D176 -0.05736 0.00033 -0.00518 0.00000 -0.00518 -0.06253

D177 0.00509 0.00002 0.00035 0.00000 0.00035 0.00544

D178 3.13928 0.00005 -0.00026 0.00000 -0.00026 3.13902

D179 -3.12887 0.00012 0.00397 0.00000 0.00396 -3.12490

D180 0.00533 0.00015 0.00336 0.00000 0.00335 0.00868

D181 3.08584 0.00040 0.00657 0.00000 0.00657 3.09241

D182 -0.06356 0.00034 0.00294 0.00000 0.00294 -0.06062

D183 -0.00002 0.00001 0.00002 0.00000 0.00002 0.00000

D184 3.13427 0.00006 -0.00053 0.00000 -0.00053 3.13374

D185 -3.13431 -0.00004 0.00056 0.00000 0.00056 -3.13374

D186 -0.00001 0.00001 0.00001 0.00000 0.00001 0.00000

D187 -0.00511 -0.00003 -0.00033 0.00000 -0.00033 -0.00544

D188 3.12885 -0.00011 -0.00395 0.00000 -0.00395 3.12490

D189 -3.13932 -0.00004 0.00029 0.00000 0.00029 -3.13902

D190 -0.00536 -0.00013 -0.00333 0.00000 -0.00333 -0.00869

D191 -3.08585 -0.00038 -0.00656 0.00000 -0.00656 -3.09241

D192 0.06355 -0.00034 -0.00293 0.00000 -0.00293 0.06062

D193 -0.01886 0.00013 0.00229 0.00000 0.00230 -0.01656

D194 3.13658 -0.00004 0.00257 0.00000 0.00257 3.13915

D195 3.11319 0.00012 0.00082 0.00000 0.00083 3.11401

D196 -0.01456 -0.00005 0.00109 0.00000 0.00110 -0.01346

D197 -3.09408 -0.00022 0.00393 0.00000 0.00393 -3.09015

D198 0.05735 -0.00033 0.00518 0.00000 0.00518 0.06253

D199 -0.00002 0.00001 0.00002 0.00000 0.00002 0.00000

D200 -3.12790 -0.00026 0.00012 0.00000 0.00011 -3.12778

D201 3.12787 0.00028 -0.00009 0.00000 -0.00009 3.12778

D202 -0.00001 0.00000 0.00001 0.00000 0.00001 0.00000

D203 0.01884 -0.00013 -0.00227 0.00000 -0.00228 0.01656

D204 -3.11319 -0.00010 -0.00081 0.00000 -0.00082 -3.11401

D205 -3.13661 0.00004 -0.00254 0.00000 -0.00254 -3.13915

D206 0.01455 0.00007 -0.00108 0.00000 -0.00108 0.01346

D207 3.09410 0.00023 -0.00395 0.00000 -0.00395 3.09015

D208 -0.05734 0.00033 -0.00518 0.00000 -0.00518 -0.06252

D209 1.09654 0.00267 0.00015 0.00000 0.00015 1.09669

D210 -1.04448 -0.00147 -0.00253 0.00000 -0.00253 -1.04700

D211 -3.11565 0.00044 -0.00135 0.00000 -0.00135 -3.11700

D212 1.04448 0.00147 0.00253 0.00000 0.00253 1.04700

D213 -1.09654 -0.00267 -0.00015 0.00000 -0.00015 -1.09669

D214 3.11564 -0.00044 0.00135 0.00000 0.00135 3.11700

D215 1.10294 0.00066 -0.00325 0.00000 -0.00325 1.09969

D216 -1.04713 -0.00017 0.00187 0.00000 0.00187 -1.04526

D217 -3.11253 -0.00005 -0.00213 0.00000 -0.00213 -3.11466

D218 1.04713 0.00018 -0.00187 0.00000 -0.00187 1.04526

D219 -1.10294 -0.00066 0.00325 0.00000 0.00325 -1.09969

D220 3.11253 0.00004 0.00214 0.00000 0.00213 3.11466

D221 1.04448 0.00147 0.00253 0.00000 0.00253 1.04700

D222 -1.09653 -0.00267 -0.00016 0.00000 -0.00016 -1.09669

D223 3.11565 -0.00044 0.00135 0.00000 0.00135 3.11700

D224 1.09654 0.00267 0.00015 0.00000 0.00015 1.09669

D225 -1.04448 -0.00147 -0.00253 0.00000 -0.00252 -1.04700

D226 -3.11564 0.00044 -0.00135 0.00000 -0.00136 -3.11700

D227 1.10294 0.00067 -0.00325 0.00000 -0.00325 1.09969

D228 -1.04713 -0.00018 0.00187 0.00000 0.00187 -1.04526

D229 -3.11252 -0.00004 -0.00214 0.00000 -0.00214 -3.11466

D230 1.04713 0.00018 -0.00188 0.00000 -0.00188 1.04526

D231 -1.10293 -0.00066 0.00325 0.00000 0.00325 -1.09969

D232 3.11253 0.00004 0.00213 0.00000 0.00213 3.11466

Item Value Threshold Converged?

Maximum Force 0.071639 0.000450 NO

RMS Force 0.012322 0.000300 NO

Maximum Displacement 0.868514 0.001800 NO

RMS Displacement 0.198716 0.001200 NO

Predicted change in Energy=-3.610518D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 00:42:40 2019, MaxMem= 1342177280 cpu: 13.1

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

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=0 Diff= 6.15D-04

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 -1.124265 2.807435 0.005991

2 7 0 -0.000162 2.048225 -0.152609

3 6 0 1.123989 2.807587 0.005999

4 6 0 0.714095 4.163948 0.307180

5 6 0 -0.714524 4.163849 0.307171

6 7 0 2.411223 2.386598 -0.102041

7 6 0 2.799166 1.132053 -0.177444

8 7 0 2.025532 -0.000143 -0.096680

9 6 0 2.799008 -1.132288 -0.177400

10 6 0 4.206528 -0.704934 -0.350121

11 6 0 4.206627 0.704537 -0.350143

12 7 0 -2.411160 2.386467 -0.102002

13 6 0 -4.206181 0.704496 -0.350021

14 6 0 -4.206084 -0.704883 -0.349998

15 6 0 -2.798606 -1.132294 -0.177291

16 7 0 -2.024886 -0.000141 -0.096558

17 6 0 -2.798761 1.132066 -0.177336

18 7 0 -2.411032 -2.386350 -0.101966

19 7 0 -0.000164 -2.047630 -0.152689

20 6 0 -1.124281 -2.807041 0.005961

21 6 0 -0.714488 -4.163419 0.307123

22 6 0 0.714050 -4.163520 0.307132

23 6 0 1.123999 -2.807197 0.005969

24 7 0 2.411090 -2.386487 -0.102004

25 30 0 0.000237 0.000171 -0.258467

26 6 0 -5.394093 1.432201 -0.489883

27 6 0 -6.584864 0.695490 -0.623239

28 6 0 -6.584774 -0.696183 -0.623227

29 6 0 -5.393909 -1.432740 -0.489854

30 6 0 1.434094 -5.343961 0.576337

31 6 0 0.700116 -6.509268 0.821250

32 6 0 -0.700863 -6.509174 0.821244

33 6 0 -1.434686 -5.343771 0.576326

34 6 0 5.394544 1.432233 -0.489989

35 6 0 6.585304 0.695491 -0.623330

36 6 0 6.585212 -0.696198 -0.623319

37 6 0 5.394356 -1.432784 -0.489960

38 6 0 -1.434715 5.344199 0.576384

39 6 0 -0.700864 6.509589 0.821313

40 6 0 0.700132 6.509681 0.821319

41 6 0 1.434135 5.344385 0.576395

42 1 0 7.532265 1.206772 -0.736908

43 1 0 7.532106 -1.207604 -0.736890

44 1 0 1.208754 7.441597 1.030656

45 1 0 -1.209608 7.441439 1.030647

46 1 0 -7.531817 1.206782 -0.736834

47 1 0 -7.531661 -1.207598 -0.736815

48 1 0 -1.209618 -7.441022 1.030566

49 1 0 1.208746 -7.441183 1.030575

50 8 0 2.781404 5.280073 0.594319

51 8 0 -2.781976 5.279717 0.594300

52 8 0 5.334566 2.779641 -0.502039

53 8 0 5.334212 -2.780183 -0.501992

54 8 0 2.781362 -5.279625 0.594256

55 8 0 -2.781946 -5.279261 0.594236

56 8 0 -5.333729 -2.780137 -0.501900

57 8 0 -5.334078 2.779606 -0.501948

58 6 0 3.512749 6.485834 0.803195

59 1 0 3.301582 6.919238 1.785667

60 1 0 3.298144 7.222646 0.022939

61 1 0 4.562377 6.201280 0.753390

62 6 0 6.554637 3.513873 -0.583473

63 1 0 7.082985 3.315095 -1.520906

64 1 0 7.212575 3.292115 0.262551

65 1 0 6.263806 4.562366 -0.549946

66 6 0 6.554193 -3.514565 -0.583422

67 1 0 7.212161 -3.292876 0.262595

68 1 0 7.082559 -3.315865 -1.520862

69 1 0 6.263232 -4.563023 -0.549879

70 6 0 -3.513474 6.485386 0.803164

71 1 0 -3.298957 7.222221 0.022905

72 1 0 -3.302369 6.918823 1.785635

73 1 0 -4.563065 6.200699 0.753353

74 6 0 -6.554128 3.513871 -0.583420

75 1 0 -7.212092 3.292140 0.262590

76 1 0 -7.082456 3.315095 -1.520865

77 1 0 -6.263270 4.562357 -0.549899

78 6 0 -6.553690 -3.514550 -0.583369

79 1 0 -7.082037 -3.315850 -1.520820

80 1 0 -7.211685 -3.292886 0.262635

81 1 0 -6.262706 -4.563001 -0.549832

82 6 0 -3.513470 -6.484921 0.803078

83 1 0 -3.302376 -6.918376 1.785543

84 1 0 -3.298963 -7.221746 0.022807

85 1 0 -4.563056 -6.200214 0.753267

86 6 0 3.512730 -6.485378 0.803110

87 1 0 3.298133 -7.222180 0.022842

88 1 0 3.301573 -6.918800 1.785575

89 1 0 4.562353 -6.200807 0.753305

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

Rotational constants (GHZ): 0.0446364 0.0438996 0.0225564

Leave Link 202 at Sat Jul 6 00:42:41 2019, MaxMem= 1342177280 cpu: 0.6

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

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

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8037.1412477894 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= 89 NActive= 89 NUniq= 89 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= -0.2277358168 Hartrees.

Nuclear repulsion after empirical dispersion term = 8036.9135119727 Hartrees.

No density basis found on file 724.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

Cavity 1st derivative terms included.

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

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

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6466

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.36D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 398

GePol: Fraction of low-weight points (<1% of avg) = 6.16%

GePol: Cavity surface area = 702.118 Ang\*\*2

GePol: Cavity volume = 801.354 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0089914110 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8036.9045205617 Hartrees.

Leave Link 301 at Sat Jul 6 00:42:41 2019, MaxMem= 1342177280 cpu: 1.3

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

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

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44278 LenP2D= 111183.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.90D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 00:42:45 2019, MaxMem= 1342177280 cpu: 41.6

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 00:42:45 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000001 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000122 -0.000151 0.000104 Ang= -0.03 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 6.82D-02

Max alpha theta= 4.932 degrees.

Max beta theta= 4.929 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0169 S= 1.0056

Leave Link 401 at Sat Jul 6 00:42:56 2019, MaxMem= 1342177280 cpu: 124.9

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 125427468.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.07D-14 for 515.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.09D-15 for 6444 6073.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.13D-14 for 498.

Iteration 1 A^-1\*A deviation from orthogonality is 1.71D-09 for 1467 1408.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.09D-14 for 535.

Iteration 2 A\*A^-1 deviation from orthogonality is 1.10D-14 for 4784 1582.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.22D-15 for 5377.

Iteration 2 A^-1\*A deviation from orthogonality is 4.56D-16 for 4448 2126.

E= -2649.79424470892

DIIS: error= 7.40D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79424470892 IErMin= 1 ErrMin= 7.40D-05

ErrMax= 7.40D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.79D-05 BMatP= 2.79D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 14.171 Goal= None Shift= 0.000

Gap= 14.033 Goal= None Shift= 0.000

RMSDP=9.79D-06 MaxDP=4.39D-04 OVMax= 4.26D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 9.75D-06 CP: 1.00D+00

E= -2649.79425179831 Delta-E= -0.000007089389 Rises=F Damp=F

DIIS: error= 4.55D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79425179831 IErMin= 2 ErrMin= 4.55D-05

ErrMax= 4.55D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.24D-06 BMatP= 2.79D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.183D+00 0.817D+00

Coeff: 0.183D+00 0.817D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.05D-06 MaxDP=1.52D-04 DE=-7.09D-06 OVMax= 2.67D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.02D-06 CP: 1.00D+00 9.97D-01

E= -2649.79425154287 Delta-E= 0.000000255443 Rises=F Damp=F

DIIS: error= 4.85D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -2649.79425179831 IErMin= 2 ErrMin= 4.55D-05

ErrMax= 4.85D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.63D-06 BMatP= 4.24D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.298D-02 0.537D+00 0.466D+00

Coeff: -0.298D-02 0.537D+00 0.466D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.19D-06 MaxDP=1.03D-04 DE= 2.55D-07 OVMax= 1.72D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.21D-07 CP: 1.00D+00 1.01D+00 4.50D-01

E= -2649.79425251979 Delta-E= -0.000000976921 Rises=F Damp=F

DIIS: error= 6.59D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79425251979 IErMin= 4 ErrMin= 6.59D-06

ErrMax= 6.59D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.36D-08 BMatP= 4.24D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.796D-02 0.201D+00 0.213D+00 0.594D+00

Coeff: -0.796D-02 0.201D+00 0.213D+00 0.594D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.71D-07 MaxDP=1.25D-05 DE=-9.77D-07 OVMax= 2.87D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.10D-07 CP: 1.00D+00 1.02D+00 4.82D-01 6.56D-01

E= -2649.79425253686 Delta-E= -0.000000017075 Rises=F Damp=F

DIIS: error= 1.47D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79425253686 IErMin= 5 ErrMin= 1.47D-06

ErrMax= 1.47D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.81D-09 BMatP= 9.36D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.318D-02 0.597D-01 0.712D-01 0.301D+00 0.571D+00

Coeff: -0.318D-02 0.597D-01 0.712D-01 0.301D+00 0.571D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.16D-08 MaxDP=4.75D-06 DE=-1.71D-08 OVMax= 7.14D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.66D-08 CP: 1.00D+00 1.02D+00 4.76D-01 7.21D-01 8.07D-01

E= -2649.79425253906 Delta-E= -0.000000002196 Rises=F Damp=F

DIIS: error= 3.14D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79425253906 IErMin= 6 ErrMin= 3.14D-07

ErrMax= 3.14D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.73D-10 BMatP= 8.81D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.995D-03 0.167D-01 0.206D-01 0.102D+00 0.243D+00 0.619D+00

Coeff: -0.995D-03 0.167D-01 0.206D-01 0.102D+00 0.243D+00 0.619D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.18D-08 MaxDP=1.03D-06 DE=-2.20D-09 OVMax= 5.26D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.01D-08 CP: 1.00D+00 1.02D+00 4.75D-01 7.19D-01 8.13D-01

CP: 7.86D-01

E= -2649.79425253897 Delta-E= 0.000000000093 Rises=F Damp=F

DIIS: error= 1.87D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 6 EnMin= -2649.79425253906 IErMin= 7 ErrMin= 1.87D-07

ErrMax= 1.87D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.57D-11 BMatP= 2.73D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.440D-06-0.192D-02-0.194D-02 0.147D-02 0.381D-01 0.393D+00

Coeff-Com: 0.572D+00

Coeff: 0.440D-06-0.192D-02-0.194D-02 0.147D-02 0.381D-01 0.393D+00

Coeff: 0.572D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=5.83D-09 MaxDP=4.95D-07 DE= 9.28D-11 OVMax= 2.80D-06

Error on total polarization charges = 0.07288

SCF Done: E(UB3LYP) = -2649.79425254 A.U. after 7 cycles

NFock= 7 Conv=0.58D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0169 S= 1.0056

<L.S>= 0.000000000000E+00

KE= 2.690075481703D+03 PE=-2.235241956318D+04 EE= 8.975645308374D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0169, after 2.0002

Leave Link 502 at Sat Jul 6 00:49:05 2019, MaxMem= 1342177280 cpu: 4324.5

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44278 LenP2D= 111183.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 284

Leave Link 701 at Sat Jul 6 00:49:24 2019, MaxMem= 1342177280 cpu: 220.5

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 00:49:24 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 00:50:58 2019, MaxMem= 1342177280 cpu: 1123.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-8.97223080D-04-1.76895211D-03 8.60108631D-02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.001776332 -0.001556253 0.002024241

2 7 0.000099877 -0.000260584 -0.000998358

3 6 0.001951860 -0.001715399 0.001994475

4 6 -0.001248447 0.000576524 -0.000687209

5 6 0.001265020 0.000603685 -0.000680788

6 7 -0.001277334 -0.001007466 0.000008231

7 6 0.000446414 0.000878450 -0.001595150

8 7 -0.000658680 0.000118029 0.004576109

9 6 0.000638804 -0.000647804 -0.001627764

10 6 -0.000823224 -0.001111028 0.000536522

11 6 -0.000845123 0.001126625 0.000538322

12 7 0.001151872 -0.000908832 0.000006628

13 6 0.000836783 0.001148659 0.000535780

14 6 0.000814697 -0.001132904 0.000533912

15 6 -0.000702393 -0.000394957 -0.001640745

16 7 0.000459305 0.000117342 0.004563265

17 6 -0.000510540 0.000627215 -0.001608162

18 7 0.001132592 0.000670745 0.000010864

19 7 0.000099070 0.000055031 -0.000964738

20 6 -0.001585095 0.001515694 0.002025678

21 6 0.001248633 -0.000610488 -0.000677411

22 6 -0.001231868 -0.000583098 -0.000683966

23 6 0.001761954 0.001674089 0.001995980

24 7 -0.001258548 0.000770301 0.000012520

25 30 0.000012126 0.000033103 -0.008361803

26 6 -0.000483124 -0.001237925 -0.000438354

27 6 0.000373985 0.000280868 0.000111026

28 6 0.000374322 -0.000279135 0.000111012

29 6 -0.000476775 0.001243501 -0.000437385

30 6 -0.001218492 0.000509760 0.000164645

31 6 -0.000036704 -0.000325116 0.000116405

32 6 0.000037895 -0.000328596 0.000117114

33 6 0.001221499 0.000520351 0.000161750

34 6 0.000482793 -0.001249563 -0.000437704

35 6 -0.000372662 0.000265623 0.000110576

36 6 -0.000373101 -0.000263878 0.000110565

37 6 0.000476548 0.001255221 -0.000436750

38 6 0.001234255 -0.000519799 0.000162000

39 6 0.000049898 0.000329394 0.000117533

40 6 -0.000048688 0.000326045 0.000116842

41 6 -0.001231119 -0.000509356 0.000164860

42 1 -0.000180695 -0.000266229 0.000034114

43 1 -0.000180150 0.000266310 0.000034145

44 1 -0.000280636 -0.000202519 -0.000123710

45 1 0.000280869 -0.000202352 -0.000123656

46 1 0.000181012 -0.000265327 0.000034224

47 1 0.000180487 0.000265417 0.000034257

48 1 0.000280103 0.000202757 -0.000123691

49 1 -0.000279865 0.000202924 -0.000123749

50 8 0.000682416 0.000669296 -0.000273440

51 8 -0.000679527 0.000672808 -0.000272906

52 8 0.000248396 -0.000258818 0.000182128

53 8 0.000253002 0.000259909 0.000182090

54 8 0.000680841 -0.000675259 -0.000271951

55 8 -0.000677891 -0.000678753 -0.000271412

56 8 -0.000264705 0.000259190 0.000180992

57 8 -0.000260115 -0.000258102 0.000181036

58 6 0.000513987 0.000236202 0.000125221

59 1 0.000034109 -0.000204995 -0.000213374

60 1 0.000095437 -0.000218597 0.000274148

61 1 -0.000095769 0.000201967 0.000032895

62 6 0.000358935 0.000436377 0.000006744

63 1 -0.000192566 0.000032250 0.000182922

64 1 -0.000277837 0.000021866 -0.000144916

65 1 0.000192935 -0.000114448 0.000003895

66 6 0.000357079 -0.000436532 0.000007375

67 1 -0.000277713 -0.000021678 -0.000144760

68 1 -0.000192281 -0.000032102 0.000182783

69 1 0.000193325 0.000114426 0.000004470

70 6 -0.000513847 0.000235122 0.000124851

71 1 -0.000095785 -0.000218338 0.000274170

72 1 -0.000034181 -0.000204798 -0.000213183

73 1 0.000096078 0.000201968 0.000032278

74 6 -0.000355565 0.000434613 0.000007001

75 1 0.000277246 0.000021795 -0.000144632

76 1 0.000191812 0.000032087 0.000182678

77 1 -0.000192731 -0.000114560 0.000004561

78 6 -0.000353721 -0.000434768 0.000007630

79 1 0.000191533 -0.000031944 0.000182544

80 1 0.000277119 -0.000021617 -0.000144479

81 1 -0.000193107 0.000114543 0.000005138

82 6 -0.000512343 -0.000232618 0.000124299

83 1 -0.000034140 0.000204219 -0.000212772

84 1 -0.000095765 0.000217830 0.000274034

85 1 0.000096401 -0.000201210 0.000031546

86 6 0.000512478 -0.000233691 0.000124676

87 1 0.000095403 0.000218095 0.000274010

88 1 0.000034064 0.000204418 -0.000212965

89 1 -0.000096087 -0.000201203 0.000032171

-------------------------------------------------------------------

Cartesian Forces: Max 0.008361803 RMS 0.000909836

Leave Link 716 at Sat Jul 6 00:50:58 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002239354 RMS 0.000417455

Search for a local minimum.

Step number 9 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .41746D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 2 3 4 6

5 8 7 9

ITU= 0 0 0 0 1 1 1 1 0

Use linear search instead of GDIIS.

Eigenvalues --- -0.42804 0.00003 0.00219 0.00690 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01316 0.01316

Eigenvalues --- 0.01316 0.01325 0.01570 0.01571 0.01582

Eigenvalues --- 0.01584 0.01600 0.01616 0.01621 0.01707

Eigenvalues --- 0.01709 0.01712 0.01715 0.01755 0.01834

Eigenvalues --- 0.01873 0.01887 0.01921 0.01923 0.01930

Eigenvalues --- 0.01943 0.01993 0.02010 0.02017 0.02020

Eigenvalues --- 0.02022 0.02026 0.02028 0.02053 0.02053

Eigenvalues --- 0.02053 0.02053 0.02057 0.02057 0.02057

Eigenvalues --- 0.02057 0.02059 0.02067 0.02067 0.02067

Eigenvalues --- 0.02069 0.02070 0.02071 0.02071 0.02071

Eigenvalues --- 0.02074 0.02084 0.02084 0.02189 0.02237

Eigenvalues --- 0.02260 0.02260 0.02260 0.02260 0.02260

Eigenvalues --- 0.02260 0.02287 0.02344 0.02351 0.02366

Eigenvalues --- 0.04115 0.09806 0.09974 0.09974 0.09974

Eigenvalues --- 0.09988 0.09988 0.09988 0.09995 0.10649

Eigenvalues --- 0.10658 0.10658 0.10658 0.10661 0.10661

Eigenvalues --- 0.10661 0.10663 0.13277 0.13464 0.13510

Eigenvalues --- 0.14594 0.15970 0.15987 0.15994 0.15998

Eigenvalues --- 0.15998 0.15999 0.15999 0.15999 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16003

Eigenvalues --- 0.16015 0.16052 0.16468 0.21477 0.21723

Eigenvalues --- 0.22473 0.22474 0.22474 0.22475 0.22653

Eigenvalues --- 0.24277 0.24410 0.24453 0.24503 0.24510

Eigenvalues --- 0.24514 0.24595 0.24708 0.24777 0.24844

Eigenvalues --- 0.24855 0.24912 0.24961 0.24997 0.24997

Eigenvalues --- 0.24997 0.24997 0.24998 0.24998 0.24998

Eigenvalues --- 0.24998 0.24998 0.24998 0.24999 0.24999

Eigenvalues --- 0.24999 0.24999 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25277 0.29313

Eigenvalues --- 0.32661 0.33627 0.33636 0.33682 0.33720

Eigenvalues --- 0.33735 0.34061 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34063 0.34063 0.34075 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34081

Eigenvalues --- 0.34090 0.34561 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34686 0.34687 0.34754

Eigenvalues --- 0.34916 0.34960 0.35381 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35632 0.35672

Eigenvalues --- 0.35990 0.37095 0.37145 0.37212 0.37779

Eigenvalues --- 0.41000 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41215 0.41215 0.41235 0.41363 0.41413

Eigenvalues --- 0.41415 0.41416 0.41418 0.42454 0.42474

Eigenvalues --- 0.42924 0.43759 0.44549 0.44571 0.44754

Eigenvalues --- 0.44847 0.44916 0.44998 0.45000 0.45001

Eigenvalues --- 0.45003 0.45364 0.45366 0.45506 0.46232

Eigenvalues --- 0.46963 0.47328 0.47972 0.49241 0.49304

Eigenvalues --- 0.49848 0.50930 0.53424 0.53554 0.53554

Eigenvalues --- 0.53554 0.53554 0.53554 0.53554 0.54923

Eigenvalues --- 0.55022 0.56072 0.57378 0.57430 0.57567

Eigenvalues --- 0.58386

Eigenvalue 1 is -4.28D-01 should be greater than 0.000000 Eigenvector:

R11 R21 R17 R28 R31

1 0.27014 0.25317 0.24752 0.23052 -0.21934

R3 R40 R7 R57 R43

1 -0.20708 -0.20184 -0.18958 0.12496 0.12373

RFO step: Lambda=-4.28060981D-01 EMin=-4.28041549D-01

I= 1 Eig= -4.28D-01 Dot1= -1.73D-03

I= 1 Stepn= -6.00D-01 RXN= 6.00D-01 EDone=F

Mixed 1 eigenvectors in step. Raw Step.Grad= 1.73D-03.

RFO eigenvector is Hessian eigenvector with negative curvature.

Taking step of 6.00D-01 in eigenvector direction(s). Step.Grad= -6.90D-04.

Quartic linear search produced a step of 0.02666.

Maximum step size ( 0.457) exceeded in Quadratic search.

-- Step size not scaled.

Iteration 1 RMS(Cart)= 0.09655565 RMS(Int)= 0.00163819

Iteration 2 RMS(Cart)= 0.00402079 RMS(Int)= 0.00023663

Iteration 3 RMS(Cart)= 0.00000319 RMS(Int)= 0.00023662

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00023662

ITry= 1 IFail=0 DXMaxC= 4.06D-01 DCOld= 1.00D+10 DXMaxT= 4.57D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58082 0.00008 0.00003 -0.00707 -0.00651 2.57431

R2 2.73747 0.00081 0.00007 -0.04094 -0.04100 2.69647

R3 2.56681 -0.00121 0.00003 0.12425 0.12388 2.69069

R4 2.58105 0.00002 0.00004 -0.00967 -0.00918 2.57187

R5 3.87543 -0.00109 0.00021 -0.02004 -0.01856 3.85687

R6 2.73745 0.00079 0.00007 -0.04233 -0.04238 2.69508

R7 2.56744 -0.00149 0.00005 0.11375 0.11324 2.68067

R8 2.69970 -0.00064 0.00009 0.01032 0.01011 2.70981

R9 2.66201 0.00042 0.00005 0.04206 0.04218 2.70419

R10 2.66202 0.00041 0.00005 0.04177 0.04189 2.70391

R11 2.48560 -0.00136 0.00022 -0.16208 -0.16261 2.32299

R12 2.59581 -0.00007 -0.00002 0.03937 0.03929 2.63511

R13 2.79880 -0.00069 0.00006 0.05771 0.05765 2.85645

R14 2.59556 0.00002 -0.00003 0.04294 0.04294 2.63850

R15 3.83944 -0.00029 0.00025 0.04515 0.04604 3.88548

R16 2.79882 -0.00068 0.00006 0.05906 0.05902 2.85784

R17 2.48496 -0.00099 0.00019 -0.14851 -0.14893 2.33603

R18 2.66351 0.00045 0.00000 0.00329 0.00294 2.66646

R19 2.64579 0.00002 0.00008 -0.02031 -0.02022 2.62557

R20 2.64578 0.00003 0.00008 -0.02016 -0.02007 2.62571

R21 2.48514 -0.00109 0.00020 -0.15190 -0.15235 2.33279

R22 2.66334 0.00050 -0.00001 0.00595 0.00568 2.66902

R23 2.79875 -0.00067 0.00005 0.05895 0.05892 2.85767

R24 2.64579 0.00004 0.00008 -0.01956 -0.01948 2.62631

R25 2.79877 -0.00065 0.00006 0.06031 0.06029 2.85906

R26 2.64579 0.00003 0.00008 -0.01972 -0.01963 2.62616

R27 2.59583 -0.00004 -0.00002 0.04073 0.04061 2.63645

R28 2.48450 -0.00072 0.00018 -0.13831 -0.13866 2.34584

R29 2.59609 -0.00013 -0.00001 0.03719 0.03700 2.63309

R30 3.83914 -0.00019 0.00025 0.05097 0.05158 3.89072

R31 2.56638 -0.00100 0.00001 0.13160 0.13131 2.69769

R32 2.58106 0.00004 0.00004 -0.00902 -0.00849 2.57257

R33 2.58130 -0.00003 0.00005 -0.01158 -0.01113 2.57017

R34 3.87494 -0.00097 0.00021 -0.01289 -0.01163 3.86331

R35 2.73742 0.00083 0.00006 -0.04019 -0.04023 2.69719

R36 2.69955 -0.00060 0.00009 0.01218 0.01202 2.71157

R37 2.66202 0.00041 0.00005 0.04199 0.04211 2.70414

R38 2.73741 0.00081 0.00006 -0.04158 -0.04162 2.69579

R39 2.66202 0.00042 0.00005 0.04229 0.04241 2.70443

R40 2.56701 -0.00129 0.00004 0.12110 0.12067 2.68767

R41 2.65805 -0.00088 -0.00002 0.02325 0.02323 2.68128

R42 2.54885 0.00010 -0.00003 -0.03960 -0.03963 2.50922

R43 2.62988 -0.00073 0.00004 -0.07424 -0.07420 2.55568

R44 2.04496 -0.00029 0.00003 -0.00784 -0.00781 2.03715

R45 2.65805 -0.00087 -0.00002 0.02345 0.02344 2.68149

R46 2.04496 -0.00029 0.00003 -0.00782 -0.00779 2.03717

R47 2.54885 0.00010 -0.00003 -0.03967 -0.03970 2.50915

R48 2.64335 -0.00005 -0.00003 -0.00788 -0.00799 2.63536

R49 2.54909 0.00119 -0.00008 -0.01688 -0.01695 2.53214

R50 2.64747 -0.00060 -0.00003 -0.02257 -0.02275 2.62472

R51 2.04491 -0.00033 0.00003 -0.00968 -0.00964 2.03527

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R53 2.04491 -0.00033 0.00003 -0.00968 -0.00964 2.03527

R54 2.54909 0.00119 -0.00008 -0.01704 -0.01712 2.53198

R55 2.65806 -0.00088 -0.00002 0.02332 0.02330 2.68136

R56 2.54885 0.00010 -0.00003 -0.03951 -0.03954 2.50931

R57 2.62991 -0.00075 0.00004 -0.07498 -0.07494 2.55497

R58 2.04496 -0.00029 0.00003 -0.00785 -0.00782 2.03715

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R64 2.64750 -0.00062 -0.00003 -0.02330 -0.02348 2.62402

R65 2.04491 -0.00033 0.00003 -0.00968 -0.00964 2.03527

R66 2.64336 -0.00005 -0.00003 -0.00791 -0.00801 2.63535

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R69 2.69401 0.00033 -0.00001 -0.00844 -0.00845 2.68556

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R71 2.69530 0.00026 -0.00002 0.00355 0.00353 2.69883

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R76 2.69530 0.00026 -0.00002 0.00340 0.00339 2.69868

R77 2.06809 -0.00028 0.00004 -0.01195 -0.01191 2.05618

R78 2.06815 -0.00036 0.00003 -0.01516 -0.01512 2.05302

R79 2.05726 -0.00015 0.00003 -0.00800 -0.00797 2.04929

R80 2.06789 -0.00026 0.00004 -0.01314 -0.01310 2.05479

R81 2.06821 -0.00028 0.00004 -0.01393 -0.01389 2.05432

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R87 2.06809 -0.00028 0.00004 -0.01194 -0.01190 2.05619

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A3 2.18305 0.00005 0.00002 0.01259 0.01175 2.19480

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A6 2.16646 -0.00010 -0.00001 0.01145 0.01170 2.17816

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A11 2.31818 0.00000 0.00006 0.02643 0.02634 2.34452

A12 2.10738 -0.00010 -0.00004 -0.01918 -0.01902 2.08836

A13 1.85763 0.00009 -0.00001 -0.00785 -0.00804 1.84959

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A15 2.10737 -0.00010 -0.00005 -0.01940 -0.01924 2.08813

A16 2.18897 0.00025 0.00009 0.01974 0.01949 2.20846

A17 2.23529 -0.00026 -0.00005 0.00990 0.00939 2.24469

A18 2.16794 0.00020 0.00005 0.01373 0.01333 2.18127

A19 1.87984 0.00005 0.00001 -0.02415 -0.02388 1.85596

A20 1.93775 -0.00003 0.00001 0.02466 0.02442 1.96217

A21 2.16108 -0.00002 -0.00002 -0.01195 -0.01172 2.14937

A22 2.16132 -0.00007 0.00000 -0.01381 -0.01385 2.14747

A23 1.87988 0.00003 0.00001 -0.02530 -0.02502 1.85486

A24 2.23531 -0.00031 -0.00006 0.00758 0.00710 2.24240

A25 2.16789 0.00027 0.00005 0.01720 0.01676 2.18465

A26 1.86357 -0.00003 -0.00001 0.01220 0.01201 1.87558

A27 2.30219 0.00046 0.00004 -0.01068 -0.01058 2.29161

A28 2.11741 -0.00043 -0.00003 -0.00157 -0.00153 2.11588

A29 1.86355 -0.00002 -0.00001 0.01284 0.01264 1.87619

A30 2.30220 0.00044 0.00004 -0.01174 -0.01163 2.29057

A31 2.11743 -0.00043 -0.00003 -0.00115 -0.00110 2.11633

A32 2.18881 0.00029 0.00008 0.02261 0.02243 2.21124

A33 1.86359 -0.00003 -0.00001 0.01245 0.01224 1.87583

A34 2.11743 -0.00043 -0.00003 -0.00131 -0.00126 2.11617

A35 2.30215 0.00046 0.00004 -0.01119 -0.01107 2.29108

A36 1.86362 -0.00005 -0.00001 0.01182 0.01162 1.87523

A37 2.11742 -0.00043 -0.00003 -0.00172 -0.00168 2.11574

A38 2.30214 0.00048 0.00004 -0.01015 -0.01003 2.29211

A39 1.87998 0.00002 0.00001 -0.02659 -0.02639 1.85359

A40 2.16771 0.00032 0.00004 0.02073 0.02045 2.18816

A41 2.23539 -0.00035 -0.00005 0.00534 0.00478 2.24016

A42 1.93747 0.00003 0.00000 0.02802 0.02796 1.96542

A43 2.16145 -0.00010 0.00001 -0.01547 -0.01559 2.14586

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A48 2.18871 0.00031 0.00007 0.02478 0.02467 2.21338

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A53 2.18293 0.00008 0.00001 0.01500 0.01421 2.19713

A54 1.88803 -0.00021 0.00002 0.01963 0.01984 1.90787

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A66 1.56664 -0.00012 -0.00001 -0.00321 -0.00384 1.56280

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A69 2.04375 0.00038 0.00004 -0.00482 -0.00483 2.03892

A70 2.07415 0.00005 0.00006 0.05376 0.05378 2.12793

A71 2.16523 -0.00043 -0.00011 -0.04877 -0.04891 2.11632

A72 2.12199 0.00005 -0.00002 0.00618 0.00614 2.12814

A73 2.09820 0.00013 -0.00001 -0.00520 -0.00520 2.09300

A74 2.06296 -0.00017 0.00002 -0.00094 -0.00091 2.06205

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A78 2.04376 0.00038 0.00004 -0.00474 -0.00474 2.03902

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A90 2.05257 0.00010 0.00004 0.01977 0.01982 2.07239

A91 2.06359 0.00045 0.00012 0.02480 0.02492 2.08851

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A93 2.04374 0.00039 0.00004 -0.00455 -0.00456 2.03918

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A110 2.06018 -0.00014 0.00002 -0.00605 -0.00593 2.05425

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A147 1.90966 -0.00008 0.00001 -0.00572 -0.00578 1.90388

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D3 3.12354 0.00064 0.00002 0.00814 0.00824 3.13177

D4 -0.20482 0.00027 0.00000 -0.02395 -0.02353 -0.22836

D5 0.00751 -0.00052 -0.00001 -0.01969 -0.01989 -0.01238

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D29 3.13269 0.00027 0.00001 0.01489 0.01491 -3.13559

D30 -0.01926 0.00027 0.00001 0.01143 0.01138 -0.00787

D31 -0.01640 -0.00002 0.00000 -0.00413 -0.00412 -0.02052

D32 3.11484 -0.00003 0.00000 -0.00759 -0.00765 3.10719

D33 -3.13269 -0.00027 -0.00001 -0.01492 -0.01497 3.13553

D34 0.01925 -0.00027 -0.00001 -0.01151 -0.01147 0.00778

D35 0.01641 0.00002 0.00000 0.00406 0.00402 0.02043

D36 -3.11484 0.00003 0.00000 0.00747 0.00752 -3.10732

D37 -0.06314 0.00026 0.00001 0.00544 0.00526 -0.05789

D38 3.09615 0.00085 0.00003 0.04900 0.04932 -3.13771

D39 -3.10804 0.00025 0.00002 0.02558 0.02549 -3.08255

D40 0.25526 0.00082 0.00006 0.03207 0.03220 0.28746

D41 0.01819 -0.00027 0.00000 -0.01197 -0.01188 0.00631

D42 -2.90170 0.00030 0.00004 -0.00549 -0.00517 -2.90687

D43 3.11621 -0.00034 -0.00002 -0.02860 -0.02864 3.08757

D44 -0.01974 -0.00020 -0.00001 -0.01838 -0.01827 -0.03801

D45 -0.01075 0.00016 0.00000 0.00717 0.00702 -0.00373

D46 3.13648 0.00029 0.00001 0.01739 0.01739 -3.12931

D47 -0.01819 0.00027 0.00000 0.01203 0.01193 -0.00626

D48 3.10806 -0.00025 -0.00002 -0.02554 -0.02539 3.08267

D49 2.90166 -0.00030 -0.00004 0.00583 0.00555 2.90721

D50 -0.25527 -0.00081 -0.00006 -0.03174 -0.03177 -0.28704

D51 -0.17635 -0.00112 -0.00008 -0.02893 -0.02878 -0.20512

D52 3.06820 0.00050 0.00004 0.02694 0.02674 3.09494

D53 -3.06825 -0.00049 -0.00004 -0.02637 -0.02611 -3.09436

D54 0.17629 0.00114 0.00008 0.02950 0.02942 0.20571

D55 0.01076 -0.00016 0.00000 -0.00733 -0.00717 0.00360

D56 -3.13647 -0.00029 -0.00001 -0.01757 -0.01759 3.12913

D57 -3.11623 0.00034 0.00002 0.02852 0.02866 -3.08757

D58 0.01973 0.00020 0.00001 0.01827 0.01824 0.03797

D59 0.06317 -0.00026 -0.00001 -0.00571 -0.00560 0.05757

D60 -3.09609 -0.00086 -0.00003 -0.04933 -0.04978 3.13731

D61 -0.00001 0.00000 0.00000 0.00008 0.00009 0.00008

D62 3.13667 -0.00011 -0.00001 -0.00887 -0.00909 3.12758

D63 -3.13669 0.00011 0.00001 0.00905 0.00928 -3.12741

D64 -0.00001 0.00000 0.00000 0.00010 0.00011 0.00010

D65 -3.12985 0.00014 0.00001 0.01295 0.01309 -3.11675

D66 0.02239 -0.00005 0.00000 -0.00274 -0.00310 0.01929

D67 0.00543 0.00000 0.00000 0.00150 0.00150 0.00693

D68 -3.12552 -0.00020 -0.00001 -0.01419 -0.01470 -3.14021

D69 3.12985 -0.00015 -0.00001 -0.01305 -0.01318 3.11667

D70 -0.02238 0.00005 0.00000 0.00257 0.00294 -0.01944

D71 -0.00541 0.00000 0.00000 -0.00162 -0.00163 -0.00705

D72 3.12554 0.00019 0.00001 0.01400 0.01449 3.14002

D73 -3.09615 -0.00085 -0.00003 -0.04864 -0.04901 3.13802

D74 0.06311 -0.00025 -0.00001 -0.00511 -0.00495 0.05817

D75 0.00001 0.00000 0.00000 -0.00008 -0.00009 -0.00008

D76 3.13671 -0.00011 -0.00001 -0.00904 -0.00930 3.12741

D77 -3.13669 0.00011 0.00001 0.00886 0.00911 -3.12758

D78 0.00001 0.00000 0.00000 -0.00010 -0.00011 -0.00010

D79 -3.11623 0.00033 0.00002 0.02840 0.02857 -3.08767

D80 0.01076 -0.00016 0.00000 -0.00735 -0.00716 0.00360

D81 0.01974 0.00020 0.00001 0.01819 0.01816 0.03790

D82 -3.13645 -0.00029 -0.00001 -0.01757 -0.01757 3.12917

D83 0.00542 0.00000 0.00000 0.00164 0.00164 0.00706

D84 -3.12552 -0.00019 -0.00001 -0.01406 -0.01457 -3.14009

D85 -3.12988 0.00014 0.00001 0.01305 0.01322 -3.11666

D86 0.02237 -0.00005 0.00000 -0.00264 -0.00299 0.01938

D87 -0.01077 0.00016 0.00000 0.00751 0.00731 -0.00346

D88 3.11625 -0.00033 -0.00002 -0.02832 -0.02859 3.08766

D89 3.13643 0.00030 0.00001 0.01775 0.01776 -3.12899

D90 -0.01973 -0.00020 -0.00001 -0.01808 -0.01814 -0.03787

D91 -0.00543 0.00000 0.00000 -0.00152 -0.00150 -0.00694

D92 3.12550 0.00020 0.00001 0.01425 0.01478 3.14028

D93 3.12987 -0.00014 -0.00001 -0.01296 -0.01313 3.11674

D94 -0.02238 0.00005 0.00000 0.00281 0.00315 -0.01923

D95 0.01820 -0.00027 0.00000 -0.01229 -0.01216 0.00604

D96 -2.90157 0.00029 0.00005 -0.00622 -0.00587 -2.90744

D97 -3.10808 0.00024 0.00002 0.02520 0.02501 -3.08307

D98 0.25533 0.00080 0.00006 0.03128 0.03129 0.28663

D99 3.09609 0.00085 0.00003 0.04897 0.04946 -3.13763

D100 -0.06314 0.00026 0.00001 0.00539 0.00529 -0.05785

D101 3.10806 -0.00024 -0.00002 -0.02525 -0.02511 3.08295

D102 -0.01820 0.00027 0.00000 0.01223 0.01210 -0.00609

D103 -0.25532 -0.00081 -0.00006 -0.03160 -0.03172 -0.28704

D104 2.90161 -0.00030 -0.00004 0.00588 0.00550 2.90710

D105 3.06815 0.00050 0.00003 0.02714 0.02702 3.09517

D106 -0.17634 -0.00114 -0.00008 -0.02951 -0.02955 -0.20589

D107 0.17639 0.00113 0.00008 0.02894 0.02891 0.20530

D108 -3.06810 -0.00052 -0.00003 -0.02771 -0.02766 -3.09576

D109 -0.19258 -0.00057 -0.00005 -0.03688 -0.03686 -0.22943

D110 2.95525 -0.00030 -0.00005 -0.00780 -0.00818 2.94707

D111 -3.12355 -0.00065 -0.00002 -0.00873 -0.00904 -3.13259

D112 0.01268 -0.00088 -0.00002 -0.03375 -0.03364 -0.02096

D113 0.20488 -0.00028 0.00000 0.02332 0.02277 0.22765

D114 -2.94208 -0.00051 0.00000 -0.00170 -0.00183 -2.94391

D115 -0.01268 0.00088 0.00002 0.03373 0.03363 0.02095

D116 3.12354 0.00065 0.00002 0.00863 0.00891 3.13245

D117 2.94212 0.00050 0.00000 0.00145 0.00152 2.94363

D118 -0.20485 0.00027 0.00000 -0.02365 -0.02320 -0.22805

D119 2.95628 -0.00132 -0.00007 -0.04263 -0.04262 2.91366

D120 -0.02605 0.00092 0.00004 0.00237 0.00200 -0.02405

D121 0.02608 -0.00093 -0.00004 -0.00282 -0.00237 0.02371

D122 -2.95624 0.00131 0.00007 0.04218 0.04225 -2.91400

D123 3.12883 0.00030 0.00001 -0.00480 -0.00500 3.12383

D124 -0.01948 0.00003 0.00000 -0.02195 -0.02234 -0.04182

D125 -0.00751 0.00052 0.00001 0.01989 0.02013 0.01262

D126 3.12736 0.00026 0.00000 0.00274 0.00279 3.13015

D127 0.00000 0.00000 0.00000 -0.00002 -0.00003 -0.00003

D128 3.13586 -0.00023 -0.00001 -0.01449 -0.01412 3.12174

D129 -3.13586 0.00023 0.00001 0.01440 0.01402 -3.12184

D130 0.00000 0.00000 0.00000 -0.00006 -0.00007 -0.00007

D131 3.13269 0.00027 0.00001 0.01499 0.01505 -3.13545

D132 -0.01925 0.00027 0.00001 0.01162 0.01161 -0.00764

D133 -0.01641 -0.00002 0.00000 -0.00409 -0.00406 -0.02047

D134 3.11484 -0.00003 0.00000 -0.00745 -0.00751 3.10733

D135 0.00751 -0.00052 -0.00001 -0.01984 -0.02010 -0.01258

D136 -3.12882 -0.00029 -0.00001 0.00490 0.00504 -3.12378

D137 -3.12737 -0.00025 0.00000 -0.00265 -0.00272 -3.13009

D138 0.01949 -0.00003 0.00000 0.02209 0.02241 0.04190

D139 0.01640 0.00003 0.00000 0.00416 0.00416 0.02056

D140 -3.11484 0.00003 0.00000 0.00757 0.00764 -3.10720

D141 -3.13268 -0.00027 -0.00001 -0.01495 -0.01500 3.13551

D142 0.01926 -0.00027 -0.00001 -0.01154 -0.01152 0.00774

D143 0.19255 0.00057 0.00005 0.03717 0.03710 0.22965

D144 -2.95529 0.00030 0.00005 0.00802 0.00838 -2.94691

D145 -0.00544 0.00000 0.00000 -0.00160 -0.00160 -0.00704

D146 -3.13902 -0.00008 0.00000 -0.00806 -0.00788 3.13629

D147 3.12489 0.00021 0.00001 0.01571 0.01518 3.14007

D148 -0.00869 0.00013 0.00001 0.00924 0.00891 0.00021

D149 -3.09243 0.00022 0.00001 0.02313 0.02315 -3.06927

D150 0.06062 0.00001 0.00001 0.00591 0.00590 0.06652

D151 0.00000 0.00000 0.00000 -0.00005 -0.00005 -0.00005

D152 -3.13373 -0.00008 0.00000 -0.00634 -0.00617 -3.13990

D153 3.13374 0.00008 0.00000 0.00627 0.00610 3.13984

D154 0.00000 0.00000 0.00000 -0.00002 -0.00002 -0.00002

D155 0.00544 0.00000 0.00000 0.00162 0.00162 0.00706

D156 -3.12488 -0.00021 -0.00001 -0.01576 -0.01524 -3.14012

D157 3.13902 0.00008 0.00000 0.00805 0.00787 -3.13630

D158 0.00870 -0.00013 -0.00001 -0.00933 -0.00899 -0.00029

D159 3.09243 -0.00022 -0.00001 -0.02328 -0.02331 3.06912

D160 -0.06062 -0.00001 -0.00001 -0.00598 -0.00598 -0.06660

D161 -0.01656 -0.00003 0.00000 -0.00434 -0.00436 -0.02093

D162 3.13915 -0.00005 0.00000 -0.00320 -0.00323 3.13592

D163 3.11401 -0.00002 0.00000 -0.00750 -0.00746 3.10656

D164 -0.01346 -0.00005 0.00000 -0.00636 -0.00632 -0.01979

D165 -3.09015 -0.00038 -0.00001 -0.02941 -0.02939 -3.11954

D166 0.06253 -0.00038 -0.00001 -0.02620 -0.02624 0.03629

D167 0.00000 0.00000 0.00000 -0.00003 -0.00003 -0.00003

D168 -3.12778 -0.00003 0.00000 0.00101 0.00099 -3.12679

D169 3.12778 0.00003 0.00000 -0.00104 -0.00103 3.12675

D170 0.00000 0.00000 0.00000 -0.00001 -0.00001 -0.00001

D171 0.01656 0.00003 0.00000 0.00435 0.00438 0.02094

D172 -3.11401 0.00002 0.00000 0.00746 0.00743 -3.10658

D173 -3.13915 0.00005 0.00000 0.00320 0.00322 -3.13593

D174 0.01346 0.00005 0.00000 0.00630 0.00627 0.01974

D175 3.09014 0.00038 0.00001 0.02933 0.02932 3.11946

D176 -0.06253 0.00038 0.00001 0.02617 0.02620 -0.03633

D177 0.00544 0.00000 0.00000 0.00158 0.00159 0.00703

D178 3.13902 0.00008 0.00000 0.00802 0.00785 -3.13632

D179 -3.12490 -0.00021 -0.00001 -0.01563 -0.01511 -3.14001

D180 0.00868 -0.00013 -0.00001 -0.00919 -0.00885 -0.00017

D181 3.09241 -0.00022 -0.00001 -0.02302 -0.02305 3.06936

D182 -0.06062 -0.00001 -0.00001 -0.00589 -0.00589 -0.06651

D183 0.00000 0.00000 0.00000 0.00005 0.00005 0.00004

D184 3.13374 0.00008 0.00000 0.00632 0.00615 3.13989

D185 -3.13374 -0.00008 0.00000 -0.00625 -0.00608 -3.13982

D186 0.00000 0.00000 0.00000 0.00002 0.00002 0.00002

D187 -0.00544 0.00000 0.00000 -0.00160 -0.00161 -0.00705

D188 3.12490 0.00021 0.00001 0.01569 0.01516 3.14006

D189 -3.13902 -0.00008 0.00000 -0.00801 -0.00784 3.13632

D190 -0.00869 0.00013 0.00001 0.00927 0.00894 0.00025

D191 -3.09241 0.00022 0.00001 0.02318 0.02320 -3.06921

D192 0.06062 0.00001 0.00001 0.00597 0.00596 0.06658

D193 -0.01656 -0.00003 0.00000 -0.00432 -0.00433 -0.02089

D194 3.13915 -0.00005 -0.00001 -0.00317 -0.00319 3.13596

D195 3.11401 -0.00002 0.00000 -0.00748 -0.00744 3.10657

D196 -0.01346 -0.00005 0.00000 -0.00633 -0.00630 -0.01976

D197 -3.09015 -0.00038 -0.00001 -0.02940 -0.02939 -3.11954

D198 0.06253 -0.00038 -0.00001 -0.02619 -0.02622 0.03631

D199 0.00000 0.00000 0.00000 0.00002 0.00003 0.00003

D200 -3.12778 -0.00003 0.00000 0.00103 0.00102 -3.12676

D201 3.12778 0.00003 0.00000 -0.00100 -0.00098 3.12680

D202 0.00000 0.00000 0.00000 0.00001 0.00001 0.00001

D203 0.01656 0.00003 0.00000 0.00431 0.00432 0.02088

D204 -3.11401 0.00002 0.00000 0.00752 0.00747 -3.10654

D205 -3.13915 0.00005 0.00000 0.00317 0.00320 -3.13595

D206 0.01346 0.00005 0.00000 0.00638 0.00635 0.01981

D207 3.09015 0.00038 0.00001 0.02948 0.02946 3.11962

D208 -0.06252 0.00038 0.00001 0.02622 0.02626 -0.03627

D209 1.09669 0.00002 0.00000 -0.00126 -0.00123 1.09546

D210 -1.04700 0.00009 0.00000 0.00888 0.00894 -1.03807

D211 -3.11700 -0.00001 0.00000 0.00135 0.00127 -3.11573

D212 1.04700 -0.00009 0.00000 -0.00888 -0.00894 1.03807

D213 -1.09669 -0.00002 0.00000 0.00123 0.00120 -1.09550

D214 3.11700 0.00001 0.00000 -0.00140 -0.00132 3.11568

D215 1.09969 -0.00005 0.00001 -0.00184 -0.00180 1.09789

D216 -1.04526 0.00002 0.00000 -0.00042 -0.00048 -1.04573

D217 -3.11466 0.00003 0.00000 0.00308 0.00311 -3.11155

D218 1.04526 -0.00002 0.00000 0.00039 0.00045 1.04570

D219 -1.09969 0.00005 -0.00001 0.00184 0.00180 -1.09789

D220 3.11466 -0.00003 0.00000 -0.00314 -0.00316 3.11150

D221 1.04700 -0.00009 0.00000 -0.00888 -0.00894 1.03807

D222 -1.09669 -0.00002 0.00000 0.00122 0.00119 -1.09550

D223 3.11700 0.00001 0.00000 -0.00140 -0.00132 3.11568

D224 1.09669 0.00002 0.00000 -0.00119 -0.00116 1.09553

D225 -1.04700 0.00009 0.00000 0.00888 0.00894 -1.03807

D226 -3.11700 -0.00001 0.00000 0.00145 0.00137 -3.11563

D227 1.09969 -0.00005 0.00001 -0.00183 -0.00179 1.09790

D228 -1.04526 0.00002 0.00000 -0.00038 -0.00043 -1.04569

D229 -3.11466 0.00003 0.00000 0.00319 0.00321 -3.11145

D230 1.04526 -0.00002 0.00000 0.00040 0.00046 1.04572

D231 -1.09969 0.00005 -0.00001 0.00183 0.00179 -1.09789

D232 3.11466 -0.00003 0.00000 -0.00313 -0.00316 3.11150

Item Value Threshold Converged?

Maximum Force 0.002239 0.000450 NO

RMS Force 0.000417 0.000300 NO

Maximum Displacement 0.405864 0.001800 NO

RMS Displacement 0.095077 0.001200 NO

Predicted change in Energy=-7.877456D-02

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 00:50:59 2019, MaxMem= 1342177280 cpu: 13.7

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=3 Diff= 8.28D-04

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 -1.108973 2.794800 -0.036189

2 7 0 0.000219 2.030393 -0.239020

3 6 0 1.110815 2.790798 -0.037493

4 6 0 0.720822 4.123572 0.287449

5 6 0 -0.713142 4.126728 0.288403

6 7 0 2.446082 2.331031 -0.171535

7 6 0 2.811581 1.160787 -0.261253

8 7 0 2.040802 0.000749 -0.192912

9 6 0 2.815859 -1.158541 -0.262178

10 6 0 4.250914 -0.701404 -0.398937

11 6 0 4.247715 0.709621 -0.398387

12 7 0 -2.449743 2.334591 -0.169954

13 6 0 -4.258106 0.709774 -0.396925

14 6 0 -4.261122 -0.702606 -0.397474

15 6 0 -2.825191 -1.159245 -0.261066

16 7 0 -2.052753 0.000504 -0.192082

17 6 0 -2.821217 1.160810 -0.260142

18 7 0 -2.452003 -2.339759 -0.171005

19 7 0 0.000489 -2.041905 -0.239254

20 6 0 -1.108898 -2.804523 -0.036929

21 6 0 -0.713076 -4.136976 0.287189

22 6 0 0.721819 -4.133646 0.286239

23 6 0 1.111478 -2.800255 -0.038228

24 7 0 2.448961 -2.335605 -0.172585

25 30 0 -0.004625 -0.004037 -0.402169

26 6 0 -5.440863 1.433269 -0.492500

27 6 0 -6.643420 0.685463 -0.581030

28 6 0 -6.646399 -0.666944 -0.581483

29 6 0 -5.447210 -1.420415 -0.493516

30 6 0 1.432884 -5.334362 0.603689

31 6 0 0.704988 -6.490540 0.883427

32 6 0 -0.683948 -6.493814 0.884296

33 6 0 -1.417787 -5.341024 0.605497

34 6 0 5.429967 1.433294 -0.494279

35 6 0 6.632941 0.686122 -0.583203

36 6 0 6.636100 -0.665905 -0.583658

37 6 0 5.436697 -1.419070 -0.495299

38 6 0 -1.417928 5.330484 0.607108

39 6 0 -0.684563 6.483447 0.886412

40 6 0 0.704003 6.480338 0.885536

41 6 0 1.431687 5.324157 0.605286

42 1 0 7.579506 1.197025 -0.654637

43 1 0 7.585116 -1.172214 -0.655423

44 1 0 1.206915 7.402525 1.123490

45 1 0 -1.182986 7.407905 1.124997

46 1 0 -7.590151 1.196106 -0.652165

47 1 0 -7.595443 -1.173249 -0.652947

48 1 0 -1.182182 -7.418462 1.122533

49 1 0 1.207925 -7.412800 1.121039

50 8 0 2.771119 5.310766 0.643069

51 8 0 -2.757271 5.323492 0.646653

52 8 0 5.440952 2.761118 -0.496672

53 8 0 5.454598 -2.746778 -0.498583

54 8 0 2.772235 -5.321387 0.641604

55 8 0 -2.757049 -5.334754 0.645156

56 8 0 -5.466352 -2.748059 -0.496831

57 8 0 -5.453456 2.761032 -0.494929

58 6 0 3.490382 6.502126 0.931082

59 1 0 3.258599 6.862523 1.931239

60 1 0 3.277823 7.284763 0.208177

61 1 0 4.543174 6.247401 0.878672

62 6 0 6.686530 3.459723 -0.507866

63 1 0 7.249822 3.249170 -1.413787

64 1 0 7.275402 3.202382 0.368939

65 1 0 6.440275 4.514728 -0.476449

66 6 0 6.703772 -3.438884 -0.510061

67 1 0 7.291168 -3.179037 0.367001

68 1 0 7.266104 -3.224807 -1.415760

69 1 0 6.463042 -4.495182 -0.479336

70 6 0 -3.470593 6.518207 0.935482

71 1 0 -3.255344 7.299807 0.212248

72 1 0 -3.235886 6.877613 1.935321

73 1 0 -4.524613 6.268370 0.884399

74 6 0 -6.699859 3.458013 -0.505707

75 1 0 -7.288120 3.199944 0.371312

76 1 0 -7.263239 3.246747 -1.411429

77 1 0 -6.454901 4.513320 -0.474358

78 6 0 -6.716147 -3.438888 -0.507890

79 1 0 -7.278624 -3.224259 -1.413390

80 1 0 -7.303003 -3.178480 0.369386

81 1 0 -6.476418 -4.495412 -0.477228

82 6 0 -3.469753 -6.529868 0.933506

83 1 0 -3.234864 -6.889628 1.933192

84 1 0 -3.254204 -7.311082 0.209926

85 1 0 -4.523864 -6.280412 0.882530

86 6 0 3.491149 -6.512983 0.929149

87 1 0 3.278476 -7.295285 0.205897

88 1 0 3.259255 -6.873787 1.929153

89 1 0 4.543977 -6.258398 0.876862

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0446646 0.0427633 0.0223168

Leave Link 202 at Sat Jul 6 00:51:00 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8004.3358328001 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= 89 NActive= 89 NUniq= 89 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= -0.2264865970 Hartrees.

Nuclear repulsion after empirical dispersion term = 8004.1093462030 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6413

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.15D-10

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 359

GePol: Fraction of low-weight points (<1% of avg) = 5.60%

GePol: Cavity surface area = 713.379 Ang\*\*2

GePol: Cavity volume = 807.786 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0094934911 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8004.0998527119 Hartrees.

Leave Link 301 at Sat Jul 6 00:51:00 2019, MaxMem= 1342177280 cpu: 1.3

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44005 LenP2D= 110416.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.73D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 00:51:04 2019, MaxMem= 1342177280 cpu: 41.6

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 00:51:05 2019, MaxMem= 1342177280 cpu: 2.5

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000176 -0.000220 -0.000032 Ang= -0.03 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>= 2.0168 S= 1.0056

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2650.00386031447

Leave Link 401 at Sat Jul 6 00:51:22 2019, MaxMem= 1342177280 cpu: 201.9

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 530000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 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= 123379707.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.33D-15 for 6405.

Iteration 1 A\*A^-1 deviation from orthogonality is 6.70D-15 for 2945 489.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.02D-14 for 2622.

Iteration 1 A^-1\*A deviation from orthogonality is 7.07D-12 for 1749 1722.

E= -2649.67108173194

DIIS: error= 5.34D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.67108173194 IErMin= 1 ErrMin= 5.34D-03

ErrMax= 5.34D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.00D-01 BMatP= 2.00D-01

IDIUse=3 WtCom= 9.47D-01 WtEn= 5.34D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.693 Goal= None Shift= 0.000

Gap= 0.735 Goal= None Shift= 0.000

GapD= 0.693 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=4.36D-04 MaxDP=2.17D-02 OVMax= 8.21D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.34D-04 CP: 9.94D-01

E= -2649.73923104870 Delta-E= -0.068149316763 Rises=F Damp=F

DIIS: error= 2.04D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.73923104870 IErMin= 2 ErrMin= 2.04D-03

ErrMax= 2.04D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.15D-02 BMatP= 2.00D-01

IDIUse=3 WtCom= 9.80D-01 WtEn= 2.04D-02

Coeff-Com: 0.113D+00 0.887D+00

Coeff-En: 0.000D+00 0.100D+01

Coeff: 0.111D+00 0.889D+00

Gap= 0.085 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.37D-04 MaxDP=1.05D-02 DE=-6.81D-02 OVMax= 2.86D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.36D-04 CP: 9.96D-01 1.03D+00

E= -2649.73683212380 Delta-E= 0.002398924895 Rises=F Damp=F

DIIS: error= 3.48D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -2649.73923104870 IErMin= 2 ErrMin= 2.04D-03

ErrMax= 3.48D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.47D-02 BMatP= 2.15D-02

IDIUse=3 WtCom= 1.45D-01 WtEn= 8.55D-01

Coeff-Com: -0.164D-01 0.569D+00 0.447D+00

Coeff-En: 0.000D+00 0.593D+00 0.407D+00

Coeff: -0.238D-02 0.590D+00 0.413D+00

Gap= 0.083 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=8.27D-05 MaxDP=7.63D-03 DE= 2.40D-03 OVMax= 2.09D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.28D-05 CP: 9.94D-01 1.06D+00 4.56D-01

E= -2649.74383160514 Delta-E= -0.006999481331 Rises=F Damp=F

DIIS: error= 7.47D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.74383160514 IErMin= 4 ErrMin= 7.47D-04

ErrMax= 7.47D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.88D-04 BMatP= 2.15D-02

IDIUse=3 WtCom= 9.93D-01 WtEn= 7.47D-03

Coeff-Com: -0.144D-01 0.214D+00 0.196D+00 0.604D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.143D-01 0.213D+00 0.195D+00 0.607D+00

Gap= 0.083 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.94D-05 MaxDP=1.48D-03 DE=-7.00D-03 OVMax= 7.85D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.72D-05 CP: 9.94D-01 1.05D+00 4.61D-01 7.44D-01

E= -2649.74400686455 Delta-E= -0.000175259416 Rises=F Damp=F

DIIS: error= 4.38D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.74400686455 IErMin= 5 ErrMin= 4.38D-04

ErrMax= 4.38D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.31D-04 BMatP= 8.88D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.38D-03

Coeff-Com: -0.570D-02 0.589D-01 0.644D-01 0.362D+00 0.520D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.170D+00 0.830D+00

Coeff: -0.568D-02 0.586D-01 0.641D-01 0.361D+00 0.522D+00

Gap= 0.083 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=8.12D-06 MaxDP=6.29D-04 DE=-1.75D-04 OVMax= 2.97D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 5.42D-06 CP: 9.94D-01 1.06D+00 4.79D-01 8.77D-01 8.25D-01

E= -2649.74406861756 Delta-E= -0.000061753006 Rises=F Damp=F

DIIS: error= 6.74D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.74406861756 IErMin= 6 ErrMin= 6.74D-05

ErrMax= 6.74D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.17D-05 BMatP= 2.31D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.355D-03-0.715D-02 0.717D-03 0.661D-01 0.189D+00 0.752D+00

Coeff: -0.355D-03-0.715D-02 0.717D-03 0.661D-01 0.189D+00 0.752D+00

Gap= 0.084 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=3.07D-06 MaxDP=1.48D-04 DE=-6.18D-05 OVMax= 2.09D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.13D-06 CP: 9.94D-01 1.06D+00 4.83D-01 9.13D-01 9.25D-01

CP: 9.83D-01

E= -2649.74407425894 Delta-E= -0.000005641381 Rises=F Damp=F

DIIS: error= 5.97D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.74407425894 IErMin= 7 ErrMin= 5.97D-05

ErrMax= 5.97D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.31D-06 BMatP= 1.17D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.966D-03-0.165D-01-0.121D-01-0.354D-01-0.270D-02 0.413D+00

Coeff-Com: 0.653D+00

Coeff: 0.966D-03-0.165D-01-0.121D-01-0.354D-01-0.270D-02 0.413D+00

Coeff: 0.653D+00

Gap= 0.084 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.11D-06 MaxDP=1.15D-04 DE=-5.64D-06 OVMax= 1.99D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.31D-06 CP: 9.94D-01 1.06D+00 4.88D-01 9.35D-01 9.57D-01

CP: 1.19D+00 1.14D+00

E= -2649.74407647856 Delta-E= -0.000002219620 Rises=F Damp=F

DIIS: error= 2.11D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.74407647856 IErMin= 8 ErrMin= 2.11D-05

ErrMax= 2.11D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.01D-06 BMatP= 4.31D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.466D-03-0.469D-02-0.448D-02-0.337D-01-0.575D-01-0.569D-01

Coeff-Com: 0.323D+00 0.834D+00

Coeff: 0.466D-03-0.469D-02-0.448D-02-0.337D-01-0.575D-01-0.569D-01

Coeff: 0.323D+00 0.834D+00

Gap= 0.084 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.22D-06 MaxDP=6.11D-05 DE=-2.22D-06 OVMax= 1.04D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 5.14D-07 CP: 9.94D-01 1.06D+00 4.88D-01 9.48D-01 9.92D-01

CP: 1.28D+00 1.45D+00 1.03D+00

E= -2649.74407708250 Delta-E= -0.000000603937 Rises=F Damp=F

DIIS: error= 1.04D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.74407708250 IErMin= 9 ErrMin= 1.04D-05

ErrMax= 1.04D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.38D-07 BMatP= 1.01D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.346D-04 0.119D-02 0.646D-03-0.763D-02-0.247D-01-0.987D-01

Coeff-Com: 0.545D-01 0.371D+00 0.704D+00

Coeff: 0.346D-04 0.119D-02 0.646D-03-0.763D-02-0.247D-01-0.987D-01

Coeff: 0.545D-01 0.371D+00 0.704D+00

Gap= 0.084 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.17D-07 MaxDP=2.25D-05 DE=-6.04D-07 OVMax= 3.49D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 2.61D-07 CP: 9.94D-01 1.06D+00 4.89D-01 9.50D-01 9.99D-01

CP: 1.30D+00 1.54D+00 1.15D+00 8.80D-01

E= -2649.74407714913 Delta-E= -0.000000066637 Rises=F Damp=F

DIIS: error= 4.96D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -2649.74407714913 IErMin=10 ErrMin= 4.96D-06

ErrMax= 4.96D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.79D-08 BMatP= 1.38D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.660D-04 0.160D-02 0.123D-02 0.113D-02-0.563D-02-0.540D-01

Coeff-Com: -0.259D-01 0.631D-01 0.439D+00 0.580D+00

Coeff: -0.660D-04 0.160D-02 0.123D-02 0.113D-02-0.563D-02-0.540D-01

Coeff: -0.259D-01 0.631D-01 0.439D+00 0.580D+00

Gap= 0.084 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.94D-07 MaxDP=1.09D-05 DE=-6.66D-08 OVMax= 1.20D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.13D-07 CP: 9.94D-01 1.06D+00 4.89D-01 9.51D-01 1.00D+00

CP: 1.31D+00 1.58D+00 1.19D+00 1.03D+00 8.44D-01

E= -2649.74407716851 Delta-E= -0.000000019381 Rises=F Damp=F

DIIS: error= 1.51D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -2649.74407716851 IErMin=11 ErrMin= 1.51D-06

ErrMax= 1.51D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.90D-09 BMatP= 5.79D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.349D-04 0.455D-03 0.426D-03 0.213D-02 0.275D-02-0.311D-02

Coeff-Com: -0.190D-01-0.479D-01 0.625D-01 0.262D+00 0.740D+00

Coeff: -0.349D-04 0.455D-03 0.426D-03 0.213D-02 0.275D-02-0.311D-02

Coeff: -0.190D-01-0.479D-01 0.625D-01 0.262D+00 0.740D+00

Gap= 0.084 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=6.23D-08 MaxDP=5.02D-06 DE=-1.94D-08 OVMax= 4.05D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 4.53D-08 CP: 9.94D-01 1.06D+00 4.89D-01 9.51D-01 1.00D+00

CP: 1.31D+00 1.59D+00 1.20D+00 1.07D+00 9.51D-01

CP: 9.78D-01

E= -2649.74407717101 Delta-E= -0.000000002501 Rises=F Damp=F

DIIS: error= 8.06D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -2649.74407717101 IErMin=12 ErrMin= 8.06D-07

ErrMax= 8.06D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.57D-09 BMatP= 5.90D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.371D-05-0.124D-03-0.569D-04 0.828D-03 0.276D-02 0.102D-01

Coeff-Com: -0.306D-02-0.393D-01-0.638D-01 0.346D-02 0.373D+00 0.716D+00

Coeff: -0.371D-05-0.124D-03-0.569D-04 0.828D-03 0.276D-02 0.102D-01

Coeff: -0.306D-02-0.393D-01-0.638D-01 0.346D-02 0.373D+00 0.716D+00

Gap= 0.084 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=3.50D-08 MaxDP=2.69D-06 DE=-2.50D-09 OVMax= 1.40D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 2.46D-08 CP: 9.94D-01 1.06D+00 4.89D-01 9.51D-01 1.00D+00

CP: 1.31D+00 1.59D+00 1.20D+00 1.10D+00 1.00D+00

CP: 1.08D+00 9.67D-01

E= -2649.74407717151 Delta-E= -0.000000000493 Rises=F Damp=F

DIIS: error= 4.84D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -2649.74407717151 IErMin=13 ErrMin= 4.84D-07

ErrMax= 4.84D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.98D-10 BMatP= 1.57D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.586D-05-0.173D-03-0.137D-03-0.940D-04 0.843D-03 0.562D-02

Coeff-Com: 0.266D-02-0.105D-01-0.476D-01-0.590D-01 0.361D-01 0.389D+00

Coeff-Com: 0.683D+00

Coeff: 0.586D-05-0.173D-03-0.137D-03-0.940D-04 0.843D-03 0.562D-02

Coeff: 0.266D-02-0.105D-01-0.476D-01-0.590D-01 0.361D-01 0.389D+00

Coeff: 0.683D+00

Gap= 0.084 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.61D-08 MaxDP=1.43D-06 DE=-4.93D-10 OVMax= 6.78D-06

Cycle 14 Pass 1 IDiag 1:

RMSU= 9.44D-09 CP: 9.94D-01 1.06D+00 4.89D-01 9.51D-01 1.00D+00

CP: 1.31D+00 1.59D+00 1.20D+00 1.10D+00 1.02D+00

CP: 1.14D+00 1.12D+00 9.05D-01

E= -2649.74407717201 Delta-E= -0.000000000502 Rises=F Damp=F

DIIS: error= 1.57D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -2649.74407717201 IErMin=14 ErrMin= 1.57D-07

ErrMax= 1.57D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.43D-11 BMatP= 3.98D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.372D-05-0.631D-04-0.576D-04-0.192D-03-0.414D-04 0.106D-02

Coeff-Com: 0.223D-02 0.258D-02-0.122D-01-0.320D-01-0.539D-01 0.566D-01

Coeff-Com: 0.343D+00 0.693D+00

Coeff: 0.372D-05-0.631D-04-0.576D-04-0.192D-03-0.414D-04 0.106D-02

Coeff: 0.223D-02 0.258D-02-0.122D-01-0.320D-01-0.539D-01 0.566D-01

Coeff: 0.343D+00 0.693D+00

Gap= 0.084 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=6.79D-09 MaxDP=6.07D-07 DE=-5.02D-10 OVMax= 1.69D-06

Error on total polarization charges = 0.07168

SCF Done: E(UB3LYP) = -2649.74407717 A.U. after 14 cycles

NFock= 14 Conv=0.68D-08 -V/T= 1.9847

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0170 S= 1.0057

<L.S>= 0.000000000000E+00

KE= 2.690914119400D+03 PE=-2.228823278516D+04 EE= 8.943474735877D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.96

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0170, after 2.0002

Leave Link 502 at Sat Jul 6 01:02:42 2019, MaxMem= 1342177280 cpu: 8057.8

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44005 LenP2D= 110416.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 281

Leave Link 701 at Sat Jul 6 01:03:01 2019, MaxMem= 1342177280 cpu: 218.8

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 01:03:01 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 01:04:31 2019, MaxMem= 1342177280 cpu: 1069.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.49309847D-02 5.13194907D-02 7.52928926D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.040536294 -0.022164490 -0.007434146

2 7 -0.000908585 0.007074605 0.003870527

3 6 0.038800794 -0.020208368 -0.007081151

4 6 0.003898623 0.019743268 0.005863834

5 6 -0.004338740 0.019157012 0.005708336

6 7 -0.058679361 0.109416442 0.009764019

7 6 0.031959592 -0.109165191 -0.004137033

8 7 0.001765314 -0.001739998 -0.001705867

9 6 0.026887253 0.100421585 -0.003247901

10 6 -0.012447494 -0.002995571 -0.000415811

11 6 -0.011882902 0.002295724 -0.000505864

12 7 0.057968501 0.103150723 0.009437629

13 6 0.012133505 0.002393769 -0.000424656

14 6 0.012689853 -0.003080138 -0.000336689

15 6 -0.024087104 0.093215358 -0.002680382

16 7 -0.000261948 -0.001744212 -0.001706277

17 6 -0.029064742 -0.101606261 -0.003545284

18 7 0.055255360 -0.094241535 0.008866177

19 7 -0.000905866 -0.005094617 0.003579940

20 6 -0.042265153 0.023391796 -0.007595328

21 6 -0.004315234 -0.019081892 0.005677592

22 6 0.003878928 -0.019663412 0.005831764

23 6 0.040618093 0.021483181 -0.007249920

24 7 -0.055928192 -0.100169160 0.009166999

25 30 -0.000347256 -0.000526974 -0.003470088

26 6 -0.017646136 -0.016919270 -0.000092968

27 6 0.006017380 0.026330123 0.000293706

28 6 0.005923728 -0.026397561 0.000293573

29 6 -0.017738931 0.016907520 -0.000109184

30 6 -0.002456497 0.006022255 -0.001131661

31 6 -0.001561472 0.001938176 -0.000722757

32 6 0.001523989 0.002037202 -0.000742367

33 6 0.002467832 0.005818552 -0.001075732

34 6 0.017809520 -0.016641498 -0.000093011

35 6 -0.006082388 0.026855448 0.000300249

36 6 -0.005984393 -0.026921812 0.000300300

37 6 0.017903249 0.016619788 -0.000109000

38 6 0.002132682 -0.005821055 -0.001068106

39 6 0.001247218 -0.002035359 -0.000745649

40 6 -0.001283611 -0.001938538 -0.000726431

41 6 -0.002132213 -0.006027450 -0.001125083

42 1 0.001850688 0.001652238 -0.000235697

43 1 0.001840605 -0.001633393 -0.000237096

44 1 0.002408789 0.001826336 0.000430287

45 1 -0.002404592 0.001839325 0.000428125

46 1 -0.001848370 0.001602993 -0.000236629

47 1 -0.001838811 -0.001584758 -0.000237931

48 1 -0.002379698 -0.001851157 0.000431128

49 1 0.002384007 -0.001838066 0.000433375

50 8 0.007608472 -0.012933071 -0.004848130

51 8 -0.007663924 -0.012865211 -0.004929927

52 8 -0.010092560 0.022882796 -0.000074992

53 8 -0.010004791 -0.022864760 0.000021033

54 8 0.007608238 0.012912082 -0.004969149

55 8 -0.007590645 0.012828708 -0.005016152

56 8 0.010041460 -0.022651192 0.000086817

57 8 0.010231553 0.022706733 0.000034833

58 6 -0.001914322 0.000848875 0.002114542

59 1 -0.000277812 0.001739842 0.003579413

60 1 -0.001253754 0.003118677 -0.003495066

61 1 0.001880434 -0.002624955 -0.000371731

62 6 -0.004486913 -0.003350592 0.000715962

63 1 0.002701903 -0.000498449 -0.002919062

64 1 0.003808114 -0.000348370 0.002746093

65 1 -0.002166477 0.002469732 -0.000074654

66 6 -0.004467783 0.003326477 0.000716334

67 1 0.003798715 0.000363144 0.002742735

68 1 0.002691849 0.000505387 -0.002910250

69 1 -0.002149091 -0.002484873 -0.000071737

70 6 0.001884807 0.000868579 0.002119550

71 1 0.001274364 0.003095730 -0.003494795

72 1 0.000284838 0.001726509 0.003574270

73 1 -0.001901260 -0.002608887 -0.000365514

74 6 0.004394219 -0.003271320 0.000723796

75 1 -0.003792312 -0.000344597 0.002732712

76 1 -0.002679449 -0.000488667 -0.002908036

77 1 0.002157179 0.002474895 -0.000071861

78 6 0.004371965 0.003244822 0.000723979

79 1 -0.002668740 0.000495905 -0.002899252

80 1 -0.003782272 0.000359465 0.002729203

81 1 0.002149906 -0.002496287 -0.000067653

82 6 0.001856174 -0.000913928 0.002131444

83 1 0.000279943 -0.001716836 0.003565145

84 1 0.001273017 -0.003087546 -0.003489798

85 1 -0.001919935 0.002601625 -0.000366225

86 6 -0.001887813 -0.000891298 0.002125153

87 1 -0.001252137 -0.003111519 -0.003490195

88 1 -0.000272875 -0.001730473 0.003570550

89 1 0.001888202 0.002611165 -0.000371248

-------------------------------------------------------------------

Cartesian Forces: Max 0.109416442 RMS 0.021193672

Leave Link 716 at Sat Jul 6 01:04:31 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.091260635 RMS 0.009572503

Search for a local minimum.

Step number 10 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .95725D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 2 3 4 6

5 8 7 10 9

ITU= 0 0 0 0 0 1 1 1 1 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.98228.

Iteration 1 RMS(Cart)= 0.09132141 RMS(Int)= 0.00147104

Iteration 2 RMS(Cart)= 0.00414402 RMS(Int)= 0.00000441

Iteration 3 RMS(Cart)= 0.00000339 RMS(Int)= 0.00000411

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000411

ITry= 1 IFail=0 DXMaxC= 3.98D-01 DCOld= 1.00D+10 DXMaxT= 4.57D-01 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.57431 0.00599 0.00639 0.00000 0.00638 2.58069

R2 2.69647 0.00328 0.04027 0.00000 0.04027 2.73674

R3 2.69069 -0.04248 -0.12168 0.00000 -0.12167 2.56901

R4 2.57187 0.00666 0.00902 0.00000 0.00901 2.58088

R5 3.85687 0.01664 0.01823 0.00000 0.01821 3.87508

R6 2.69508 0.00371 0.04163 0.00000 0.04163 2.73671

R7 2.68067 -0.03954 -0.11123 0.00000 -0.11122 2.56945

R8 2.70981 -0.00122 -0.00993 0.00000 -0.00993 2.69988

R9 2.70419 -0.01686 -0.04143 0.00000 -0.04144 2.66276

R10 2.70391 -0.01669 -0.04115 0.00000 -0.04115 2.66276

R11 2.32299 0.09126 0.15973 0.00000 0.15974 2.48273

R12 2.63511 -0.01296 -0.03860 0.00000 -0.03860 2.59651

R13 2.85645 -0.01009 -0.05663 0.00000 -0.05663 2.79982

R14 2.63850 -0.01396 -0.04218 0.00000 -0.04218 2.59632

R15 3.88548 -0.00135 -0.04522 0.00000 -0.04523 3.84025

R16 2.85784 -0.01060 -0.05797 0.00000 -0.05797 2.79987

R17 2.33603 0.08017 0.14629 0.00000 0.14630 2.48233

R18 2.66646 -0.00390 -0.00289 0.00000 -0.00289 2.66357

R19 2.62557 0.00326 0.01986 0.00000 0.01986 2.64543

R20 2.62571 0.00312 0.01971 0.00000 0.01971 2.64543

R21 2.33279 0.08282 0.14965 0.00000 0.14966 2.48245

R22 2.66902 -0.00457 -0.00558 0.00000 -0.00557 2.66344

R23 2.85767 -0.01072 -0.05788 0.00000 -0.05788 2.79980

R24 2.62631 0.00281 0.01913 0.00000 0.01913 2.64544

R25 2.85906 -0.01101 -0.05922 0.00000 -0.05922 2.79984

R26 2.62616 0.00306 0.01928 0.00000 0.01928 2.64545

R27 2.63645 -0.01370 -0.03989 0.00000 -0.03989 2.59656

R28 2.34584 0.07220 0.13620 0.00000 0.13621 2.48205

R29 2.63309 -0.01276 -0.03634 0.00000 -0.03634 2.59675

R30 3.89072 -0.00290 -0.05067 0.00000 -0.05067 3.84005

R31 2.69769 -0.04428 -0.12898 0.00000 -0.12898 2.56871

R32 2.57257 0.00589 0.00834 0.00000 0.00833 2.58090

R33 2.57017 0.00651 0.01093 0.00000 0.01092 2.58109

R34 3.86331 0.01391 0.01143 0.00000 0.01141 3.87472

R35 2.69719 0.00332 0.03952 0.00000 0.03952 2.73671

R36 2.71157 -0.00139 -0.01181 0.00000 -0.01180 2.69976

R37 2.70414 -0.01671 -0.04137 0.00000 -0.04137 2.66277

R38 2.69579 0.00363 0.04088 0.00000 0.04089 2.73667

R39 2.70443 -0.01687 -0.04166 0.00000 -0.04166 2.66277

R40 2.68767 -0.04154 -0.11853 0.00000 -0.11852 2.56915

R41 2.68128 -0.00140 -0.02282 0.00000 -0.02282 2.65846

R42 2.50922 0.02098 0.03893 0.00000 0.03893 2.54815

R43 2.55568 0.03189 0.07288 0.00000 0.07288 2.62857

R44 2.03715 0.00240 0.00767 0.00000 0.00767 2.04482

R45 2.68149 -0.00142 -0.02302 0.00000 -0.02302 2.65847

R46 2.03717 0.00238 0.00765 0.00000 0.00765 2.04482

R47 2.50915 0.02090 0.03900 0.00000 0.03900 2.54815

R48 2.63536 0.00440 0.00785 0.00000 0.00785 2.64321

R49 2.53214 0.00608 0.01665 0.00000 0.01665 2.54879

R50 2.62472 0.00951 0.02235 0.00000 0.02235 2.64707

R51 2.03527 0.00278 0.00947 0.00000 0.00947 2.04474

R52 2.63559 0.00434 0.00762 0.00000 0.00762 2.64322

R53 2.03527 0.00279 0.00947 0.00000 0.00947 2.04474

R54 2.53198 0.00605 0.01681 0.00000 0.01681 2.54879

R55 2.68136 -0.00138 -0.02289 0.00000 -0.02289 2.65847

R56 2.50931 0.02107 0.03884 0.00000 0.03884 2.54815

R57 2.55497 0.03258 0.07361 0.00000 0.07361 2.62858

R58 2.03715 0.00242 0.00768 0.00000 0.00768 2.04482

R59 2.68157 -0.00144 -0.02309 0.00000 -0.02309 2.65848

R60 2.03717 0.00240 0.00766 0.00000 0.00766 2.04482

R61 2.50924 0.02102 0.03891 0.00000 0.03891 2.54815

R62 2.63558 0.00441 0.00765 0.00000 0.00765 2.64323

R63 2.53213 0.00608 0.01666 0.00000 0.01666 2.54879

R64 2.62402 0.00999 0.02306 0.00000 0.02307 2.64708

R65 2.03527 0.00279 0.00947 0.00000 0.00947 2.04474

R66 2.63535 0.00448 0.00787 0.00000 0.00787 2.64322

R67 2.03527 0.00278 0.00947 0.00000 0.00947 2.04474

R68 2.53229 0.00605 0.01650 0.00000 0.01650 2.54880

R69 2.68556 0.00216 0.00830 0.00000 0.00830 2.69386

R70 2.68554 0.00219 0.00832 0.00000 0.00832 2.69386

R71 2.69883 -0.00097 -0.00347 0.00000 -0.00347 2.69536

R72 2.69879 -0.00094 -0.00343 0.00000 -0.00343 2.69536

R73 2.68542 0.00222 0.00844 0.00000 0.00844 2.69386

R74 2.68540 0.00225 0.00846 0.00000 0.00846 2.69386

R75 2.69864 -0.00084 -0.00328 0.00000 -0.00328 2.69536

R76 2.69868 -0.00087 -0.00333 0.00000 -0.00333 2.69536

R77 2.05618 0.00392 0.01170 0.00000 0.01170 2.06788

R78 2.05302 0.00482 0.01486 0.00000 0.01486 2.06788

R79 2.04929 0.00246 0.00783 0.00000 0.00783 2.05712

R80 2.05479 0.00393 0.01287 0.00000 0.01287 2.06765

R81 2.05432 0.00436 0.01364 0.00000 0.01364 2.06796

R82 2.04812 0.00289 0.00887 0.00000 0.00887 2.05699

R83 2.05433 0.00435 0.01363 0.00000 0.01363 2.06796

R84 2.05480 0.00391 0.01285 0.00000 0.01285 2.06765

R85 2.04812 0.00290 0.00888 0.00000 0.00888 2.05699

R86 2.05303 0.00481 0.01485 0.00000 0.01485 2.06788

R87 2.05619 0.00391 0.01169 0.00000 0.01169 2.06788

R88 2.04927 0.00247 0.00785 0.00000 0.00785 2.05712

R89 2.05434 0.00434 0.01361 0.00000 0.01361 2.06796

R90 2.05482 0.00391 0.01283 0.00000 0.01283 2.06765

R91 2.04812 0.00290 0.00887 0.00000 0.00887 2.05699

R92 2.05483 0.00389 0.01282 0.00000 0.01282 2.06766

R93 2.05436 0.00433 0.01360 0.00000 0.01360 2.06796

R94 2.04811 0.00291 0.00888 0.00000 0.00888 2.05699

R95 2.05622 0.00391 0.01166 0.00000 0.01166 2.06788

R96 2.05305 0.00480 0.01483 0.00000 0.01483 2.06788

R97 2.04926 0.00248 0.00785 0.00000 0.00785 2.05712

R98 2.05305 0.00481 0.01483 0.00000 0.01483 2.06788

R99 2.05621 0.00392 0.01167 0.00000 0.01167 2.06788

R100 2.04928 0.00246 0.00784 0.00000 0.00784 2.05712

A1 1.90898 0.00214 -0.02066 0.00000 -0.02067 1.88832

A2 2.17896 0.00762 0.03262 0.00000 0.03262 2.21158

A3 2.19480 -0.00976 -0.01154 0.00000 -0.01153 2.18327

A4 1.90590 -0.00486 0.02720 0.00000 0.02722 1.93312

A5 2.17645 0.00224 -0.00950 0.00000 -0.00950 2.16695

A6 2.17816 0.00283 -0.01149 0.00000 -0.01149 2.16667

A7 1.90998 0.00183 -0.02169 0.00000 -0.02169 1.88829

A8 2.18101 0.00689 0.03060 0.00000 0.03060 2.21161

A9 2.19175 -0.00872 -0.00850 0.00000 -0.00848 2.18327

A10 1.85008 0.00040 0.00740 0.00000 0.00740 1.85748

A11 2.34452 -0.00680 -0.02588 0.00000 -0.02588 2.31865

A12 2.08836 0.00640 0.01869 0.00000 0.01868 2.10704

A13 1.84959 0.00051 0.00790 0.00000 0.00790 1.85749

A14 2.34524 -0.00679 -0.02659 0.00000 -0.02659 2.31865

A15 2.08813 0.00629 0.01890 0.00000 0.01890 2.10703

A16 2.20846 -0.00927 -0.01914 0.00000 -0.01914 2.18932

A17 2.24469 -0.00442 -0.00923 0.00000 -0.00922 2.23547

A18 2.18127 -0.00178 -0.01309 0.00000 -0.01308 2.16819

A19 1.85596 0.00625 0.02346 0.00000 0.02346 1.87941

A20 1.96217 -0.00544 -0.02399 0.00000 -0.02399 1.93819

A21 2.14937 0.00255 0.01151 0.00000 0.01150 2.16087

A22 2.14747 0.00291 0.01360 0.00000 0.01360 2.16108

A23 1.85486 0.00662 0.02458 0.00000 0.02458 1.87943

A24 2.24240 -0.00312 -0.00697 0.00000 -0.00696 2.23544

A25 2.18465 -0.00345 -0.01646 0.00000 -0.01645 2.16819

A26 1.87558 -0.00363 -0.01180 0.00000 -0.01180 1.86379

A27 2.29161 -0.00122 0.01039 0.00000 0.01039 2.30200

A28 2.11588 0.00485 0.00150 0.00000 0.00150 2.11738

A29 1.87619 -0.00380 -0.01241 0.00000 -0.01241 1.86377

A30 2.29057 -0.00110 0.01143 0.00000 0.01142 2.30199

A31 2.11633 0.00489 0.00108 0.00000 0.00108 2.11741

A32 2.21124 -0.00933 -0.02203 0.00000 -0.02203 2.18921

A33 1.87583 -0.00361 -0.01202 0.00000 -0.01202 1.86381

A34 2.11617 0.00491 0.00124 0.00000 0.00124 2.11741

A35 2.29108 -0.00130 0.01087 0.00000 0.01087 2.30195

A36 1.87523 -0.00351 -0.01141 0.00000 -0.01141 1.86383

A37 2.11574 0.00471 0.00165 0.00000 0.00165 2.11739

A38 2.29211 -0.00119 0.00985 0.00000 0.00985 2.30196

A39 1.85359 0.00661 0.02592 0.00000 0.02592 1.87951

A40 2.18816 -0.00462 -0.02008 0.00000 -0.02008 2.16808

A41 2.24016 -0.00195 -0.00469 0.00000 -0.00468 2.23548

A42 1.96542 -0.00581 -0.02746 0.00000 -0.02746 1.93796

A43 2.14586 0.00314 0.01531 0.00000 0.01532 2.16118

A44 2.14777 0.00269 0.01321 0.00000 0.01321 2.16097

A45 2.18480 -0.00314 -0.01672 0.00000 -0.01672 2.16808

A46 2.24244 -0.00313 -0.00694 0.00000 -0.00693 2.23551

A47 1.85468 0.00631 0.02481 0.00000 0.02481 1.87949

A48 2.21338 -0.00930 -0.02423 0.00000 -0.02423 2.18915

A49 1.90853 -0.00462 0.02438 0.00000 0.02439 1.93293

A50 2.17513 0.00217 -0.00809 0.00000 -0.00810 2.16704

A51 2.17685 0.00267 -0.01009 0.00000 -0.01009 2.16676

A52 2.17776 0.00797 0.03385 0.00000 0.03385 2.21160

A53 2.19713 -0.00990 -0.01395 0.00000 -0.01394 2.18319

A54 1.90787 0.00192 -0.01949 0.00000 -0.01950 1.88837

A55 1.84939 0.00058 0.00814 0.00000 0.00814 1.85753

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D157 -3.13630 -0.00024 -0.00773 0.00000 -0.00773 3.13916

D158 -0.00029 0.00005 0.00883 0.00000 0.00882 0.00853

D159 3.06912 0.00040 0.02289 0.00000 0.02289 3.09202

D160 -0.06660 0.00005 0.00587 0.00000 0.00587 -0.06072

D161 -0.02093 0.00033 0.00429 0.00000 0.00429 -0.01664

D162 3.13592 0.00003 0.00317 0.00000 0.00317 3.13909

D163 3.10656 0.00045 0.00733 0.00000 0.00733 3.11388

D164 -0.01979 0.00014 0.00621 0.00000 0.00621 -0.01358

D165 -3.11954 -0.00031 0.02887 0.00000 0.02887 -3.09067

D166 0.03629 -0.00045 0.02577 0.00000 0.02577 0.06206

D167 -0.00003 -0.00001 0.00003 0.00000 0.00003 0.00000

D168 -3.12679 -0.00028 -0.00098 0.00000 -0.00098 -3.12777

D169 3.12675 0.00026 0.00102 0.00000 0.00102 3.12777

D170 -0.00001 -0.00001 0.00001 0.00000 0.00001 0.00000

D171 0.02094 -0.00032 -0.00430 0.00000 -0.00430 0.01664

D172 -3.10658 -0.00046 -0.00730 0.00000 -0.00730 -3.11388

D173 -3.13593 -0.00003 -0.00316 0.00000 -0.00316 -3.13909

D174 0.01974 -0.00016 -0.00616 0.00000 -0.00616 0.01357

D175 3.11946 0.00029 -0.02880 0.00000 -0.02880 3.09066

D176 -0.03633 0.00045 -0.02574 0.00000 -0.02574 -0.06207

D177 0.00703 -0.00021 -0.00156 0.00000 -0.00156 0.00547

D178 -3.13632 -0.00023 -0.00771 0.00000 -0.00770 3.13916

D179 -3.14001 0.00012 0.01484 0.00000 0.01483 -3.12518

D180 -0.00017 0.00011 0.00870 0.00000 0.00869 0.00852

D181 3.06936 0.00043 0.02264 0.00000 0.02264 3.09200

D182 -0.06651 0.00004 0.00578 0.00000 0.00578 -0.06072

D183 0.00004 0.00002 -0.00005 0.00000 -0.00005 0.00000

D184 3.13989 -0.00001 -0.00604 0.00000 -0.00604 3.13385

D185 -3.13982 0.00004 0.00597 0.00000 0.00597 -3.13385

D186 0.00002 0.00001 -0.00002 0.00000 -0.00002 0.00000

D187 -0.00705 0.00020 0.00158 0.00000 0.00158 -0.00547

D188 3.14006 -0.00010 -0.01489 0.00000 -0.01488 3.12518

D189 3.13632 0.00023 0.00770 0.00000 0.00769 -3.13917

D190 0.00025 -0.00007 -0.00878 0.00000 -0.00877 -0.00852

D191 -3.06921 -0.00038 -0.02279 0.00000 -0.02279 -3.09200

D192 0.06658 -0.00003 -0.00586 0.00000 -0.00586 0.06073

D193 -0.02089 0.00028 0.00426 0.00000 0.00426 -0.01664

D194 3.13596 0.00002 0.00313 0.00000 0.00313 3.13909

D195 3.10657 0.00041 0.00731 0.00000 0.00731 3.11388

D196 -0.01976 0.00014 0.00619 0.00000 0.00619 -0.01357

D197 -3.11954 -0.00027 0.02887 0.00000 0.02887 -3.09067

D198 0.03631 -0.00041 0.02576 0.00000 0.02576 0.06207

D199 0.00003 0.00002 -0.00003 0.00000 -0.00003 0.00000

D200 -3.12676 -0.00023 -0.00100 0.00000 -0.00100 -3.12777

D201 3.12680 0.00026 0.00096 0.00000 0.00096 3.12777

D202 0.00001 0.00001 -0.00001 0.00000 -0.00001 0.00000

D203 0.02088 -0.00029 -0.00424 0.00000 -0.00424 0.01664

D204 -3.10654 -0.00039 -0.00734 0.00000 -0.00734 -3.11388

D205 -3.13595 -0.00001 -0.00314 0.00000 -0.00314 -3.13909

D206 0.01981 -0.00011 -0.00624 0.00000 -0.00624 0.01358

D207 3.11962 0.00029 -0.02894 0.00000 -0.02894 3.09068

D208 -0.03627 0.00041 -0.02579 0.00000 -0.02579 -0.06206

D209 1.09546 0.00054 0.00121 0.00000 0.00121 1.09667

D210 -1.03807 -0.00083 -0.00878 0.00000 -0.00878 -1.04685

D211 -3.11573 0.00010 -0.00125 0.00000 -0.00125 -3.11698

D212 1.03807 0.00083 0.00878 0.00000 0.00878 1.04685

D213 -1.09550 -0.00054 -0.00118 0.00000 -0.00118 -1.09667

D214 3.11568 -0.00010 0.00130 0.00000 0.00129 3.11697

D215 1.09789 0.00071 0.00177 0.00000 0.00177 1.09965

D216 -1.04573 -0.00028 0.00047 0.00000 0.00047 -1.04527

D217 -3.11155 -0.00034 -0.00306 0.00000 -0.00306 -3.11461

D218 1.04570 0.00029 -0.00044 0.00000 -0.00044 1.04526

D219 -1.09789 -0.00072 -0.00177 0.00000 -0.00177 -1.09965

D220 3.11150 0.00033 0.00311 0.00000 0.00311 3.11461

D221 1.03807 0.00082 0.00878 0.00000 0.00878 1.04685

D222 -1.09550 -0.00054 -0.00117 0.00000 -0.00117 -1.09667

D223 3.11568 -0.00010 0.00130 0.00000 0.00130 3.11697

D224 1.09553 0.00055 0.00114 0.00000 0.00114 1.09667

D225 -1.03807 -0.00082 -0.00878 0.00000 -0.00878 -1.04685

D226 -3.11563 0.00010 -0.00135 0.00000 -0.00134 -3.11697

D227 1.09790 0.00073 0.00176 0.00000 0.00176 1.09965

D228 -1.04569 -0.00028 0.00043 0.00000 0.00043 -1.04526

D229 -3.11145 -0.00033 -0.00316 0.00000 -0.00316 -3.11461

D230 1.04572 0.00028 -0.00045 0.00000 -0.00045 1.04526

D231 -1.09789 -0.00073 -0.00176 0.00000 -0.00176 -1.09965

D232 3.11150 0.00034 0.00310 0.00000 0.00310 3.11461

Item Value Threshold Converged?

Maximum Force 0.091261 0.000450 NO

RMS Force 0.009573 0.000300 NO

Maximum Displacement 0.398456 0.001800 NO

RMS Displacement 0.093368 0.001200 NO

Predicted change in Energy=-1.922040D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 01:04:32 2019, MaxMem= 1342177280 cpu: 12.9

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=0 Diff= 8.28D-04

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 -1.123992 2.807229 0.005223

2 7 0 -0.000149 2.047913 -0.154144

3 6 0 1.123765 2.807304 0.005227

4 6 0 0.714221 4.163254 0.306826

5 6 0 -0.714494 4.163215 0.306821

6 7 0 2.411861 2.385616 -0.103237

7 6 0 2.799402 1.132555 -0.178909

8 7 0 2.025811 -0.000134 -0.098369

9 6 0 2.799318 -1.132762 -0.178866

10 6 0 4.207341 -0.704885 -0.350947

11 6 0 4.207383 0.704617 -0.350968

12 7 0 -2.411850 2.385560 -0.103211

13 6 0 -4.207118 0.704595 -0.350888

14 6 0 -4.207080 -0.704840 -0.350866

15 6 0 -2.799087 -1.132770 -0.178785

16 7 0 -2.025381 -0.000128 -0.098267

17 6 0 -2.799165 1.132579 -0.178828

18 7 0 -2.411774 -2.385531 -0.103162

19 7 0 -0.000154 -2.047531 -0.154202

20 6 0 -1.124016 -2.807008 0.005216

21 6 0 -0.714474 -4.162964 0.306806

22 6 0 0.714179 -4.163008 0.306811

23 6 0 1.123775 -2.807089 0.005221

24 7 0 2.411773 -2.385601 -0.103189

25 30 0 0.000158 0.000098 -0.261011

26 6 0 -5.394952 1.432226 -0.489972

27 6 0 -6.585948 0.695321 -0.622542

28 6 0 -6.585917 -0.695656 -0.622529

29 6 0 -5.394890 -1.432515 -0.489944

30 6 0 1.434061 -5.343824 0.576879

31 6 0 0.700182 -6.508972 0.822420

32 6 0 -0.700586 -6.508935 0.822418

33 6 0 -1.434409 -5.343750 0.576875

34 6 0 5.395217 1.432238 -0.490024

35 6 0 6.586208 0.695308 -0.622568

36 6 0 6.586174 -0.695678 -0.622556

37 6 0 5.395148 -1.432555 -0.489995

38 6 0 -1.434419 5.344001 0.576890

39 6 0 -0.700572 6.509176 0.822437

40 6 0 0.700205 6.509209 0.822439

41 6 0 1.434101 5.344066 0.576894

42 1 0 7.533180 1.206580 -0.735390

43 1 0 7.533122 -1.206996 -0.735371

44 1 0 1.208723 7.440961 1.032291

45 1 0 -1.209131 7.440906 1.032288

46 1 0 -7.532912 1.206603 -0.735390

47 1 0 -7.532860 -1.206979 -0.735370

48 1 0 -1.209156 -7.440661 1.032263

49 1 0 1.208705 -7.440723 1.032266

50 8 0 2.781252 5.280677 0.595153

51 8 0 -2.781565 5.280562 0.595148

52 8 0 5.336524 2.779331 -0.501959

53 8 0 5.336412 -2.779646 -0.501911

54 8 0 2.781210 -5.280424 0.595134

55 8 0 -2.781553 -5.280292 0.595128

56 8 0 -5.336147 -2.779604 -0.501875

57 8 0 -5.336245 2.779318 -0.501923

58 6 0 3.512384 6.486225 0.805458

59 1 0 3.300823 6.918345 1.788286

60 1 0 3.297842 7.223887 0.026186

61 1 0 4.562075 6.202201 0.755603

62 6 0 6.557092 3.512940 -0.582142

63 1 0 7.086095 3.313953 -1.519018

64 1 0 7.213817 3.290533 0.264485

65 1 0 6.267053 4.561567 -0.548692

66 6 0 6.556957 -3.513292 -0.582087

67 1 0 7.213690 -3.290893 0.264535

68 1 0 7.085963 -3.314336 -1.518968

69 1 0 6.266885 -4.561910 -0.548621

70 6 0 -3.512743 6.486084 0.805444

71 1 0 -3.298228 7.223749 0.026168

72 1 0 -3.301202 6.918219 1.788270

73 1 0 -4.562423 6.202018 0.755587

74 6 0 -6.556804 3.512935 -0.582155

75 1 0 -7.213558 3.290544 0.264453

76 1 0 -7.085777 3.313939 -1.519047

77 1 0 -6.266758 4.561561 -0.548710

78 6 0 -6.556686 -3.513253 -0.582100

79 1 0 -7.085661 -3.314285 -1.518996

80 1 0 -7.213448 -3.290866 0.264503

81 1 0 -6.266613 -4.561871 -0.548638

82 6 0 -3.512750 -6.485805 0.805409

83 1 0 -3.301219 -6.917953 1.788231

84 1 0 -3.298243 -7.223465 0.026126

85 1 0 -4.562425 -6.201723 0.755551

86 6 0 3.512354 -6.485968 0.805424

87 1 0 3.297815 -7.223623 0.026146

88 1 0 3.300800 -6.918099 1.788249

89 1 0 4.562042 -6.201934 0.755568

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0446364 0.0438785 0.0225517

Leave Link 202 at Sat Jul 6 01:04:33 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8036.4951838633 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= 89 NActive= 89 NUniq= 89 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= -0.2277141490 Hartrees.

Nuclear repulsion after empirical dispersion term = 8036.2674697143 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6466

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.59D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 390

GePol: Fraction of low-weight points (<1% of avg) = 6.03%

GePol: Cavity surface area = 702.387 Ang\*\*2

GePol: Cavity volume = 801.542 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0090050875 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8036.2584646268 Hartrees.

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(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44271 LenP2D= 111168.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.90D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

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(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 01:04:37 2019, MaxMem= 1342177280 cpu: 2.5

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000176 0.000220 0.000032 Ang= 0.03 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 1.77D-02

Max alpha theta= 7.742 degrees.

Max beta theta= 5.758 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0169 S= 1.0056

Leave Link 401 at Sat Jul 6 01:04:48 2019, MaxMem= 1342177280 cpu: 124.0

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 125427468.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.13D-14 for 6436.

Iteration 1 A\*A^-1 deviation from orthogonality is 8.32D-15 for 3971 2140.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.13D-14 for 6436.

Iteration 1 A^-1\*A deviation from orthogonality is 1.55D-08 for 2627 2569.

Iteration 2 A\*A^-1 deviation from unit magnitude is 1.31D-14 for 490.

Iteration 2 A\*A^-1 deviation from orthogonality is 1.13D-14 for 2850 1074.

Iteration 2 A^-1\*A deviation from unit magnitude is 2.22D-15 for 2152.

Iteration 2 A^-1\*A deviation from orthogonality is 7.83D-16 for 6433 2101.

E= -2649.79426753170

DIIS: error= 1.36D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79426753170 IErMin= 1 ErrMin= 1.36D-05

ErrMax= 1.36D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.51D-07 BMatP= 7.51D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 14.963 Goal= None Shift= 0.000

Gap= 15.006 Goal= None Shift= 0.000

RMSDP=1.14D-06 MaxDP=5.33D-05 OVMax= 1.73D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.12D-06 CP: 1.00D+00

E= -2649.79426761759 Delta-E= -0.000000085889 Rises=F Damp=F

DIIS: error= 1.35D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79426761759 IErMin= 2 ErrMin= 1.35D-05

ErrMax= 1.35D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.01D-07 BMatP= 7.51D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.340D+00 0.660D+00

Coeff: 0.340D+00 0.660D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.70D-07 MaxDP=3.95D-05 DE=-8.59D-08 OVMax= 9.71D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.23D-07 CP: 1.00D+00 8.38D-01

E= -2649.79426762643 Delta-E= -0.000000008838 Rises=F Damp=F

DIIS: error= 1.28D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79426762643 IErMin= 3 ErrMin= 1.28D-05

ErrMax= 1.28D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.49D-07 BMatP= 3.01D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.391D-02 0.475D+00 0.521D+00

Coeff: 0.391D-02 0.475D+00 0.521D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.72D-07 MaxDP=1.56D-05 DE=-8.84D-09 OVMax= 5.11D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 8.40D-08 CP: 1.00D+00 9.47D-01 4.77D-01

E= -2649.79426767623 Delta-E= -0.000000049798 Rises=F Damp=F

DIIS: error= 1.77D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79426767623 IErMin= 4 ErrMin= 1.77D-06

ErrMax= 1.77D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.64D-09 BMatP= 2.49D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.597D-02 0.245D+00 0.295D+00 0.466D+00

Coeff: -0.597D-02 0.245D+00 0.295D+00 0.466D+00

Gap= 0.046 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 320071 IAlg= 4 N= 1128 NDim= 1128 NE2= 1186103 trying DSYEV.

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.06D-08 MaxDP=4.46D-06 DE=-4.98D-08 OVMax= 1.16D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.45D-08 CP: 1.00D+00 9.53D-01 4.88D-01 7.63D-01

E= -2649.79426767751 Delta-E= -0.000000001282 Rises=F Damp=F

DIIS: error= 4.42D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79426767751 IErMin= 5 ErrMin= 4.42D-07

ErrMax= 4.42D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.05D-10 BMatP= 6.64D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.271D-02 0.459D-01 0.645D-01 0.227D+00 0.666D+00

Coeff: -0.271D-02 0.459D-01 0.645D-01 0.227D+00 0.666D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.56D-08 MaxDP=1.17D-06 DE=-1.28D-09 OVMax= 5.49D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.31D-08 CP: 1.00D+00 9.54D-01 4.99D-01 8.44D-01 9.50D-01

E= -2649.79426767756 Delta-E= -0.000000000042 Rises=F Damp=F

DIIS: error= 3.40D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79426767756 IErMin= 6 ErrMin= 3.40D-07

ErrMax= 3.40D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D-10 BMatP= 5.05D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.890D-04-0.278D-01-0.309D-01 0.199D-01 0.328D+00 0.711D+00

Coeff: -0.890D-04-0.278D-01-0.309D-01 0.199D-01 0.328D+00 0.711D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=8.80D-09 MaxDP=6.51D-07 DE=-4.18D-11 OVMax= 3.73D-06

Error on total polarization charges = 0.07286

SCF Done: E(UB3LYP) = -2649.79426768 A.U. after 6 cycles

NFock= 6 Conv=0.88D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0169 S= 1.0056

<L.S>= 0.000000000000E+00

KE= 2.690084777001D+03 PE=-2.235114722368D+04 EE= 8.975009714373D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.65

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0169, after 2.0002

Leave Link 502 at Sat Jul 6 01:10:14 2019, MaxMem= 1342177280 cpu: 3808.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44271 LenP2D= 111168.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 284

Leave Link 701 at Sat Jul 6 01:10:33 2019, MaxMem= 1342177280 cpu: 220.7

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 01:10:33 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 01:12:04 2019, MaxMem= 1342177280 cpu: 1093.5

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-4.82045647D-04-7.45900971D-04 9.67743479D-02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.002591499 -0.001959051 0.001859254

2 7 0.000080490 -0.000124990 -0.000900380

3 6 0.002711705 -0.002071183 0.001837491

4 6 -0.001146091 0.000916617 -0.000580599

5 6 0.001152612 0.000932709 -0.000576646

6 7 -0.002269230 0.000530237 0.000126060

7 6 0.000866217 -0.000671721 -0.001597027

8 7 -0.000591057 0.000085779 0.004462475

9 6 0.000991475 0.000818129 -0.001619587

10 6 -0.001050769 -0.001142995 0.000531392

11 6 -0.001062348 0.001147741 0.000531844

12 7 0.002170779 0.000585562 0.000125402

13 6 0.001059016 0.001170066 0.000530420

14 6 0.001047353 -0.001165310 0.000529945

15 6 -0.001017989 0.000989740 -0.001627046

16 7 0.000424918 0.000085672 0.004450172

17 6 -0.000892832 -0.000842875 -0.001604519

18 7 0.002144597 -0.000735419 0.000126426

19 7 0.000080353 -0.000042860 -0.000870736

20 6 -0.002450908 0.001945273 0.001856992

21 6 0.001135674 -0.000937067 -0.000574157

22 6 -0.001129109 -0.000920844 -0.000578177

23 6 0.002571532 0.002057212 0.001835239

24 7 -0.002243319 -0.000679787 0.000127136

25 30 0.000005053 0.000022460 -0.008316062

26 6 -0.000802626 -0.001490498 -0.000442465

27 6 0.000479653 0.000685819 0.000119648

28 6 0.000480465 -0.000684969 0.000119720

29 6 -0.000799533 0.001494983 -0.000441867

30 6 -0.001253418 0.000609806 0.000142209

31 6 -0.000056568 -0.000275391 0.000101156

32 6 0.000057226 -0.000277120 0.000101555

33 6 0.001256741 0.000616367 0.000140281

34 6 0.000804327 -0.001496842 -0.000442073

35 6 -0.000479272 0.000677833 0.000119361

36 6 -0.000480120 -0.000676988 0.000119430

37 6 0.000801265 0.001501356 -0.000441483

38 6 0.001263484 -0.000616023 0.000140598

39 6 0.000064803 0.000277934 0.000101878

40 6 -0.000064134 0.000276252 0.000101487

41 6 -0.001260110 -0.000609512 0.000142512

42 1 -0.000146561 -0.000230143 0.000028044

43 1 -0.000146580 0.000230213 0.000028087

44 1 -0.000231870 -0.000168313 -0.000115034

45 1 0.000231903 -0.000168380 -0.000115050

46 1 0.000146910 -0.000229920 0.000028171

47 1 0.000146945 0.000229995 0.000028212

48 1 0.000231532 0.000168580 -0.000115056

49 1 -0.000231489 0.000168518 -0.000115045

50 8 0.000802266 0.000430866 -0.000339137

51 8 -0.000802940 0.000432058 -0.000339131

52 8 0.000049604 0.000109000 0.000180950

53 8 0.000050065 -0.000110274 0.000181498

54 8 0.000803040 -0.000433441 -0.000338186

55 8 -0.000803675 -0.000434673 -0.000338153

56 8 -0.000054756 -0.000111015 0.000181087

57 8 -0.000054267 0.000109755 0.000180538

58 6 0.000463823 0.000248394 0.000162962

59 1 0.000029883 -0.000166821 -0.000150028

60 1 0.000072583 -0.000164560 0.000206518

61 1 -0.000062035 0.000150408 0.000029595

62 6 0.000277697 0.000362764 0.000023760

63 1 -0.000144495 0.000024227 0.000127527

64 1 -0.000201023 0.000020046 -0.000100624

65 1 0.000148376 -0.000071028 0.000002898

66 6 0.000276782 -0.000363134 0.000024055

67 1 -0.000200930 -0.000020146 -0.000100595

68 1 -0.000144470 -0.000024270 0.000127541

69 1 0.000148587 0.000070896 0.000003091

70 6 -0.000464190 0.000248145 0.000162796

71 1 -0.000072615 -0.000164598 0.000206546

72 1 -0.000029960 -0.000166891 -0.000150035

73 1 0.000062014 0.000150572 0.000029476

74 6 -0.000276195 0.000362146 0.000023881

75 1 0.000200757 0.000020107 -0.000100507

76 1 0.000144151 0.000024280 0.000127518

77 1 -0.000148244 -0.000071044 0.000003170

78 6 -0.000275281 -0.000362494 0.000024161

79 1 0.000144130 -0.000024329 0.000127534

80 1 0.000200657 -0.000020222 -0.000100478

81 1 -0.000148442 0.000070909 0.000003363

82 6 -0.000463173 -0.000246640 0.000162387

83 1 -0.000030020 0.000166511 -0.000149805

84 1 -0.000072615 0.000164230 0.000206522

85 1 0.000062035 -0.000150154 0.000029167

86 6 0.000462824 -0.000246903 0.000162564

87 1 0.000072563 0.000164207 0.000206495

88 1 0.000029939 0.000166450 -0.000149808

89 1 -0.000062046 -0.000149991 0.000029297

-------------------------------------------------------------------

Cartesian Forces: Max 0.008316062 RMS 0.000982171

Leave Link 716 at Sat Jul 6 01:12:04 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002237391 RMS 0.000421542

Search for a local minimum.

Step number 11 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .42154D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 2 3 4 6

5 8 7 10 9

11

ITU= 0 0 0 0 0 0 1 1 1 1 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.00002 0.00061 0.00851 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01316 0.01316

Eigenvalues --- 0.01322 0.01570 0.01571 0.01582 0.01585

Eigenvalues --- 0.01600 0.01616 0.01621 0.01707 0.01709

Eigenvalues --- 0.01712 0.01715 0.01753 0.01834 0.01873

Eigenvalues --- 0.01881 0.01888 0.01923 0.01926 0.01930

Eigenvalues --- 0.01943 0.02010 0.02020 0.02021 0.02022

Eigenvalues --- 0.02028 0.02030 0.02048 0.02053 0.02053

Eigenvalues --- 0.02053 0.02053 0.02057 0.02057 0.02057

Eigenvalues --- 0.02057 0.02066 0.02067 0.02067 0.02069

Eigenvalues --- 0.02070 0.02071 0.02071 0.02071 0.02079

Eigenvalues --- 0.02083 0.02084 0.02161 0.02228 0.02260

Eigenvalues --- 0.02260 0.02260 0.02260 0.02260 0.02260

Eigenvalues --- 0.02265 0.02344 0.02351 0.02366 0.03334

Eigenvalues --- 0.09816 0.09975 0.09975 0.09975 0.09988

Eigenvalues --- 0.09988 0.09988 0.09993 0.10650 0.10656

Eigenvalues --- 0.10656 0.10656 0.10661 0.10661 0.10661

Eigenvalues --- 0.10661 0.13261 0.13467 0.13539 0.14724

Eigenvalues --- 0.15978 0.15985 0.15997 0.15998 0.15998

Eigenvalues --- 0.15999 0.15999 0.15999 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16002 0.16019

Eigenvalues --- 0.16062 0.16376 0.21445 0.21691 0.22471

Eigenvalues --- 0.22473 0.22474 0.22475 0.22550 0.24277

Eigenvalues --- 0.24408 0.24432 0.24480 0.24508 0.24514

Eigenvalues --- 0.24575 0.24705 0.24713 0.24844 0.24853

Eigenvalues --- 0.24903 0.24912 0.24993 0.24996 0.24997

Eigenvalues --- 0.24997 0.24997 0.24998 0.24998 0.24998

Eigenvalues --- 0.24998 0.24998 0.24999 0.24999 0.24999

Eigenvalues --- 0.24999 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25154 0.26093 0.31249

Eigenvalues --- 0.33632 0.33637 0.33682 0.33720 0.33893

Eigenvalues --- 0.34042 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34063 0.34063 0.34077 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34081

Eigenvalues --- 0.34141 0.34577 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34686 0.34687 0.34908

Eigenvalues --- 0.34953 0.35077 0.35591 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35632 0.35718

Eigenvalues --- 0.36554 0.37104 0.37156 0.38726 0.41002

Eigenvalues --- 0.41175 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41215 0.41215 0.41412 0.41414 0.41415

Eigenvalues --- 0.41417 0.41447 0.42405 0.42470 0.42636

Eigenvalues --- 0.43581 0.44544 0.44567 0.44772 0.44827

Eigenvalues --- 0.44901 0.44955 0.44998 0.45000 0.45001

Eigenvalues --- 0.45003 0.45364 0.45366 0.45866 0.46930

Eigenvalues --- 0.47328 0.48561 0.49238 0.49299 0.49848

Eigenvalues --- 0.50607 0.53394 0.53554 0.53554 0.53554

Eigenvalues --- 0.53554 0.53554 0.53554 0.54741 0.54984

Eigenvalues --- 0.56071 0.56596 0.57409 0.57568 0.57729

Eigenvalues --- 0.76783

RFO step: Lambda=-6.66924686D-03 EMin= 2.12859708D-05

Quartic linear search produced a step of -0.00328.

Maximum step size ( 0.457) exceeded in Quadratic search.

-- Step size scaled by 0.984

Iteration 1 RMS(Cart)= 0.15173150 RMS(Int)= 0.00594936

Iteration 2 RMS(Cart)= 0.02321589 RMS(Int)= 0.00364159

Iteration 3 RMS(Cart)= 0.00024275 RMS(Int)= 0.00364096

Iteration 4 RMS(Cart)= 0.00000531 RMS(Int)= 0.00364096

Iteration 5 RMS(Cart)= 0.00000011 RMS(Int)= 0.00364096

ITry= 1 IFail=0 DXMaxC= 1.07D+00 DCOld= 1.00D+10 DXMaxT= 4.57D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58069 0.00015 0.00000 0.00925 0.01217 2.59286

R2 2.73674 0.00085 0.00000 0.03114 0.02974 2.76648

R3 2.56901 -0.00202 -0.00001 -0.03352 -0.04163 2.52739

R4 2.58088 0.00010 0.00000 0.00837 0.00921 2.59009

R5 3.87508 -0.00091 0.00000 -0.01924 -0.00292 3.87215

R6 2.73671 0.00085 0.00000 0.03063 0.02926 2.76597

R7 2.56945 -0.00222 -0.00001 -0.03679 -0.04911 2.52035

R8 2.69988 -0.00061 0.00000 -0.02637 -0.03114 2.66874

R9 2.66276 0.00010 0.00000 0.00691 0.00696 2.66972

R10 2.66276 0.00009 0.00000 0.00682 0.00688 2.66964

R11 2.48273 -0.00012 0.00001 -0.00838 -0.02012 2.46261

R12 2.59651 -0.00034 0.00000 -0.00022 0.00305 2.59956

R13 2.79982 -0.00088 0.00000 -0.02751 -0.02917 2.77065

R14 2.59632 -0.00028 0.00000 0.00096 0.00632 2.60264

R15 3.84025 -0.00041 0.00000 0.01060 0.02819 3.86843

R16 2.79987 -0.00088 0.00000 -0.02698 -0.02870 2.77117

R17 2.48233 0.00012 0.00001 -0.00408 -0.01165 2.47068

R18 2.66357 0.00037 0.00000 0.00887 0.00317 2.66675

R19 2.64543 0.00006 0.00000 0.00899 0.00915 2.65458

R20 2.64543 0.00007 0.00000 0.00903 0.00918 2.65461

R21 2.48245 0.00005 0.00001 -0.00521 -0.01413 2.46832

R22 2.66344 0.00040 0.00000 0.00980 0.00610 2.66954

R23 2.79980 -0.00087 0.00000 -0.02706 -0.02813 2.77167

R24 2.64544 0.00007 0.00000 0.00922 0.00931 2.65475

R25 2.79984 -0.00087 0.00000 -0.02653 -0.02765 2.77219

R26 2.64545 0.00007 0.00000 0.00919 0.00927 2.65472

R27 2.59656 -0.00033 0.00000 0.00028 0.00307 2.59962

R28 2.48205 0.00028 0.00001 -0.00091 -0.00564 2.47641

R29 2.59675 -0.00039 0.00000 -0.00089 -0.00021 2.59654

R30 3.84005 -0.00035 0.00000 0.01032 0.02064 3.86069

R31 2.56871 -0.00189 -0.00001 -0.03126 -0.03656 2.53216

R32 2.58090 0.00010 0.00000 0.00863 0.00930 2.59020

R33 2.58109 0.00005 0.00000 0.00777 0.00635 2.58744

R34 3.87472 -0.00083 0.00000 -0.01972 -0.01081 3.86391

R35 2.73671 0.00086 0.00000 0.03141 0.03060 2.76731

R36 2.69976 -0.00059 0.00000 -0.02567 -0.02852 2.67124

R37 2.66277 0.00010 0.00000 0.00690 0.00689 2.66965

R38 2.73667 0.00085 0.00000 0.03090 0.03011 2.76679

R39 2.66277 0.00010 0.00000 0.00698 0.00697 2.66974

R40 2.56915 -0.00209 -0.00001 -0.03453 -0.04406 2.52510

R41 2.65846 -0.00089 0.00000 -0.02129 -0.02138 2.63708

R42 2.54815 0.00044 0.00000 0.00144 0.00144 2.54959

R43 2.62857 -0.00021 0.00000 -0.00626 -0.00643 2.62214

R44 2.04482 -0.00024 0.00000 -0.00393 -0.00393 2.04089

R45 2.65847 -0.00089 0.00000 -0.02121 -0.02130 2.63716

R46 2.04482 -0.00024 0.00000 -0.00393 -0.00393 2.04090

R47 2.54815 0.00044 0.00000 0.00141 0.00141 2.54956

R48 2.64321 0.00002 0.00000 -0.00439 -0.00437 2.63884

R49 2.54879 0.00128 0.00000 0.01349 0.01349 2.56228

R50 2.64707 -0.00042 0.00000 -0.00843 -0.00841 2.63866

R51 2.04474 -0.00028 0.00000 -0.00358 -0.00358 2.04117

R52 2.64322 0.00002 0.00000 -0.00430 -0.00430 2.63892

R53 2.04474 -0.00028 0.00000 -0.00358 -0.00358 2.04117

R54 2.54879 0.00128 0.00000 0.01343 0.01343 2.56222

R55 2.65847 -0.00089 0.00000 -0.02126 -0.02142 2.63705

R56 2.54815 0.00044 0.00000 0.00147 0.00148 2.54963

R57 2.62858 -0.00022 0.00000 -0.00649 -0.00679 2.62179

R58 2.04482 -0.00024 0.00000 -0.00393 -0.00393 2.04089

R59 2.65848 -0.00089 0.00000 -0.02118 -0.02134 2.63713

R60 2.04482 -0.00024 0.00000 -0.00393 -0.00393 2.04090

R61 2.54815 0.00044 0.00000 0.00144 0.00144 2.54959

R62 2.64323 0.00002 0.00000 -0.00431 -0.00436 2.63886

R63 2.54879 0.00128 0.00000 0.01349 0.01349 2.56228

R64 2.64708 -0.00044 0.00000 -0.00865 -0.00876 2.63833

R65 2.04474 -0.00028 0.00000 -0.00358 -0.00357 2.04117

R66 2.64322 0.00001 0.00000 -0.00439 -0.00444 2.63878

R67 2.04474 -0.00028 0.00000 -0.00358 -0.00358 2.04117

R68 2.54880 0.00128 0.00000 0.01355 0.01355 2.56235

R69 2.69386 0.00035 0.00000 0.00376 0.00376 2.69761

R70 2.69386 0.00035 0.00000 0.00375 0.00375 2.69760

R71 2.69536 0.00024 0.00000 0.00433 0.00433 2.69969

R72 2.69536 0.00024 0.00000 0.00431 0.00431 2.69967

R73 2.69386 0.00035 0.00000 0.00372 0.00372 2.69757

R74 2.69386 0.00035 0.00000 0.00371 0.00371 2.69756

R75 2.69536 0.00024 0.00000 0.00427 0.00427 2.69963

R76 2.69536 0.00024 0.00000 0.00428 0.00428 2.69964

R77 2.06788 -0.00021 0.00000 -0.00312 -0.00312 2.06476

R78 2.06788 -0.00027 0.00000 -0.00489 -0.00489 2.06299

R79 2.05712 -0.00010 0.00000 -0.00148 -0.00148 2.05564

R80 2.06765 -0.00018 0.00000 -0.00281 -0.00281 2.06484

R81 2.06796 -0.00020 0.00000 -0.00349 -0.00349 2.06447

R82 2.05699 -0.00011 0.00000 -0.00184 -0.00184 2.05515

R83 2.06796 -0.00020 0.00000 -0.00348 -0.00348 2.06448

R84 2.06765 -0.00018 0.00000 -0.00281 -0.00281 2.06485

R85 2.05699 -0.00011 0.00000 -0.00184 -0.00184 2.05515

R86 2.06788 -0.00027 0.00000 -0.00489 -0.00489 2.06299

R87 2.06788 -0.00021 0.00000 -0.00312 -0.00312 2.06476

R88 2.05712 -0.00010 0.00000 -0.00148 -0.00148 2.05564

R89 2.06796 -0.00020 0.00000 -0.00348 -0.00348 2.06448

R90 2.06765 -0.00018 0.00000 -0.00280 -0.00280 2.06485

R91 2.05699 -0.00011 0.00000 -0.00184 -0.00184 2.05515

R92 2.06766 -0.00018 0.00000 -0.00280 -0.00280 2.06486

R93 2.06796 -0.00020 0.00000 -0.00348 -0.00347 2.06448

R94 2.05699 -0.00011 0.00000 -0.00184 -0.00184 2.05515

R95 2.06788 -0.00021 0.00000 -0.00311 -0.00311 2.06477

R96 2.06788 -0.00027 0.00000 -0.00489 -0.00488 2.06300

R97 2.05712 -0.00010 0.00000 -0.00149 -0.00149 2.05563

R98 2.06788 -0.00027 0.00000 -0.00489 -0.00489 2.06299

R99 2.06788 -0.00021 0.00000 -0.00311 -0.00311 2.06477

R100 2.05712 -0.00010 0.00000 -0.00148 -0.00148 2.05564

A1 1.88832 -0.00019 0.00000 -0.00102 0.00387 1.89218

A2 2.21158 0.00027 0.00000 0.01772 0.01853 2.23012

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D105 3.06863 0.00051 0.00000 0.07671 0.07188 3.14051

D106 -0.17686 -0.00114 0.00000 -0.17021 -0.16691 -0.34377

D107 0.17690 0.00113 0.00000 0.17019 0.16720 0.34410

D108 -3.06859 -0.00051 0.00000 -0.07673 -0.07160 -3.14018

D109 -0.19323 -0.00057 0.00000 -0.01572 -0.01473 -0.20796

D110 2.95511 -0.00031 0.00000 -0.02643 -0.02502 2.93009

D111 -3.12370 -0.00062 0.00000 -0.09352 -0.09236 3.06712

D112 0.01208 -0.00083 0.00000 -0.08434 -0.08347 -0.07139

D113 0.20529 -0.00026 0.00000 -0.11549 -0.11498 0.09031

D114 -2.94211 -0.00048 0.00000 -0.10632 -0.10608 -3.04819

D115 -0.01208 0.00083 0.00000 0.08433 0.08349 0.07141

D116 3.12369 0.00062 0.00000 0.09354 0.09273 -3.06676

D117 2.94214 0.00048 0.00000 0.10609 0.10502 3.04717

D118 -0.20527 0.00026 0.00000 0.11530 0.11427 -0.09100

D119 2.95552 -0.00131 0.00000 -0.14805 -0.14368 2.81185

D120 -0.02601 0.00093 0.00000 0.17224 0.16816 0.14215

D121 0.02603 -0.00094 0.00000 -0.17220 -0.16718 -0.14115

D122 -2.95550 0.00130 0.00000 0.14809 0.14465 -2.81084

D123 3.12875 0.00028 0.00000 0.05908 0.05836 -3.09608

D124 -0.01987 0.00002 0.00000 0.03472 0.03420 0.01433

D125 -0.00715 0.00049 0.00000 0.04996 0.04972 0.04257

D126 3.12741 0.00023 0.00000 0.02560 0.02556 -3.13022

D127 0.00000 0.00000 0.00000 -0.00002 0.00000 0.00000

D128 3.13560 -0.00023 0.00000 -0.02082 -0.02074 3.11486

D129 -3.13560 0.00023 0.00000 0.02077 0.02066 -3.11495

D130 0.00000 0.00000 0.00000 -0.00003 -0.00009 -0.00009

D131 3.13295 0.00027 0.00000 0.03185 0.03172 -3.11851

D132 -0.01905 0.00026 0.00000 0.02812 0.02795 0.00890

D133 -0.01648 -0.00002 0.00000 0.00468 0.00478 -0.01170

D134 3.11471 -0.00003 0.00000 0.00095 0.00101 3.11571

D135 0.00716 -0.00049 0.00000 -0.04992 -0.04978 -0.04262

D136 -3.12873 -0.00028 0.00000 -0.05908 -0.05875 3.09570

D137 -3.12741 -0.00023 0.00000 -0.02555 -0.02552 3.13025

D138 0.01988 -0.00002 0.00000 -0.03471 -0.03449 -0.01461

D139 0.01648 0.00002 0.00000 -0.00464 -0.00466 0.01181

D140 -3.11471 0.00003 0.00000 -0.00090 -0.00089 -3.11560

D141 -3.13295 -0.00027 0.00000 -0.03182 -0.03171 3.11853

D142 0.01905 -0.00026 0.00000 -0.02808 -0.02794 -0.00889

D143 0.19321 0.00057 0.00000 0.01568 0.01450 0.20770

D144 -2.95514 0.00032 0.00000 0.02645 0.02517 -2.92997

D145 -0.00547 0.00000 0.00000 0.00147 0.00144 -0.00403

D146 -3.13916 -0.00007 0.00000 -0.00104 -0.00106 -3.14022

D147 3.12516 0.00019 0.00000 0.00853 0.00852 3.13368

D148 -0.00853 0.00012 0.00000 0.00603 0.00601 -0.00251

D149 -3.09202 0.00020 0.00000 -0.00655 -0.00659 -3.09861

D150 0.06072 0.00000 0.00000 -0.01387 -0.01383 0.04689

D151 0.00000 0.00000 0.00000 -0.00001 -0.00002 -0.00001

D152 -3.13384 -0.00007 0.00000 -0.00254 -0.00253 -3.13637

D153 3.13385 0.00007 0.00000 0.00253 0.00250 3.13635

D154 0.00000 0.00000 0.00000 0.00000 -0.00001 -0.00001

D155 0.00547 0.00000 0.00000 -0.00146 -0.00145 0.00402

D156 -3.12516 -0.00019 0.00000 -0.00855 -0.00855 -3.13371

D157 3.13916 0.00007 0.00000 0.00104 0.00105 3.14021

D158 0.00853 -0.00012 0.00000 -0.00605 -0.00605 0.00248

D159 3.09202 -0.00020 0.00000 0.00649 0.00653 3.09855

D160 -0.06072 0.00000 0.00000 0.01384 0.01380 -0.04692

D161 -0.01664 -0.00002 0.00000 0.00472 0.00478 -0.01186

D162 3.13909 -0.00005 0.00000 -0.00046 -0.00047 3.13862

D163 3.11388 -0.00003 0.00000 0.00094 0.00104 3.11492

D164 -0.01358 -0.00005 0.00000 -0.00425 -0.00421 -0.01779

D165 -3.09067 -0.00039 0.00000 -0.03581 -0.03581 -3.12647

D166 0.06206 -0.00038 0.00000 -0.03194 -0.03194 0.03012

D167 0.00000 0.00000 0.00000 -0.00002 -0.00003 -0.00003

D168 -3.12777 -0.00003 0.00000 -0.00514 -0.00518 -3.13295

D169 3.12777 0.00003 0.00000 0.00512 0.00514 3.13291

D170 0.00000 0.00000 0.00000 0.00000 -0.00001 -0.00001

D171 0.01664 0.00002 0.00000 -0.00471 -0.00478 0.01186

D172 -3.11388 0.00003 0.00000 -0.00095 -0.00103 -3.11491

D173 -3.13909 0.00005 0.00000 0.00046 0.00044 -3.13865

D174 0.01357 0.00005 0.00000 0.00422 0.00419 0.01777

D175 3.09066 0.00039 0.00000 0.03576 0.03576 3.12642

D176 -0.06207 0.00038 0.00000 0.03190 0.03189 -0.03018

D177 0.00547 -0.00001 0.00000 -0.00149 -0.00144 0.00403

D178 3.13916 0.00007 0.00000 0.00104 0.00107 3.14024

D179 -3.12518 -0.00019 0.00000 -0.00857 -0.00852 -3.13370

D180 0.00852 -0.00012 0.00000 -0.00604 -0.00602 0.00250

D181 3.09200 -0.00020 0.00000 0.00653 0.00657 3.09857

D182 -0.06072 0.00000 0.00000 0.01387 0.01383 -0.04690

D183 0.00000 0.00000 0.00000 0.00001 0.00002 0.00001

D184 3.13385 0.00007 0.00000 0.00257 0.00253 3.13638

D185 -3.13385 -0.00007 0.00000 -0.00255 -0.00250 -3.13635

D186 0.00000 0.00000 0.00000 0.00000 0.00001 0.00001

D187 -0.00547 0.00001 0.00000 0.00148 0.00145 -0.00402

D188 3.12518 0.00019 0.00000 0.00858 0.00855 3.13373

D189 -3.13917 -0.00007 0.00000 -0.00104 -0.00106 -3.14022

D190 -0.00852 0.00012 0.00000 0.00606 0.00605 -0.00247

D191 -3.09200 0.00020 0.00000 -0.00647 -0.00652 -3.09851

D192 0.06073 0.00000 0.00000 -0.01383 -0.01379 0.04693

D193 -0.01664 -0.00002 0.00000 0.00475 0.00492 -0.01172

D194 3.13909 -0.00005 0.00000 -0.00043 -0.00038 3.13871

D195 3.11388 -0.00003 0.00000 0.00096 0.00114 3.11502

D196 -0.01357 -0.00005 0.00000 -0.00422 -0.00416 -0.01774

D197 -3.09067 -0.00039 0.00000 -0.03581 -0.03582 -3.12648

D198 0.06207 -0.00038 0.00000 -0.03193 -0.03192 0.03014

D199 0.00000 0.00000 0.00000 0.00002 0.00003 0.00003

D200 -3.12777 -0.00003 0.00000 -0.00513 -0.00522 -3.13298

D201 3.12777 0.00003 0.00000 0.00515 0.00525 3.13302

D202 0.00000 0.00000 0.00000 0.00000 0.00001 0.00001

D203 0.01664 0.00002 0.00000 -0.00476 -0.00492 0.01172

D204 -3.11388 0.00003 0.00000 -0.00094 -0.00114 -3.11502

D205 -3.13909 0.00005 0.00000 0.00043 0.00040 -3.13869

D206 0.01358 0.00005 0.00000 0.00425 0.00419 0.01776

D207 3.09068 0.00039 0.00000 0.03587 0.03586 3.12654

D208 -0.06206 0.00038 0.00000 0.03196 0.03197 -0.03009

D209 1.09667 0.00003 0.00000 -0.00135 -0.00135 1.09532

D210 -1.04685 0.00007 0.00000 -0.00023 -0.00022 -1.04707

D211 -3.11698 -0.00001 0.00000 -0.00389 -0.00390 -3.12088

D212 1.04685 -0.00007 0.00000 0.00023 0.00021 1.04706

D213 -1.09667 -0.00003 0.00000 0.00133 0.00133 -1.09534

D214 3.11697 0.00001 0.00000 0.00386 0.00387 3.12085

D215 1.09965 -0.00003 0.00000 -0.00751 -0.00750 1.09215

D216 -1.04527 0.00002 0.00000 -0.00336 -0.00337 -1.04863

D217 -3.11461 0.00002 0.00000 -0.00457 -0.00457 -3.11918

D218 1.04526 -0.00002 0.00000 0.00334 0.00335 1.04861

D219 -1.09965 0.00003 0.00000 0.00751 0.00750 -1.09216

D220 3.11461 -0.00002 0.00000 0.00454 0.00454 3.11915

D221 1.04685 -0.00007 0.00000 0.00023 0.00021 1.04706

D222 -1.09667 -0.00003 0.00000 0.00134 0.00134 -1.09533

D223 3.11697 0.00001 0.00000 0.00386 0.00388 3.12085

D224 1.09667 0.00003 0.00000 -0.00132 -0.00132 1.09535

D225 -1.04685 0.00007 0.00000 -0.00022 -0.00021 -1.04705

D226 -3.11697 -0.00001 0.00000 -0.00384 -0.00385 -3.12083

D227 1.09965 -0.00003 0.00000 -0.00750 -0.00749 1.09217

D228 -1.04526 0.00002 0.00000 -0.00333 -0.00334 -1.04860

D229 -3.11461 0.00002 0.00000 -0.00453 -0.00452 -3.11913

D230 1.04526 -0.00002 0.00000 0.00335 0.00336 1.04862

D231 -1.09965 0.00003 0.00000 0.00751 0.00750 -1.09216

D232 3.11461 -0.00002 0.00000 0.00455 0.00455 3.11916

Item Value Threshold Converged?

Maximum Force 0.002237 0.000450 NO

RMS Force 0.000422 0.000300 NO

Maximum Displacement 1.071226 0.001800 NO

RMS Displacement 0.161622 0.001200 NO

Predicted change in Energy=-5.584128D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 01:12:06 2019, MaxMem= 1342177280 cpu: 14.7

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=3 Diff= 4.40D-04

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 -1.120380 2.761327 -0.146081

2 7 0 0.002657 2.010579 -0.386443

3 6 0 1.124906 2.760062 -0.146811

4 6 0 0.709395 4.123179 0.187323

5 6 0 -0.702842 4.124173 0.187825

6 7 0 2.397288 2.362993 -0.193341

7 6 0 2.784132 1.120702 -0.266041

8 7 0 1.982054 0.003122 -0.260239

9 6 0 2.785934 -1.115168 -0.266834

10 6 0 4.192686 -0.701580 -0.287770

11 6 0 4.191324 0.709600 -0.287184

12 7 0 -2.396684 2.364294 -0.192417

13 6 0 -4.198031 0.709425 -0.286183

14 6 0 -4.199072 -0.703235 -0.286759

15 6 0 -2.791707 -1.116663 -0.265990

16 7 0 -1.992075 0.002708 -0.259570

17 6 0 -2.790414 1.121003 -0.265217

18 7 0 -2.397594 -2.364349 -0.193457

19 7 0 0.003129 -2.020543 -0.387089

20 6 0 -1.120624 -2.767660 -0.146784

21 6 0 -0.702560 -4.130779 0.187256

22 6 0 0.710999 -4.129477 0.186737

23 6 0 1.126428 -2.765904 -0.147537

24 7 0 2.399288 -2.362014 -0.194416

25 30 0 -0.007200 -0.007142 -0.743284

26 6 0 -5.407258 1.424444 -0.294977

27 6 0 -6.599274 0.698875 -0.299266

28 6 0 -6.600343 -0.688701 -0.299791

29 6 0 -5.409468 -1.416231 -0.296067

30 6 0 1.433966 -5.300225 0.507010

31 6 0 0.704873 -6.452704 0.807314

32 6 0 -0.691443 -6.454032 0.807767

33 6 0 -1.422984 -5.302920 0.507967

34 6 0 5.400141 1.425166 -0.296094

35 6 0 6.592535 0.700247 -0.300501

36 6 0 6.593919 -0.687146 -0.301035

37 6 0 5.402998 -1.414570 -0.297203

38 6 0 -1.423769 5.296114 0.508086

39 6 0 -0.692808 6.447604 0.807707

40 6 0 0.703335 6.446579 0.807271

41 6 0 1.432353 5.294039 0.507162

42 1 0 7.547686 1.204236 -0.308611

43 1 0 7.550103 -1.189175 -0.309523

44 1 0 1.208910 7.368225 1.055590

45 1 0 -1.196853 7.370004 1.056340

46 1 0 -7.554610 1.202518 -0.307296

47 1 0 -7.556481 -1.190820 -0.308192

48 1 0 -1.195178 -7.376528 1.056670

49 1 0 1.210544 -7.374227 1.055893

50 8 0 2.787318 5.246208 0.525690

51 8 0 -2.778761 5.250436 0.527506

52 8 0 5.349973 2.773413 -0.304290

53 8 0 5.355824 -2.762900 -0.306408

54 8 0 2.788898 -5.252473 0.525733

55 8 0 -2.777961 -5.257904 0.527613

56 8 0 -5.362698 -2.764556 -0.305293

57 8 0 -5.358111 2.772710 -0.303211

58 6 0 3.505810 6.441060 0.832120

59 1 0 3.282427 6.788260 1.843742

60 1 0 3.288919 7.235901 0.115905

61 1 0 4.559376 6.177715 0.769236

62 6 0 6.582593 3.494207 -0.259148

63 1 0 7.198640 3.287017 -1.137488

64 1 0 7.144176 3.258469 0.647797

65 1 0 6.311253 4.547324 -0.251213

66 6 0 6.590031 -3.480986 -0.261721

67 1 0 7.151030 -3.244655 0.645432

68 1 0 7.205674 -3.271783 -1.139871

69 1 0 6.321041 -4.534710 -0.254560

70 6 0 -3.495206 6.446417 0.834298

71 1 0 -3.277554 7.240873 0.117885

72 1 0 -3.270658 6.793357 1.845753

73 1 0 -4.549210 6.184686 0.772084

74 6 0 -6.591268 3.492532 -0.257993

75 1 0 -7.152604 3.256370 0.648998

76 1 0 -7.207223 3.284848 -1.136288

77 1 0 -6.320740 4.545857 -0.250086

78 6 0 -6.597112 -3.482233 -0.260521

79 1 0 -7.212758 -3.272831 -1.138628

80 1 0 -7.157973 -3.245724 0.646676

81 1 0 -6.328451 -4.536040 -0.253373

82 6 0 -3.493782 -6.454136 0.834786

83 1 0 -3.268918 -6.800753 1.846286

84 1 0 -3.275874 -7.248653 0.118512

85 1 0 -4.547910 -6.192890 0.772661

86 6 0 3.507289 -6.447267 0.832528

87 1 0 3.290468 -7.242262 0.116458

88 1 0 3.283760 -6.794240 1.844200

89 1 0 4.560864 -6.183954 0.769710

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0453953 0.0438382 0.0226901

Leave Link 202 at Sat Jul 6 01:12:07 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8061.8549293396 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= 89 NActive= 89 NUniq= 89 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= -0.2282865049 Hartrees.

Nuclear repulsion after empirical dispersion term = 8061.6266428347 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6304

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.12D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 318

GePol: Fraction of low-weight points (<1% of avg) = 5.04%

GePol: Cavity surface area = 702.167 Ang\*\*2

GePol: Cavity volume = 800.901 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0083795065 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8061.6182633282 Hartrees.

Leave Link 301 at Sat Jul 6 01:12:07 2019, MaxMem= 1342177280 cpu: 1.4

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44528 LenP2D= 111829.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.55D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 01:12:11 2019, MaxMem= 1342177280 cpu: 42.0

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 01:12:12 2019, MaxMem= 1342177280 cpu: 2.7

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000083 -0.000134 -0.000056 Ang= -0.02 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>= 2.0169 S= 1.0056

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2650.03022258191

Leave Link 401 at Sat Jul 6 01:12:29 2019, MaxMem= 1342177280 cpu: 204.9

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 119221248.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.77D-15 for 6287.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.93D-15 for 4822 2065.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.77D-15 for 6287.

Iteration 1 A^-1\*A deviation from orthogonality is 4.28D-14 for 1906 1904.

E= -2649.67039209079

DIIS: error= 7.65D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.67039209079 IErMin= 1 ErrMin= 7.65D-03

ErrMax= 7.65D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.71D-01 BMatP= 2.71D-01

IDIUse=3 WtCom= 9.23D-01 WtEn= 7.65D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.665 Goal= None Shift= 0.000

Gap= 0.730 Goal= None Shift= 0.000

GapD= 0.665 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=4.58D-04 MaxDP=2.30D-02 OVMax= 4.28D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.58D-04 CP: 9.99D-01

E= -2649.78682812605 Delta-E= -0.116436035258 Rises=F Damp=F

DIIS: error= 1.31D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.78682812605 IErMin= 2 ErrMin= 1.31D-03

ErrMax= 1.31D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.47D-03 BMatP= 2.71D-01

IDIUse=3 WtCom= 9.87D-01 WtEn= 1.31D-02

Coeff-Com: -0.339D-01 0.103D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.335D-01 0.103D+01

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=8.25D-05 MaxDP=6.17D-03 DE=-1.16D-01 OVMax= 1.71D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 8.07D-05 CP: 9.99D-01 1.04D+00

E= -2649.78659229318 Delta-E= 0.000235832867 Rises=F Damp=F

DIIS: error= 2.61D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -2649.78682812605 IErMin= 2 ErrMin= 1.31D-03

ErrMax= 2.61D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.23D-02 BMatP= 6.47D-03

IDIUse=3 WtCom= 1.64D-01 WtEn= 8.36D-01

Coeff-Com: -0.389D-01 0.628D+00 0.411D+00

Coeff-En: 0.000D+00 0.534D+00 0.466D+00

Coeff: -0.638D-02 0.549D+00 0.457D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=5.99D-05 MaxDP=5.58D-03 DE= 2.36D-04 OVMax= 1.15D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.44D-05 CP: 9.99D-01 1.05D+00 3.95D-01

E= -2649.78872191204 Delta-E= -0.002129618861 Rises=F Damp=F

DIIS: error= 1.05D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.78872191204 IErMin= 4 ErrMin= 1.05D-03

ErrMax= 1.05D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.61D-03 BMatP= 6.47D-03

IDIUse=3 WtCom= 9.90D-01 WtEn= 1.05D-02

Coeff-Com: -0.113D-01 0.128D+00 0.280D+00 0.603D+00

Coeff-En: 0.000D+00 0.000D+00 0.136D+00 0.864D+00

Coeff: -0.112D-01 0.127D+00 0.279D+00 0.606D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.86D-05 MaxDP=1.62D-03 DE=-2.13D-03 OVMax= 4.66D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 9.20D-06 CP: 9.99D-01 1.05D+00 5.50D-01 7.03D-01

E= -2649.78904510566 Delta-E= -0.000323193619 Rises=F Damp=F

DIIS: error= 1.42D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.78904510566 IErMin= 5 ErrMin= 1.42D-04

ErrMax= 1.42D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.87D-05 BMatP= 1.61D-03

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.42D-03

Coeff-Com: -0.313D-02 0.198D-01 0.119D+00 0.329D+00 0.536D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.313D-02 0.198D-01 0.118D+00 0.329D+00 0.536D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.74D-06 MaxDP=2.92D-04 DE=-3.23D-04 OVMax= 1.13D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.48D-06 CP: 9.99D-01 1.05D+00 5.52D-01 7.52D-01 7.15D-01

E= -2649.78905791099 Delta-E= -0.000012805329 Rises=F Damp=F

DIIS: error= 4.90D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.78905791099 IErMin= 6 ErrMin= 4.90D-05

ErrMax= 4.90D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.67D-06 BMatP= 6.87D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.262D-03-0.136D-01 0.147D-01 0.741D-01 0.294D+00 0.630D+00

Coeff: 0.262D-03-0.136D-01 0.147D-01 0.741D-01 0.294D+00 0.630D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.85D-06 MaxDP=1.03D-04 DE=-1.28D-05 OVMax= 8.59D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.17D-06 CP: 9.99D-01 1.05D+00 5.55D-01 7.66D-01 8.00D-01

CP: 7.07D-01

E= -2649.78905989858 Delta-E= -0.000001987590 Rises=F Damp=F

DIIS: error= 1.92D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.78905989858 IErMin= 7 ErrMin= 1.92D-05

ErrMax= 1.92D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.26D-06 BMatP= 8.67D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.425D-03-0.100D-01-0.138D-02 0.165D-01 0.128D+00 0.370D+00

Coeff-Com: 0.497D+00

Coeff: 0.425D-03-0.100D-01-0.138D-02 0.165D-01 0.128D+00 0.370D+00

Coeff: 0.497D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=6.20D-07 MaxDP=3.60D-05 DE=-1.99D-06 OVMax= 2.45D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 4.90D-07 CP: 9.99D-01 1.05D+00 5.57D-01 7.69D-01 8.02D-01

CP: 7.95D-01 9.01D-01

E= -2649.78906022581 Delta-E= -0.000000327238 Rises=F Damp=F

DIIS: error= 9.52D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.78906022581 IErMin= 8 ErrMin= 9.52D-06

ErrMax= 9.52D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.04D-08 BMatP= 1.26D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.785D-04-0.248D-03-0.347D-02-0.100D-01-0.225D-01-0.163D-01

Coeff-Com: 0.147D+00 0.906D+00

Coeff: 0.785D-04-0.248D-03-0.347D-02-0.100D-01-0.225D-01-0.163D-01

Coeff: 0.147D+00 0.906D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.11D-07 MaxDP=2.67D-05 DE=-3.27D-07 OVMax= 4.37D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.20D-07 CP: 9.99D-01 1.05D+00 5.57D-01 7.72D-01 8.12D-01

CP: 8.26D-01 1.14D+00 1.21D+00

E= -2649.78906030771 Delta-E= -0.000000081898 Rises=F Damp=F

DIIS: error= 5.16D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.78906030771 IErMin= 9 ErrMin= 5.16D-06

ErrMax= 5.16D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.89D-08 BMatP= 9.04D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.511D-04 0.215D-02-0.155D-02-0.901D-02-0.408D-01-0.915D-01

Coeff-Com: -0.378D-01 0.521D+00 0.657D+00

Coeff: -0.511D-04 0.215D-02-0.155D-02-0.901D-02-0.408D-01-0.915D-01

Coeff: -0.378D-01 0.521D+00 0.657D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.17D-07 MaxDP=1.46D-05 DE=-8.19D-08 OVMax= 1.71D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.20D-07 CP: 9.99D-01 1.05D+00 5.57D-01 7.73D-01 8.17D-01

CP: 8.41D-01 1.24D+00 1.44D+00 9.74D-01

E= -2649.78906033338 Delta-E= -0.000000025666 Rises=F Damp=F

DIIS: error= 2.85D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -2649.78906033338 IErMin=10 ErrMin= 2.85D-06

ErrMax= 2.85D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.34D-08 BMatP= 4.89D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.573D-04 0.142D-02 0.226D-03-0.215D-02-0.174D-01-0.500D-01

Coeff-Com: -0.754D-01 0.413D-01 0.408D+00 0.694D+00

Coeff: -0.573D-04 0.142D-02 0.226D-03-0.215D-02-0.174D-01-0.500D-01

Coeff: -0.754D-01 0.413D-01 0.408D+00 0.694D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.20D-07 MaxDP=9.53D-06 DE=-2.57D-08 OVMax= 1.11D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.69D-08 CP: 9.99D-01 1.05D+00 5.57D-01 7.73D-01 8.18D-01

CP: 8.49D-01 1.31D+00 1.55D+00 1.16D+00 8.56D-01

E= -2649.78906034020 Delta-E= -0.000000006823 Rises=F Damp=F

DIIS: error= 1.05D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -2649.78906034020 IErMin=11 ErrMin= 1.05D-06

ErrMax= 1.05D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.15D-09 BMatP= 1.34D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.162D-04 0.224D-03 0.384D-03 0.695D-03-0.135D-03-0.532D-02

Coeff-Com: -0.288D-01-0.821D-01 0.571D-01 0.335D+00 0.723D+00

Coeff: -0.162D-04 0.224D-03 0.384D-03 0.695D-03-0.135D-03-0.532D-02

Coeff: -0.288D-01-0.821D-01 0.571D-01 0.335D+00 0.723D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.32D-08 MaxDP=3.50D-06 DE=-6.82D-09 OVMax= 3.67D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.30D-08 CP: 9.99D-01 1.05D+00 5.57D-01 7.73D-01 8.19D-01

CP: 8.52D-01 1.32D+00 1.59D+00 1.23D+00 1.02D+00

CP: 1.02D+00

E= -2649.78906034148 Delta-E= -0.000000001275 Rises=F Damp=F

DIIS: error= 4.48D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -2649.78906034148 IErMin=12 ErrMin= 4.48D-07

ErrMax= 4.48D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.91D-10 BMatP= 2.15D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.492D-05-0.221D-03 0.135D-03 0.837D-03 0.409D-02 0.906D-02

Coeff-Com: 0.345D-02-0.520D-01-0.673D-01 0.159D-01 0.376D+00 0.710D+00

Coeff: 0.492D-05-0.221D-03 0.135D-03 0.837D-03 0.409D-02 0.906D-02

Coeff: 0.345D-02-0.520D-01-0.673D-01 0.159D-01 0.376D+00 0.710D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.66D-08 MaxDP=1.42D-06 DE=-1.28D-09 OVMax= 8.34D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.10D-08 CP: 9.99D-01 1.05D+00 5.57D-01 7.73D-01 8.19D-01

CP: 8.52D-01 1.32D+00 1.59D+00 1.26D+00 1.06D+00

CP: 1.16D+00 9.74D-01

E= -2649.78906034145 Delta-E= 0.000000000025 Rises=F Damp=F

DIIS: error= 2.02D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=12 EnMin= -2649.78906034148 IErMin=13 ErrMin= 2.02D-07

ErrMax= 2.02D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.49D-11 BMatP= 4.91D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.392D-05-0.108D-03-0.529D-05 0.197D-03 0.147D-02 0.392D-02

Coeff-Com: 0.546D-02-0.823D-02-0.328D-01-0.409D-01 0.341D-01 0.259D+00

Coeff-Com: 0.778D+00

Coeff: 0.392D-05-0.108D-03-0.529D-05 0.197D-03 0.147D-02 0.392D-02

Coeff: 0.546D-02-0.823D-02-0.328D-01-0.409D-01 0.341D-01 0.259D+00

Coeff: 0.778D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=7.63D-09 MaxDP=6.08D-07 DE= 2.55D-11 OVMax= 4.31D-06

Error on total polarization charges = 0.07271

SCF Done: E(UB3LYP) = -2649.78906034 A.U. after 13 cycles

NFock= 13 Conv=0.76D-08 -V/T= 1.9849

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0177 S= 1.0059

<L.S>= 0.000000000000E+00

KE= 2.690527149394D+03 PE=-2.240244796574D+04 EE= 9.000513492673D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.26

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0177, after 2.0002

Leave Link 502 at Sat Jul 6 01:23:07 2019, MaxMem= 1342177280 cpu: 7561.0

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44528 LenP2D= 111829.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 272

Leave Link 701 at Sat Jul 6 01:23:26 2019, MaxMem= 1342177280 cpu: 216.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 01:23:26 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 01:24:59 2019, MaxMem= 1342177280 cpu: 1106.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-4.62561052D-03 9.76995101D-03 1.78511005D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.013965409 0.012666139 -0.001181790

2 7 -0.001252033 0.006690261 0.007656450

3 6 -0.016414764 0.014422054 -0.000958611

4 6 0.009116906 -0.003927047 0.000128070

5 6 -0.009448008 -0.004230276 0.000059822

6 7 0.009526686 0.005699665 -0.001669795

7 6 -0.002519844 -0.002492041 0.001475792

8 7 0.013574338 -0.001695514 -0.001375988

9 6 -0.004883849 -0.000626241 0.001787455

10 6 0.007815977 0.006431182 -0.001380045

11 6 0.008123433 -0.006751325 -0.001411085

12 7 -0.008252773 0.004306205 -0.001697820

13 6 -0.007919845 -0.006824871 -0.001360147

14 6 -0.007615247 0.006510537 -0.001329203

15 6 0.005911384 -0.003365422 0.001971358

16 7 -0.011635363 -0.001696557 -0.001315084

17 6 0.003559960 0.000350447 0.001663207

18 7 -0.008101911 -0.001545412 -0.001741710

19 7 -0.001243744 -0.004579584 0.007251301

20 6 0.012015860 -0.011913749 -0.001129126

21 6 -0.009327375 0.004341351 0.000067096

22 6 0.009000450 0.004040383 0.000134309

23 6 -0.014389833 -0.013656609 -0.000904337

24 7 0.009337046 -0.002872067 -0.001715601

25 30 0.000982551 0.000840828 -0.001938841

26 6 0.007792460 0.006438597 0.000335636

27 6 -0.003493809 -0.002395332 0.000025754

28 6 -0.003480111 0.002377028 0.000025111

29 6 0.007687163 -0.006506795 0.000331919

30 6 0.004101932 0.000207983 0.001376988

31 6 0.001386263 0.000710625 -0.000587296

32 6 -0.001400006 0.000759845 -0.000598984

33 6 -0.004117113 0.000074373 0.001415708

34 6 -0.007735019 0.006633431 0.000337567

35 6 0.003448342 -0.002167849 0.000029941

36 6 0.003434639 0.002150103 0.000029031

37 6 -0.007629057 -0.006701475 0.000333699

38 6 -0.004321318 -0.000072498 0.001419493

39 6 -0.001551512 -0.000782739 -0.000608402

40 6 0.001537089 -0.000732723 -0.000596811

41 6 0.004306751 -0.000207249 0.001380718

42 1 0.000236377 0.001351404 -0.000014533

43 1 0.000223859 -0.001344520 -0.000014556

44 1 0.000920663 0.000585831 0.000119529

45 1 -0.000923738 0.000585953 0.000117220

46 1 -0.000235756 0.001331550 -0.000014713

47 1 -0.000224896 -0.001326198 -0.000014581

48 1 -0.000912628 -0.000592028 0.000117340

49 1 0.000909134 -0.000591763 0.000119972

50 8 -0.001413022 -0.001488993 -0.001569896

51 8 0.001351676 -0.001565329 -0.001562561

52 8 0.000415672 0.002903422 -0.000154111

53 8 0.000358964 -0.002958427 -0.000197842

54 8 -0.001394760 0.001638138 -0.001585614

55 8 0.001343134 0.001703568 -0.001591001

56 8 -0.000195314 -0.002922424 -0.000176659

57 8 -0.000244048 0.002879277 -0.000148221

58 6 -0.001235289 -0.002269892 0.000536217

59 1 -0.000226442 0.000691545 0.000800895

60 1 -0.000413063 0.001022245 -0.000887094

61 1 0.000255128 -0.000788097 -0.000191994

62 6 -0.001597917 -0.000749326 -0.000028611

63 1 0.000522195 -0.000014055 -0.000569294

64 1 0.000844398 0.000177034 0.000564277

65 1 -0.000919711 0.000277015 -0.000025208

66 6 -0.001573449 0.000746723 -0.000022495

67 1 0.000842374 -0.000178105 0.000561692

68 1 0.000522845 0.000005245 -0.000568162

69 1 -0.000927205 -0.000278252 -0.000024260

70 6 0.001222461 -0.002260482 0.000534841

71 1 0.000417384 0.001016615 -0.000886514

72 1 0.000226663 0.000686683 0.000799597

73 1 -0.000264452 -0.000782078 -0.000187447

74 6 0.001537009 -0.000712201 -0.000023097

75 1 -0.000834033 0.000180138 0.000558000

76 1 -0.000509705 -0.000008089 -0.000564049

77 1 0.000921511 0.000279234 -0.000024627

78 6 0.001514227 0.000708137 -0.000017014

79 1 -0.000509556 0.000000433 -0.000562791

80 1 -0.000832033 -0.000180656 0.000555279

81 1 0.000924120 -0.000277290 -0.000024048

82 6 0.001192386 0.002220497 0.000540662

83 1 0.000225049 -0.000677107 0.000793592

84 1 0.000416966 -0.001007603 -0.000883923

85 1 -0.000267034 0.000765496 -0.000183737

86 6 -0.001206316 0.002230637 0.000541539

87 1 -0.000412399 -0.001014005 -0.000884724

88 1 -0.000224806 -0.000682327 0.000794835

89 1 0.000261273 0.000774764 -0.000187859

-------------------------------------------------------------------

Cartesian Forces: Max 0.016414764 RMS 0.003906625

Leave Link 716 at Sat Jul 6 01:24:59 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.013375513 RMS 0.002299242

Search for a local minimum.

Step number 12 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .22992D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 2 3 4 6

5 8 7 10 9

12 11

DE= 5.21D-03 DEPred=-5.58D-03 R=-9.33D-01

Trust test=-9.33D-01 RLast= 9.22D-01 DXMaxT set to 2.28D-01

ITU= -1 0 0 0 0 0 0 1 1 1 1 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.75173.

Iteration 1 RMS(Cart)= 0.11956302 RMS(Int)= 0.00264279

Iteration 2 RMS(Cart)= 0.01134935 RMS(Int)= 0.00066826

Iteration 3 RMS(Cart)= 0.00001900 RMS(Int)= 0.00066823

Iteration 4 RMS(Cart)= 0.00000003 RMS(Int)= 0.00066823

ITry= 1 IFail=0 DXMaxC= 8.07D-01 DCOld= 1.00D+10 DXMaxT= 2.28D-01 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.59286 -0.00076 -0.00915 0.00000 -0.00971 2.58315

R2 2.76648 -0.00779 -0.02236 0.00000 -0.02209 2.74440

R3 2.52739 0.00968 0.03129 0.00000 0.03283 2.56021

R4 2.59009 -0.00035 -0.00692 0.00000 -0.00710 2.58299

R5 3.87215 0.01191 0.00220 0.00000 -0.00090 3.87126

R6 2.76597 -0.00734 -0.02200 0.00000 -0.02173 2.74423

R7 2.52035 0.01338 0.03691 0.00000 0.03924 2.55959

R8 2.66874 0.00505 0.02341 0.00000 0.02433 2.69307

R9 2.66972 -0.00358 -0.00523 0.00000 -0.00525 2.66447

R10 2.66964 -0.00354 -0.00517 0.00000 -0.00518 2.66446

R11 2.46261 0.01076 0.01512 0.00000 0.01733 2.47994

R12 2.59956 0.00158 -0.00229 0.00000 -0.00288 2.59668

R13 2.77065 0.00448 0.02193 0.00000 0.02224 2.79290

R14 2.60264 0.00073 -0.00475 0.00000 -0.00574 2.59690

R15 3.86843 0.00859 -0.02119 0.00000 -0.02459 3.84384

R16 2.77117 0.00404 0.02158 0.00000 0.02190 2.79307

R17 2.47068 0.00597 0.00876 0.00000 0.01018 2.48086

R18 2.66675 0.00004 -0.00239 0.00000 -0.00132 2.66543

R19 2.65458 -0.00282 -0.00688 0.00000 -0.00690 2.64767

R20 2.65461 -0.00286 -0.00690 0.00000 -0.00693 2.64768

R21 2.46832 0.00700 0.01063 0.00000 0.01229 2.48060

R22 2.66954 -0.00075 -0.00458 0.00000 -0.00390 2.66564

R23 2.77167 0.00396 0.02114 0.00000 0.02134 2.79301

R24 2.65475 -0.00307 -0.00700 0.00000 -0.00701 2.64774

R25 2.77219 0.00357 0.02079 0.00000 0.02100 2.79319

R26 2.65472 -0.00301 -0.00697 0.00000 -0.00699 2.64773

R27 2.59962 0.00117 -0.00231 0.00000 -0.00282 2.59680

R28 2.47641 0.00234 0.00424 0.00000 0.00512 2.48153

R29 2.59654 0.00202 0.00015 0.00000 0.00004 2.59658

R30 3.86069 0.00785 -0.01552 0.00000 -0.01753 3.84316

R31 2.53216 0.00701 0.02748 0.00000 0.02848 2.56064

R32 2.59020 -0.00046 -0.00699 0.00000 -0.00712 2.58308

R33 2.58744 -0.00006 -0.00477 0.00000 -0.00452 2.58292

R34 3.86391 0.01079 0.00813 0.00000 0.00646 3.87037

R35 2.76731 -0.00807 -0.02300 0.00000 -0.02284 2.74447

R36 2.67124 0.00439 0.02144 0.00000 0.02200 2.69324

R37 2.66965 -0.00366 -0.00518 0.00000 -0.00517 2.66448

R38 2.76679 -0.00766 -0.02264 0.00000 -0.02248 2.74430

R39 2.66974 -0.00371 -0.00524 0.00000 -0.00524 2.66450

R40 2.52510 0.01060 0.03312 0.00000 0.03491 2.56001

R41 2.63708 0.00674 0.01607 0.00000 0.01609 2.65317

R42 2.54959 0.00265 -0.00108 0.00000 -0.00108 2.54851

R43 2.62214 0.00572 0.00483 0.00000 0.00486 2.62700

R44 2.04089 0.00083 0.00296 0.00000 0.00296 2.04385

R45 2.63716 0.00667 0.01601 0.00000 0.01603 2.65319

R46 2.04090 0.00082 0.00295 0.00000 0.00295 2.04385

R47 2.54956 0.00270 -0.00106 0.00000 -0.00106 2.54850

R48 2.63884 0.00134 0.00329 0.00000 0.00329 2.64212

R49 2.56228 -0.00289 -0.01014 0.00000 -0.01014 2.55214

R50 2.63866 0.00521 0.00632 0.00000 0.00632 2.64498

R51 2.04117 0.00096 0.00269 0.00000 0.00269 2.04385

R52 2.63892 0.00126 0.00323 0.00000 0.00323 2.64215

R53 2.04117 0.00096 0.00269 0.00000 0.00269 2.04385

R54 2.56222 -0.00283 -0.01009 0.00000 -0.01009 2.55212

R55 2.63705 0.00671 0.01610 0.00000 0.01613 2.65318

R56 2.54963 0.00262 -0.00111 0.00000 -0.00111 2.54852

R57 2.62179 0.00600 0.00510 0.00000 0.00516 2.62695

R58 2.04089 0.00084 0.00296 0.00000 0.00296 2.04385

R59 2.63713 0.00664 0.01604 0.00000 0.01607 2.65321

R60 2.04090 0.00082 0.00295 0.00000 0.00295 2.04385

R61 2.54959 0.00269 -0.00109 0.00000 -0.00109 2.54851

R62 2.63886 0.00126 0.00328 0.00000 0.00329 2.64216

R63 2.56228 -0.00287 -0.01014 0.00000 -0.01014 2.55214

R64 2.63833 0.00542 0.00658 0.00000 0.00661 2.64493

R65 2.04117 0.00096 0.00269 0.00000 0.00269 2.04385

R66 2.63878 0.00134 0.00334 0.00000 0.00335 2.64213

R67 2.04117 0.00096 0.00269 0.00000 0.00269 2.04385

R68 2.56235 -0.00295 -0.01019 0.00000 -0.01019 2.55216

R69 2.69761 -0.00188 -0.00282 0.00000 -0.00282 2.69479

R70 2.69760 -0.00187 -0.00282 0.00000 -0.00282 2.69479

R71 2.69969 -0.00115 -0.00325 0.00000 -0.00325 2.69643

R72 2.69967 -0.00113 -0.00324 0.00000 -0.00324 2.69643

R73 2.69757 -0.00184 -0.00279 0.00000 -0.00279 2.69478

R74 2.69756 -0.00182 -0.00279 0.00000 -0.00279 2.69478

R75 2.69963 -0.00108 -0.00321 0.00000 -0.00321 2.69642

R76 2.69964 -0.00110 -0.00322 0.00000 -0.00322 2.69642

R77 2.06476 0.00101 0.00235 0.00000 0.00235 2.06710

R78 2.06299 0.00141 0.00368 0.00000 0.00368 2.06667

R79 2.05564 0.00045 0.00111 0.00000 0.00111 2.05675

R80 2.06484 0.00075 0.00211 0.00000 0.00211 2.06696

R81 2.06447 0.00086 0.00262 0.00000 0.00262 2.06709

R82 2.05515 0.00050 0.00138 0.00000 0.00138 2.05654

R83 2.06448 0.00086 0.00262 0.00000 0.00262 2.06709

R84 2.06485 0.00075 0.00211 0.00000 0.00211 2.06696

R85 2.05515 0.00050 0.00138 0.00000 0.00138 2.05654

R86 2.06299 0.00140 0.00368 0.00000 0.00368 2.06667

R87 2.06476 0.00100 0.00234 0.00000 0.00234 2.06711

R88 2.05564 0.00046 0.00111 0.00000 0.00111 2.05675

R89 2.06448 0.00085 0.00261 0.00000 0.00261 2.06710

R90 2.06485 0.00074 0.00211 0.00000 0.00211 2.06696

R91 2.05515 0.00050 0.00138 0.00000 0.00138 2.05653

R92 2.06486 0.00074 0.00210 0.00000 0.00210 2.06696

R93 2.06448 0.00085 0.00261 0.00000 0.00261 2.06710

R94 2.05515 0.00050 0.00139 0.00000 0.00139 2.05653

R95 2.06477 0.00100 0.00234 0.00000 0.00234 2.06711

R96 2.06300 0.00140 0.00367 0.00000 0.00367 2.06667

R97 2.05563 0.00045 0.00112 0.00000 0.00112 2.05675

R98 2.06299 0.00140 0.00367 0.00000 0.00367 2.06667

R99 2.06477 0.00100 0.00234 0.00000 0.00234 2.06711

R100 2.05564 0.00045 0.00111 0.00000 0.00111 2.05675

A1 1.89218 0.00176 -0.00291 0.00000 -0.00385 1.88833

A2 2.23012 -0.00164 -0.01393 0.00000 -0.01411 2.21601

A3 2.16088 -0.00012 0.01683 0.00000 0.01795 2.17884

A4 1.91808 -0.00157 0.01130 0.00000 0.01343 1.93151

A5 2.17167 0.00118 -0.00355 0.00000 -0.00387 2.16780

A6 2.18077 0.00063 -0.01060 0.00000 -0.01239 2.16838

A7 1.89307 0.00150 -0.00359 0.00000 -0.00463 1.88844

A8 2.22969 -0.00230 -0.01359 0.00000 -0.01360 2.21609

A9 2.16042 0.00080 0.01718 0.00000 0.01822 2.17865

A10 1.85940 -0.00080 -0.00145 0.00000 -0.00117 1.85824

A11 2.31616 -0.00053 0.00187 0.00000 0.00174 2.31791

A12 2.10723 0.00133 -0.00014 0.00000 -0.00025 2.10697

A13 1.85926 -0.00070 -0.00132 0.00000 -0.00104 1.85822

A14 2.31642 -0.00072 0.00167 0.00000 0.00155 2.31797

A15 2.10712 0.00144 -0.00007 0.00000 -0.00019 2.10693

A16 2.17604 -0.00002 0.00999 0.00000 0.01151 2.18755

A17 2.21574 0.00165 0.01483 0.00000 0.01471 2.23045

A18 2.15677 0.00111 0.00858 0.00000 0.01013 2.16690

A19 1.90909 -0.00273 -0.02231 0.00000 -0.02358 1.88551

A20 1.89580 0.00338 0.03186 0.00000 0.03399 1.92979

A21 2.17690 -0.00201 -0.01205 0.00000 -0.01355 2.16335

A22 2.16759 -0.00133 -0.00489 0.00000 -0.00494 2.16265

A23 1.90815 -0.00237 -0.02159 0.00000 -0.02275 1.88539

A24 2.21613 0.00232 0.01451 0.00000 0.01422 2.23035

A25 2.15730 0.00009 0.00819 0.00000 0.00982 2.16712

A26 1.85574 0.00092 0.00605 0.00000 0.00622 1.86196

A27 2.32330 -0.00477 -0.01601 0.00000 -0.01605 2.30725

A28 2.10411 0.00385 0.00997 0.00000 0.00984 2.11396

A29 1.85597 0.00079 0.00587 0.00000 0.00602 1.86199

A30 2.32289 -0.00452 -0.01571 0.00000 -0.01574 2.30715

A31 2.10430 0.00372 0.00985 0.00000 0.00973 2.11403

A32 2.17993 -0.00059 0.00698 0.00000 0.00798 2.18791

A33 1.85597 0.00087 0.00589 0.00000 0.00604 1.86201

A34 2.10404 0.00378 0.01005 0.00000 0.00996 2.11400

A35 2.32314 -0.00465 -0.01593 0.00000 -0.01598 2.30716

A36 1.85575 0.00100 0.00607 0.00000 0.00623 1.86198

A37 2.10386 0.00387 0.01017 0.00000 0.01007 2.11393

A38 2.32355 -0.00487 -0.01623 0.00000 -0.01629 2.30726

A39 1.90540 -0.00201 -0.01947 0.00000 -0.02021 1.88519

A40 2.16232 -0.00095 0.00433 0.00000 0.00527 2.16759

A41 2.21386 0.00299 0.01626 0.00000 0.01622 2.23007

A42 1.90128 0.00248 0.02757 0.00000 0.02887 1.93015

A43 2.16483 -0.00089 -0.00274 0.00000 -0.00238 2.16245

A44 2.17419 -0.00157 -0.00994 0.00000 -0.01103 2.16317

A45 2.16180 0.00003 0.00472 0.00000 0.00558 2.16738

A46 2.21345 0.00235 0.01658 0.00000 0.01671 2.23017

A47 1.90634 -0.00234 -0.02019 0.00000 -0.02103 1.88531

A48 2.18353 -0.00100 0.00423 0.00000 0.00474 2.18827

A49 1.92326 -0.00229 0.00727 0.00000 0.00861 1.93187

A50 2.16897 0.00155 -0.00145 0.00000 -0.00137 2.16759

A51 2.17811 0.00100 -0.00853 0.00000 -0.00992 2.16819

A52 2.22831 -0.00120 -0.01255 0.00000 -0.01250 2.21580

A53 2.16540 -0.00088 0.01337 0.00000 0.01386 2.17926

A54 1.88947 0.00208 -0.00083 0.00000 -0.00136 1.88811

A55 1.85933 -0.00066 -0.00135 0.00000 -0.00107 1.85826

A56 2.31655 -0.00078 0.00155 0.00000 0.00140 2.31794

A57 2.10691 0.00145 0.00009 0.00000 0.00000 2.10692

A58 1.85947 -0.00075 -0.00147 0.00000 -0.00120 1.85827

A59 2.10702 0.00138 0.00002 0.00000 -0.00006 2.10696

A60 2.31630 -0.00062 0.00174 0.00000 0.00159 2.31788

A61 1.89036 0.00184 -0.00151 0.00000 -0.00214 1.88822

A62 2.22788 -0.00185 -0.01222 0.00000 -0.01200 2.21589

A63 2.16494 0.00001 0.01372 0.00000 0.01413 2.17907

A64 2.17963 -0.00044 0.00724 0.00000 0.00827 2.18790

A65 1.52007 0.00209 0.03519 0.00000 0.04009 1.56016

A66 1.52948 0.00037 0.02789 0.00000 0.03143 1.56091

A67 1.52971 0.00040 0.02778 0.00000 0.03131 1.56102

A68 1.53920 -0.00128 0.02042 0.00000 0.02259 1.56179

A69 2.06082 -0.00403 -0.01289 0.00000 -0.01287 2.04795

A70 2.06838 -0.00065 0.00505 0.00000 0.00504 2.07342

A71 2.15398 0.00468 0.00781 0.00000 0.00780 2.16178

A72 2.11835 0.00023 0.00282 0.00000 0.00289 2.12124

A73 2.10965 -0.00120 -0.00868 0.00000 -0.00871 2.10094

A74 2.05517 0.00097 0.00585 0.00000 0.00581 2.06098

A75 2.11843 0.00020 0.00276 0.00000 0.00283 2.12126

A76 2.05512 0.00099 0.00588 0.00000 0.00585 2.06097

A77 2.10962 -0.00119 -0.00865 0.00000 -0.00869 2.10093

A78 2.06085 -0.00405 -0.01291 0.00000 -0.01289 2.04796

A79 2.06849 -0.00069 0.00498 0.00000 0.00497 2.07345

A80 2.15384 0.00474 0.00790 0.00000 0.00789 2.16173

A81 2.05499 -0.00152 -0.00156 0.00000 -0.00152 2.05347

A82 2.07752 -0.00312 -0.01014 0.00000 -0.01016 2.06736

A83 2.15058 0.00465 0.01173 0.00000 0.01171 2.16229

A84 2.12113 0.00013 0.00148 0.00000 0.00152 2.12266

A85 2.10503 -0.00060 -0.00384 0.00000 -0.00386 2.10117

A86 2.05699 0.00047 0.00232 0.00000 0.00230 2.05929

A87 2.12116 0.00011 0.00146 0.00000 0.00150 2.12267

A88 2.05697 0.00048 0.00233 0.00000 0.00231 2.05929

A89 2.10502 -0.00059 -0.00383 0.00000 -0.00385 2.10116

A90 2.05503 -0.00154 -0.00158 0.00000 -0.00154 2.05349

A91 2.07757 -0.00317 -0.01018 0.00000 -0.01020 2.06738

A92 2.15049 0.00472 0.01179 0.00000 0.01177 2.16226

A93 2.06087 -0.00411 -0.01294 0.00000 -0.01292 2.04795

A94 2.06811 -0.00041 0.00526 0.00000 0.00525 2.07336

A95 2.15420 0.00451 0.00765 0.00000 0.00764 2.16184

A96 2.11804 0.00036 0.00306 0.00000 0.00317 2.12121

A97 2.10983 -0.00129 -0.00881 0.00000 -0.00887 2.10096

A98 2.05531 0.00093 0.00574 0.00000 0.00569 2.06099

A99 2.11812 0.00032 0.00301 0.00000 0.00311 2.12123

A100 2.05525 0.00095 0.00577 0.00000 0.00572 2.06098

A101 2.10979 -0.00127 -0.00879 0.00000 -0.00884 2.10095

A102 2.06091 -0.00414 -0.01296 0.00000 -0.01294 2.04797

A103 2.06821 -0.00046 0.00518 0.00000 0.00517 2.07339

A104 2.15406 0.00460 0.00775 0.00000 0.00774 2.16180

A105 2.05508 -0.00162 -0.00163 0.00000 -0.00159 2.05349

A106 2.07747 -0.00301 -0.01009 0.00000 -0.01011 2.06736

A107 2.15054 0.00463 0.01176 0.00000 0.01174 2.16228

A108 2.12090 0.00021 0.00167 0.00000 0.00175 2.12265

A109 2.10517 -0.00065 -0.00395 0.00000 -0.00399 2.10118

A110 2.05708 0.00045 0.00224 0.00000 0.00221 2.05929

A111 2.12087 0.00023 0.00169 0.00000 0.00177 2.12264

A112 2.05711 0.00043 0.00223 0.00000 0.00219 2.05930

A113 2.10518 -0.00066 -0.00396 0.00000 -0.00400 2.10118

A114 2.05505 -0.00159 -0.00161 0.00000 -0.00157 2.05348

A115 2.07742 -0.00295 -0.01006 0.00000 -0.01008 2.06734

A116 2.15063 0.00454 0.01170 0.00000 0.01168 2.16230

A117 2.06731 -0.00062 -0.00157 0.00000 -0.00157 2.06574

A118 2.06735 -0.00062 -0.00160 0.00000 -0.00160 2.06575

A119 2.06225 0.00331 0.00441 0.00000 0.00441 2.06667

A120 2.06225 0.00334 0.00441 0.00000 0.00441 2.06666

A121 2.06733 -0.00062 -0.00159 0.00000 -0.00159 2.06574

A122 2.06738 -0.00063 -0.00162 0.00000 -0.00162 2.06576

A123 2.06223 0.00338 0.00443 0.00000 0.00443 2.06666

A124 2.06223 0.00337 0.00443 0.00000 0.00443 2.06666

A125 1.94102 0.00065 0.00442 0.00000 0.00442 1.94544

A126 1.94829 -0.00007 -0.00333 0.00000 -0.00333 1.94496

A127 1.84672 -0.00112 -0.00412 0.00000 -0.00412 1.84260

A128 1.91287 -0.00019 0.00005 0.00000 0.00004 1.91292

A129 1.90547 0.00034 0.00170 0.00000 0.00169 1.90717

A130 1.90790 0.00039 0.00125 0.00000 0.00125 1.90915

A131 1.94484 0.00030 0.00239 0.00000 0.00239 1.94722

A132 1.94001 0.00109 0.00375 0.00000 0.00375 1.94376

A133 1.84786 -0.00153 -0.00608 0.00000 -0.00608 1.84178

A134 1.91410 -0.00022 -0.00101 0.00000 -0.00100 1.91310

A135 1.90726 0.00021 0.00015 0.00000 0.00015 1.90741

A136 1.90832 0.00011 0.00061 0.00000 0.00061 1.90893

A137 1.94000 0.00109 0.00375 0.00000 0.00375 1.94376

A138 1.94484 0.00032 0.00238 0.00000 0.00238 1.94723

A139 1.84787 -0.00155 -0.00609 0.00000 -0.00609 1.84178

A140 1.91410 -0.00022 -0.00100 0.00000 -0.00100 1.91309

A141 1.90831 0.00011 0.00062 0.00000 0.00062 1.90893

A142 1.90727 0.00021 0.00014 0.00000 0.00014 1.90741

A143 1.94830 -0.00008 -0.00334 0.00000 -0.00334 1.94496

A144 1.94103 0.00064 0.00441 0.00000 0.00441 1.94544

A145 1.84670 -0.00110 -0.00411 0.00000 -0.00411 1.84259

A146 1.91287 -0.00019 0.00005 0.00000 0.00005 1.91292

A147 1.90789 0.00039 0.00126 0.00000 0.00126 1.90915

A148 1.90548 0.00034 0.00169 0.00000 0.00169 1.90717

A149 1.94001 0.00108 0.00374 0.00000 0.00375 1.94376

A150 1.94484 0.00030 0.00238 0.00000 0.00238 1.94722

A151 1.84785 -0.00153 -0.00607 0.00000 -0.00607 1.84178

A152 1.91410 -0.00021 -0.00100 0.00000 -0.00100 1.91310

A153 1.90832 0.00011 0.00062 0.00000 0.00062 1.90893

A154 1.90727 0.00021 0.00014 0.00000 0.00014 1.90741

A155 1.94485 0.00031 0.00238 0.00000 0.00238 1.94723

A156 1.94000 0.00108 0.00375 0.00000 0.00375 1.94376

A157 1.84786 -0.00154 -0.00608 0.00000 -0.00608 1.84178

A158 1.91409 -0.00021 -0.00100 0.00000 -0.00100 1.91309

A159 1.90728 0.00020 0.00014 0.00000 0.00014 1.90741

A160 1.90831 0.00011 0.00062 0.00000 0.00062 1.90893

A161 1.94104 0.00063 0.00440 0.00000 0.00440 1.94545

A162 1.94830 -0.00009 -0.00334 0.00000 -0.00334 1.94496

A163 1.84667 -0.00108 -0.00409 0.00000 -0.00409 1.84259

A164 1.91287 -0.00019 0.00005 0.00000 0.00005 1.91292

A165 1.90550 0.00033 0.00168 0.00000 0.00168 1.90718

A166 1.90789 0.00038 0.00126 0.00000 0.00126 1.90915

A167 1.94829 -0.00008 -0.00333 0.00000 -0.00333 1.94496

A168 1.94103 0.00064 0.00441 0.00000 0.00441 1.94544

A169 1.84669 -0.00109 -0.00410 0.00000 -0.00410 1.84259

A170 1.91287 -0.00019 0.00005 0.00000 0.00005 1.91292

A171 1.90790 0.00038 0.00125 0.00000 0.00125 1.90915

A172 1.90549 0.00034 0.00168 0.00000 0.00168 1.90717

A173 3.06868 -0.00091 0.04831 0.00000 0.05402 3.12270

A174 3.06891 -0.00088 0.04820 0.00000 0.05390 3.12281

A175 3.48428 -0.00128 -0.17951 0.00000 -0.17878 3.30550

A176 2.66969 0.00348 0.23442 0.00000 0.23355 2.90325

D1 0.07005 -0.00249 -0.06175 0.00000 -0.06150 0.00855

D2 3.04821 -0.00086 -0.07973 0.00000 -0.07980 2.96841

D3 -3.06899 -0.00212 -0.06804 0.00000 -0.06772 -3.13671

D4 -0.09083 -0.00049 -0.08601 0.00000 -0.08602 -0.17685

D5 -0.04192 0.00146 0.03690 0.00000 0.03685 -0.00507

D6 3.13049 0.00104 0.01902 0.00000 0.01901 -3.13369

D7 3.09724 0.00110 0.04300 0.00000 0.04285 3.14009

D8 -0.01353 0.00068 0.02512 0.00000 0.02501 0.01148

D9 0.20744 -0.00005 -0.01066 0.00000 -0.01058 0.19686

D10 -2.93124 0.00037 -0.01792 0.00000 -0.01774 -2.94898

D11 -0.07007 0.00249 0.06177 0.00000 0.06152 -0.00854

D12 3.06864 0.00214 0.06831 0.00000 0.06804 3.13669

D13 -3.04719 0.00079 0.07893 0.00000 0.07885 -2.96834

D14 0.09152 0.00043 0.08547 0.00000 0.08537 0.17689

D15 -2.81393 -0.00227 -0.10647 0.00000 -0.10559 -2.91952

D16 -0.14091 0.00064 0.12542 0.00000 0.12478 -0.01613

D17 0.13991 -0.00058 -0.12470 0.00000 -0.12384 0.01607

D18 2.81294 0.00232 0.10719 0.00000 0.10653 2.91946

D19 0.04197 -0.00145 -0.03694 0.00000 -0.03691 0.00506

D20 -3.13053 -0.00103 -0.01899 0.00000 -0.01898 3.13367

D21 -3.09688 -0.00110 -0.04329 0.00000 -0.04319 -3.14007

D22 0.01381 -0.00068 -0.02533 0.00000 -0.02526 -0.01146

D23 -0.20717 0.00004 0.01048 0.00000 0.01035 -0.19682

D24 2.93113 -0.00037 0.01803 0.00000 0.01785 2.94898

D25 0.00001 -0.00001 0.00000 0.00000 0.00000 0.00001

D26 3.11526 0.00031 0.01529 0.00000 0.01527 3.13052

D27 -3.11517 -0.00034 -0.01536 0.00000 -0.01534 -3.13051

D28 0.00009 -0.00002 -0.00007 0.00000 -0.00008 0.00001

D29 -3.11880 -0.00042 -0.02363 0.00000 -0.02360 3.14078

D30 0.00858 -0.00019 -0.02077 0.00000 -0.02074 -0.01216

D31 -0.01168 0.00002 -0.00361 0.00000 -0.00361 -0.01529

D32 3.11570 0.00024 -0.00075 0.00000 -0.00075 3.11495

D33 3.11878 0.00044 0.02364 0.00000 0.02361 -3.14079

D34 -0.00860 0.00022 0.02078 0.00000 0.02074 0.01215

D35 0.01156 0.00001 0.00369 0.00000 0.00372 0.01528

D36 -3.11582 -0.00022 0.00083 0.00000 0.00085 -3.11497

D37 -0.04350 -0.00055 -0.01469 0.00000 -0.01486 -0.05836

D38 -3.11801 -0.00129 -0.05123 0.00000 -0.05117 3.11401

D39 -3.07502 -0.00015 -0.02448 0.00000 -0.02457 -3.09959

D40 0.36731 -0.00015 -0.08380 0.00000 -0.08388 0.28343

D41 0.00733 0.00060 0.00800 0.00000 0.00789 0.01522

D42 -2.83353 0.00060 -0.05132 0.00000 -0.05142 -2.88495

D43 3.08037 0.00040 0.02656 0.00000 0.02660 3.10697

D44 -0.05262 0.00025 0.02447 0.00000 0.02450 -0.02812

D45 -0.00440 -0.00035 -0.00468 0.00000 -0.00465 -0.00904

D46 -3.13739 -0.00050 -0.00677 0.00000 -0.00675 3.13905

D47 -0.00739 -0.00060 -0.00796 0.00000 -0.00784 -0.01522

D48 3.07465 0.00012 0.02478 0.00000 0.02495 3.09960

D49 2.83544 -0.00075 0.04985 0.00000 0.04961 2.88506

D50 -0.36570 -0.00003 0.08259 0.00000 0.08240 -0.28330

D51 -0.34237 0.00045 0.12442 0.00000 0.12392 -0.21846

D52 3.13737 0.00002 -0.05164 0.00000 -0.05051 3.08686

D53 -3.13771 -0.00028 0.05186 0.00000 0.05076 -3.08695

D54 0.34204 -0.00072 -0.12420 0.00000 -0.12366 0.21838

D55 0.00455 0.00036 0.00457 0.00000 0.00451 0.00906

D56 3.13736 0.00053 0.00680 0.00000 0.00679 -3.13904

D57 -3.07992 -0.00043 -0.02691 0.00000 -0.02705 -3.10697

D58 0.05288 -0.00026 -0.02468 0.00000 -0.02477 0.02812

D59 0.04363 0.00067 0.01461 0.00000 0.01477 0.05840

D60 3.11774 0.00143 0.05148 0.00000 0.05149 -3.11396

D61 -0.00009 0.00000 0.00007 0.00000 0.00009 -0.00001

D62 3.13421 0.00007 0.00174 0.00000 0.00176 3.13596

D63 -3.13424 -0.00010 -0.00172 0.00000 -0.00174 -3.13597

D64 0.00006 -0.00002 -0.00005 0.00000 -0.00007 -0.00001

D65 -3.12785 -0.00014 -0.00133 0.00000 -0.00137 -3.12922

D66 0.01739 0.00009 0.00372 0.00000 0.00369 0.02108

D67 0.00395 0.00003 0.00113 0.00000 0.00115 0.00510

D68 -3.13399 0.00026 0.00618 0.00000 0.00620 -3.12779

D69 3.12797 0.00014 0.00124 0.00000 0.00125 3.12923

D70 -0.01728 -0.00009 -0.00380 0.00000 -0.00379 -0.02107

D71 -0.00403 -0.00001 -0.00106 0.00000 -0.00106 -0.00509

D72 3.13389 -0.00023 -0.00610 0.00000 -0.00610 3.12779

D73 3.11801 0.00123 0.05124 0.00000 0.05123 -3.11394

D74 0.04359 0.00049 0.01461 0.00000 0.01479 0.05837

D75 0.00010 0.00000 -0.00007 0.00000 -0.00009 0.00001

D76 3.13427 0.00009 0.00171 0.00000 0.00174 3.13601

D77 -3.13423 -0.00008 -0.00173 0.00000 -0.00177 -3.13600

D78 -0.00006 0.00001 0.00005 0.00000 0.00006 0.00001

D79 -3.08026 -0.00043 -0.02666 0.00000 -0.02677 -3.10703

D80 0.00440 0.00035 0.00468 0.00000 0.00463 0.00903

D81 0.05276 -0.00028 -0.02458 0.00000 -0.02465 0.02811

D82 3.13742 0.00050 0.00677 0.00000 0.00675 -3.13901

D83 0.00402 0.00001 0.00107 0.00000 0.00107 0.00510

D84 -3.13388 0.00022 0.00610 0.00000 0.00611 -3.12777

D85 -3.12802 -0.00014 -0.00123 0.00000 -0.00125 -3.12927

D86 0.01727 0.00008 0.00380 0.00000 0.00378 0.02104

D87 -0.00455 -0.00034 -0.00457 0.00000 -0.00449 -0.00905

D88 3.07982 0.00047 0.02701 0.00000 0.02721 3.10703

D89 -3.13739 -0.00052 -0.00680 0.00000 -0.00679 3.13901

D90 -0.05302 0.00030 0.02479 0.00000 0.02491 -0.02811

D91 -0.00395 -0.00003 -0.00114 0.00000 -0.00116 -0.00511

D92 3.13397 -0.00025 -0.00618 0.00000 -0.00621 3.12777

D93 3.12789 0.00015 0.00132 0.00000 0.00137 3.12926

D94 -0.01737 -0.00007 -0.00373 0.00000 -0.00368 -0.02105

D95 0.00742 0.00058 0.00794 0.00000 0.00779 0.01521

D96 -2.83518 0.00071 -0.04999 0.00000 -0.04979 -2.88497

D97 -3.07481 -0.00010 -0.02467 0.00000 -0.02486 -3.09968

D98 0.36577 0.00004 -0.08260 0.00000 -0.08245 0.28332

D99 -3.11776 -0.00137 -0.05147 0.00000 -0.05153 3.11389

D100 -0.04372 -0.00061 -0.01452 0.00000 -0.01468 -0.05841

D101 3.07517 0.00012 0.02439 0.00000 0.02449 3.09966

D102 -0.00736 -0.00058 -0.00798 0.00000 -0.00784 -0.01521

D103 -0.36739 0.00013 0.08382 0.00000 0.08393 -0.28346

D104 2.83326 -0.00057 0.05146 0.00000 0.05160 2.88486

D105 3.14051 -0.00024 -0.05403 0.00000 -0.05349 3.08702

D106 -0.34377 0.00104 0.12547 0.00000 0.12529 -0.21849

D107 0.34410 -0.00078 -0.12569 0.00000 -0.12553 0.21857

D108 -3.14018 0.00050 0.05382 0.00000 0.05325 -3.08693

D109 -0.20796 0.00007 0.01108 0.00000 0.01108 -0.19688

D110 2.93009 -0.00025 0.01881 0.00000 0.01880 2.94889

D111 3.06712 0.00238 0.06943 0.00000 0.06937 3.13649

D112 -0.07139 0.00266 0.06274 0.00000 0.06267 -0.00872

D113 0.09031 0.00070 0.08644 0.00000 0.08656 0.17687

D114 -3.04819 0.00098 0.07975 0.00000 0.07987 -2.96833

D115 0.07141 -0.00266 -0.06276 0.00000 -0.06270 0.00871

D116 -3.06676 -0.00240 -0.06971 0.00000 -0.06970 -3.13646

D117 3.04717 -0.00091 -0.07895 0.00000 -0.07892 2.96825

D118 -0.09100 -0.00065 -0.08590 0.00000 -0.08592 -0.17692

D119 2.81185 0.00253 0.10801 0.00000 0.10748 2.91933

D120 0.14215 -0.00096 -0.12641 0.00000 -0.12607 0.01608

D121 -0.14115 0.00089 0.12568 0.00000 0.12512 -0.01603

D122 -2.81084 -0.00259 -0.10874 0.00000 -0.10843 -2.91928

D123 -3.09608 -0.00125 -0.04387 0.00000 -0.04386 -3.13993

D124 0.01433 -0.00079 -0.02571 0.00000 -0.02569 -0.01136

D125 0.04257 -0.00152 -0.03738 0.00000 -0.03739 0.00517

D126 -3.13022 -0.00106 -0.01921 0.00000 -0.01923 3.13374

D127 0.00000 0.00000 0.00000 0.00000 0.00000 -0.00001

D128 3.11486 0.00037 0.01559 0.00000 0.01561 3.13047

D129 -3.11495 -0.00035 -0.01553 0.00000 -0.01554 -3.13049

D130 -0.00009 0.00001 0.00007 0.00000 0.00008 -0.00001

D131 -3.11851 -0.00047 -0.02385 0.00000 -0.02385 3.14082

D132 0.00890 -0.00025 -0.02101 0.00000 -0.02101 -0.01211

D133 -0.01170 0.00001 -0.00359 0.00000 -0.00360 -0.01530

D134 3.11571 0.00023 -0.00076 0.00000 -0.00075 3.11496

D135 -0.04262 0.00153 0.03742 0.00000 0.03746 -0.00516

D136 3.09570 0.00127 0.04416 0.00000 0.04421 3.13991

D137 3.13025 0.00106 0.01918 0.00000 0.01920 -3.13373

D138 -0.01461 0.00080 0.02593 0.00000 0.02596 0.01134

D139 0.01181 -0.00003 0.00351 0.00000 0.00350 0.01531

D140 -3.11560 -0.00024 0.00067 0.00000 0.00066 -3.11494

D141 3.11853 0.00046 0.02384 0.00000 0.02385 -3.14081

D142 -0.00889 0.00024 0.02100 0.00000 0.02101 0.01212

D143 0.20770 -0.00005 -0.01090 0.00000 -0.01086 0.19684

D144 -2.92997 0.00025 -0.01892 0.00000 -0.01892 -2.94889

D145 -0.00403 -0.00001 -0.00109 0.00000 -0.00110 -0.00513

D146 -3.14022 0.00009 0.00080 0.00000 0.00080 -3.13943

D147 3.13368 -0.00025 -0.00641 0.00000 -0.00642 3.12726

D148 -0.00251 -0.00016 -0.00452 0.00000 -0.00452 -0.00704

D149 -3.09861 -0.00045 0.00495 0.00000 0.00496 -3.09364

D150 0.04689 -0.00020 0.01040 0.00000 0.01039 0.05728

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D152 -3.13637 0.00010 0.00190 0.00000 0.00191 -3.13446

D153 3.13635 -0.00009 -0.00188 0.00000 -0.00189 3.13446

D154 -0.00001 0.00000 0.00001 0.00000 0.00001 0.00000

D155 0.00402 0.00001 0.00109 0.00000 0.00111 0.00513

D156 -3.13371 0.00026 0.00643 0.00000 0.00645 -3.12726

D157 3.14021 -0.00008 -0.00079 0.00000 -0.00078 3.13943

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D159 3.09855 0.00044 -0.00491 0.00000 -0.00492 3.09363

D160 -0.04692 0.00019 -0.01037 0.00000 -0.01036 -0.05729

D161 -0.01186 0.00003 -0.00360 0.00000 -0.00359 -0.01545

D162 3.13862 -0.00007 0.00035 0.00000 0.00036 3.13898

D163 3.11492 0.00019 -0.00078 0.00000 -0.00078 3.11413

D164 -0.01779 0.00009 0.00317 0.00000 0.00317 -0.01462

D165 -3.12647 -0.00024 0.02692 0.00000 0.02691 -3.09956

D166 0.03012 -0.00041 0.02401 0.00000 0.02401 0.05413

D167 -0.00003 0.00000 0.00002 0.00000 0.00002 -0.00001

D168 -3.13295 -0.00009 0.00389 0.00000 0.00389 -3.12905

D169 3.13291 0.00009 -0.00387 0.00000 -0.00386 3.12905

D170 -0.00001 0.00000 0.00000 0.00000 0.00000 0.00000

D171 0.01186 -0.00003 0.00359 0.00000 0.00359 0.01545

D172 -3.11491 -0.00019 0.00078 0.00000 0.00078 -3.11413

D173 -3.13865 0.00007 -0.00033 0.00000 -0.00033 -3.13898

D174 0.01777 -0.00009 -0.00315 0.00000 -0.00315 0.01462

D175 3.12642 0.00024 -0.02688 0.00000 -0.02688 3.09954

D176 -0.03018 0.00041 -0.02398 0.00000 -0.02398 -0.05415

D177 0.00403 0.00001 0.00108 0.00000 0.00109 0.00512

D178 3.14024 -0.00009 -0.00081 0.00000 -0.00081 3.13943

D179 -3.13370 0.00026 0.00641 0.00000 0.00642 -3.12728

D180 0.00250 0.00016 0.00452 0.00000 0.00452 0.00703

D181 3.09857 0.00045 -0.00494 0.00000 -0.00495 3.09362

D182 -0.04690 0.00020 -0.01039 0.00000 -0.01039 -0.05728

D183 0.00001 -0.00001 -0.00001 0.00000 -0.00001 0.00000

D184 3.13638 -0.00010 -0.00190 0.00000 -0.00191 3.13447

D185 -3.13635 0.00010 0.00188 0.00000 0.00188 -3.13447

D186 0.00001 0.00000 -0.00001 0.00000 -0.00001 0.00000

D187 -0.00402 -0.00001 -0.00109 0.00000 -0.00110 -0.00512

D188 3.13373 -0.00027 -0.00643 0.00000 -0.00644 3.12729

D189 -3.14022 0.00008 0.00079 0.00000 0.00079 -3.13943

D190 -0.00247 -0.00017 -0.00455 0.00000 -0.00455 -0.00702

D191 -3.09851 -0.00045 0.00490 0.00000 0.00491 -3.09361

D192 0.04693 -0.00019 0.01037 0.00000 0.01036 0.05729

D193 -0.01172 0.00001 -0.00370 0.00000 -0.00371 -0.01543

D194 3.13871 -0.00008 0.00029 0.00000 0.00028 3.13899

D195 3.11502 0.00018 -0.00086 0.00000 -0.00088 3.11414

D196 -0.01774 0.00008 0.00313 0.00000 0.00312 -0.01461

D197 -3.12648 -0.00024 0.02692 0.00000 0.02693 -3.09956

D198 0.03014 -0.00042 0.02400 0.00000 0.02399 0.05414

D199 0.00003 -0.00001 -0.00002 0.00000 -0.00002 0.00001

D200 -3.13298 -0.00009 0.00392 0.00000 0.00393 -3.12905

D201 3.13302 0.00008 -0.00395 0.00000 -0.00396 3.12906

D202 0.00001 0.00000 0.00000 0.00000 0.00000 0.00000

D203 0.01172 -0.00001 0.00370 0.00000 0.00371 0.01543

D204 -3.11502 -0.00018 0.00086 0.00000 0.00088 -3.11414

D205 -3.13869 0.00008 -0.00030 0.00000 -0.00030 -3.13899

D206 0.01776 -0.00009 -0.00315 0.00000 -0.00314 0.01462

D207 3.12654 0.00024 -0.02696 0.00000 -0.02696 3.09958

D208 -0.03009 0.00042 -0.02403 0.00000 -0.02403 -0.05412

D209 1.09532 -0.00007 0.00101 0.00000 0.00101 1.09633

D210 -1.04707 -0.00024 0.00016 0.00000 0.00016 -1.04690

D211 -3.12088 0.00002 0.00293 0.00000 0.00293 -3.11794

D212 1.04706 0.00023 -0.00016 0.00000 -0.00016 1.04690

D213 -1.09534 0.00007 -0.00100 0.00000 -0.00100 -1.09634

D214 3.12085 -0.00002 -0.00291 0.00000 -0.00291 3.11793

D215 1.09215 0.00042 0.00564 0.00000 0.00564 1.09779

D216 -1.04863 -0.00029 0.00253 0.00000 0.00254 -1.04610

D217 -3.11918 -0.00009 0.00343 0.00000 0.00343 -3.11574

D218 1.04861 0.00030 -0.00252 0.00000 -0.00252 1.04609

D219 -1.09216 -0.00043 -0.00563 0.00000 -0.00563 -1.09779

D220 3.11915 0.00008 -0.00341 0.00000 -0.00341 3.11573

D221 1.04706 0.00023 -0.00016 0.00000 -0.00016 1.04690

D222 -1.09533 0.00007 -0.00100 0.00000 -0.00100 -1.09634

D223 3.12085 -0.00002 -0.00292 0.00000 -0.00292 3.11794

D224 1.09535 -0.00008 0.00099 0.00000 0.00099 1.09634

D225 -1.04705 -0.00023 0.00016 0.00000 0.00015 -1.04690

D226 -3.12083 0.00002 0.00290 0.00000 0.00290 -3.11793

D227 1.09217 0.00043 0.00563 0.00000 0.00563 1.09779

D228 -1.04860 -0.00030 0.00251 0.00000 0.00251 -1.04609

D229 -3.11913 -0.00008 0.00340 0.00000 0.00340 -3.11573

D230 1.04862 0.00029 -0.00253 0.00000 -0.00253 1.04610

D231 -1.09216 -0.00043 -0.00564 0.00000 -0.00563 -1.09779

D232 3.11916 0.00009 -0.00342 0.00000 -0.00342 3.11574

Item Value Threshold Converged?

Maximum Force 0.013376 0.000450 NO

RMS Force 0.002299 0.000300 NO

Maximum Displacement 0.806898 0.001800 NO

RMS Displacement 0.121960 0.001200 NO

Predicted change in Energy=-9.135853D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 01:25:00 2019, MaxMem= 1342177280 cpu: 12.9

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=3 Diff= 4.31D-04

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 -1.124143 2.797533 -0.032039

2 7 0 0.000084 2.040871 -0.211241

3 6 0 1.124352 2.797329 -0.032098

4 6 0 0.712848 4.155174 0.277364

5 6 0 -0.712264 4.155360 0.277407

6 7 0 2.409837 2.380848 -0.125279

7 6 0 2.798840 1.129742 -0.200194

8 7 0 2.018898 0.000172 -0.137553

9 6 0 2.799117 -1.129349 -0.200199

10 6 0 4.208450 -0.704816 -0.334843

11 6 0 4.208212 0.705666 -0.334827

12 7 0 -2.409965 2.381028 -0.125244

13 6 0 -4.209003 0.705579 -0.334895

14 6 0 -4.209188 -0.705016 -0.334911

15 6 0 -2.799796 -1.129540 -0.200188

16 7 0 -2.019858 0.000109 -0.137510

17 6 0 -2.799603 1.129751 -0.200184

18 7 0 -2.410032 -2.381290 -0.125221

19 7 0 0.000162 -2.041892 -0.211348

20 6 0 -1.124148 -2.798341 -0.032046

21 6 0 -0.712159 -4.156164 0.277447

22 6 0 0.713041 -4.155932 0.277402

23 6 0 1.124565 -2.798065 -0.032106

24 7 0 2.410081 -2.380953 -0.125259

25 30 0 -0.000663 -0.000742 -0.380083

26 6 0 -5.403526 1.429951 -0.442339

27 6 0 -6.595991 0.695747 -0.543211

28 6 0 -6.596192 -0.694401 -0.543232

29 6 0 -5.403946 -1.428991 -0.442382

30 6 0 1.433524 -5.334571 0.559882

31 6 0 0.700720 -6.496780 0.818916

32 6 0 -0.698942 -6.497021 0.818954

33 6 0 -1.432182 -5.335062 0.559966

34 6 0 5.402672 1.430097 -0.442160

35 6 0 6.595201 0.695968 -0.542936

36 6 0 6.595453 -0.694156 -0.542957

37 6 0 5.403200 -1.428760 -0.442203

38 6 0 -1.432337 5.334232 0.559840

39 6 0 -0.699154 6.496244 0.818777

40 6 0 0.700484 6.496047 0.818741

41 6 0 1.433305 5.333833 0.559759

42 1 0 7.545317 1.205337 -0.630046

43 1 0 7.545764 -1.203163 -0.630084

44 1 0 1.208201 7.425493 1.038122

45 1 0 -1.206592 7.425836 1.038186

46 1 0 -7.546123 1.205072 -0.630409

47 1 0 -7.546479 -1.203436 -0.630447

48 1 0 -1.206345 -7.426620 1.038413

49 1 0 1.208463 -7.426199 1.038347

50 8 0 2.782420 5.274461 0.578062

51 8 0 -2.781459 5.275292 0.578223

52 8 0 5.346432 2.777495 -0.453487

53 8 0 5.347544 -2.776176 -0.453577

54 8 0 2.782629 -5.275196 0.578201

55 8 0 -2.781299 -5.276205 0.578368

56 8 0 -5.348357 -2.776404 -0.453786

57 8 0 -5.347454 2.777350 -0.453696

58 6 0 3.510267 6.478180 0.812235

59 1 0 3.295558 6.889511 1.802815

60 1 0 3.295190 7.230422 0.048098

61 1 0 4.560986 6.199350 0.759067

62 6 0 6.571309 3.507729 -0.503014

63 1 0 7.122344 3.306491 -1.426178

64 1 0 7.205066 3.282003 0.359498

65 1 0 6.285861 4.557560 -0.476368

66 6 0 6.572737 -3.505874 -0.503114

67 1 0 7.206386 -3.279895 0.359411

68 1 0 7.123695 -3.304368 -1.426267

69 1 0 6.287748 -4.555831 -0.476499

70 6 0 -3.508921 6.479239 0.812410

71 1 0 -3.293658 7.231400 0.048246

72 1 0 -3.294037 6.890528 1.802970

73 1 0 -4.559727 6.200729 0.759298

74 6 0 -6.572418 3.507417 -0.503363

75 1 0 -7.206232 3.281627 0.359092

76 1 0 -7.123335 3.306082 -1.426578

77 1 0 -6.287111 4.557286 -0.476712

78 6 0 -6.573582 -3.506028 -0.503464

79 1 0 -7.124437 -3.304466 -1.426668

80 1 0 -7.207305 -3.280033 0.359004

81 1 0 -6.288655 -4.556000 -0.476844

82 6 0 -3.508687 -6.480179 0.812612

83 1 0 -3.293769 -6.891417 1.803186

84 1 0 -3.293391 -7.232359 0.048474

85 1 0 -4.559507 -6.201724 0.759497

86 6 0 3.510479 -6.478896 0.812430

87 1 0 3.295416 -7.231171 0.048320

88 1 0 3.295765 -6.890191 1.803025

89 1 0 4.561194 -6.200056 0.759257

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0448203 0.0438123 0.0225569

Leave Link 202 at Sat Jul 6 01:25:01 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8040.2218670695 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= 89 NActive= 89 NUniq= 89 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= -0.2278249461 Hartrees.

Nuclear repulsion after empirical dispersion term = 8039.9940421234 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6440

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.79D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 412

GePol: Fraction of low-weight points (<1% of avg) = 6.40%

GePol: Cavity surface area = 703.655 Ang\*\*2

GePol: Cavity volume = 802.261 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0089273233 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8039.9851148000 Hartrees.

Leave Link 301 at Sat Jul 6 01:25:01 2019, MaxMem= 1342177280 cpu: 1.9

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44303 LenP2D= 111295.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.82D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 01:25:05 2019, MaxMem= 1342177280 cpu: 41.6

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 01:25:06 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000004 -0.000003 -0.000009 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000076 0.000131 0.000047 Ang= 0.02 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 2.48D-01

Max alpha theta= 4.071 degrees.

Max beta theta= 4.088 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0171 S= 1.0057

Leave Link 401 at Sat Jul 6 01:25:16 2019, MaxMem= 1342177280 cpu: 124.6

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 124420800.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.10D-15 for 6422.

Iteration 1 A\*A^-1 deviation from orthogonality is 7.86D-15 for 4261 1019.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.31D-14 for 504.

Iteration 1 A^-1\*A deviation from orthogonality is 2.72D-11 for 5491 4014.

E= -2649.79502970540

DIIS: error= 3.84D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79502970540 IErMin= 1 ErrMin= 3.84D-04

ErrMax= 3.84D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.39D-04 BMatP= 1.39D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.84D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 13.591 Goal= None Shift= 0.000

Gap= 15.246 Goal= None Shift= 0.000

RMSDP=3.55D-05 MaxDP=3.21D-03 OVMax= 1.78D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.53D-05 CP: 1.00D+00

E= -2649.79506380732 Delta-E= -0.000034101915 Rises=F Damp=F

DIIS: error= 3.38D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79506380732 IErMin= 2 ErrMin= 3.38D-04

ErrMax= 3.38D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.70D-05 BMatP= 1.39D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.38D-03

Coeff-Com: 0.336D+00 0.664D+00

Coeff-En: 0.000D+00 0.100D+01

Coeff: 0.335D+00 0.665D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.76D-06 MaxDP=3.21D-04 DE=-3.41D-05 OVMax= 4.97D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.53D-06 CP: 1.00D+00 9.60D-01

E= -2649.79506767505 Delta-E= -0.000003867730 Rises=F Damp=F

DIIS: error= 2.04D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79506767505 IErMin= 3 ErrMin= 2.04D-04

ErrMax= 2.04D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.11D-05 BMatP= 5.70D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.04D-03

Coeff-Com: -0.607D-02 0.377D+00 0.629D+00

Coeff-En: 0.000D+00 0.283D+00 0.717D+00

Coeff: -0.606D-02 0.377D+00 0.629D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.85D-06 MaxDP=1.12D-04 DE=-3.87D-06 OVMax= 3.21D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 8.49D-07 CP: 1.00D+00 9.89D-01 7.22D-01

E= -2649.79506979044 Delta-E= -0.000002115397 Rises=F Damp=F

DIIS: error= 1.19D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79506979044 IErMin= 4 ErrMin= 1.19D-05

ErrMax= 1.19D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.78D-07 BMatP= 2.11D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.713D-02 0.211D+00 0.354D+00 0.443D+00

Coeff: -0.713D-02 0.211D+00 0.354D+00 0.443D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.21D-07 MaxDP=4.37D-05 DE=-2.12D-06 OVMax= 7.80D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.17D-07 CP: 1.00D+00 9.90D-01 7.32D-01 6.85D-01

E= -2649.79506991419 Delta-E= -0.000000123746 Rises=F Damp=F

DIIS: error= 4.67D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79506991419 IErMin= 5 ErrMin= 4.67D-06

ErrMax= 4.67D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.18D-08 BMatP= 6.78D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.263D-02 0.408D-01 0.597D-01 0.234D+00 0.668D+00

Coeff: -0.263D-02 0.408D-01 0.597D-01 0.234D+00 0.668D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.44D-07 MaxDP=1.17D-05 DE=-1.24D-07 OVMax= 3.81D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.45D-08 CP: 1.00D+00 9.91D-01 7.19D-01 7.35D-01 7.56D-01

E= -2649.79506992714 Delta-E= -0.000000012946 Rises=F Damp=F

DIIS: error= 1.40D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79506992714 IErMin= 6 ErrMin= 1.40D-06

ErrMax= 1.40D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.35D-09 BMatP= 6.18D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.943D-03 0.107D-01 0.135D-01 0.901D-01 0.331D+00 0.556D+00

Coeff: -0.943D-03 0.107D-01 0.135D-01 0.901D-01 0.331D+00 0.556D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.52D-08 MaxDP=3.01D-06 DE=-1.29D-08 OVMax= 1.84D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.74D-08 CP: 1.00D+00 9.91D-01 7.19D-01 7.45D-01 7.96D-01

CP: 7.97D-01

E= -2649.79506992797 Delta-E= -0.000000000839 Rises=F Damp=F

DIIS: error= 7.75D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79506992797 IErMin= 7 ErrMin= 7.75D-07

ErrMax= 7.75D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.42D-09 BMatP= 4.35D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.942D-04-0.440D-02-0.739D-02-0.454D-02 0.468D-01 0.371D+00

Coeff-Com: 0.598D+00

Coeff: 0.942D-04-0.440D-02-0.739D-02-0.454D-02 0.468D-01 0.371D+00

Coeff: 0.598D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.14D-08 MaxDP=2.09D-06 DE=-8.39D-10 OVMax= 7.42D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.70D-08 CP: 1.00D+00 9.91D-01 7.19D-01 7.46D-01 8.08D-01

CP: 9.00D-01 8.08D-01

E= -2649.79506992840 Delta-E= -0.000000000422 Rises=F Damp=F

DIIS: error= 2.48D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.79506992840 IErMin= 8 ErrMin= 2.48D-07

ErrMax= 2.48D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D-10 BMatP= 1.42D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.161D-03-0.313D-02-0.401D-02-0.174D-01-0.381D-01 0.468D-01

Coeff-Com: 0.180D+00 0.836D+00

Coeff: 0.161D-03-0.313D-02-0.401D-02-0.174D-01-0.381D-01 0.468D-01

Coeff: 0.180D+00 0.836D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.10D-08 MaxDP=1.15D-06 DE=-4.22D-10 OVMax= 5.30D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 7.49D-09 CP: 1.00D+00 9.91D-01 7.20D-01 7.47D-01 8.14D-01

CP: 9.38D-01 9.28D-01 1.26D+00

E= -2649.79506992854 Delta-E= -0.000000000147 Rises=F Damp=F

DIIS: error= 1.49D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.79506992854 IErMin= 9 ErrMin= 1.49D-07

ErrMax= 1.49D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.87D-11 BMatP= 1.13D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.649D-04-0.153D-03 0.419D-03-0.785D-02-0.344D-01-0.940D-01

Coeff-Com: -0.109D+00 0.475D+00 0.770D+00

Coeff: 0.649D-04-0.153D-03 0.419D-03-0.785D-02-0.344D-01-0.940D-01

Coeff: -0.109D+00 0.475D+00 0.770D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=7.61D-09 MaxDP=9.09D-07 DE=-1.47D-10 OVMax= 4.80D-06

Error on total polarization charges = 0.07288

SCF Done: E(UB3LYP) = -2649.79506993 A.U. after 9 cycles

NFock= 9 Conv=0.76D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0171 S= 1.0057

<L.S>= 0.000000000000E+00

KE= 2.690163347634D+03 PE=-2.235867463445D+04 EE= 8.978731102083D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.60

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0171, after 2.0002

Leave Link 502 at Sat Jul 6 01:32:37 2019, MaxMem= 1342177280 cpu: 5185.1

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44303 LenP2D= 111295.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 286

Leave Link 701 at Sat Jul 6 01:32:56 2019, MaxMem= 1342177280 cpu: 220.5

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 01:32:56 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 01:34:28 2019, MaxMem= 1342177280 cpu: 1096.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.31410141D-04 2.76005931D-03 1.15633910D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.001128061 0.001489018 0.001162800

2 7 -0.000072037 0.000099380 0.001587404

3 6 -0.001312189 0.001626146 0.001184952

4 6 0.001289596 -0.000415641 -0.000396569

5 6 -0.001338481 -0.000457203 -0.000405245

6 7 0.000086893 0.001171265 -0.000477482

7 6 -0.000400707 -0.000327805 -0.000500767

8 7 0.001361888 -0.000143785 -0.000331689

9 6 -0.000633231 0.000004294 -0.000468945

10 6 0.001137914 0.000835313 -0.000205722

11 6 0.001179494 -0.000888068 -0.000212377

12 7 -0.000051468 0.000994725 -0.000477902

13 6 -0.001157251 -0.000867713 -0.000207169

14 6 -0.001115790 0.000814627 -0.000200571

15 6 0.000799259 -0.000265900 -0.000449885

16 7 -0.001297984 -0.000145000 -0.000316807

17 6 0.000565031 -0.000059283 -0.000481338

18 7 -0.000114742 -0.000677827 -0.000489892

19 7 -0.000072194 -0.000011115 0.001601861

20 6 0.001006674 -0.001367524 0.001144890

21 6 -0.001355453 0.000467789 -0.000405502

22 6 0.001306074 0.000426465 -0.000396830

23 6 -0.001192244 -0.001505296 0.001166882

24 7 0.000150840 -0.000855773 -0.000489638

25 30 0.000065571 0.000083038 -0.001454260

26 6 0.001286521 0.000394144 -0.000032696

27 6 -0.000465631 -0.000106453 0.000008046

28 6 -0.000462245 0.000103011 0.000008434

29 6 0.001272814 -0.000396549 -0.000033620

30 6 0.000096210 0.000528844 0.000438754

31 6 0.000258969 -0.000046674 -0.000061697

32 6 -0.000261222 -0.000039048 -0.000063100

33 6 -0.000091525 0.000512814 0.000442442

34 6 -0.001273350 0.000418407 -0.000032893

35 6 0.000459715 -0.000075625 0.000008694

36 6 0.000456454 0.000072263 0.000009153

37 6 -0.001259739 -0.000420813 -0.000033825

38 6 -0.000117756 -0.000512800 0.000443659

39 6 -0.000277541 0.000038401 -0.000063818

40 6 0.000275197 0.000046107 -0.000062427

41 6 0.000122445 -0.000528907 0.000439958

42 1 -0.000056662 0.000165461 -0.000003876

43 1 -0.000059589 -0.000165055 -0.000003953

44 1 0.000049693 0.000017072 -0.000061516

45 1 -0.000050536 0.000016171 -0.000061926

46 1 0.000057315 0.000162133 -0.000003708

47 1 0.000059995 -0.000161830 -0.000003737

48 1 -0.000048972 -0.000016899 -0.000061907

49 1 0.000048067 -0.000017853 -0.000061456

50 8 0.000151160 0.000004239 -0.000821304

51 8 -0.000169303 -0.000008353 -0.000818403

52 8 0.000190678 0.000741641 0.000285456

53 8 0.000168410 -0.000757466 0.000284688

54 8 0.000162814 0.000014914 -0.000822011

55 8 -0.000180840 0.000027364 -0.000819008

56 8 -0.000132598 -0.000759292 0.000284738

57 8 -0.000154333 0.000743969 0.000285690

58 6 0.000003821 -0.000409449 0.000330229

59 1 -0.000028532 0.000059168 0.000066582

60 1 -0.000033636 0.000119979 -0.000053004

61 1 0.000028876 -0.000107135 -0.000035175

62 6 -0.000255175 0.000096980 0.000015679

63 1 0.000041448 0.000025722 -0.000015318

64 1 0.000107603 0.000070580 0.000028889

65 1 -0.000139680 0.000025584 0.000038286

66 6 -0.000251585 -0.000098017 0.000014964

67 1 0.000107567 -0.000071924 0.000028493

68 1 0.000040485 -0.000026796 -0.000014633

69 1 -0.000139828 -0.000026181 0.000037129

70 6 -0.000006550 -0.000406262 0.000330609

71 1 0.000034969 0.000118555 -0.000052841

72 1 0.000028408 0.000057911 0.000065778

73 1 -0.000030466 -0.000105864 -0.000033204

74 6 0.000246307 0.000102732 0.000015282

75 1 -0.000106181 0.000071424 0.000028183

76 1 -0.000039579 0.000026921 -0.000014026

77 1 0.000139270 0.000025985 0.000037161

78 6 0.000242762 -0.000104064 0.000014761

79 1 -0.000038614 -0.000027912 -0.000013367

80 1 -0.000106076 -0.000072546 0.000027772

81 1 0.000139342 -0.000026530 0.000035980

82 6 -0.000009254 0.000401635 0.000331046

83 1 0.000027917 -0.000056950 0.000064910

84 1 0.000034974 -0.000117870 -0.000052167

85 1 -0.000031716 0.000104137 -0.000031518

86 6 0.000006350 0.000404920 0.000330633

87 1 -0.000033470 -0.000119420 -0.000052348

88 1 -0.000028013 -0.000058255 0.000065770

89 1 0.000030118 0.000105477 -0.000033566

-------------------------------------------------------------------

Cartesian Forces: Max 0.001626146 RMS 0.000520695

Leave Link 716 at Sat Jul 6 01:34:28 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.001503982 RMS 0.000381874

Search for a local minimum.

Step number 13 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .38187D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 4 6 5 8 7

10 9 11 13

ITU= 0 -1 0 0 0 0 0 0 1 1 1 1 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.00060 0.01044 0.01225 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01316 0.01316

Eigenvalues --- 0.01358 0.01569 0.01572 0.01573 0.01583

Eigenvalues --- 0.01599 0.01617 0.01619 0.01683 0.01707

Eigenvalues --- 0.01709 0.01711 0.01715 0.01836 0.01873

Eigenvalues --- 0.01890 0.01920 0.01924 0.01928 0.01947

Eigenvalues --- 0.01959 0.02015 0.02021 0.02023 0.02024

Eigenvalues --- 0.02039 0.02047 0.02053 0.02053 0.02053

Eigenvalues --- 0.02053 0.02057 0.02057 0.02057 0.02057

Eigenvalues --- 0.02063 0.02067 0.02067 0.02069 0.02070

Eigenvalues --- 0.02070 0.02070 0.02071 0.02071 0.02083

Eigenvalues --- 0.02083 0.02143 0.02235 0.02260 0.02260

Eigenvalues --- 0.02260 0.02260 0.02260 0.02260 0.02303

Eigenvalues --- 0.02345 0.02356 0.02363 0.02533 0.03216

Eigenvalues --- 0.08863 0.09986 0.09986 0.09986 0.09990

Eigenvalues --- 0.09990 0.09990 0.09995 0.10506 0.10649

Eigenvalues --- 0.10649 0.10649 0.10652 0.10653 0.10653

Eigenvalues --- 0.10653 0.10678 0.13324 0.13462 0.14447

Eigenvalues --- 0.15858 0.15977 0.15993 0.15997 0.15998

Eigenvalues --- 0.15998 0.15999 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16005

Eigenvalues --- 0.16032 0.16231 0.18768 0.21481 0.21730

Eigenvalues --- 0.22474 0.22474 0.22474 0.22475 0.23782

Eigenvalues --- 0.24178 0.24351 0.24432 0.24505 0.24512

Eigenvalues --- 0.24518 0.24628 0.24755 0.24809 0.24838

Eigenvalues --- 0.24868 0.24905 0.24979 0.24992 0.24992

Eigenvalues --- 0.24995 0.24995 0.24998 0.24998 0.24998

Eigenvalues --- 0.24998 0.24998 0.24998 0.24999 0.24999

Eigenvalues --- 0.24999 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25004 0.25121 0.28671

Eigenvalues --- 0.33592 0.33632 0.33673 0.33676 0.33712

Eigenvalues --- 0.33717 0.34061 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34063 0.34063 0.34077 0.34080

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34081

Eigenvalues --- 0.34081 0.34606 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34686 0.34686 0.34851

Eigenvalues --- 0.34944 0.35016 0.35324 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35632 0.35634

Eigenvalues --- 0.36633 0.37064 0.37138 0.38283 0.40619

Eigenvalues --- 0.41161 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41215 0.41215 0.41351 0.41397 0.41399

Eigenvalues --- 0.41407 0.41409 0.42066 0.42372 0.42474

Eigenvalues --- 0.42763 0.43403 0.44515 0.44560 0.44748

Eigenvalues --- 0.44807 0.44872 0.44998 0.45000 0.45000

Eigenvalues --- 0.45002 0.45308 0.45365 0.45372 0.45917

Eigenvalues --- 0.47263 0.47274 0.48413 0.49222 0.49298

Eigenvalues --- 0.49834 0.52928 0.53554 0.53554 0.53554

Eigenvalues --- 0.53554 0.53554 0.53554 0.54324 0.54968

Eigenvalues --- 0.56061 0.57105 0.57400 0.57560 0.59352

Eigenvalues --- 0.62130

RFO step: Lambda=-8.81047669D-04 EMin= 5.99768664D-04

Quartic linear search produced a step of -0.05771.

Iteration 1 RMS(Cart)= 0.23892841 RMS(Int)= 0.00346769

Iteration 2 RMS(Cart)= 0.01588602 RMS(Int)= 0.00020905

Iteration 3 RMS(Cart)= 0.00004074 RMS(Int)= 0.00020890

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00020890

ITry= 1 IFail=0 DXMaxC= 9.22D-01 DCOld= 1.00D+10 DXMaxT= 2.28D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58315 -0.00022 -0.00014 -0.00113 -0.00130 2.58185

R2 2.74440 -0.00147 -0.00044 -0.00290 -0.00323 2.74116

R3 2.56021 0.00018 0.00051 -0.00293 -0.00199 2.55823

R4 2.58299 -0.00020 -0.00012 -0.00176 -0.00197 2.58102

R5 3.87126 0.00085 0.00022 -0.00152 -0.00147 3.86979

R6 2.74423 -0.00138 -0.00043 -0.00279 -0.00312 2.74112

R7 2.55959 0.00048 0.00057 -0.00453 -0.00366 2.55593

R8 2.69307 0.00045 0.00039 -0.00179 -0.00107 2.69200

R9 2.66447 -0.00089 -0.00010 -0.00424 -0.00437 2.66011

R10 2.66446 -0.00089 -0.00010 -0.00427 -0.00440 2.66006

R11 2.47994 0.00131 0.00016 -0.00775 -0.00744 2.47250

R12 2.59668 -0.00002 -0.00001 -0.00157 -0.00207 2.59461

R13 2.79290 0.00043 0.00040 -0.00404 -0.00351 2.78938

R14 2.59690 -0.00010 -0.00003 -0.00089 -0.00135 2.59555

R15 3.84384 0.00037 -0.00021 0.00385 0.00299 3.84683

R16 2.79307 0.00032 0.00039 -0.00422 -0.00370 2.78937

R17 2.48086 0.00080 0.00009 -0.00603 -0.00567 2.47519

R18 2.66543 -0.00003 -0.00011 0.00252 0.00282 2.66824

R19 2.64767 -0.00070 -0.00013 -0.00273 -0.00289 2.64478

R20 2.64768 -0.00069 -0.00013 -0.00269 -0.00285 2.64483

R21 2.48060 0.00090 0.00011 -0.00657 -0.00624 2.47437

R22 2.66564 -0.00011 -0.00013 0.00287 0.00320 2.66884

R23 2.79301 0.00035 0.00039 -0.00403 -0.00349 2.78952

R24 2.64774 -0.00074 -0.00013 -0.00274 -0.00290 2.64484

R25 2.79319 0.00024 0.00038 -0.00421 -0.00368 2.78951

R26 2.64773 -0.00075 -0.00013 -0.00278 -0.00294 2.64479

R27 2.59680 -0.00012 -0.00001 -0.00156 -0.00207 2.59473

R28 2.48153 0.00039 0.00003 -0.00486 -0.00447 2.47706

R29 2.59658 -0.00004 0.00001 -0.00223 -0.00279 2.59380

R30 3.84316 0.00031 -0.00018 0.00415 0.00308 3.84624

R31 2.56064 -0.00006 0.00047 -0.00187 -0.00089 2.55975

R32 2.58308 -0.00026 -0.00013 -0.00177 -0.00199 2.58110

R33 2.58292 -0.00024 -0.00011 -0.00240 -0.00266 2.58026

R34 3.87037 0.00074 0.00025 -0.00130 -0.00146 3.86891

R35 2.74447 -0.00150 -0.00045 -0.00285 -0.00318 2.74129

R36 2.69324 0.00041 0.00038 -0.00147 -0.00072 2.69252

R37 2.66448 -0.00091 -0.00010 -0.00430 -0.00442 2.66006

R38 2.74430 -0.00142 -0.00044 -0.00275 -0.00306 2.74124

R39 2.66450 -0.00091 -0.00010 -0.00427 -0.00440 2.66010

R40 2.56001 0.00025 0.00053 -0.00347 -0.00256 2.55746

R41 2.65317 0.00096 0.00031 0.00065 0.00099 2.65415

R42 2.54851 0.00097 -0.00002 0.00337 0.00335 2.55186

R43 2.62700 0.00122 0.00009 0.00374 0.00388 2.63088

R44 2.04385 0.00003 0.00006 -0.00059 -0.00054 2.04331

R45 2.65319 0.00094 0.00030 0.00064 0.00097 2.65416

R46 2.04385 0.00002 0.00006 -0.00060 -0.00054 2.04331

R47 2.54850 0.00099 -0.00002 0.00340 0.00338 2.55187

R48 2.64212 0.00036 0.00006 0.00155 0.00164 2.64376

R49 2.55214 0.00015 -0.00019 0.00398 0.00378 2.55593

R50 2.64498 0.00092 0.00012 0.00361 0.00378 2.64876

R51 2.04385 0.00003 0.00005 -0.00045 -0.00039 2.04346

R52 2.64215 0.00034 0.00006 0.00154 0.00163 2.64378

R53 2.04385 0.00002 0.00005 -0.00045 -0.00040 2.04346

R54 2.55212 0.00017 -0.00019 0.00399 0.00380 2.55592

R55 2.65318 0.00095 0.00031 0.00061 0.00095 2.65413

R56 2.54852 0.00096 -0.00002 0.00337 0.00335 2.55187

R57 2.62695 0.00124 0.00009 0.00365 0.00379 2.63074

R58 2.04385 0.00003 0.00006 -0.00059 -0.00053 2.04331

R59 2.65321 0.00093 0.00030 0.00060 0.00093 2.65414

R60 2.04385 0.00003 0.00006 -0.00060 -0.00054 2.04331

R61 2.54851 0.00098 -0.00002 0.00339 0.00337 2.55188

R62 2.64216 0.00034 0.00006 0.00152 0.00160 2.64376

R63 2.55214 0.00015 -0.00019 0.00399 0.00379 2.55593

R64 2.64493 0.00094 0.00012 0.00352 0.00369 2.64862

R65 2.04385 0.00003 0.00005 -0.00045 -0.00040 2.04346

R66 2.64213 0.00035 0.00006 0.00152 0.00161 2.64374

R67 2.04385 0.00003 0.00005 -0.00045 -0.00039 2.04346

R68 2.55216 0.00013 -0.00019 0.00397 0.00378 2.55594

R69 2.69479 -0.00025 -0.00005 -0.00044 -0.00049 2.69430

R70 2.69479 -0.00025 -0.00005 -0.00043 -0.00049 2.69430

R71 2.69643 -0.00010 -0.00006 0.00037 0.00031 2.69674

R72 2.69643 -0.00010 -0.00006 0.00037 0.00031 2.69674

R73 2.69478 -0.00024 -0.00005 -0.00044 -0.00049 2.69429

R74 2.69478 -0.00024 -0.00005 -0.00044 -0.00049 2.69429

R75 2.69642 -0.00009 -0.00006 0.00038 0.00032 2.69673

R76 2.69642 -0.00009 -0.00006 0.00037 0.00031 2.69673

R77 2.06710 0.00009 0.00004 0.00034 0.00039 2.06749

R78 2.06667 0.00013 0.00007 0.00033 0.00040 2.06707

R79 2.05675 0.00006 0.00002 0.00018 0.00021 2.05696

R80 2.06696 0.00003 0.00004 0.00017 0.00021 2.06716

R81 2.06709 0.00007 0.00005 0.00035 0.00040 2.06750

R82 2.05654 0.00006 0.00003 0.00015 0.00018 2.05671

R83 2.06709 0.00007 0.00005 0.00035 0.00040 2.06750

R84 2.06696 0.00003 0.00004 0.00017 0.00021 2.06716

R85 2.05654 0.00006 0.00003 0.00015 0.00018 2.05671

R86 2.06667 0.00013 0.00007 0.00033 0.00040 2.06706

R87 2.06711 0.00009 0.00004 0.00034 0.00039 2.06749

R88 2.05675 0.00006 0.00002 0.00019 0.00021 2.05696

R89 2.06710 0.00007 0.00005 0.00035 0.00040 2.06750

R90 2.06696 0.00003 0.00004 0.00017 0.00021 2.06716

R91 2.05653 0.00006 0.00003 0.00015 0.00018 2.05671

R92 2.06696 0.00003 0.00004 0.00016 0.00020 2.06717

R93 2.06710 0.00007 0.00005 0.00035 0.00040 2.06750

R94 2.05653 0.00006 0.00003 0.00015 0.00018 2.05671

R95 2.06711 0.00009 0.00004 0.00034 0.00039 2.06749

R96 2.06667 0.00012 0.00007 0.00033 0.00040 2.06707

R97 2.05675 0.00006 0.00002 0.00019 0.00021 2.05696

R98 2.06667 0.00013 0.00007 0.00033 0.00040 2.06707

R99 2.06711 0.00009 0.00004 0.00034 0.00039 2.06749

R100 2.05675 0.00006 0.00002 0.00019 0.00021 2.05696

A1 1.88833 0.00035 0.00000 -0.00274 -0.00353 1.88480

A2 2.21601 -0.00022 -0.00026 0.00206 0.00174 2.21775

A3 2.17884 -0.00013 0.00026 0.00076 0.00157 2.18041

A4 1.93151 -0.00042 0.00009 0.00364 0.00328 1.93479

A5 2.16780 0.00024 -0.00005 0.00010 -0.00002 2.16778

A6 2.16838 0.00025 -0.00010 0.00090 0.00098 2.16936

A7 1.88844 0.00031 -0.00001 -0.00269 -0.00347 1.88497

A8 2.21609 -0.00029 -0.00026 0.00205 0.00170 2.21779

A9 2.17865 -0.00002 0.00027 0.00073 0.00156 2.18021

A10 1.85824 -0.00012 -0.00004 0.00127 0.00101 1.85925

A11 2.31791 -0.00023 0.00004 -0.00390 -0.00370 2.31421

A12 2.10697 0.00035 0.00000 0.00249 0.00249 2.10946

A13 1.85822 -0.00012 -0.00004 0.00115 0.00089 1.85911

A14 2.31797 -0.00026 0.00004 -0.00386 -0.00366 2.31430

A15 2.10693 0.00038 0.00001 0.00258 0.00258 2.10951

A16 2.18755 -0.00005 0.00010 -0.00579 -0.00649 2.18106

A17 2.23045 0.00018 0.00029 -0.00451 -0.00469 2.22575

A18 2.16690 0.00020 0.00007 0.00525 0.00631 2.17321

A19 1.88551 -0.00039 -0.00035 -0.00105 -0.00196 1.88355

A20 1.92979 0.00053 0.00048 0.00133 0.00190 1.93169

A21 2.16335 -0.00025 -0.00014 -0.00046 -0.00052 2.16284

A22 2.16265 -0.00024 -0.00009 -0.00137 -0.00163 2.16102

A23 1.88539 -0.00033 -0.00034 -0.00108 -0.00201 1.88339

A24 2.23035 0.00028 0.00029 -0.00443 -0.00458 2.22577

A25 2.16712 0.00004 0.00006 0.00521 0.00624 2.17335

A26 1.86196 0.00010 0.00011 -0.00009 -0.00019 1.86177

A27 2.30725 -0.00082 -0.00030 -0.00136 -0.00152 2.30573

A28 2.11396 0.00072 0.00020 0.00137 0.00155 2.11551

A29 1.86199 0.00009 0.00010 0.00001 -0.00009 1.86191

A30 2.30715 -0.00076 -0.00030 -0.00132 -0.00148 2.30567

A31 2.11403 0.00067 0.00019 0.00123 0.00141 2.11543

A32 2.18791 -0.00011 0.00008 -0.00565 -0.00629 2.18162

A33 1.86201 0.00009 0.00010 -0.00011 -0.00021 1.86180

A34 2.11400 0.00069 0.00020 0.00124 0.00141 2.11541

A35 2.30716 -0.00077 -0.00030 -0.00120 -0.00135 2.30580

A36 1.86198 0.00010 0.00011 -0.00022 -0.00032 1.86166

A37 2.11393 0.00073 0.00020 0.00138 0.00155 2.11549

A38 2.30726 -0.00083 -0.00031 -0.00124 -0.00139 2.30586

A39 1.88519 -0.00030 -0.00033 -0.00121 -0.00219 1.88301

A40 2.16759 -0.00008 0.00003 0.00544 0.00654 2.17414

A41 2.23007 0.00037 0.00031 -0.00453 -0.00471 2.22536

A42 1.93015 0.00047 0.00045 0.00184 0.00251 1.93267

A43 2.16245 -0.00021 -0.00007 -0.00166 -0.00196 2.16049

A44 2.16317 -0.00022 -0.00013 -0.00075 -0.00086 2.16231

A45 2.16738 0.00008 0.00004 0.00548 0.00662 2.17400

A46 2.23017 0.00027 0.00031 -0.00461 -0.00482 2.22535

A47 1.88531 -0.00036 -0.00034 -0.00118 -0.00214 1.88317

A48 2.18827 -0.00014 0.00005 -0.00557 -0.00617 2.18210

A49 1.93187 -0.00046 0.00006 0.00414 0.00387 1.93574

A50 2.16759 0.00026 -0.00003 -0.00014 -0.00030 2.16729

A51 2.16819 0.00026 -0.00008 0.00066 0.00069 2.16888

A52 2.21580 -0.00017 -0.00024 0.00199 0.00165 2.21745

A53 2.17926 -0.00020 0.00023 0.00095 0.00183 2.18109

A54 1.88811 0.00038 0.00001 -0.00285 -0.00369 1.88442

A55 1.85826 -0.00012 -0.00004 0.00102 0.00076 1.85902

A56 2.31794 -0.00026 0.00004 -0.00374 -0.00354 2.31440

A57 2.10692 0.00038 0.00001 0.00258 0.00257 2.10949

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D4 -0.17685 -0.00006 -0.00164 -0.01232 -0.01396 -0.19081

D5 -0.00507 0.00012 0.00071 0.03872 0.03934 0.03427

D6 -3.13369 0.00007 0.00036 0.05158 0.05188 -3.08181

D7 3.14009 0.00036 0.00083 0.01373 0.01446 -3.12864

D8 0.01148 0.00031 0.00049 0.02658 0.02699 0.03847

D9 0.19686 0.00020 -0.00021 0.03378 0.03342 0.23029

D10 -2.94898 -0.00009 -0.00035 0.06349 0.06308 -2.88590

D11 -0.00854 0.00020 0.00119 0.06487 0.06608 0.05754

D12 3.13669 0.00045 0.00132 0.03910 0.04041 -3.10609

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D147 3.12726 0.00027 -0.00012 0.00106 0.00091 3.12817

D148 -0.00704 0.00015 -0.00009 0.00235 0.00225 -0.00479

D149 -3.09364 0.00011 0.00009 -0.00375 -0.00366 -3.09730

D150 0.05728 -0.00006 0.00020 0.00118 0.00139 0.05866

D151 0.00000 0.00000 0.00000 0.00008 0.00008 0.00008

D152 -3.13446 -0.00012 0.00004 0.00130 0.00135 -3.13311

D153 3.13446 0.00012 -0.00004 -0.00119 -0.00124 3.13322

D154 0.00000 0.00000 0.00000 0.00003 0.00003 0.00003

D155 0.00513 -0.00011 0.00002 -0.00598 -0.00595 -0.00082

D156 -3.12726 -0.00027 0.00012 -0.00100 -0.00085 -3.12812

D157 3.13943 0.00002 -0.00002 -0.00722 -0.00723 3.13219

D158 0.00704 -0.00014 0.00009 -0.00224 -0.00214 0.00490

D159 3.09363 -0.00010 -0.00009 0.00393 0.00384 3.09747

D160 -0.05729 0.00006 -0.00020 -0.00110 -0.00130 -0.05859

D161 -0.01545 0.00008 -0.00007 -0.00552 -0.00561 -0.02106

D162 3.13898 -0.00004 0.00001 -0.00224 -0.00224 3.13674

D163 3.11413 0.00015 -0.00001 -0.01080 -0.01084 3.10329

D164 -0.01462 0.00004 0.00006 -0.00752 -0.00747 -0.02210

D165 -3.09956 -0.00041 0.00051 -0.01834 -0.01783 -3.11739

D166 0.05413 -0.00049 0.00046 -0.01302 -0.01256 0.04157

D167 -0.00001 0.00000 0.00000 0.00008 0.00008 0.00007

D168 -3.12905 -0.00011 0.00007 0.00326 0.00335 -3.12570

D169 3.12905 0.00011 -0.00007 -0.00316 -0.00325 3.12579

D170 0.00000 0.00000 0.00000 0.00002 0.00002 0.00002

D171 0.01545 -0.00008 0.00007 0.00549 0.00558 0.02103

D172 -3.11413 -0.00015 0.00001 0.01085 0.01089 -3.10324

D173 -3.13898 0.00004 -0.00001 0.00227 0.00227 -3.13671

D174 0.01462 -0.00003 -0.00006 0.00763 0.00759 0.02221

D175 3.09954 0.00042 -0.00051 0.01844 0.01794 3.11747

D176 -0.05415 0.00049 -0.00046 0.01304 0.01258 -0.04157

D177 0.00512 -0.00011 0.00002 -0.00601 -0.00598 -0.00086

D178 3.13943 0.00002 -0.00002 -0.00725 -0.00727 3.13216

D179 -3.12728 -0.00027 0.00012 -0.00117 -0.00103 -3.12831

D180 0.00703 -0.00015 0.00009 -0.00241 -0.00231 0.00471

D181 3.09362 -0.00011 -0.00009 0.00374 0.00365 3.09727

D182 -0.05728 0.00006 -0.00020 -0.00114 -0.00134 -0.05863

D183 0.00000 0.00000 0.00000 -0.00008 -0.00008 -0.00008

D184 3.13447 0.00012 -0.00004 -0.00125 -0.00130 3.13318

D185 -3.13447 -0.00012 0.00004 0.00114 0.00119 -3.13329

D186 0.00000 0.00000 0.00000 -0.00003 -0.00003 -0.00003

D187 -0.00512 0.00011 -0.00002 0.00605 0.00602 0.00090

D188 3.12729 0.00027 -0.00012 0.00112 0.00097 3.12826

D189 -3.13943 -0.00002 0.00002 0.00724 0.00725 -3.13218

D190 -0.00702 0.00015 -0.00009 0.00230 0.00220 -0.00482

D191 -3.09361 0.00010 0.00009 -0.00393 -0.00384 -3.09745

D192 0.05729 -0.00006 0.00020 0.00105 0.00125 0.05855

D193 -0.01543 0.00008 -0.00007 -0.00545 -0.00553 -0.02096

D194 3.13899 -0.00004 0.00001 -0.00224 -0.00224 3.13675

D195 3.11414 0.00015 -0.00002 -0.01080 -0.01083 3.10331

D196 -0.01461 0.00003 0.00006 -0.00760 -0.00755 -0.02216

D197 -3.09956 -0.00042 0.00051 -0.01849 -0.01799 -3.11754

D198 0.05414 -0.00049 0.00046 -0.01310 -0.01264 0.04150

D199 0.00001 0.00000 0.00000 -0.00008 -0.00008 -0.00008

D200 -3.12905 -0.00011 0.00007 0.00314 0.00323 -3.12582

D201 3.12906 0.00011 -0.00007 -0.00324 -0.00333 3.12573

D202 0.00000 0.00000 0.00000 -0.00002 -0.00002 -0.00002

D203 0.01543 -0.00008 0.00007 0.00548 0.00556 0.02099

D204 -3.11414 -0.00015 0.00002 0.01074 0.01078 -3.10336

D205 -3.13899 0.00004 -0.00001 0.00221 0.00221 -3.13678

D206 0.01462 -0.00004 -0.00006 0.00748 0.00743 0.02205

D207 3.09958 0.00042 -0.00051 0.01839 0.01788 3.11746

D208 -0.05412 0.00049 -0.00046 0.01309 0.01262 -0.04150

D209 1.09633 0.00002 0.00002 0.00251 0.00253 1.09886

D210 -1.04690 0.00001 0.00000 0.00215 0.00216 -1.04475

D211 -3.11794 0.00002 0.00006 0.00203 0.00209 -3.11585

D212 1.04690 -0.00001 0.00000 -0.00213 -0.00213 1.04477

D213 -1.09634 -0.00002 -0.00002 -0.00247 -0.00249 -1.09883

D214 3.11793 -0.00002 -0.00006 -0.00199 -0.00205 3.11588

D215 1.09779 0.00008 0.00011 0.00607 0.00618 1.10397

D216 -1.04610 -0.00006 0.00005 0.00127 0.00130 -1.04480

D217 -3.11574 0.00001 0.00007 0.00353 0.00359 -3.11215

D218 1.04609 0.00006 -0.00005 -0.00121 -0.00125 1.04485

D219 -1.09779 -0.00008 -0.00011 -0.00602 -0.00614 -1.10393

D220 3.11573 -0.00001 -0.00007 -0.00347 -0.00354 3.11220

D221 1.04690 -0.00001 0.00000 -0.00212 -0.00212 1.04478

D222 -1.09634 -0.00002 -0.00002 -0.00247 -0.00249 -1.09883

D223 3.11794 -0.00002 -0.00006 -0.00200 -0.00205 3.11588

D224 1.09634 0.00002 0.00002 0.00244 0.00245 1.09880

D225 -1.04690 0.00001 0.00000 0.00210 0.00210 -1.04480

D226 -3.11793 0.00001 0.00006 0.00196 0.00202 -3.11591

D227 1.09779 0.00008 0.00011 0.00599 0.00611 1.10390

D228 -1.04609 -0.00006 0.00005 0.00117 0.00121 -1.04488

D229 -3.11573 0.00001 0.00006 0.00343 0.00350 -3.11223

D230 1.04610 0.00006 -0.00005 -0.00122 -0.00126 1.04484

D231 -1.09779 -0.00008 -0.00011 -0.00603 -0.00615 -1.10394

D232 3.11574 -0.00001 -0.00007 -0.00349 -0.00355 3.11218

Item Value Threshold Converged?

Maximum Force 0.001504 0.000450 NO

RMS Force 0.000382 0.000300 NO

Maximum Displacement 0.922139 0.001800 NO

RMS Displacement 0.246456 0.001200 NO

Predicted change in Energy=-5.151850D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 01:34:29 2019, MaxMem= 1342177280 cpu: 15.2

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=3 Diff= 3.22D-05

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 -1.124312 2.772963 -0.038462

2 7 0 0.000542 2.025669 -0.245623

3 6 0 1.125304 2.772381 -0.038782

4 6 0 0.713130 4.089242 0.408480

5 6 0 -0.711414 4.089595 0.408889

6 7 0 2.408550 2.372448 -0.189449

7 6 0 2.795699 1.130062 -0.325369

8 7 0 2.016881 0.000630 -0.270758

9 6 0 2.796237 -1.129027 -0.325563

10 6 0 4.197088 -0.705184 -0.517296

11 6 0 4.196745 0.706788 -0.516982

12 7 0 -2.408840 2.373094 -0.189274

13 6 0 -4.198500 0.706991 -0.517374

14 6 0 -4.198857 -0.705297 -0.517680

15 6 0 -2.797941 -1.129020 -0.325589

16 7 0 -2.019390 0.000654 -0.270612

17 6 0 -2.797384 1.130121 -0.325396

18 7 0 -2.409340 -2.373455 -0.189285

19 7 0 0.000524 -2.028054 -0.245355

20 6 0 -1.124377 -2.774531 -0.038145

21 6 0 -0.711596 -4.091183 0.409475

22 6 0 0.713225 -4.090846 0.409070

23 6 0 1.125316 -2.773978 -0.038465

24 7 0 2.409005 -2.372866 -0.189463

25 30 0 -0.001422 -0.001447 -0.535981

26 6 0 -5.387048 1.432430 -0.658574

27 6 0 -6.575439 0.697536 -0.801155

28 6 0 -6.575740 -0.694667 -0.801593

29 6 0 -5.387670 -1.430156 -0.659377

30 6 0 1.435708 -5.225958 0.822669

31 6 0 0.702366 -6.353851 1.206492

32 6 0 -0.699298 -6.354113 1.207016

33 6 0 -1.433351 -5.226515 0.823653

34 6 0 5.385336 1.432241 -0.657703

35 6 0 6.573808 0.697435 -0.799928

36 6 0 6.574096 -0.694694 -0.800381

37 6 0 5.385931 -1.430077 -0.658532

38 6 0 -1.433176 5.225020 0.822811

39 6 0 -0.699188 6.352703 1.206008

40 6 0 0.702404 6.352425 1.205476

41 6 0 1.435651 5.224431 0.821811

42 1 0 7.519442 1.207649 -0.920820

43 1 0 7.519933 -1.204442 -0.921629

44 1 0 1.212455 7.250271 1.526478

45 1 0 -1.208644 7.250742 1.527414

46 1 0 -7.521041 1.207718 -0.922410

47 1 0 -7.521556 -1.204367 -0.923192

48 1 0 -1.208737 -7.252103 1.528586

49 1 0 1.212377 -7.251658 1.527666

50 8 0 2.786111 5.152156 0.841970

51 8 0 -2.783645 5.153263 0.844048

52 8 0 5.319958 2.781030 -0.664414

53 8 0 5.321043 -2.778891 -0.666164

54 8 0 2.786162 -5.153709 0.842913

55 8 0 -2.783813 -5.154755 0.844956

56 8 0 -5.322839 -2.778970 -0.667138

57 8 0 -5.321701 2.781218 -0.665445

58 6 0 3.518423 6.311663 1.231913

59 1 0 3.299105 6.593768 2.265985

60 1 0 3.313394 7.157785 0.569693

61 1 0 4.566897 6.031414 1.148344

62 6 0 6.535076 3.524146 -0.752446

63 1 0 7.056489 3.336958 -1.695684

64 1 0 7.202967 3.305277 0.086012

65 1 0 6.232877 4.568841 -0.709684

66 6 0 6.536396 -3.521535 -0.754942

67 1 0 7.204359 -3.303062 0.083562

68 1 0 7.057584 -3.333490 -1.698134

69 1 0 6.234555 -4.566363 -0.712895

70 6 0 -3.515215 6.313000 1.234701

71 1 0 -3.310414 7.159108 0.572393

72 1 0 -3.294938 6.594926 2.268618

73 1 0 -4.563863 6.033155 1.151974

74 6 0 -6.536787 3.524317 -0.754004

75 1 0 -7.204956 3.305589 0.084270

76 1 0 -7.057886 3.336979 -1.697387

77 1 0 -6.234599 4.569017 -0.711313

78 6 0 -6.538175 -3.521574 -0.756413

79 1 0 -7.059053 -3.333390 -1.699749

80 1 0 -7.206403 -3.303205 0.081907

81 1 0 -6.236368 -4.566412 -0.714413

82 6 0 -3.515367 -6.314437 1.235784

83 1 0 -3.295013 -6.596263 2.269712

84 1 0 -3.310625 -7.160615 0.573545

85 1 0 -4.564018 -6.034590 1.153110

86 6 0 3.518433 -6.313173 1.233042

87 1 0 3.313460 -7.159364 0.570891

88 1 0 3.299018 -6.595173 2.267123

89 1 0 4.566916 -6.032939 1.149539

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0454820 0.0432213 0.0230344

Leave Link 202 at Sat Jul 6 01:34:30 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8053.5996875372 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= 89 NActive= 89 NUniq= 89 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= -0.2275100022 Hartrees.

Nuclear repulsion after empirical dispersion term = 8053.3721775350 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6350

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.25D-10

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 347

GePol: Fraction of low-weight points (<1% of avg) = 5.46%

GePol: Cavity surface area = 704.294 Ang\*\*2

GePol: Cavity volume = 800.389 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0095658140 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8053.3626117210 Hartrees.

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(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44547 LenP2D= 111731.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.97D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 01:34:34 2019, MaxMem= 1342177280 cpu: 41.9

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 01:34:35 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000005 0.000001 0.000011 Ang= 0.00 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>= 2.0172 S= 1.0057

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2650.02652051094

Leave Link 401 at Sat Jul 6 01:34:52 2019, MaxMem= 1342177280 cpu: 203.6

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 120967500.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.88D-15 for 6341.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.31D-15 for 6343 4374.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.66D-15 for 6338.

Iteration 1 A^-1\*A deviation from orthogonality is 3.94D-13 for 4039 3999.

E= -2649.68654874514

DIIS: error= 7.69D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.68654874514 IErMin= 1 ErrMin= 7.69D-03

ErrMax= 7.69D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.32D-01 BMatP= 2.32D-01

IDIUse=3 WtCom= 9.23D-01 WtEn= 7.69D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.672 Goal= None Shift= 0.000

Gap= 0.735 Goal= None Shift= 0.000

GapD= 0.672 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=3.25D-04 MaxDP=1.08D-02 OVMax= 4.69D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.24D-04 CP: 9.98D-01

E= -2649.79167314804 Delta-E= -0.105124402895 Rises=F Damp=F

DIIS: error= 1.06D-03 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79167314804 IErMin= 2 ErrMin= 1.06D-03

ErrMax= 1.06D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.54D-03 BMatP= 2.32D-01

IDIUse=3 WtCom= 9.89D-01 WtEn= 1.06D-02

Coeff-Com: -0.634D-01 0.106D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.627D-01 0.106D+01

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=4.37D-05 MaxDP=1.78D-03 DE=-1.05D-01 OVMax= 6.71D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.78D-05 CP: 9.98D-01 1.07D+00

E= -2649.79284946628 Delta-E= -0.001176318245 Rises=F Damp=F

DIIS: error= 5.13D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79284946628 IErMin= 3 ErrMin= 5.13D-04

ErrMax= 5.13D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-03 BMatP= 2.54D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.13D-03

Coeff-Com: -0.307D-01 0.443D+00 0.587D+00

Coeff-En: 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.306D-01 0.441D+00 0.589D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=2.16D-05 MaxDP=1.53D-03 DE=-1.18D-03 OVMax= 4.75D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.92D-05 CP: 9.98D-01 1.08D+00 7.44D-01

E= -2649.79298013894 Delta-E= -0.000130672657 Rises=F Damp=F

DIIS: error= 3.78D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79298013894 IErMin= 4 ErrMin= 3.78D-04

ErrMax= 3.78D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.22D-04 BMatP= 1.02D-03

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.78D-03

Coeff-Com: -0.686D-02 0.748D-01 0.388D+00 0.544D+00

Coeff-En: 0.000D+00 0.000D+00 0.312D+00 0.688D+00

Coeff: -0.683D-02 0.746D-01 0.387D+00 0.545D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=9.26D-06 MaxDP=7.77D-04 DE=-1.31D-04 OVMax= 2.28D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.74D-06 CP: 9.98D-01 1.08D+00 8.50D-01 6.42D-01

E= -2649.79306695367 Delta-E= -0.000086814733 Rises=F Damp=F

DIIS: error= 7.85D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79306695367 IErMin= 5 ErrMin= 7.85D-05

ErrMax= 7.85D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.31D-05 BMatP= 4.22D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.706D-03-0.246D-02 0.121D+00 0.233D+00 0.649D+00

Coeff: -0.706D-03-0.246D-02 0.121D+00 0.233D+00 0.649D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=2.37D-06 MaxDP=1.53D-04 DE=-8.68D-05 OVMax= 5.35D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.85D-06 CP: 9.97D-01 1.08D+00 8.64D-01 6.77D-01 7.50D-01

E= -2649.79306886257 Delta-E= -0.000001908902 Rises=F Damp=F

DIIS: error= 4.85D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79306886257 IErMin= 6 ErrMin= 4.85D-05

ErrMax= 4.85D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.80D-06 BMatP= 1.31D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.492D-03-0.125D-01 0.231D-01 0.730D-01 0.418D+00 0.498D+00

Coeff: 0.492D-03-0.125D-01 0.231D-01 0.730D-01 0.418D+00 0.498D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=1.09D-06 MaxDP=7.35D-05 DE=-1.91D-06 OVMax= 2.00D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 4.75D-07 CP: 9.98D-01 1.08D+00 8.67D-01 6.82D-01 8.00D-01

CP: 4.99D-01

E= -2649.79306985659 Delta-E= -0.000000994014 Rises=F Damp=F

DIIS: error= 9.92D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79306985659 IErMin= 7 ErrMin= 9.92D-06

ErrMax= 9.92D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.80D-07 BMatP= 4.80D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.282D-03-0.600D-02 0.378D-02 0.213D-01 0.164D+00 0.248D+00

Coeff-Com: 0.569D+00

Coeff: 0.282D-03-0.600D-02 0.378D-02 0.213D-01 0.164D+00 0.248D+00

Coeff: 0.569D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=2.53D-07 MaxDP=1.58D-05 DE=-9.94D-07 OVMax= 8.06D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.00D-07 CP: 9.98D-01 1.08D+00 8.68D-01 6.82D-01 8.06D-01

CP: 5.52D-01 7.76D-01

E= -2649.79306989258 Delta-E= -0.000000035992 Rises=F Damp=F

DIIS: error= 2.87D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.79306989258 IErMin= 8 ErrMin= 2.87D-06

ErrMax= 2.87D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.59D-08 BMatP= 1.80D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.611D-04-0.857D-03-0.264D-02-0.265D-02 0.911D-02 0.422D-01

Coeff-Com: 0.326D+00 0.629D+00

Coeff: 0.611D-04-0.857D-03-0.264D-02-0.265D-02 0.911D-02 0.422D-01

Coeff: 0.326D+00 0.629D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=1.00D-07 MaxDP=7.06D-06 DE=-3.60D-08 OVMax= 2.94D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 7.96D-08 CP: 9.98D-01 1.08D+00 8.68D-01 6.83D-01 8.08D-01

CP: 5.51D-01 8.78D-01 8.60D-01

E= -2649.79306990064 Delta-E= -0.000000008062 Rises=F Damp=F

DIIS: error= 1.12D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.79306990064 IErMin= 9 ErrMin= 1.12D-06

ErrMax= 1.12D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.72D-09 BMatP= 3.59D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.825D-05 0.416D-03-0.178D-02-0.412D-02-0.178D-01-0.130D-01

Coeff-Com: 0.882D-01 0.298D+00 0.651D+00

Coeff: -0.825D-05 0.416D-03-0.178D-02-0.412D-02-0.178D-01-0.130D-01

Coeff: 0.882D-01 0.298D+00 0.651D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=4.65D-08 MaxDP=3.32D-06 DE=-8.06D-09 OVMax= 2.12D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 3.69D-08 CP: 9.98D-01 1.08D+00 8.68D-01 6.83D-01 8.08D-01

CP: 5.58D-01 9.13D-01 9.32D-01 8.66D-01

E= -2649.79306990146 Delta-E= -0.000000000824 Rises=F Damp=F

DIIS: error= 8.65D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -2649.79306990146 IErMin=10 ErrMin= 8.65D-07

ErrMax= 8.65D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.18D-09 BMatP= 3.72D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.162D-04 0.409D-03-0.579D-03-0.200D-02-0.123D-01-0.156D-01

Coeff-Com: -0.425D-02 0.610D-01 0.394D+00 0.579D+00

Coeff: -0.162D-04 0.409D-03-0.579D-03-0.200D-02-0.123D-01-0.156D-01

Coeff: -0.425D-02 0.610D-01 0.394D+00 0.579D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=2.24D-08 MaxDP=1.69D-06 DE=-8.24D-10 OVMax= 1.03D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.73D-08 CP: 9.98D-01 1.08D+00 8.68D-01 6.83D-01 8.08D-01

CP: 5.59D-01 9.25D-01 9.66D-01 9.87D-01 8.59D-01

E= -2649.79306990193 Delta-E= -0.000000000466 Rises=F Damp=F

DIIS: error= 3.34D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -2649.79306990193 IErMin=11 ErrMin= 3.34D-07

ErrMax= 3.34D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.45D-10 BMatP= 1.18D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.535D-05 0.860D-04 0.156D-03 0.362D-04-0.141D-02-0.418D-02

Coeff-Com: -0.224D-01-0.420D-01 0.341D-01 0.265D+00 0.770D+00

Coeff: -0.535D-05 0.860D-04 0.156D-03 0.362D-04-0.141D-02-0.418D-02

Coeff: -0.224D-01-0.420D-01 0.341D-01 0.265D+00 0.770D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=1.28D-08 MaxDP=6.49D-07 DE=-4.66D-10 OVMax= 7.63D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 7.51D-09 CP: 9.98D-01 1.08D+00 8.68D-01 6.83D-01 8.08D-01

CP: 5.59D-01 9.33D-01 9.85D-01 1.06D+00 1.04D+00

CP: 9.92D-01

E= -2649.79306990217 Delta-E= -0.000000000240 Rises=F Damp=F

DIIS: error= 1.31D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -2649.79306990217 IErMin=12 ErrMin= 1.31D-07

ErrMax= 1.31D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.70D-11 BMatP= 1.45D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.508D-06-0.400D-04 0.217D-03 0.450D-03 0.179D-02 0.921D-03

Coeff-Com: -0.116D-01-0.378D-01-0.616D-01 0.314D-01 0.443D+00 0.634D+00

Coeff: 0.508D-06-0.400D-04 0.217D-03 0.450D-03 0.179D-02 0.921D-03

Coeff: -0.116D-01-0.378D-01-0.616D-01 0.314D-01 0.443D+00 0.634D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=5.80D-09 MaxDP=2.87D-07 DE=-2.40D-10 OVMax= 3.98D-06

Error on total polarization charges = 0.07318

SCF Done: E(UB3LYP) = -2649.79306990 A.U. after 12 cycles

NFock= 12 Conv=0.58D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0169 S= 1.0056

<L.S>= 0.000000000000E+00

KE= 2.690229919230D+03 PE=-2.238553588542D+04 EE= 8.992150284564D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.00

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0169, after 2.0002

Leave Link 502 at Sat Jul 6 01:44:39 2019, MaxMem= 1342177280 cpu: 6945.6

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44547 LenP2D= 111731.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 273

Leave Link 701 at Sat Jul 6 01:44:59 2019, MaxMem= 1342177280 cpu: 218.8

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 01:44:59 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 01:46:31 2019, MaxMem= 1342177280 cpu: 1104.7

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.48544939D-03 5.35043008D-03 2.92270357D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.002351716 0.000682369 0.005632385

2 7 -0.000357043 -0.000993838 -0.008232025

3 6 -0.003037272 0.001238486 0.005762716

4 6 0.001253227 0.000239725 -0.001552030

5 6 -0.001316271 0.000119523 -0.001608005

6 7 0.000208590 0.003295088 -0.000524681

7 6 0.000369016 -0.003584978 -0.002033207

8 7 -0.000159817 -0.000483436 0.002712516

9 6 -0.000395333 0.002568130 -0.001876640

10 6 0.001734532 0.002193678 0.000894549

11 6 0.001852210 -0.002257175 0.000866717

12 7 0.000217950 0.002800949 -0.000525014

13 6 -0.001812410 -0.002298660 0.000885375

14 6 -0.001694786 0.002235639 0.000912954

15 6 0.000716500 0.001570350 -0.001777798

16 7 0.000676205 -0.000483596 0.002754798

17 6 -0.000043777 -0.002576925 -0.001934735

18 7 0.000229093 -0.001769463 -0.000576606

19 7 -0.000358213 0.001505912 -0.008349323

20 6 0.001665812 -0.000478173 0.005588484

21 6 -0.001279618 -0.000099030 -0.001618654

22 6 0.001216865 -0.000219476 -0.001563067

23 6 -0.002345515 -0.001031141 0.005718913

24 7 0.000195149 -0.002256042 -0.000576225

25 30 0.000099840 0.000109084 0.002741689

26 6 0.001066536 0.000864690 -0.000456473

27 6 -0.000173938 -0.000458413 0.000032501

28 6 -0.000170705 0.000446922 0.000034911

29 6 0.001031851 -0.000889763 -0.000463848

30 6 0.000513373 -0.000191270 0.000339491

31 6 0.000075877 0.000272883 0.000012132

32 6 -0.000082919 0.000289404 0.000004686

33 6 -0.000520876 -0.000238995 0.000356858

34 6 -0.001056475 0.000903691 -0.000454916

35 6 0.000169951 -0.000396236 0.000034689

36 6 0.000166672 0.000384551 0.000037095

37 6 -0.001021768 -0.000928903 -0.000462462

38 6 -0.000568577 0.000236546 0.000357595

39 6 -0.000128077 -0.000289041 0.000003108

40 6 0.000121016 -0.000272668 0.000010587

41 6 0.000560767 0.000188833 0.000340210

42 1 0.000376900 0.000248087 0.000007632

43 1 0.000376556 -0.000249214 0.000007423

44 1 -0.000084192 0.000445360 0.000124066

45 1 0.000082807 0.000445024 0.000123861

46 1 -0.000379456 0.000246071 0.000008210

47 1 -0.000378905 -0.000247090 0.000007990

48 1 0.000085154 -0.000447081 0.000124539

49 1 -0.000086321 -0.000447479 0.000124730

50 8 -0.002062156 0.000708995 -0.000967535

51 8 0.002062932 0.000691379 -0.000983308

52 8 0.000783741 -0.000731663 0.000140591

53 8 0.000777434 0.000742790 0.000147496

54 8 -0.002062854 -0.000686100 -0.000982185

55 8 0.002063507 -0.000668026 -0.000997089

56 8 -0.000747211 0.000760439 0.000160565

57 8 -0.000753271 -0.000750189 0.000154364

58 6 0.000552212 -0.000494138 0.000072143

59 1 -0.000100986 0.000019711 0.000021449

60 1 0.000000044 0.000044491 -0.000070417

61 1 0.000087691 0.000527248 0.000207826

62 6 -0.000394769 0.000441754 0.000141769

63 1 -0.000173490 -0.000231015 -0.000058570

64 1 -0.000337057 -0.000310647 0.000107418

65 1 0.000577021 0.000164169 -0.000086440

66 6 -0.000385844 -0.000440305 0.000140712

67 1 -0.000338803 0.000312156 0.000107610

68 1 -0.000175260 0.000231593 -0.000058150

69 1 0.000576049 -0.000166462 -0.000086839

70 6 -0.000552130 -0.000488503 0.000071883

71 1 0.000000167 0.000044124 -0.000070328

72 1 0.000100141 0.000020337 0.000021379

73 1 -0.000087109 0.000525309 0.000211137

74 6 0.000377283 0.000447122 0.000140567

75 1 0.000340196 -0.000311942 0.000107102

76 1 0.000176399 -0.000231303 -0.000057755

77 1 -0.000577590 0.000166332 -0.000088464

78 6 0.000368413 -0.000445405 0.000139325

79 1 0.000178119 0.000231747 -0.000057326

80 1 0.000341788 0.000313190 0.000107277

81 1 -0.000576422 -0.000168566 -0.000088918

82 6 -0.000555174 0.000478381 0.000075380

83 1 0.000099179 -0.000019113 0.000020546

84 1 0.000000497 -0.000042566 -0.000070144

85 1 -0.000087684 -0.000524492 0.000213241

86 6 0.000555433 0.000484001 0.000075640

87 1 -0.000000499 -0.000042787 -0.000070247

88 1 -0.000100091 -0.000018451 0.000020545

89 1 0.000088250 -0.000526501 0.000210049

-------------------------------------------------------------------

Cartesian Forces: Max 0.008349323 RMS 0.001358542

Leave Link 716 at Sat Jul 6 01:46:31 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.004658725 RMS 0.000730473

Search for a local minimum.

Step number 14 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .73047D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 6 7 9 11 13

14

DE= 2.00D-03 DEPred=-5.15D-04 R=-3.88D+00

Trust test=-3.88D+00 RLast= 4.43D-01 DXMaxT set to 1.14D-01

ITU= -1 0 -1 0 0 0 0 0 0 1 1 1 1 0

Eigenvalues --- 0.00087 0.01092 0.01300 0.01315 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01316 0.01316

Eigenvalues --- 0.01470 0.01571 0.01572 0.01577 0.01587

Eigenvalues --- 0.01604 0.01621 0.01622 0.01708 0.01711

Eigenvalues --- 0.01713 0.01717 0.01792 0.01844 0.01877

Eigenvalues --- 0.01902 0.01936 0.01938 0.01956 0.01966

Eigenvalues --- 0.01994 0.02005 0.02021 0.02022 0.02048

Eigenvalues --- 0.02051 0.02053 0.02053 0.02053 0.02057

Eigenvalues --- 0.02057 0.02057 0.02057 0.02059 0.02062

Eigenvalues --- 0.02067 0.02067 0.02069 0.02070 0.02071

Eigenvalues --- 0.02071 0.02071 0.02072 0.02084 0.02085

Eigenvalues --- 0.02134 0.02175 0.02242 0.02260 0.02260

Eigenvalues --- 0.02260 0.02260 0.02260 0.02260 0.02352

Eigenvalues --- 0.02364 0.02382 0.02551 0.02682 0.03304

Eigenvalues --- 0.09650 0.09947 0.09947 0.09947 0.09987

Eigenvalues --- 0.09987 0.09987 0.10024 0.10488 0.10669

Eigenvalues --- 0.10669 0.10669 0.10675 0.10681 0.10681

Eigenvalues --- 0.10681 0.10737 0.13390 0.13440 0.14633

Eigenvalues --- 0.15967 0.15983 0.15994 0.15998 0.15998

Eigenvalues --- 0.15998 0.15999 0.15999 0.15999 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16009

Eigenvalues --- 0.16220 0.16376 0.18399 0.21239 0.21717

Eigenvalues --- 0.22472 0.22473 0.22473 0.22474 0.24053

Eigenvalues --- 0.24109 0.24176 0.24348 0.24500 0.24505

Eigenvalues --- 0.24511 0.24656 0.24715 0.24759 0.24816

Eigenvalues --- 0.24865 0.24873 0.24936 0.24963 0.24964

Eigenvalues --- 0.24970 0.24972 0.24984 0.24985 0.24991

Eigenvalues --- 0.24991 0.24996 0.24997 0.24997 0.24997

Eigenvalues --- 0.24998 0.24998 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25420 0.28289

Eigenvalues --- 0.33534 0.33609 0.33639 0.33642 0.33704

Eigenvalues --- 0.33851 0.33982 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34063 0.34063 0.34074 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34081

Eigenvalues --- 0.34086 0.34134 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34686 0.34686 0.34701

Eigenvalues --- 0.34856 0.34927 0.35165 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35632 0.35634

Eigenvalues --- 0.35843 0.37004 0.37100 0.37127 0.40451

Eigenvalues --- 0.41177 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41215 0.41215 0.41404 0.41408 0.41414

Eigenvalues --- 0.41417 0.41471 0.41932 0.42103 0.42454

Eigenvalues --- 0.42765 0.42994 0.44506 0.44553 0.44730

Eigenvalues --- 0.44791 0.44843 0.44998 0.44999 0.44999

Eigenvalues --- 0.45000 0.45361 0.45364 0.45412 0.45946

Eigenvalues --- 0.46280 0.47231 0.48356 0.49158 0.49261

Eigenvalues --- 0.49817 0.52498 0.53553 0.53554 0.53554

Eigenvalues --- 0.53554 0.53554 0.53554 0.53630 0.54851

Eigenvalues --- 0.55786 0.56029 0.57320 0.57447 0.57543

Eigenvalues --- 0.61209

En-DIIS/RFO-DIIS IScMMF= 0 using points: 14 13

RFO step: Lambda=-9.35015583D-04.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=T DC= -2.00D-03 SmlDif= 1.00D-05

RMS Error= 0.3488976133D-02 NUsed= 2 EDIIS=F

DidBck=T Rises=T RFO-DIIS coefs: 0.17943 0.82057

Iteration 1 RMS(Cart)= 0.45984270 RMS(Int)= 0.02222948

Iteration 2 RMS(Cart)= 0.11797290 RMS(Int)= 0.00622449

Iteration 3 RMS(Cart)= 0.00369233 RMS(Int)= 0.00617433

Iteration 4 RMS(Cart)= 0.00007142 RMS(Int)= 0.00617431

Iteration 5 RMS(Cart)= 0.00000242 RMS(Int)= 0.00617431

Iteration 6 RMS(Cart)= 0.00000008 RMS(Int)= 0.00617431

ITry= 1 IFail=0 DXMaxC= 2.05D+00 DCOld= 1.00D+10 DXMaxT= 1.14D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58185 0.00087 0.00106 0.01120 0.01680 2.59866

R2 2.74116 0.00038 0.00265 0.00530 0.00579 2.74695

R3 2.55823 0.00112 0.00163 -0.00497 -0.01602 2.54221

R4 2.58102 0.00106 0.00162 0.01176 0.01440 2.59542

R5 3.86979 0.00171 0.00120 0.08037 0.10594 3.97573

R6 2.74112 0.00047 0.00256 0.00645 0.00680 2.74792

R7 2.55593 0.00213 0.00300 -0.00183 -0.01840 2.53753

R8 2.69200 0.00029 0.00088 -0.00451 -0.01155 2.68044

R9 2.66011 0.00078 0.00358 0.00704 0.01056 2.67067

R10 2.66006 0.00080 0.00361 0.00704 0.01058 2.67064

R11 2.47250 0.00466 0.00611 0.00906 -0.00325 2.46924

R12 2.59461 0.00060 0.00170 0.00485 0.01197 2.60658

R13 2.78938 0.00174 0.00288 -0.00117 -0.00088 2.78850

R14 2.59555 0.00029 0.00111 0.00354 0.01345 2.60900

R15 3.84683 0.00061 -0.00246 0.09101 0.11616 3.96299

R16 2.78937 0.00168 0.00304 -0.00276 -0.00229 2.78708

R17 2.47519 0.00316 0.00465 0.00481 -0.00216 2.47303

R18 2.66824 -0.00120 -0.00231 -0.00086 -0.01165 2.65659

R19 2.64478 0.00029 0.00237 0.00428 0.00701 2.65179

R20 2.64483 0.00025 0.00234 0.00443 0.00712 2.65195

R21 2.47437 0.00358 0.00512 0.00584 -0.00295 2.47142

R22 2.66884 -0.00134 -0.00262 -0.00225 -0.01023 2.65861

R23 2.78952 0.00166 0.00286 -0.00237 -0.00116 2.78836

R24 2.64484 0.00022 0.00238 0.00396 0.00657 2.65141

R25 2.78951 0.00160 0.00302 -0.00397 -0.00257 2.78694

R26 2.64479 0.00025 0.00241 0.00381 0.00646 2.65125

R27 2.59473 0.00042 0.00170 0.00410 0.01036 2.60509

R28 2.47706 0.00209 0.00367 0.00152 -0.00188 2.47518

R29 2.59380 0.00073 0.00229 0.00542 0.00886 2.60265

R30 3.84624 0.00028 -0.00253 0.08807 0.10150 3.94774

R31 2.55975 0.00040 0.00073 -0.00755 -0.01498 2.54477

R32 2.58110 0.00098 0.00163 0.01168 0.01421 2.59531

R33 2.58026 0.00117 0.00218 0.01225 0.01178 2.59205

R34 3.86891 0.00137 0.00120 0.07641 0.09050 3.95941

R35 2.74129 0.00034 0.00261 0.00456 0.00594 2.74723

R36 2.69252 0.00019 0.00059 -0.00563 -0.00984 2.68268

R37 2.66006 0.00078 0.00363 0.00686 0.01033 2.67038

R38 2.74124 0.00042 0.00251 0.00573 0.00697 2.74821

R39 2.66010 0.00076 0.00361 0.00686 0.01030 2.67040

R40 2.55746 0.00141 0.00210 -0.00436 -0.01735 2.54010

R41 2.65415 0.00030 -0.00081 -0.00768 -0.00873 2.64543

R42 2.55186 -0.00070 -0.00275 -0.00314 -0.00589 2.54597

R43 2.63088 -0.00054 -0.00319 -0.00104 -0.00469 2.62619

R44 2.04331 0.00045 0.00044 0.00006 0.00050 2.04381

R45 2.65416 0.00028 -0.00079 -0.00788 -0.00891 2.64525

R46 2.04331 0.00045 0.00045 0.00002 0.00047 2.04377

R47 2.55187 -0.00071 -0.00277 -0.00295 -0.00572 2.54615

R48 2.64376 -0.00025 -0.00134 -0.00979 -0.01096 2.63280

R49 2.55593 -0.00157 -0.00310 -0.00598 -0.00909 2.54684

R50 2.64876 -0.00083 -0.00310 -0.00574 -0.00851 2.64025

R51 2.04346 0.00037 0.00032 0.00156 0.00188 2.04534

R52 2.64378 -0.00027 -0.00134 -0.00993 -0.01109 2.63269

R53 2.04346 0.00037 0.00032 0.00155 0.00187 2.04533

R54 2.55592 -0.00157 -0.00312 -0.00582 -0.00894 2.54698

R55 2.65413 0.00030 -0.00078 -0.00779 -0.00893 2.64520

R56 2.55187 -0.00069 -0.00275 -0.00323 -0.00597 2.54589

R57 2.63074 -0.00045 -0.00311 -0.00091 -0.00471 2.62603

R58 2.04331 0.00045 0.00044 0.00009 0.00053 2.04384

R59 2.65414 0.00029 -0.00076 -0.00799 -0.00911 2.64502

R60 2.04331 0.00045 0.00044 0.00005 0.00049 2.04380

R61 2.55188 -0.00070 -0.00276 -0.00304 -0.00581 2.54607

R62 2.64376 -0.00027 -0.00131 -0.00994 -0.01118 2.63258

R63 2.55593 -0.00158 -0.00311 -0.00595 -0.00906 2.54687

R64 2.64862 -0.00077 -0.00303 -0.00563 -0.00852 2.64010

R65 2.04346 0.00037 0.00032 0.00155 0.00188 2.04534

R66 2.64374 -0.00024 -0.00132 -0.00980 -0.01106 2.63268

R67 2.04346 0.00037 0.00032 0.00156 0.00189 2.04535

R68 2.55594 -0.00157 -0.00310 -0.00611 -0.00921 2.54672

R69 2.69430 0.00042 0.00040 -0.00535 -0.00495 2.68935

R70 2.69430 0.00042 0.00040 -0.00531 -0.00491 2.68939

R71 2.69674 -0.00025 -0.00025 -0.00124 -0.00150 2.69524

R72 2.69674 -0.00025 -0.00026 -0.00119 -0.00145 2.69529

R73 2.69429 0.00043 0.00041 -0.00528 -0.00487 2.68941

R74 2.69429 0.00043 0.00040 -0.00524 -0.00483 2.68945

R75 2.69673 -0.00024 -0.00026 -0.00109 -0.00135 2.69539

R76 2.69673 -0.00024 -0.00026 -0.00114 -0.00139 2.69534

R77 2.06749 0.00005 -0.00032 0.00076 0.00044 2.06793

R78 2.06707 0.00008 -0.00033 -0.00134 -0.00167 2.06540

R79 2.05696 -0.00007 -0.00017 -0.00010 -0.00027 2.05668

R80 2.06716 0.00001 -0.00017 -0.00014 -0.00031 2.06686

R81 2.06750 -0.00006 -0.00033 -0.00048 -0.00081 2.06668

R82 2.05671 -0.00001 -0.00015 -0.00019 -0.00034 2.05637

R83 2.06750 -0.00006 -0.00033 -0.00050 -0.00083 2.06667

R84 2.06716 0.00001 -0.00017 -0.00015 -0.00032 2.06684

R85 2.05671 0.00000 -0.00015 -0.00019 -0.00033 2.05638

R86 2.06706 0.00008 -0.00033 -0.00135 -0.00168 2.06539

R87 2.06749 0.00005 -0.00032 0.00074 0.00043 2.06792

R88 2.05696 -0.00007 -0.00017 -0.00009 -0.00026 2.05669

R89 2.06750 -0.00006 -0.00033 -0.00050 -0.00083 2.06666

R90 2.06716 0.00001 -0.00017 -0.00017 -0.00034 2.06682

R91 2.05671 0.00000 -0.00015 -0.00019 -0.00034 2.05637

R92 2.06717 0.00000 -0.00017 -0.00019 -0.00036 2.06681

R93 2.06750 -0.00006 -0.00033 -0.00052 -0.00084 2.06665

R94 2.05671 0.00000 -0.00015 -0.00019 -0.00033 2.05638

R95 2.06749 0.00004 -0.00032 0.00072 0.00040 2.06789

R96 2.06707 0.00008 -0.00033 -0.00136 -0.00169 2.06538

R97 2.05696 -0.00007 -0.00017 -0.00009 -0.00026 2.05670

R98 2.06707 0.00008 -0.00033 -0.00135 -0.00168 2.06539

R99 2.06749 0.00004 -0.00032 0.00073 0.00042 2.06791

R100 2.05696 -0.00007 -0.00017 -0.00010 -0.00027 2.05669

A1 1.88480 0.00148 0.00290 0.01209 0.01928 1.90408

A2 2.21775 -0.00116 -0.00143 0.00277 0.00004 2.21779

A3 2.18041 -0.00030 -0.00129 -0.01256 -0.02516 2.15525

A4 1.93479 -0.00204 -0.00269 -0.01442 -0.03748 1.89731

A5 2.16778 0.00097 0.00002 0.01887 0.01886 2.18664

A6 2.16936 0.00092 -0.00080 0.01781 0.02967 2.19903

A7 1.88497 0.00143 0.00285 0.01133 0.01938 1.90434

A8 2.21779 -0.00134 -0.00139 0.00177 -0.00270 2.21509

A9 2.18021 -0.00007 -0.00128 -0.01080 -0.02244 2.15777

A10 1.85925 -0.00040 -0.00083 -0.00011 -0.00421 1.85504

A11 2.31421 0.00095 0.00303 0.00635 0.01155 2.32576

A12 2.10946 -0.00055 -0.00204 -0.00589 -0.00708 2.10238

A13 1.85911 -0.00034 -0.00073 -0.00029 -0.00426 1.85485

A14 2.31430 0.00090 0.00301 0.00603 0.01118 2.32548

A15 2.10951 -0.00056 -0.00211 -0.00538 -0.00666 2.10285

A16 2.18106 0.00017 0.00533 0.00027 -0.00624 2.17482

A17 2.22575 -0.00016 0.00385 -0.02241 -0.02025 2.20550

A18 2.17321 0.00000 -0.00518 -0.00057 -0.02189 2.15132

A19 1.88355 0.00015 0.00161 0.01742 0.02692 1.91047

A20 1.93169 -0.00041 -0.00156 -0.02205 -0.04164 1.89005

A21 2.16284 0.00004 0.00042 0.00042 0.01430 2.17713

A22 2.16102 0.00023 0.00134 0.00111 0.00326 2.16428

A23 1.88339 0.00022 0.00165 0.01844 0.02710 1.91048

A24 2.22577 0.00002 0.00376 -0.02099 -0.01725 2.20852

A25 2.17335 -0.00025 -0.00512 -0.00305 -0.02521 2.14815

A26 1.86177 0.00010 0.00016 -0.00443 -0.00541 1.85636

A27 2.30573 -0.00014 0.00125 0.00806 0.00755 2.31328

A28 2.11551 0.00005 -0.00127 -0.00511 -0.00568 2.10983

A29 1.86191 0.00003 0.00007 -0.00442 -0.00552 1.85639

A30 2.30567 -0.00009 0.00121 0.00906 0.00856 2.31423

A31 2.11543 0.00006 -0.00115 -0.00611 -0.00654 2.10890

A32 2.18162 0.00010 0.00516 -0.00252 -0.00455 2.17707

A33 1.86180 0.00007 0.00018 -0.00448 -0.00550 1.85630

A34 2.11541 0.00006 -0.00116 -0.00589 -0.00659 2.10882

A35 2.30580 -0.00013 0.00111 0.00892 0.00865 2.31445

A36 1.86166 0.00014 0.00026 -0.00449 -0.00539 1.85627

A37 2.11549 0.00004 -0.00128 -0.00488 -0.00573 2.10976

A38 2.30586 -0.00018 0.00114 0.00792 0.00764 2.31350

A39 1.88301 0.00024 0.00179 0.01964 0.02501 1.90802

A40 2.17414 -0.00042 -0.00537 -0.00582 -0.02245 2.15169

A41 2.22536 0.00018 0.00386 -0.01940 -0.01795 2.20741

A42 1.93267 -0.00053 -0.00206 -0.02434 -0.03748 1.89518

A43 2.16049 0.00029 0.00161 0.00193 0.00088 2.16137

A44 2.16231 0.00010 0.00070 0.00122 0.01201 2.17432

A45 2.17400 -0.00017 -0.00543 -0.00331 -0.01912 2.15488

A46 2.22535 0.00000 0.00396 -0.02084 -0.02096 2.20438

A47 1.88317 0.00017 0.00176 0.01861 0.02483 1.90800

A48 2.18210 0.00005 0.00506 -0.00512 -0.00288 2.17921

A49 1.93574 -0.00214 -0.00318 -0.01660 -0.03332 1.90242

A50 2.16729 0.00102 0.00025 0.01998 0.01673 2.18401

A51 2.16888 0.00097 -0.00056 0.01892 0.02763 2.19651

A52 2.21745 -0.00106 -0.00135 0.00384 -0.00092 2.21653

A53 2.18109 -0.00041 -0.00150 -0.01482 -0.02203 2.15906

A54 1.88442 0.00150 0.00303 0.01330 0.01708 1.90150

A55 1.85902 -0.00030 -0.00063 -0.00045 -0.00420 1.85482

A56 2.31440 0.00087 0.00290 0.00607 0.01129 2.32570

A57 2.10949 -0.00056 -0.00211 -0.00525 -0.00682 2.10267

A58 1.85916 -0.00037 -0.00073 -0.00026 -0.00415 1.85502

A59 2.10944 -0.00056 -0.00204 -0.00577 -0.00725 2.10219

A60 2.31431 0.00093 0.00293 0.00639 0.01167 2.32598

A61 1.88458 0.00145 0.00299 0.01253 0.01716 1.90175

A62 2.21749 -0.00124 -0.00132 0.00283 -0.00367 2.21382

A63 2.18089 -0.00018 -0.00149 -0.01304 -0.01929 2.16160

A64 2.18154 0.00012 0.00522 -0.00232 -0.00461 2.17693

A65 1.55036 0.00052 0.00804 -0.05573 -0.08814 1.46222

A66 1.55224 0.00014 0.00712 -0.05820 -0.08011 1.47213

A67 1.55237 0.00007 0.00710 -0.05802 -0.08000 1.47237

A68 1.55425 -0.00031 0.00618 -0.06052 -0.07183 1.48242

A69 2.04606 0.00009 0.00155 0.00844 0.00966 2.05572

A70 2.06818 0.00116 0.00430 0.00408 0.00739 2.07557

A71 2.16886 -0.00124 -0.00581 -0.01169 -0.01841 2.15045

A72 2.12169 -0.00014 -0.00037 -0.00281 -0.00375 2.11795

A73 2.09955 0.00003 0.00114 0.00310 0.00405 2.10360

A74 2.06191 0.00011 -0.00076 0.00004 -0.00089 2.06102

A75 2.12168 -0.00014 -0.00034 -0.00312 -0.00403 2.11765

A76 2.06192 0.00011 -0.00078 0.00023 -0.00073 2.06119

A77 2.09955 0.00003 0.00113 0.00322 0.00416 2.10371

A78 2.04604 0.00009 0.00158 0.00820 0.00948 2.05551

A79 2.06816 0.00116 0.00434 0.00366 0.00702 2.07519

A80 2.16890 -0.00124 -0.00588 -0.01105 -0.01782 2.15107

A81 2.05068 0.00066 0.00229 0.00816 0.00948 2.06016

A82 2.06438 0.00034 0.00245 0.02415 0.02660 2.09097

A83 2.16800 -0.00100 -0.00469 -0.03169 -0.03632 2.13168

A84 2.12285 -0.00010 -0.00016 -0.00166 -0.00252 2.12033

A85 2.09858 0.00035 0.00212 0.00080 0.00243 2.10101

A86 2.06165 -0.00025 -0.00193 0.00168 -0.00072 2.06092

A87 2.12285 -0.00010 -0.00015 -0.00176 -0.00261 2.12024

A88 2.06165 -0.00024 -0.00194 0.00177 -0.00065 2.06101

A89 2.09858 0.00035 0.00212 0.00081 0.00243 2.10101

A90 2.05067 0.00067 0.00231 0.00799 0.00934 2.06001

A91 2.06439 0.00031 0.00245 0.02409 0.02654 2.09093

A92 2.16800 -0.00098 -0.00471 -0.03147 -0.03612 2.13188

A93 2.04611 0.00006 0.00151 0.00847 0.00968 2.05579

A94 2.06815 0.00119 0.00427 0.00492 0.00817 2.07632

A95 2.16883 -0.00125 -0.00574 -0.01257 -0.01923 2.14960

A96 2.12162 -0.00011 -0.00033 -0.00262 -0.00383 2.11778

A97 2.09959 0.00001 0.00113 0.00292 0.00401 2.10359

A98 2.06195 0.00010 -0.00079 0.00004 -0.00077 2.06118

A99 2.12161 -0.00012 -0.00031 -0.00293 -0.00411 2.11749

A100 2.06196 0.00010 -0.00081 0.00023 -0.00061 2.06135

A101 2.09959 0.00002 0.00112 0.00304 0.00411 2.10370

A102 2.04609 0.00006 0.00154 0.00824 0.00950 2.05559

A103 2.06814 0.00119 0.00431 0.00450 0.00780 2.07594

A104 2.16887 -0.00125 -0.00581 -0.01192 -0.01865 2.15022

A105 2.05072 0.00065 0.00228 0.00797 0.00929 2.06000

A106 2.06438 0.00035 0.00245 0.02447 0.02692 2.09130

A107 2.16797 -0.00099 -0.00467 -0.03183 -0.03645 2.13152

A108 2.12279 -0.00009 -0.00011 -0.00161 -0.00273 2.12005

A109 2.09861 0.00034 0.00211 0.00068 0.00244 2.10105

A110 2.06168 -0.00025 -0.00196 0.00176 -0.00054 2.06114

A111 2.12279 -0.00009 -0.00012 -0.00151 -0.00265 2.12014

A112 2.06168 -0.00025 -0.00195 0.00166 -0.00061 2.06107

A113 2.09861 0.00034 0.00211 0.00067 0.00244 2.10105

A114 2.05073 0.00064 0.00226 0.00814 0.00941 2.06014

A115 2.06436 0.00037 0.00245 0.02454 0.02699 2.09135

A116 2.16797 -0.00101 -0.00465 -0.03206 -0.03666 2.13131

A117 2.06401 -0.00023 0.00142 -0.02271 -0.02129 2.04272

A118 2.06402 -0.00023 0.00142 -0.02276 -0.02135 2.04268

A119 2.07054 -0.00144 -0.00318 0.00054 -0.00264 2.06790

A120 2.07057 -0.00146 -0.00320 0.00070 -0.00251 2.06806

A121 2.06402 -0.00023 0.00142 -0.02271 -0.02129 2.04272

A122 2.06403 -0.00023 0.00142 -0.02278 -0.02137 2.04266

A123 2.07059 -0.00147 -0.00322 0.00088 -0.00235 2.06824

A124 2.07056 -0.00145 -0.00320 0.00073 -0.00247 2.06809

A125 1.94468 -0.00023 0.00062 -0.00889 -0.00827 1.93641

A126 1.94682 -0.00017 -0.00153 0.00596 0.00443 1.95125

A127 1.83834 0.00094 0.00350 -0.00034 0.00315 1.84149

A128 1.91259 -0.00007 0.00027 -0.00094 -0.00067 1.91192

A129 1.90926 -0.00021 -0.00172 0.00289 0.00117 1.91044

A130 1.91052 -0.00024 -0.00112 0.00152 0.00039 1.91091

A131 1.94975 -0.00049 -0.00207 -0.00034 -0.00241 1.94734

A132 1.94803 -0.00083 -0.00351 -0.00020 -0.00371 1.94433

A133 1.83484 0.00120 0.00569 -0.00352 0.00217 1.83701

A134 1.91304 0.00025 0.00005 0.00221 0.00226 1.91530

A135 1.90761 -0.00008 -0.00017 0.00254 0.00238 1.90999

A136 1.90860 -0.00001 0.00027 -0.00086 -0.00059 1.90801

A137 1.94804 -0.00083 -0.00352 -0.00010 -0.00362 1.94442

A138 1.94975 -0.00049 -0.00207 -0.00036 -0.00243 1.94732

A139 1.83484 0.00120 0.00569 -0.00355 0.00214 1.83698

A140 1.91304 0.00025 0.00004 0.00224 0.00229 1.91533

A141 1.90860 0.00000 0.00027 -0.00086 -0.00059 1.90801

A142 1.90760 -0.00008 -0.00016 0.00246 0.00230 1.90991

A143 1.94682 -0.00017 -0.00152 0.00589 0.00436 1.95118

A144 1.94468 -0.00023 0.00063 -0.00897 -0.00834 1.93634

A145 1.83835 0.00094 0.00348 -0.00020 0.00328 1.84163

A146 1.91259 -0.00007 0.00027 -0.00094 -0.00067 1.91192

A147 1.91052 -0.00024 -0.00112 0.00159 0.00045 1.91097

A148 1.90926 -0.00021 -0.00171 0.00283 0.00112 1.91038

A149 1.94803 -0.00083 -0.00351 -0.00021 -0.00371 1.94432

A150 1.94976 -0.00049 -0.00208 -0.00035 -0.00243 1.94733

A151 1.83484 0.00120 0.00569 -0.00351 0.00219 1.83703

A152 1.91305 0.00025 0.00004 0.00227 0.00232 1.91536

A153 1.90860 0.00000 0.00028 -0.00087 -0.00059 1.90800

A154 1.90761 -0.00008 -0.00016 0.00248 0.00232 1.90993

A155 1.94975 -0.00050 -0.00207 -0.00038 -0.00246 1.94730

A156 1.94804 -0.00083 -0.00352 -0.00012 -0.00364 1.94440

A157 1.83484 0.00120 0.00569 -0.00353 0.00217 1.83701

A158 1.91305 0.00025 0.00004 0.00230 0.00235 1.91539

A159 1.90760 -0.00008 -0.00015 0.00241 0.00225 1.90985

A160 1.90859 0.00000 0.00028 -0.00085 -0.00058 1.90801

A161 1.94468 -0.00023 0.00063 -0.00901 -0.00838 1.93630

A162 1.94681 -0.00017 -0.00152 0.00584 0.00432 1.95113

A163 1.83836 0.00094 0.00347 -0.00006 0.00341 1.84177

A164 1.91259 -0.00006 0.00027 -0.00095 -0.00067 1.91191

A165 1.90926 -0.00021 -0.00171 0.00278 0.00107 1.91033

A166 1.91052 -0.00024 -0.00112 0.00159 0.00046 1.91098

A167 1.94682 -0.00017 -0.00153 0.00593 0.00440 1.95122

A168 1.94468 -0.00023 0.00062 -0.00893 -0.00831 1.93638

A169 1.83834 0.00094 0.00349 -0.00022 0.00327 1.84161

A170 1.91259 -0.00006 0.00027 -0.00094 -0.00067 1.91192

A171 1.91052 -0.00024 -0.00112 0.00152 0.00039 1.91091

A172 1.90926 -0.00021 -0.00172 0.00284 0.00112 1.91039

A173 3.10649 -0.00017 0.01330 -0.11873 -0.15193 2.95455

A174 3.10662 -0.00024 0.01328 -0.11854 -0.15183 2.95479

A175 3.42415 -0.00196 -0.09735 0.46020 0.34075 3.76490

A176 2.88251 -0.00023 0.01702 -0.38166 -0.33979 2.54272

D1 -0.05768 0.00209 0.05435 0.13235 0.18358 0.12590

D2 2.92888 0.00115 0.03244 0.28566 0.31757 -3.03674

D3 3.10581 0.00080 0.03336 0.01916 0.04591 -3.13146

D4 -0.19081 -0.00015 0.01146 0.17247 0.17990 -0.01091

D5 0.03427 -0.00119 -0.03228 -0.07691 -0.10951 -0.07524

D6 -3.08181 -0.00126 -0.04257 -0.09402 -0.13729 3.06409

D7 -3.12864 0.00005 -0.01186 0.03348 0.02254 -3.10610

D8 0.03847 -0.00001 -0.02215 0.01637 -0.00524 0.03323

D9 0.23029 -0.00015 -0.02743 0.05658 0.02749 0.25778

D10 -2.88590 -0.00166 -0.05176 -0.07507 -0.12918 -3.01507

D11 0.05754 -0.00209 -0.05423 -0.13334 -0.18443 -0.12689

D12 -3.10609 -0.00080 -0.03316 -0.02074 -0.04762 3.12948

D13 -2.92885 -0.00115 -0.03240 -0.28692 -0.31840 3.03593

D14 0.19071 0.00014 -0.01133 -0.17433 -0.18159 0.00911

D15 -2.92456 0.00083 0.00413 0.10522 0.09130 -2.83326

D16 -0.04148 0.00046 0.02080 -0.27615 -0.24248 -0.28396

D17 0.04148 -0.00050 -0.02084 0.27610 0.24222 0.28370

D18 2.92456 -0.00086 -0.00418 -0.10527 -0.09155 2.83300

D19 -0.03390 0.00118 0.03198 0.07947 0.11188 0.07798

D20 3.08211 0.00125 0.04231 0.09634 0.13944 -3.06164

D21 3.12913 -0.00005 0.01148 -0.03029 -0.01976 3.10937

D22 -0.03804 0.00002 0.02181 -0.01342 0.00780 -0.03024

D23 -0.23010 0.00017 0.02730 -0.05524 -0.02620 -0.25630

D24 2.88594 0.00167 0.05173 0.07565 0.12969 3.01563

D25 -0.00023 0.00001 0.00019 -0.00150 -0.00133 -0.00156

D26 3.11948 0.00009 0.00906 0.01336 0.02247 -3.14124

D27 -3.11988 -0.00007 -0.00872 -0.01617 -0.02494 3.13836

D28 -0.00017 0.00000 0.00015 -0.00131 -0.00114 -0.00132

D29 -3.13372 0.00010 -0.00712 0.02812 0.02062 -3.11311

D30 -0.00832 0.00034 -0.00315 0.06829 0.06574 0.05742

D31 -0.02070 0.00018 0.00444 0.04706 0.05139 0.03069

D32 3.10471 0.00042 0.00841 0.08723 0.09651 -3.08197

D33 3.13400 -0.00011 0.00688 -0.02622 -0.01892 3.11508

D34 0.00868 -0.00035 0.00285 -0.06577 -0.06349 -0.05482

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D36 -3.10441 -0.00042 -0.00866 -0.08498 -0.09452 3.08426

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D38 3.11858 0.00041 -0.00375 0.23795 0.22959 -2.93502

D39 -3.03695 -0.00120 -0.05140 0.09090 0.03937 -2.99758

D40 0.34734 -0.00065 -0.05244 0.17948 0.12674 0.47407

D41 0.06625 -0.00132 -0.04187 -0.06689 -0.10917 -0.04293

D42 -2.83265 -0.00077 -0.04291 0.02170 -0.02180 -2.85445

D43 3.06546 0.00065 0.03406 -0.11242 -0.07647 2.98899

D44 -0.05549 0.00043 0.02246 -0.02636 -0.00257 -0.05806

D45 -0.03918 0.00077 0.02473 0.04006 0.06652 0.02734

D46 3.12305 0.00055 0.01312 0.12613 0.14042 -3.01971

D47 -0.06638 0.00132 0.04198 0.06591 0.10822 0.04184

D48 3.03673 0.00119 0.05159 -0.09245 -0.04145 2.99528

D49 2.83282 0.00074 0.04287 -0.02267 0.02355 2.85636

D50 -0.34726 0.00061 0.05248 -0.18103 -0.12613 -0.47338

D51 -0.27797 0.00054 0.04883 -0.28121 -0.22062 -0.49859

D52 -3.13750 -0.00133 -0.04827 0.17891 0.11446 -3.02303

D53 3.13767 0.00125 0.04806 -0.17808 -0.11436 3.02331

D54 0.27814 -0.00061 -0.04904 0.28204 0.22073 0.49887

D55 0.03952 -0.00077 -0.02500 -0.03751 -0.06392 -0.02439

D56 -3.12276 -0.00055 -0.01335 -0.12378 -0.13816 3.02226

D57 -3.06503 -0.00066 -0.03442 0.11544 0.07937 -2.98565

D58 0.05587 -0.00044 -0.02277 0.02917 0.00513 0.06100

D59 0.06736 -0.00025 -0.00736 -0.05547 -0.06190 0.00547

D60 -3.11868 -0.00038 0.00387 -0.23805 -0.22951 2.93500

D61 -0.00022 0.00001 0.00017 -0.00149 -0.00150 -0.00171

D62 3.12347 0.00019 0.01025 -0.07592 -0.06461 3.05887

D63 -3.12386 -0.00018 -0.00994 0.07315 0.06203 -3.06183

D64 -0.00017 0.00000 0.00013 -0.00128 -0.00108 -0.00125

D65 -3.11919 -0.00008 -0.00823 0.05968 0.05120 -3.06799

D66 0.03579 -0.00034 -0.01207 -0.00478 -0.01781 0.01798

D67 -0.00078 0.00017 0.00482 -0.03691 -0.03181 -0.03258

D68 -3.12898 -0.00009 0.00098 -0.10137 -0.10081 3.05339

D69 3.11946 0.00007 0.00802 -0.05786 -0.04943 3.07003

D70 -0.03543 0.00033 0.01179 0.00730 0.02023 -0.01521

D71 0.00098 -0.00017 -0.00498 0.03848 0.03313 0.03411

D72 3.12927 0.00009 -0.00122 0.10364 0.10279 -3.05112

D73 -3.11830 -0.00045 0.00357 -0.23711 -0.22941 2.93548

D74 0.06758 -0.00030 -0.00756 -0.05524 -0.06215 0.00543

D75 0.00021 -0.00001 -0.00016 0.00144 0.00146 0.00167

D76 3.12400 0.00017 0.00986 -0.07242 -0.06155 3.06245

D77 -3.12363 -0.00018 -0.01015 0.07510 0.06406 -3.05957

D78 0.00016 0.00000 -0.00013 0.00124 0.00105 0.00121

D79 -3.06555 -0.00063 -0.03403 0.11251 0.07730 -2.98825

D80 0.03912 -0.00076 -0.02469 -0.03988 -0.06608 -0.02695

D81 0.05557 -0.00042 -0.02253 0.02734 0.00399 0.05956

D82 -3.12294 -0.00055 -0.01319 -0.12505 -0.13939 3.02085

D83 -0.00090 0.00017 0.00492 -0.03796 -0.03275 -0.03364

D84 -3.12913 -0.00010 0.00111 -0.10269 -0.10197 3.05209

D85 -3.11956 -0.00006 -0.00797 0.05739 0.04916 -3.07040

D86 0.03539 -0.00033 -0.01177 -0.00735 -0.02006 0.01533

D87 -0.03946 0.00076 0.02495 0.03740 0.06354 0.02408

D88 3.06513 0.00064 0.03438 -0.11548 -0.08015 2.98498

D89 3.12266 0.00055 0.01341 0.12278 0.13720 -3.02333

D90 -0.05594 0.00042 0.02284 -0.03010 -0.00649 -0.06243

D91 0.00070 -0.00017 -0.00477 0.03644 0.03146 0.03216

D92 3.12885 0.00010 -0.00089 0.10049 0.10006 -3.05428

D93 3.11930 0.00007 0.00817 -0.05916 -0.05088 3.06842

D94 -0.03574 0.00034 0.01205 0.00490 0.01771 -0.01802

D95 0.06632 -0.00131 -0.04194 -0.06583 -0.10775 -0.04143

D96 -2.83249 -0.00074 -0.04307 0.02545 -0.02132 -2.85381

D97 -3.03685 -0.00117 -0.05155 0.09245 0.04177 -2.99508

D98 0.34752 -0.00059 -0.05267 0.18373 0.12820 0.47572

D99 3.11839 0.00043 -0.00370 0.23723 0.22930 -2.93549

D100 -0.06760 0.00027 0.00754 0.05472 0.06120 -0.00640

D101 3.03708 0.00117 0.05136 -0.09089 -0.03970 2.99738

D102 -0.06619 0.00131 0.04184 0.06678 0.10868 0.04249

D103 -0.34760 0.00063 0.05263 -0.18217 -0.12885 -0.47645

D104 2.83232 0.00076 0.04311 -0.02450 0.01953 2.85185

D105 -3.13754 -0.00131 -0.04811 0.17643 0.11679 -3.02075

D106 -0.27850 0.00065 0.04925 -0.28377 -0.22397 -0.50247

D107 0.27833 -0.00058 -0.04904 0.28295 0.22387 0.50220

D108 3.13737 0.00138 0.04832 -0.17725 -0.11688 3.02048

D109 -0.23057 0.00016 0.02764 -0.05764 -0.02947 -0.26003

D110 2.88560 0.00171 0.05193 0.07513 0.12777 3.01338

D111 -3.10598 -0.00075 -0.03341 -0.01750 -0.04666 3.13055

D112 0.05752 -0.00206 -0.05435 -0.13155 -0.18443 -0.12691

D113 0.19081 0.00019 -0.01143 -0.17103 -0.17933 0.01147

D114 -2.92889 -0.00112 -0.03236 -0.28508 -0.31710 3.03720

D115 -0.05738 0.00206 0.05423 0.13252 0.18526 0.12789

D116 3.10625 0.00075 0.03321 0.01908 0.04839 -3.12854

D117 2.92886 0.00112 0.03232 0.28633 0.31790 -3.03643

D118 -0.19070 -0.00018 0.01131 0.17289 0.18103 -0.00967

D119 2.92424 -0.00076 -0.00403 -0.10545 -0.09509 2.82915

D120 0.04173 -0.00053 -0.02105 0.27622 0.24470 0.28643

D121 -0.04173 0.00056 0.02109 -0.27617 -0.24444 -0.28617

D122 -2.92424 0.00080 0.00407 0.10549 0.09535 -2.82889

D123 3.12878 -0.00010 0.01187 -0.03501 -0.02281 3.10597

D124 -0.03839 -0.00002 0.02217 -0.01765 0.00477 -0.03362

D125 -0.03414 0.00117 0.03226 0.07635 0.10974 0.07559

D126 3.08188 0.00125 0.04256 0.09371 0.13731 -3.06400

D127 0.00022 -0.00001 -0.00019 0.00148 0.00131 0.00153

D128 3.11983 0.00009 0.00873 0.01637 0.02475 -3.13861

D129 -3.11944 -0.00010 -0.00906 -0.01360 -0.02231 3.14143

D130 0.00017 0.00000 -0.00015 0.00129 0.00112 0.00129

D131 -3.13401 0.00010 -0.00686 0.02572 0.01881 -3.11519

D132 -0.00868 0.00033 -0.00282 0.06517 0.06327 0.05460

D133 -0.02098 0.00019 0.00466 0.04520 0.04961 0.02863

D134 3.10435 0.00043 0.00871 0.08465 0.09407 -3.08476

D135 0.03379 -0.00116 -0.03196 -0.07886 -0.11207 -0.07828

D136 -3.12926 0.00009 -0.01150 0.03184 0.02003 -3.10923

D137 -3.08217 -0.00124 -0.04231 -0.09599 -0.13943 3.06159

D138 0.03797 0.00001 -0.02184 0.01472 -0.00733 0.03064

D139 0.02077 -0.00019 -0.00448 -0.04682 -0.05103 -0.03026

D140 -3.10463 -0.00042 -0.00846 -0.08687 -0.09604 3.08251

D141 3.13373 -0.00010 0.00709 -0.02759 -0.02048 3.11325

D142 0.00833 -0.00033 0.00311 -0.06764 -0.06549 -0.05716

D143 0.23038 -0.00018 -0.02752 0.05632 0.02820 0.25858

D144 -2.88564 -0.00171 -0.05190 -0.07568 -0.12823 -3.01387

D145 0.00078 -0.00017 -0.00485 0.03719 0.03214 0.03292

D146 -3.13218 -0.00019 -0.00595 -0.00901 -0.01492 3.13609

D147 3.12817 0.00014 -0.00074 0.10618 0.10479 -3.05023

D148 -0.00479 0.00011 -0.00184 0.05998 0.05773 0.05294

D149 -3.09730 0.00039 0.00300 0.02967 0.03241 -3.06489

D150 0.05866 0.00009 -0.00114 -0.04016 -0.04104 0.01763

D151 0.00008 0.00000 -0.00007 0.00061 0.00054 0.00062

D152 -3.13311 -0.00002 -0.00111 -0.04505 -0.04580 3.10428

D153 3.13322 0.00002 0.00102 0.04586 0.04651 -3.10346

D154 0.00003 0.00000 -0.00002 0.00021 0.00017 0.00020

D155 -0.00082 0.00017 0.00488 -0.03749 -0.03241 -0.03323

D156 -3.12812 -0.00014 0.00070 -0.10574 -0.10444 3.05063

D157 3.13219 0.00019 0.00594 0.00913 0.01503 -3.13597

D158 0.00490 -0.00011 0.00176 -0.05913 -0.05701 -0.05211

D159 3.09747 -0.00039 -0.00315 -0.02827 -0.03118 3.06629

D160 -0.05859 -0.00009 0.00107 0.04082 0.04164 -0.01695

D161 -0.02106 0.00019 0.00460 0.04623 0.05072 0.02966

D162 3.13674 -0.00004 0.00184 -0.01443 -0.01240 3.12434

D163 3.10329 0.00045 0.00889 0.08948 0.09749 -3.08240

D164 -0.02210 0.00022 0.00613 0.02882 0.03438 0.01228

D165 -3.11739 -0.00005 0.01463 -0.12949 -0.11503 3.05077

D166 0.04157 -0.00031 0.01031 -0.17290 -0.16243 -0.12086

D167 0.00007 0.00000 -0.00007 0.00057 0.00050 0.00058

D168 -3.12570 -0.00023 -0.00275 -0.05926 -0.06161 3.09587

D169 3.12579 0.00023 0.00267 0.05998 0.06225 -3.09515

D170 0.00002 0.00000 -0.00002 0.00015 0.00014 0.00015

D171 0.02103 -0.00019 -0.00458 -0.04644 -0.05089 -0.02986

D172 -3.10324 -0.00045 -0.00894 -0.08905 -0.09711 3.08283

D173 -3.13671 0.00004 -0.00186 0.01465 0.01259 -3.12412

D174 0.02221 -0.00022 -0.00623 -0.02796 -0.03363 -0.01142

D175 3.11747 0.00005 -0.01472 0.13027 0.11571 -3.05000

D176 -0.04157 0.00031 -0.01032 0.17304 0.16256 0.12099

D177 -0.00086 0.00017 0.00491 -0.03768 -0.03249 -0.03335

D178 3.13216 0.00019 0.00596 0.00894 0.01488 -3.13614

D179 -3.12831 -0.00013 0.00084 -0.10714 -0.10554 3.04934

D180 0.00471 -0.00011 0.00190 -0.06052 -0.05817 -0.05345

D181 3.09727 -0.00039 -0.00299 -0.02990 -0.03263 3.06464

D182 -0.05863 -0.00009 0.00110 0.04040 0.04124 -0.01739

D183 -0.00008 0.00000 0.00007 -0.00063 -0.00056 -0.00064

D184 3.13318 0.00002 0.00106 0.04544 0.04609 -3.10392

D185 -3.13329 -0.00002 -0.00097 -0.04630 -0.04684 3.10306

D186 -0.00003 0.00000 0.00002 -0.00022 -0.00018 -0.00021

D187 0.00090 -0.00017 -0.00494 0.03799 0.03277 0.03368

D188 3.12826 0.00013 -0.00080 0.10669 0.10518 -3.04975

D189 -3.13218 -0.00019 -0.00595 -0.00905 -0.01498 3.13603

D190 -0.00482 0.00011 -0.00181 0.05965 0.05743 0.05260

D191 -3.09745 0.00039 0.00315 0.02844 0.03134 -3.06611

D192 0.05855 0.00009 -0.00103 -0.04109 -0.04188 0.01667

D193 -0.02096 0.00018 0.00453 0.04667 0.05124 0.03028

D194 3.13675 -0.00005 0.00184 -0.01448 -0.01240 3.12435

D195 3.10331 0.00044 0.00889 0.08940 0.09756 -3.08231

D196 -0.02216 0.00022 0.00620 0.02825 0.03392 0.01175

D197 -3.11754 -0.00004 0.01476 -0.13057 -0.11597 3.04967

D198 0.04150 -0.00031 0.01037 -0.17345 -0.16292 -0.12142

D199 -0.00008 0.00000 0.00007 -0.00058 -0.00051 -0.00059

D200 -3.12582 -0.00023 -0.00265 -0.06006 -0.06240 3.09496

D201 3.12573 0.00023 0.00274 0.05932 0.06175 -3.09571

D202 -0.00002 0.00000 0.00002 -0.00016 -0.00014 -0.00016

D203 0.02099 -0.00018 -0.00456 -0.04646 -0.05106 -0.03007

D204 -3.10336 -0.00045 -0.00884 -0.08984 -0.09794 3.08188

D205 -3.13678 0.00005 -0.00181 0.01427 0.01220 -3.12458

D206 0.02205 -0.00022 -0.00610 -0.02911 -0.03467 -0.01262

D207 3.11746 0.00004 -0.01467 0.12979 0.11528 -3.05044

D208 -0.04150 0.00031 -0.01036 0.17333 0.16280 0.12130

D209 1.09886 -0.00028 -0.00207 -0.00387 -0.00594 1.09292

D210 -1.04475 0.00010 -0.00177 -0.00053 -0.00228 -1.04703

D211 -3.11585 -0.00009 -0.00172 -0.00529 -0.00702 -3.12287

D212 1.04477 -0.00009 0.00175 0.00073 0.00247 1.04724

D213 -1.09883 0.00028 0.00204 0.00419 0.00623 -1.09260

D214 3.11588 0.00009 0.00168 0.00563 0.00733 3.12321

D215 1.10397 -0.00038 -0.00507 -0.00626 -0.01133 1.09263

D216 -1.04480 0.00026 -0.00107 -0.00874 -0.00981 -1.05460

D217 -3.11215 -0.00002 -0.00295 -0.00550 -0.00846 -3.12060

D218 1.04485 -0.00026 0.00102 0.00915 0.01017 1.05501

D219 -1.10393 0.00038 0.00504 0.00657 0.01161 -1.09232

D220 3.11220 0.00002 0.00290 0.00595 0.00885 3.12105

D221 1.04478 -0.00010 0.00174 0.00078 0.00251 1.04729

D222 -1.09883 0.00028 0.00204 0.00418 0.00622 -1.09261

D223 3.11588 0.00009 0.00169 0.00561 0.00730 3.12318

D224 1.09880 -0.00028 -0.00201 -0.00449 -0.00650 1.09229

D225 -1.04480 0.00009 -0.00173 -0.00097 -0.00269 -1.04748

D226 -3.11591 -0.00010 -0.00166 -0.00593 -0.00760 -3.12351

D227 1.10390 -0.00038 -0.00501 -0.00683 -0.01184 1.09206

D228 -1.04488 0.00026 -0.00099 -0.00945 -0.01044 -1.05532

D229 -3.11223 -0.00002 -0.00287 -0.00626 -0.00914 -3.12137

D230 1.04484 -0.00026 0.00103 0.00907 0.01010 1.05494

D231 -1.10394 0.00038 0.00505 0.00653 0.01157 -1.09237

D232 3.11218 0.00002 0.00292 0.00584 0.00876 3.12094

Item Value Threshold Converged?

Maximum Force 0.004659 0.000450 NO

RMS Force 0.000730 0.000300 NO

Maximum Displacement 2.050093 0.001800 NO

RMS Displacement 0.536042 0.001200 NO

Predicted change in Energy=-2.686898D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 01:46:32 2019, MaxMem= 1342177280 cpu: 15.2

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.25D-04

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 -1.113828 2.741484 -0.176278

2 7 0 0.004266 1.987418 -0.445152

3 6 0 1.119760 2.742664 -0.177560

4 6 0 0.711170 4.105548 0.122628

5 6 0 -0.707257 4.104245 0.124732

6 7 0 2.401113 2.360413 -0.300596

7 6 0 2.796508 1.122383 -0.435951

8 7 0 1.988543 0.005008 -0.471401

9 6 0 2.795686 -1.114602 -0.437949

10 6 0 4.206143 -0.700208 -0.319196

11 6 0 4.206977 0.705594 -0.316386

12 7 0 -2.398016 2.360053 -0.299335

13 6 0 -4.208483 0.705433 -0.316563

14 6 0 -4.207388 -0.701437 -0.319306

15 6 0 -2.796806 -1.115428 -0.437024

16 7 0 -1.993936 0.004716 -0.470038

17 6 0 -2.798034 1.122331 -0.435073

18 7 0 -2.397939 -2.355598 -0.301053

19 7 0 0.004637 -1.991940 -0.445657

20 6 0 -1.113939 -2.741869 -0.176284

21 6 0 -0.707165 -4.104338 0.126474

22 6 0 0.712446 -4.105431 0.124362

23 6 0 1.120841 -2.742719 -0.177613

24 7 0 2.401879 -2.355230 -0.302400

25 30 0 -0.007156 -0.006733 -1.115585

26 6 0 -5.397579 1.423104 -0.117584

27 6 0 -6.582328 0.693337 0.035808

28 6 0 -6.581113 -0.696376 0.031984

29 6 0 -5.394862 -1.422815 -0.124694

30 6 0 1.427994 -5.295885 0.384572

31 6 0 0.699762 -6.447150 0.676662

32 6 0 -0.697392 -6.445667 0.679782

33 6 0 -1.424341 -5.293007 0.390276

34 6 0 5.395843 1.423715 -0.115649

35 6 0 6.580600 0.694418 0.038825

36 6 0 6.579651 -0.695213 0.034897

37 6 0 5.393671 -1.421613 -0.122947

38 6 0 -1.424908 5.293182 0.386769

39 6 0 -0.698385 6.446340 0.675071

40 6 0 0.698692 6.448031 0.671934

41 6 0 1.426843 5.296482 0.381048

42 1 0 7.521419 1.202695 0.200925

43 1 0 7.519704 -1.205834 0.193899

44 1 0 1.207623 7.384495 0.860368

45 1 0 -1.208803 7.381496 0.865933

46 1 0 -7.523524 1.201287 0.196628

47 1 0 -7.521346 -1.207003 0.189797

48 1 0 -1.207536 -7.380731 0.871809

49 1 0 1.208696 -7.383370 0.866278

50 8 0 2.772529 5.299063 0.308038

51 8 0 -2.771007 5.292049 0.320190

52 8 0 5.338188 2.765924 -0.014789

53 8 0 5.333117 -2.764382 -0.030288

54 8 0 2.773771 -5.297975 0.312106

55 8 0 -2.770527 -5.291791 0.324209

56 8 0 -5.333400 -2.765652 -0.033025

57 8 0 -5.339546 2.765431 -0.017933

58 6 0 3.438869 6.497143 0.690040

59 1 0 3.254455 6.728524 1.743583

60 1 0 3.135690 7.345275 0.070912

61 1 0 4.499021 6.300335 0.542226

62 6 0 6.537485 3.477678 0.284071

63 1 0 7.288056 3.348502 -0.500919

64 1 0 6.954114 3.170800 1.247553

65 1 0 6.243968 4.524260 0.335669

66 6 0 6.531149 -3.480895 0.262332

67 1 0 6.949819 -3.181384 1.227240

68 1 0 7.280946 -3.348389 -0.522831

69 1 0 6.235220 -4.527103 0.307413

70 6 0 -3.438829 6.487945 0.706504

71 1 0 -3.141079 7.337386 0.086549

72 1 0 -3.249708 6.718973 1.759282

73 1 0 -4.499191 6.288363 0.563966

74 6 0 -6.538820 3.478171 0.278907

75 1 0 -6.956490 3.172718 1.242380

76 1 0 -7.288668 3.348404 -0.506651

77 1 0 -6.244857 4.524680 0.329451

78 6 0 -6.531116 -3.483535 0.257770

79 1 0 -7.280286 -3.350852 -0.527938

80 1 0 -6.950878 -3.185417 1.222624

81 1 0 -6.234357 -4.529544 0.301978

82 6 0 -3.438321 -6.487320 0.711834

83 1 0 -3.248535 -6.717580 1.764647

84 1 0 -3.141043 -7.337244 0.092319

85 1 0 -4.498774 -6.287793 0.569883

86 6 0 3.440472 -6.495471 0.695435

87 1 0 3.138072 -7.344195 0.076742

88 1 0 3.255457 -6.726141 1.749016

89 1 0 4.500655 -6.298362 0.548224

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0452147 0.0441988 0.0227528

Leave Link 202 at Sat Jul 6 01:46:33 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8068.0737343199 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= 89 NActive= 89 NUniq= 89 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= -0.2288323368 Hartrees.

Nuclear repulsion after empirical dispersion term = 8067.8449019831 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6332

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.19D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 384

GePol: Fraction of low-weight points (<1% of avg) = 6.06%

GePol: Cavity surface area = 694.624 Ang\*\*2

GePol: Cavity volume = 798.124 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0086993377 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8067.8362026453 Hartrees.

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(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44663 LenP2D= 112223.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 6.02D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

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(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 01:46:38 2019, MaxMem= 1342177280 cpu: 2.8

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000058 -0.000074 -0.000044 Ang= -0.01 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>= 2.0170 S= 1.0056

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2650.01200820494

Leave Link 401 at Sat Jul 6 01:46:55 2019, MaxMem= 1342177280 cpu: 206.2

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 120282672.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.07D-14 for 6330.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.20D-15 for 4868 1371.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.09D-14 for 6330.

Iteration 1 A^-1\*A deviation from orthogonality is 1.81D-10 for 5909 5864.

Iteration 2 A\*A^-1 deviation from unit magnitude is 5.33D-15 for 6314.

Iteration 2 A\*A^-1 deviation from orthogonality is 4.22D-15 for 3548 674.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 87.

Iteration 2 A^-1\*A deviation from orthogonality is 5.54D-16 for 6314 86.

E= -2649.18923249822

DIIS: error= 2.13D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.18923249822 IErMin= 1 ErrMin= 2.13D-02

ErrMax= 2.13D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.30D+00 BMatP= 1.30D+00

IDIUse=3 WtCom= 7.87D-01 WtEn= 2.13D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Recover alternate guess density for next cycle.

RMSDP=1.64D-03 MaxDP=7.96D-02 OVMax= 0.00D+00

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.60D-03 CP: 9.48D-01

E= -2648.68338495350 Delta-E= 0.505847544722 Rises=F Damp=F

Switch densities from cycles 1 and 2 for lowest energy.

DIIS: error= 4.17D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 1 EnMin= -2649.18923249822 IErMin= 1 ErrMin= 2.13D-02

ErrMax= 4.17D-02 0.00D+00 EMaxC= 1.00D+00 BMatC= 6.06D+00 BMatP= 1.30D+00

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.825D+00 0.175D+00

Coeff: 0.825D+00 0.175D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.063 Goal= None Shift= 0.000

RMSDP=5.50D-03 MaxDP=3.64D-01 DE= 5.06D-01 OVMax= 1.65D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 9.05D-04 CP: 9.91D-01 2.33D-01

E= -2649.73255340552 Delta-E= -1.049168452022 Rises=F Damp=F

DIIS: error= 7.07D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.73255340552 IErMin= 3 ErrMin= 7.07D-03

ErrMax= 7.07D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.15D-01 BMatP= 1.30D+00

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.678D-02 0.145D+00 0.862D+00

Coeff: -0.678D-02 0.145D+00 0.862D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.067 Goal= None Shift= 0.000

RMSDP=2.70D-04 MaxDP=1.90D-02 DE=-1.05D+00 OVMax= 5.02D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.69D-04 CP: 9.84D-01 3.43D-01 8.83D-01

E= -2649.76448765287 Delta-E= -0.031934247349 Rises=F Damp=F

DIIS: error= 4.16D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.76448765287 IErMin= 4 ErrMin= 4.16D-03

ErrMax= 4.16D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 6.05D-02 BMatP= 2.15D-01

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.247D-01 0.619D-01 0.478D+00 0.485D+00

Coeff: -0.247D-01 0.619D-01 0.478D+00 0.485D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.17D-04 MaxDP=9.12D-03 DE=-3.19D-02 OVMax= 2.84D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 8.22D-05 CP: 9.84D-01 3.42D-01 9.01D-01 5.19D-01

E= -2649.77576139658 Delta-E= -0.011273743710 Rises=F Damp=F

DIIS: error= 1.37D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.77576139658 IErMin= 5 ErrMin= 1.37D-03

ErrMax= 1.37D-03 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.73D-03 BMatP= 6.05D-02

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.911D-02 0.111D-01 0.146D+00 0.269D+00 0.584D+00

Coeff: -0.911D-02 0.111D-01 0.146D+00 0.269D+00 0.584D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=3.84D-05 MaxDP=2.47D-03 DE=-1.13D-02 OVMax= 9.20D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.04D-05 CP: 9.84D-01 3.39D-01 9.06D-01 6.18D-01 6.67D-01

E= -2649.77685908743 Delta-E= -0.001097690849 Rises=F Damp=F

DIIS: error= 4.85D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.77685908743 IErMin= 6 ErrMin= 4.85D-04

ErrMax= 4.85D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.37D-04 BMatP= 5.73D-03

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.302D-02 0.104D-02 0.376D-01 0.103D+00 0.317D+00 0.544D+00

Coeff: -0.302D-02 0.104D-02 0.376D-01 0.103D+00 0.317D+00 0.544D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.11D-05 MaxDP=7.65D-04 DE=-1.10D-03 OVMax= 3.73D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 7.99D-06 CP: 9.84D-01 3.40D-01 9.05D-01 6.14D-01 7.13D-01

CP: 6.74D-01

E= -2649.77697098373 Delta-E= -0.000111896303 Rises=F Damp=F

DIIS: error= 1.89D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.77697098373 IErMin= 7 ErrMin= 1.89D-04

ErrMax= 1.89D-04 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.37D-05 BMatP= 5.37D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.827D-03-0.494D-03 0.614D-02 0.289D-01 0.114D+00 0.293D+00

Coeff-Com: 0.559D+00

Coeff: -0.827D-03-0.494D-03 0.614D-02 0.289D-01 0.114D+00 0.293D+00

Coeff: 0.559D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=4.50D-06 MaxDP=2.45D-04 DE=-1.12D-04 OVMax= 1.05D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 3.11D-06 CP: 9.84D-01 3.38D-01 9.07D-01 6.18D-01 7.13D-01

CP: 7.37D-01 7.70D-01

E= -2649.77698217964 Delta-E= -0.000011195907 Rises=F Damp=F

DIIS: error= 6.32D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.77698217964 IErMin= 8 ErrMin= 6.32D-05

ErrMax= 6.32D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 8.71D-06 BMatP= 5.37D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.336D-05-0.421D-03-0.271D-02-0.110D-02 0.122D-01 0.768D-01

Coeff-Com: 0.308D+00 0.607D+00

Coeff: 0.336D-05-0.421D-03-0.271D-02-0.110D-02 0.122D-01 0.768D-01

Coeff: 0.308D+00 0.607D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.75D-06 MaxDP=1.25D-04 DE=-1.12D-05 OVMax= 7.32D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.40D-06 CP: 9.84D-01 3.39D-01 9.07D-01 6.19D-01 7.18D-01

CP: 7.51D-01 8.48D-01 8.60D-01

E= -2649.77698506595 Delta-E= -0.000002886312 Rises=F Damp=F

DIIS: error= 2.43D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.77698506595 IErMin= 9 ErrMin= 2.43D-05

ErrMax= 2.43D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.14D-06 BMatP= 8.71D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.169D-03-0.157D-04-0.193D-02-0.639D-02-0.195D-01-0.378D-01

Coeff-Com: -0.354D-01 0.196D+00 0.905D+00

Coeff: 0.169D-03-0.157D-04-0.193D-02-0.639D-02-0.195D-01-0.378D-01

Coeff: -0.354D-01 0.196D+00 0.905D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.065 Goal= None Shift= 0.000

RMSDP=1.11D-06 MaxDP=8.70D-05 DE=-2.89D-06 OVMax= 5.07D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 8.09D-07 CP: 9.84D-01 3.39D-01 9.07D-01 6.19D-01 7.20D-01

CP: 7.66D-01 8.85D-01 1.01D+00 1.23D+00

E= -2649.77698588395 Delta-E= -0.000000818003 Rises=F Damp=F

DIIS: error= 1.44D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -2649.77698588395 IErMin=10 ErrMin= 1.44D-05

ErrMax= 1.44D-05 0.00D+00 EMaxC= 1.00D+00 BMatC= 5.25D-07 BMatP= 1.14D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.103D-03 0.100D-03-0.471D-03-0.355D-02-0.146D-01-0.417D-01

Coeff-Com: -0.104D+00-0.430D-01 0.538D+00 0.669D+00

Coeff: 0.103D-03 0.100D-03-0.471D-03-0.355D-02-0.146D-01-0.417D-01

Coeff: -0.104D+00-0.430D-01 0.538D+00 0.669D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=6.46D-07 MaxDP=5.13D-05 DE=-8.18D-07 OVMax= 2.96D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 3.61D-07 CP: 9.84D-01 3.39D-01 9.07D-01 6.19D-01 7.20D-01

CP: 7.73D-01 9.10D-01 1.11D+00 1.49D+00 8.93D-01

E= -2649.77698614565 Delta-E= -0.000000261698 Rises=F Damp=F

DIIS: error= 7.89D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -2649.77698614565 IErMin=11 ErrMin= 7.89D-06

ErrMax= 7.89D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 9.51D-08 BMatP= 5.25D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.606D-05 0.502D-04 0.338D-03 0.218D-04-0.176D-02-0.101D-01

Coeff-Com: -0.434D-01-0.751D-01 0.246D-01 0.327D+00 0.778D+00

Coeff: 0.606D-05 0.502D-04 0.338D-03 0.218D-04-0.176D-02-0.101D-01

Coeff: -0.434D-01-0.751D-01 0.246D-01 0.327D+00 0.778D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=3.28D-07 MaxDP=3.27D-05 DE=-2.62D-07 OVMax= 1.55D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.92D-07 CP: 9.84D-01 3.39D-01 9.07D-01 6.20D-01 7.20D-01

CP: 7.74D-01 9.17D-01 1.15D+00 1.59D+00 1.07D+00

CP: 8.94D-01

E= -2649.77698619607 Delta-E= -0.000000050419 Rises=F Damp=F

DIIS: error= 4.09D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -2649.77698619607 IErMin=12 ErrMin= 4.09D-06

ErrMax= 4.09D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 4.33D-08 BMatP= 9.51D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.146D-04 0.125D-04 0.325D-03 0.694D-03 0.168D-02 0.169D-02

Coeff-Com: -0.702D-02-0.400D-01-0.966D-01 0.646D-01 0.515D+00 0.560D+00

Coeff: -0.146D-04 0.125D-04 0.325D-03 0.694D-03 0.168D-02 0.169D-02

Coeff: -0.702D-02-0.400D-01-0.966D-01 0.646D-01 0.515D+00 0.560D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.34D-07 MaxDP=1.47D-05 DE=-5.04D-08 OVMax= 5.45D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 7.34D-08 CP: 9.84D-01 3.39D-01 9.07D-01 6.19D-01 7.20D-01

CP: 7.74D-01 9.18D-01 1.15D+00 1.64D+00 1.13D+00

CP: 1.07D+00 8.06D-01

E= -2649.77698620952 Delta-E= -0.000000013455 Rises=F Damp=F

DIIS: error= 1.18D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -2649.77698620952 IErMin=13 ErrMin= 1.18D-06

ErrMax= 1.18D-06 0.00D+00 EMaxC= 1.00D+00 BMatC= 3.03D-09 BMatP= 4.33D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.734D-05-0.104D-05 0.106D-03 0.323D-03 0.106D-02 0.225D-02

Coeff-Com: 0.260D-02-0.972D-02-0.485D-01-0.132D-01 0.151D+00 0.258D+00

Coeff-Com: 0.656D+00

Coeff: -0.734D-05-0.104D-05 0.106D-03 0.323D-03 0.106D-02 0.225D-02

Coeff: 0.260D-02-0.972D-02-0.485D-01-0.132D-01 0.151D+00 0.258D+00

Coeff: 0.656D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.33D-08 MaxDP=3.81D-06 DE=-1.35D-08 OVMax= 1.68D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 3.08D-08 CP: 9.84D-01 3.39D-01 9.07D-01 6.19D-01 7.20D-01

CP: 7.75D-01 9.19D-01 1.15D+00 1.64D+00 1.14D+00

CP: 1.12D+00 8.94D-01 8.12D-01

E= -2649.77698621024 Delta-E= -0.000000000715 Rises=F Damp=F

DIIS: error= 5.61D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -2649.77698621024 IErMin=14 ErrMin= 5.61D-07

ErrMax= 5.61D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 1.03D-09 BMatP= 3.03D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.186D-05-0.323D-05-0.582D-05 0.518D-04 0.302D-03 0.101D-02

Coeff-Com: 0.304D-02 0.249D-02-0.706D-02-0.218D-01-0.224D-01 0.229D-01

Coeff-Com: 0.391D+00 0.630D+00

Coeff: -0.186D-05-0.323D-05-0.582D-05 0.518D-04 0.302D-03 0.101D-02

Coeff: 0.304D-02 0.249D-02-0.706D-02-0.218D-01-0.224D-01 0.229D-01

Coeff: 0.391D+00 0.630D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.08D-08 MaxDP=1.47D-06 DE=-7.15D-10 OVMax= 8.12D-06

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.32D-08 CP: 9.84D-01 3.39D-01 9.07D-01 6.19D-01 7.20D-01

CP: 7.74D-01 9.19D-01 1.15D+00 1.64D+00 1.15D+00

CP: 1.13D+00 9.24D-01 9.86D-01 9.18D-01

E= -2649.77698621061 Delta-E= -0.000000000375 Rises=F Damp=F

DIIS: error= 1.69D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -2649.77698621061 IErMin=15 ErrMin= 1.69D-07

ErrMax= 1.69D-07 0.00D+00 EMaxC= 1.00D+00 BMatC= 8.90D-11 BMatP= 1.03D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.108D-05-0.784D-06-0.265D-04-0.618D-04-0.151D-03-0.185D-03

Coeff-Com: 0.478D-03 0.321D-02 0.923D-02-0.490D-02-0.432D-01-0.545D-01

Coeff-Com: -0.618D-02 0.215D+00 0.881D+00

Coeff: 0.108D-05-0.784D-06-0.265D-04-0.618D-04-0.151D-03-0.185D-03

Coeff: 0.478D-03 0.321D-02 0.923D-02-0.490D-02-0.432D-01-0.545D-01

Coeff: -0.618D-02 0.215D+00 0.881D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.02D-08 MaxDP=7.52D-07 DE=-3.75D-10 OVMax= 4.92D-06

Cycle 16 Pass 1 IDiag 1:

RMSU= 4.60D-09 CP: 9.84D-01 3.39D-01 9.07D-01 6.19D-01 7.20D-01

CP: 7.74D-01 9.19D-01 1.15D+00 1.64D+00 1.15D+00

CP: 1.14D+00 9.42D-01 1.05D+00 1.10D+00 1.02D+00

E= -2649.77698621047 Delta-E= 0.000000000146 Rises=F Damp=F

DIIS: error= 8.24D-08 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=15 EnMin= -2649.77698621061 IErMin=16 ErrMin= 8.24D-08

ErrMax= 8.24D-08 0.00D+00 EMaxC= 1.00D+00 BMatC= 2.37D-11 BMatP= 8.90D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.730D-06-0.174D-07-0.128D-04-0.371D-04-0.109D-03-0.201D-03

Coeff-Com: -0.941D-04 0.133D-02 0.538D-02-0.211D-03-0.191D-01-0.299D-01

Coeff-Com: -0.458D-01 0.359D-01 0.452D+00 0.601D+00

Coeff: 0.730D-06-0.174D-07-0.128D-04-0.371D-04-0.109D-03-0.201D-03

Coeff: -0.941D-04 0.133D-02 0.538D-02-0.211D-03-0.191D-01-0.299D-01

Coeff: -0.458D-01 0.359D-01 0.452D+00 0.601D+00

Gap= 0.043 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=3.09D-09 MaxDP=2.59D-07 DE= 1.46D-10 OVMax= 1.44D-06

Error on total polarization charges = 0.07240

SCF Done: E(UB3LYP) = -2649.77698621 A.U. after 16 cycles

NFock= 16 Conv=0.31D-08 -V/T= 1.9848

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0180 S= 1.0060

<L.S>= 0.000000000000E+00

KE= 2.690550358035D+03 PE=-2.241510883612D+04 EE= 9.006945289231D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.46

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0180, after 2.0002

Leave Link 502 at Sat Jul 6 02:00:15 2019, MaxMem= 1342177280 cpu: 9489.2

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44663 LenP2D= 112223.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 278

Leave Link 701 at Sat Jul 6 02:00:34 2019, MaxMem= 1342177280 cpu: 217.8

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 02:00:34 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 02:02:07 2019, MaxMem= 1342177280 cpu: 1108.9

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-2.48080961D-02-3.12005914D-02 5.57356723D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.004932897 0.004723686 -0.017965564

2 7 -0.001516961 0.008299188 0.016079316

3 6 -0.006348361 0.005693814 -0.017904832

4 6 0.003792836 -0.000309793 0.003737414

5 6 -0.003660368 -0.000495856 0.003607782

6 7 0.007588672 0.005097041 0.001408038

7 6 -0.006304753 -0.002316569 0.013843796

8 7 0.016054571 -0.001465609 -0.011802301

9 6 -0.007274881 0.000823853 0.014000348

10 6 0.002744756 0.001255003 -0.004706265

11 6 0.002790542 -0.001075100 -0.004747469

12 7 -0.006405755 0.004493357 0.001372660

13 6 -0.002821710 -0.001432811 -0.004719789

14 6 -0.002773504 0.001615842 -0.004675287

15 6 0.007225939 -0.000786302 0.014224928

16 7 -0.013650550 -0.001481690 -0.011791085

17 6 0.006262148 -0.000663224 0.014063319

18 7 -0.005763806 -0.003288054 0.001269772

19 7 -0.001522461 -0.006118814 0.015747056

20 6 0.003691529 -0.004871568 -0.017861142

21 6 -0.003412641 0.000534069 0.003635294

22 6 0.003547816 0.000344102 0.003766609

23 6 -0.005071890 -0.005837612 -0.017795290

24 7 0.006930363 -0.003873026 0.001308903

25 30 0.001174735 0.001142459 0.006707983

26 6 0.003083469 0.002590144 0.003457457

27 6 -0.001756036 -0.002042692 0.000238707

28 6 -0.001775503 0.002006537 0.000270829

29 6 0.003070384 -0.002724979 0.003419904

30 6 -0.000392241 0.001750667 -0.000477409

31 6 -0.003043228 -0.002550043 -0.000253133

32 6 0.003027894 -0.002546330 -0.000278804

33 6 0.000311185 0.001669762 -0.000478566

34 6 -0.003122519 0.002594457 0.003472020

35 6 0.001760299 -0.002039605 0.000230969

36 6 0.001779160 0.002003722 0.000263238

37 6 -0.003108883 -0.002734891 0.003433649

38 6 0.000289357 -0.001666018 -0.000479341

39 6 0.002985693 0.002527321 -0.000279831

40 6 -0.003000373 0.002530522 -0.000254157

41 6 -0.000376482 -0.001745879 -0.000477654

42 1 -0.000248840 0.000204506 -0.000542660

43 1 -0.000215969 -0.000213280 -0.000532017

44 1 -0.001854695 -0.001152237 0.000875680

45 1 0.001863580 -0.001137114 0.000874154

46 1 0.000231955 0.000230826 -0.000533883

47 1 0.000199109 -0.000238677 -0.000523575

48 1 0.001850602 0.001132190 0.000870866

49 1 -0.001840613 0.001147033 0.000872214

50 8 0.002102696 -0.003518692 0.000429435

51 8 -0.002017800 -0.003523612 0.000542178

52 8 -0.000707856 0.003198171 -0.003040821

53 8 -0.000632401 -0.003088825 -0.003149565

54 8 0.002060111 0.003526576 0.000559505

55 8 -0.001979256 0.003542184 0.000684323

56 8 0.000566592 -0.003078606 -0.003231809

57 8 0.000634680 0.003173902 -0.003115205

58 6 0.004040036 -0.000737742 0.000185938

59 1 0.000076365 0.000603851 -0.000153333

60 1 0.001699966 0.000065931 -0.000788690

61 1 0.000294633 0.000278506 0.000148876

62 6 -0.001174937 0.000168072 -0.000314465

63 1 0.000234483 0.000353759 0.000017686

64 1 0.000155671 -0.000149923 0.000083631

65 1 0.000327623 0.000261243 -0.000106973

66 6 -0.001200739 -0.000108652 -0.000326511

67 1 0.000146103 0.000159593 0.000081971

68 1 0.000243228 -0.000342914 0.000023393

69 1 0.000330381 -0.000235367 -0.000077131

70 6 -0.003996811 -0.000752806 0.000203909

71 1 -0.001720922 0.000078403 -0.000788983

72 1 -0.000076379 0.000615434 -0.000145399

73 1 -0.000273034 0.000274976 0.000121201

74 6 0.001169730 0.000138942 -0.000314252

75 1 -0.000153936 -0.000161713 0.000083110

76 1 -0.000239544 0.000341342 0.000013755

77 1 -0.000338194 0.000245170 -0.000085381

78 6 0.001194583 -0.000077332 -0.000327742

79 1 -0.000248551 -0.000331801 0.000019308

80 1 -0.000144911 0.000169305 0.000081814

81 1 -0.000341021 -0.000217990 -0.000057575

82 6 -0.003988987 0.000733954 0.000220486

83 1 -0.000078083 -0.000616356 -0.000140124

84 1 -0.001711259 -0.000075058 -0.000789297

85 1 -0.000247921 -0.000282703 0.000094451

86 6 0.004032298 0.000719908 0.000202055

87 1 0.001689491 -0.000062427 -0.000789097

88 1 0.000077004 -0.000604029 -0.000148253

89 1 0.000270402 -0.000285002 0.000120731

-------------------------------------------------------------------

Cartesian Forces: Max 0.017965564 RMS 0.004258084

Leave Link 716 at Sat Jul 6 02:02:07 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.016008365 RMS 0.003027383

Search for a local minimum.

Step number 15 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .30274D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 4 6 5 8 7

10 9 11 14 15

13

DE= 1.81D-02 DEPred=-2.69D-03 R=-6.73D+00

Trust test=-6.73D+00 RLast= 1.69D+00 DXMaxT set to 5.71D-02

ITU= -1 -1 0 -1 0 0 0 0 0 0 1 1 1 1 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.92075.

Iteration 1 RMS(Cart)= 0.29129961 RMS(Int)= 0.01666078

Iteration 2 RMS(Cart)= 0.06239582 RMS(Int)= 0.00074061

Iteration 3 RMS(Cart)= 0.00170094 RMS(Int)= 0.00062541

Iteration 4 RMS(Cart)= 0.00000115 RMS(Int)= 0.00062541

Iteration 5 RMS(Cart)= 0.00000000 RMS(Int)= 0.00062541

ITry= 1 IFail=0 DXMaxC= 1.54D+00 DCOld= 1.00D+10 DXMaxT= 5.71D-02 DXLimC= 3.00D+00 Rises=T

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.59866 -0.00249 -0.01428 0.00000 -0.01505 2.58361

R2 2.74695 -0.00274 -0.00235 0.00000 -0.00206 2.74489

R3 2.54221 0.00413 0.01658 0.00000 0.01795 2.56016

R4 2.59542 -0.00187 -0.01145 0.00000 -0.01184 2.58358

R5 3.97573 0.00721 -0.09619 0.00000 -0.09921 3.87652

R6 2.74792 -0.00303 -0.00339 0.00000 -0.00310 2.74482

R7 2.53753 0.00628 0.02031 0.00000 0.02242 2.55995

R8 2.68044 0.00271 0.01163 0.00000 0.01263 2.69307

R9 2.67067 -0.00387 -0.00570 0.00000 -0.00571 2.66495

R10 2.67064 -0.00374 -0.00570 0.00000 -0.00571 2.66493

R11 2.46924 0.00576 0.00985 0.00000 0.01194 2.48118

R12 2.60658 -0.00076 -0.00912 0.00000 -0.00950 2.59709

R13 2.78850 -0.00005 0.00405 0.00000 0.00432 2.79282

R14 2.60900 -0.00137 -0.01114 0.00000 -0.01189 2.59711

R15 3.96299 0.00408 -0.10971 0.00000 -0.11269 3.85030

R16 2.78708 0.00035 0.00552 0.00000 0.00580 2.79288

R17 2.47303 0.00359 0.00721 0.00000 0.00857 2.48160

R18 2.65659 0.00212 0.00814 0.00000 0.00903 2.66562

R19 2.65179 -0.00151 -0.00379 0.00000 -0.00383 2.64796

R20 2.65195 -0.00162 -0.00393 0.00000 -0.00397 2.64798

R21 2.47142 0.00422 0.00845 0.00000 0.01005 2.48147

R22 2.65861 0.00169 0.00648 0.00000 0.00702 2.66562

R23 2.78836 0.00007 0.00428 0.00000 0.00444 2.79281

R24 2.65141 -0.00145 -0.00338 0.00000 -0.00341 2.64800

R25 2.78694 0.00046 0.00576 0.00000 0.00593 2.79287

R26 2.65125 -0.00135 -0.00324 0.00000 -0.00326 2.64799

R27 2.60509 -0.00034 -0.00763 0.00000 -0.00795 2.59714

R28 2.47518 0.00209 0.00584 0.00000 0.00671 2.48190

R29 2.60265 0.00029 -0.00559 0.00000 -0.00553 2.59712

R30 3.94774 0.00386 -0.09630 0.00000 -0.09797 3.84978

R31 2.54477 0.00266 0.01461 0.00000 0.01548 2.56026

R32 2.59531 -0.00173 -0.01126 0.00000 -0.01162 2.58369

R33 2.59205 -0.00109 -0.00840 0.00000 -0.00839 2.58365

R34 3.95941 0.00699 -0.08198 0.00000 -0.08369 3.87573

R35 2.74723 -0.00280 -0.00254 0.00000 -0.00235 2.74488

R36 2.68268 0.00220 0.00972 0.00000 0.01038 2.69306

R37 2.67038 -0.00368 -0.00544 0.00000 -0.00544 2.66495

R38 2.74821 -0.00308 -0.00360 0.00000 -0.00341 2.74480

R39 2.67040 -0.00381 -0.00544 0.00000 -0.00544 2.66497

R40 2.54010 0.00478 0.01833 0.00000 0.01994 2.56004

R41 2.64543 0.00370 0.00713 0.00000 0.00715 2.65258

R42 2.54597 0.00352 0.00233 0.00000 0.00233 2.54831

R43 2.62619 0.00290 0.00075 0.00000 0.00080 2.62699

R44 2.04381 -0.00017 0.00003 0.00000 0.00003 2.04385

R45 2.64525 0.00375 0.00732 0.00000 0.00734 2.65259

R46 2.04377 -0.00014 0.00007 0.00000 0.00007 2.04384

R47 2.54615 0.00333 0.00216 0.00000 0.00216 2.54831

R48 2.63280 0.00606 0.00859 0.00000 0.00859 2.64139

R49 2.54684 0.00812 0.00489 0.00000 0.00489 2.55172

R50 2.64025 0.00429 0.00436 0.00000 0.00436 2.64460

R51 2.04534 -0.00171 -0.00137 0.00000 -0.00137 2.04397

R52 2.63269 0.00610 0.00871 0.00000 0.00871 2.64140

R53 2.04533 -0.00170 -0.00136 0.00000 -0.00136 2.04397

R54 2.54698 0.00800 0.00473 0.00000 0.00473 2.55172

R55 2.64520 0.00379 0.00735 0.00000 0.00739 2.65259

R56 2.54589 0.00361 0.00242 0.00000 0.00242 2.54831

R57 2.62603 0.00308 0.00085 0.00000 0.00092 2.62696

R58 2.04384 -0.00020 0.00000 0.00000 0.00000 2.04385

R59 2.64502 0.00384 0.00754 0.00000 0.00758 2.65260

R60 2.04380 -0.00017 0.00004 0.00000 0.00004 2.04385

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R62 2.63258 0.00615 0.00882 0.00000 0.00883 2.64141

R63 2.54687 0.00808 0.00485 0.00000 0.00485 2.55172

R64 2.64010 0.00445 0.00445 0.00000 0.00448 2.64458

R65 2.04534 -0.00171 -0.00136 0.00000 -0.00136 2.04397

R66 2.63268 0.00611 0.00870 0.00000 0.00871 2.64140

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R68 2.54672 0.00821 0.00501 0.00000 0.00501 2.55173

R69 2.68935 0.00288 0.00501 0.00000 0.00501 2.69436

R70 2.68939 0.00287 0.00497 0.00000 0.00497 2.69436

R71 2.69524 -0.00014 0.00109 0.00000 0.00109 2.69634

R72 2.69529 -0.00020 0.00105 0.00000 0.00105 2.69634

R73 2.68941 0.00287 0.00494 0.00000 0.00494 2.69435

R74 2.68945 0.00286 0.00490 0.00000 0.00490 2.69436

R75 2.69539 -0.00021 0.00095 0.00000 0.00095 2.69634

R76 2.69534 -0.00015 0.00099 0.00000 0.00099 2.69634

R77 2.06793 -0.00003 -0.00076 0.00000 -0.00076 2.06717

R78 2.06540 0.00002 0.00117 0.00000 0.00117 2.06656

R79 2.05668 0.00022 0.00006 0.00000 0.00006 2.05675

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A2 2.21779 0.00105 -0.00164 0.00000 -0.00177 2.21602

A3 2.15525 -0.00018 0.02172 0.00000 0.02319 2.17844

A4 1.89731 0.00205 0.03150 0.00000 0.03362 1.93092

A5 2.18664 -0.00038 -0.01735 0.00000 -0.01731 2.16933

A6 2.19903 -0.00163 -0.02822 0.00000 -0.02954 2.16949

A7 1.90434 -0.00041 -0.01464 0.00000 -0.01566 1.88868

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A10 1.85504 -0.00037 0.00294 0.00000 0.00315 1.85818

A11 2.32576 -0.00328 -0.00723 0.00000 -0.00733 2.31843

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A13 1.85485 -0.00022 0.00310 0.00000 0.00331 1.85816

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A31 2.10890 0.00245 0.00472 0.00000 0.00466 2.11356

A32 2.17707 -0.00207 0.00999 0.00000 0.01086 2.18793

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A62 2.21382 0.00123 0.00190 0.00000 0.00216 2.21598

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A65 1.46222 0.00272 0.09017 0.00000 0.09466 1.55689

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A67 1.47237 0.00136 0.08162 0.00000 0.08487 1.55724

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A70 2.07557 -0.00102 -0.00198 0.00000 -0.00191 2.07366

A71 2.15045 0.00424 0.01043 0.00000 0.01049 2.16094

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A73 2.10360 -0.00076 -0.00245 0.00000 -0.00245 2.10115

A74 2.06102 -0.00003 -0.00003 0.00000 -0.00004 2.06098

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A78 2.05551 -0.00308 -0.00695 0.00000 -0.00694 2.04858

A79 2.07519 -0.00088 -0.00160 0.00000 -0.00154 2.07365

A80 2.15107 0.00405 0.00982 0.00000 0.00988 2.16095

A81 2.06016 -0.00440 -0.00615 0.00000 -0.00610 2.05406

A82 2.09097 -0.00985 -0.02174 0.00000 -0.02174 2.06923

A83 2.13168 0.01426 0.02818 0.00000 0.02818 2.15986

A84 2.12033 0.00085 0.00214 0.00000 0.00222 2.12255

A85 2.10101 0.00082 0.00014 0.00000 0.00015 2.10117

A86 2.06092 -0.00164 -0.00150 0.00000 -0.00148 2.05944

A87 2.12024 0.00090 0.00224 0.00000 0.00232 2.12255

A88 2.06101 -0.00167 -0.00158 0.00000 -0.00157 2.05944

A89 2.10101 0.00081 0.00014 0.00000 0.00016 2.10117

A90 2.06001 -0.00436 -0.00601 0.00000 -0.00595 2.05406

A91 2.09093 -0.00979 -0.02169 0.00000 -0.02169 2.06924

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A93 2.05579 -0.00325 -0.00722 0.00000 -0.00720 2.04859

A94 2.07632 -0.00118 -0.00273 0.00000 -0.00266 2.07366

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A109 2.10105 0.00079 0.00012 0.00000 0.00012 2.10117

A110 2.06114 -0.00171 -0.00171 0.00000 -0.00171 2.05944

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A112 2.06107 -0.00168 -0.00163 0.00000 -0.00163 2.05944

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A130 1.91091 -0.00136 -0.00162 0.00000 -0.00162 1.90929

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D3 -3.13146 -0.00019 -0.00483 0.00000 -0.00454 -3.13600

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D47 0.04184 -0.00221 -0.05254 0.00000 -0.05243 -0.01059

D48 2.99528 0.00250 0.09606 0.00000 0.09628 3.09156

D49 2.85636 -0.00155 0.02642 0.00000 0.02630 2.88267

D50 -0.47338 0.00315 0.17502 0.00000 0.17502 -0.29836

D51 -0.49859 0.00326 0.25793 0.00000 0.25736 -0.24123

D52 -3.02303 -0.00107 -0.15956 0.00000 -0.15853 3.10162

D53 3.02331 0.00105 0.15923 0.00000 0.15824 -3.10164

D54 0.49887 -0.00328 -0.25826 0.00000 -0.25765 0.24121

D55 -0.02439 0.00143 0.03080 0.00000 0.03078 0.00639

D56 3.02226 0.00280 0.11223 0.00000 0.11225 3.13452

D57 -2.98565 -0.00359 -0.11171 0.00000 -0.11183 -3.09749

D58 0.06100 -0.00222 -0.03028 0.00000 -0.03036 0.03065

D59 0.00547 0.00052 0.04873 0.00000 0.04891 0.05438

D60 2.93500 0.00560 0.21566 0.00000 0.21565 -3.13254

D61 -0.00171 -0.00001 0.00157 0.00000 0.00158 -0.00013

D62 3.05887 0.00081 0.07099 0.00000 0.07097 3.12984

D63 -3.06183 -0.00086 -0.06827 0.00000 -0.06825 -3.13008

D64 -0.00125 -0.00004 0.00115 0.00000 0.00114 -0.00011

D65 -3.06799 -0.00094 -0.05637 0.00000 -0.05641 -3.12441

D66 0.01798 0.00096 0.00285 0.00000 0.00284 0.02082

D67 -0.03258 0.00047 0.03470 0.00000 0.03471 0.00213

D68 3.05339 0.00237 0.09392 0.00000 0.09396 -3.13583

D69 3.07003 0.00096 0.05451 0.00000 0.05453 3.12456

D70 -0.01521 -0.00094 -0.00540 0.00000 -0.00540 -0.02061

D71 0.03411 -0.00042 -0.03610 0.00000 -0.03610 -0.00198

D72 -3.05112 -0.00233 -0.09601 0.00000 -0.09604 3.13603

D73 2.93548 0.00561 0.21524 0.00000 0.21524 -3.13247

D74 0.00543 0.00045 0.04874 0.00000 0.04895 0.05439

D75 0.00167 0.00002 -0.00153 0.00000 -0.00154 0.00012

D76 3.06245 0.00090 0.06773 0.00000 0.06772 3.13017

D77 -3.05957 -0.00083 -0.07037 0.00000 -0.07036 -3.12993

D78 0.00121 0.00005 -0.00111 0.00000 -0.00110 0.00011

D79 -2.98825 -0.00368 -0.10936 0.00000 -0.10947 -3.09772

D80 -0.02695 0.00142 0.03313 0.00000 0.03314 0.00619

D81 0.05956 -0.00230 -0.02895 0.00000 -0.02903 0.03053

D82 3.02085 0.00280 0.11354 0.00000 0.11359 3.13444

D83 -0.03364 0.00045 0.03567 0.00000 0.03567 0.00203

D84 3.05209 0.00234 0.09514 0.00000 0.09517 -3.13593

D85 -3.07040 -0.00097 -0.05421 0.00000 -0.05424 -3.12464

D86 0.01533 0.00091 0.00526 0.00000 0.00526 0.02059

D87 0.02408 -0.00144 -0.03050 0.00000 -0.03048 -0.00640

D88 2.98498 0.00366 0.11238 0.00000 0.11253 3.09751

D89 -3.02333 -0.00283 -0.11128 0.00000 -0.11131 -3.13464

D90 -0.06243 0.00226 0.03160 0.00000 0.03170 -0.03072

D91 0.03216 -0.00051 -0.03432 0.00000 -0.03433 -0.00217

D92 -3.05428 -0.00239 -0.09313 0.00000 -0.09317 3.13574

D93 3.06842 0.00094 0.05602 0.00000 0.05607 3.12448

D94 -0.01802 -0.00094 -0.00279 0.00000 -0.00277 -0.02079

D95 -0.04143 0.00225 0.05215 0.00000 0.05205 0.01062

D96 -2.85381 0.00157 -0.02869 0.00000 -0.02860 -2.88241

D97 -2.99508 -0.00243 -0.09631 0.00000 -0.09650 -3.09158

D98 0.47572 -0.00311 -0.17715 0.00000 -0.17715 0.29857

D99 -2.93549 -0.00562 -0.21528 0.00000 -0.21528 3.13241

D100 -0.00640 -0.00045 -0.04789 0.00000 -0.04805 -0.05445

D101 2.99738 0.00240 0.09418 0.00000 0.09428 3.09166

D102 0.04249 -0.00223 -0.05312 0.00000 -0.05303 -0.01054

D103 -0.47645 0.00339 0.17769 0.00000 0.17790 -0.29855

D104 2.85185 -0.00125 0.03040 0.00000 0.03059 2.88244

D105 -3.02075 -0.00159 -0.16151 0.00000 -0.16089 3.10154

D106 -0.50247 0.00362 0.26147 0.00000 0.26109 -0.24137

D107 0.50220 -0.00359 -0.26115 0.00000 -0.26080 0.24140

D108 3.02048 0.00162 0.16184 0.00000 0.16118 -3.10152

D109 -0.26003 0.00265 0.05815 0.00000 0.05825 -0.20178

D110 3.01338 -0.00161 -0.05938 0.00000 -0.05921 2.95417

D111 3.13055 0.00049 0.00547 0.00000 0.00538 3.13593

D112 -0.12691 0.00417 0.10883 0.00000 0.10885 -0.01806

D113 0.01147 -0.00155 0.15229 0.00000 0.15236 0.16383

D114 3.03720 0.00214 0.25565 0.00000 0.25582 -2.99016

D115 0.12789 -0.00415 -0.10973 0.00000 -0.10975 0.01814

D116 -3.12854 -0.00046 -0.00729 0.00000 -0.00723 -3.13577

D117 -3.03643 -0.00207 -0.25644 0.00000 -0.25655 2.99021

D118 -0.00967 0.00162 -0.15400 0.00000 -0.15403 -0.16370

D119 2.82915 0.00295 0.08303 0.00000 0.08224 2.91139

D120 0.28643 -0.00062 -0.24892 0.00000 -0.24853 0.03790

D121 -0.28617 0.00054 0.24873 0.00000 0.24825 -0.03792

D122 -2.82889 -0.00303 -0.08322 0.00000 -0.08251 -2.91140

D123 3.10597 0.00111 0.03432 0.00000 0.03419 3.14017

D124 -0.03362 0.00104 0.02049 0.00000 0.02040 -0.01321

D125 0.07559 -0.00258 -0.06484 0.00000 -0.06495 0.01064

D126 -3.06400 -0.00265 -0.07868 0.00000 -0.07874 3.14045

D127 0.00153 0.00002 -0.00142 0.00000 -0.00142 0.00012

D128 -3.13861 -0.00002 -0.01299 0.00000 -0.01294 3.13164

D129 3.14143 0.00008 0.01038 0.00000 0.01033 -3.13143

D130 0.00129 0.00003 -0.00120 0.00000 -0.00120 0.00009

D131 -3.11519 -0.00027 -0.02502 0.00000 -0.02505 -3.14024

D132 0.05460 -0.00117 -0.06142 0.00000 -0.06150 -0.00690

D133 0.02863 -0.00034 -0.04045 0.00000 -0.04042 -0.01179

D134 -3.08476 -0.00124 -0.07685 0.00000 -0.07688 3.12154

D135 -0.07828 0.00256 0.06733 0.00000 0.06745 -0.01084

D136 -3.10923 -0.00116 -0.03134 0.00000 -0.03121 -3.14044

D137 3.06159 0.00262 0.08090 0.00000 0.08098 -3.14062

D138 0.03064 -0.00110 -0.01776 0.00000 -0.01768 0.01296

D139 -0.03026 0.00030 0.04196 0.00000 0.04193 0.01167

D140 3.08251 0.00119 0.07894 0.00000 0.07896 -3.12171

D141 3.11325 0.00024 0.02682 0.00000 0.02684 3.14009

D142 -0.05716 0.00113 0.06379 0.00000 0.06387 0.00671

D143 0.25858 -0.00263 -0.05685 0.00000 -0.05692 0.20166

D144 -3.01387 0.00165 0.05983 0.00000 0.05968 -2.95418

D145 0.03292 -0.00051 -0.03503 0.00000 -0.03504 -0.00212

D146 3.13609 0.00075 0.00707 0.00000 0.00706 -3.14004

D147 -3.05023 -0.00229 -0.09731 0.00000 -0.09731 3.13564

D148 0.05294 -0.00103 -0.05522 0.00000 -0.05521 -0.00228

D149 -3.06489 -0.00104 -0.02647 0.00000 -0.02646 -3.09135

D150 0.01763 0.00069 0.03651 0.00000 0.03650 0.05412

D151 0.00062 0.00001 -0.00057 0.00000 -0.00057 0.00005

D152 3.10428 0.00121 0.04092 0.00000 0.04093 -3.13798

D153 -3.10346 -0.00120 -0.04168 0.00000 -0.04168 3.13805

D154 0.00020 0.00000 -0.00018 0.00000 -0.00018 0.00002

D155 -0.03323 0.00052 0.03532 0.00000 0.03533 0.00210

D156 3.05063 0.00230 0.09695 0.00000 0.09695 -3.13561

D157 -3.13597 -0.00074 -0.00717 0.00000 -0.00717 3.14005

D158 -0.05211 0.00105 0.05446 0.00000 0.05446 0.00234

D159 3.06629 0.00101 0.02517 0.00000 0.02516 3.09145

D160 -0.01695 -0.00073 -0.03714 0.00000 -0.03713 -0.05408

D161 0.02966 -0.00037 -0.04154 0.00000 -0.04152 -0.01185

D162 3.12434 0.00066 0.01348 0.00000 0.01347 3.13781

D163 -3.08240 -0.00085 -0.07979 0.00000 -0.07972 3.12106

D164 0.01228 0.00018 -0.02477 0.00000 -0.02474 -0.01246

D165 3.05077 0.00129 0.12233 0.00000 0.12233 -3.11008

D166 -0.12086 0.00188 0.16112 0.00000 0.16112 0.04026

D167 0.00058 0.00001 -0.00053 0.00000 -0.00053 0.00004

D168 3.09587 0.00108 0.05364 0.00000 0.05362 -3.13370

D169 -3.09515 -0.00106 -0.05432 0.00000 -0.05429 3.13375

D170 0.00015 0.00001 -0.00014 0.00000 -0.00014 0.00001

D171 -0.02986 0.00037 0.04173 0.00000 0.04171 0.01184

D172 3.08283 0.00087 0.07939 0.00000 0.07932 -3.12103

D173 -3.12412 -0.00066 -0.01369 0.00000 -0.01368 -3.13779

D174 -0.01142 -0.00016 0.02397 0.00000 0.02394 0.01252

D175 -3.05000 -0.00132 -0.12305 0.00000 -0.12306 3.11012

D176 0.12099 -0.00193 -0.16126 0.00000 -0.16125 -0.04026

D177 -0.03335 0.00047 0.03542 0.00000 0.03543 0.00208

D178 -3.13614 -0.00076 -0.00701 0.00000 -0.00701 3.14004

D179 3.04934 0.00225 0.09812 0.00000 0.09811 -3.13574

D180 -0.05345 0.00102 0.05569 0.00000 0.05568 0.00222

D181 3.06464 0.00108 0.02669 0.00000 0.02667 3.09131

D182 -0.01739 -0.00065 -0.03673 0.00000 -0.03672 -0.05411

D183 -0.00064 -0.00001 0.00059 0.00000 0.00059 -0.00005

D184 -3.10392 -0.00119 -0.04125 0.00000 -0.04125 3.13802

D185 3.10306 0.00118 0.04203 0.00000 0.04203 -3.13810

D186 -0.00021 0.00000 0.00019 0.00000 0.00019 -0.00002

D187 0.03368 -0.00048 -0.03572 0.00000 -0.03573 -0.00205

D188 -3.04975 -0.00226 -0.09774 0.00000 -0.09773 3.13571

D189 3.13603 0.00075 0.00712 0.00000 0.00711 -3.14005

D190 0.05260 -0.00103 -0.05490 0.00000 -0.05489 -0.00229

D191 -3.06611 -0.00104 -0.02532 0.00000 -0.02531 -3.09142

D192 0.01667 0.00069 0.03740 0.00000 0.03739 0.05406

D193 0.03028 -0.00035 -0.04209 0.00000 -0.04208 -0.01180

D194 3.12435 0.00067 0.01348 0.00000 0.01347 3.13782

D195 -3.08231 -0.00085 -0.07985 0.00000 -0.07980 3.12107

D196 0.01175 0.00017 -0.02428 0.00000 -0.02425 -0.01250

D197 3.04967 0.00126 0.12334 0.00000 0.12335 -3.11017

D198 -0.12142 0.00187 0.16165 0.00000 0.16164 0.04022

D199 -0.00059 0.00000 0.00055 0.00000 0.00055 -0.00004

D200 3.09496 0.00105 0.05448 0.00000 0.05446 -3.13376

D201 -3.09571 -0.00107 -0.05379 0.00000 -0.05377 3.13371

D202 -0.00016 -0.00001 0.00015 0.00000 0.00015 -0.00001

D203 -0.03007 0.00034 0.04190 0.00000 0.04189 0.01181

D204 3.08188 0.00083 0.08025 0.00000 0.08020 -3.12110

D205 -3.12458 -0.00067 -0.01327 0.00000 -0.01326 -3.13784

D206 -0.01262 -0.00019 0.02508 0.00000 0.02505 0.01243

D207 -3.05044 -0.00123 -0.12261 0.00000 -0.12262 3.11013

D208 0.12130 -0.00183 -0.16152 0.00000 -0.16151 -0.04021

D209 1.09292 -0.00091 0.00315 0.00000 0.00315 1.09606

D210 -1.04703 -0.00221 0.00012 0.00000 0.00012 -1.04692

D211 -3.12287 -0.00094 0.00454 0.00000 0.00454 -3.11833

D212 1.04724 0.00222 -0.00031 0.00000 -0.00031 1.04693

D213 -1.09260 0.00091 -0.00344 0.00000 -0.00344 -1.09605

D214 3.12321 0.00092 -0.00486 0.00000 -0.00486 3.11835

D215 1.09263 0.00011 0.00475 0.00000 0.00475 1.09738

D216 -1.05460 0.00017 0.00783 0.00000 0.00783 -1.04677

D217 -3.12060 0.00001 0.00448 0.00000 0.00448 -3.11613

D218 1.05501 -0.00018 -0.00821 0.00000 -0.00821 1.04680

D219 -1.09232 -0.00010 -0.00504 0.00000 -0.00504 -1.09736

D220 3.12105 -0.00004 -0.00489 0.00000 -0.00489 3.11615

D221 1.04729 0.00219 -0.00036 0.00000 -0.00036 1.04693

D222 -1.09261 0.00090 -0.00343 0.00000 -0.00344 -1.09604

D223 3.12318 0.00089 -0.00483 0.00000 -0.00483 3.11835

D224 1.09229 -0.00089 0.00373 0.00000 0.00373 1.09602

D225 -1.04748 -0.00221 0.00054 0.00000 0.00054 -1.04695

D226 -3.12351 -0.00087 0.00514 0.00000 0.00514 -3.11837

D227 1.09206 0.00010 0.00528 0.00000 0.00528 1.09734

D228 -1.05532 0.00019 0.00850 0.00000 0.00850 -1.04682

D229 -3.12137 0.00006 0.00519 0.00000 0.00519 -3.11618

D230 1.05494 -0.00018 -0.00814 0.00000 -0.00814 1.04680

D231 -1.09237 -0.00011 -0.00500 0.00000 -0.00500 -1.09736

D232 3.12094 -0.00003 -0.00479 0.00000 -0.00479 3.11615

Item Value Threshold Converged?

Maximum Force 0.016008 0.000450 NO

RMS Force 0.003027 0.000300 NO

Maximum Displacement 1.538753 0.001800 NO

RMS Displacement 0.325109 0.001200 NO

Predicted change in Energy=-1.376483D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 02:02:08 2019, MaxMem= 1342177280 cpu: 13.4

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=3 Diff= 1.06D-04

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 -1.124274 2.795968 -0.042445

2 7 0 -0.000075 2.040503 -0.228607

3 6 0 1.124222 2.795900 -0.042899

4 6 0 0.712652 4.154214 0.265860

5 6 0 -0.712461 4.154265 0.266255

6 7 0 2.409998 2.380366 -0.139014

7 6 0 2.800196 1.129249 -0.218923

8 7 0 2.018746 0.000076 -0.163622

9 6 0 2.800272 -1.129041 -0.219289

10 6 0 4.211413 -0.705109 -0.334329

11 6 0 4.211349 0.705474 -0.333986

12 7 0 -2.410196 2.380454 -0.138231

13 6 0 -4.211698 0.705414 -0.332909

14 6 0 -4.211735 -0.705172 -0.333247

15 6 0 -2.800575 -1.129079 -0.218428

16 7 0 -2.019035 0.000057 -0.162903

17 6 0 -2.800542 1.129219 -0.218066

18 7 0 -2.410197 -2.380559 -0.138898

19 7 0 -0.000032 -2.040670 -0.229293

20 6 0 -1.124253 -2.796192 -0.043209

21 6 0 -0.712391 -4.154529 0.265213

22 6 0 0.712715 -4.154461 0.264817

23 6 0 1.124304 -2.796099 -0.043665

24 7 0 2.410087 -2.380413 -0.139688

25 30 0 -0.000332 -0.000259 -0.436907

26 6 0 -5.408655 1.429222 -0.416176

27 6 0 -6.602444 0.695287 -0.497031

28 6 0 -6.602468 -0.694854 -0.497458

29 6 0 -5.408706 -1.428885 -0.416992

30 6 0 1.432717 -5.334241 0.544981

31 6 0 0.700162 -6.495623 0.806310

32 6 0 -0.699302 -6.495670 0.806776

33 6 0 -1.432117 -5.334344 0.545887

34 6 0 5.408277 1.429296 -0.417326

35 6 0 6.602079 0.695388 -0.498317

36 6 0 6.602129 -0.694737 -0.498752

37 6 0 5.408383 -1.428789 -0.418156

38 6 0 -1.432192 5.334017 0.547143

39 6 0 -0.699386 6.495296 0.808291

40 6 0 0.700064 6.495265 0.807824

41 6 0 1.432635 5.333946 0.546236

42 1 0 7.553845 1.204637 -0.565944

43 1 0 7.553931 -1.203873 -0.566714

44 1 0 1.207900 7.425315 1.024666

45 1 0 -1.207035 7.425365 1.025483

46 1 0 -7.554226 1.204513 -0.564597

47 1 0 -7.554266 -1.204004 -0.565353

48 1 0 -1.206943 -7.425789 1.023772

49 1 0 1.208010 -7.425711 1.022957

50 8 0 2.781814 5.279624 0.557147

51 8 0 -2.781363 5.279764 0.558992

52 8 0 5.354108 2.776714 -0.419817

53 8 0 5.354302 -2.776210 -0.421522

54 8 0 2.781891 -5.279876 0.555942

55 8 0 -2.781283 -5.280076 0.557784

56 8 0 -5.354586 -2.776303 -0.420464

57 8 0 -5.354499 2.776639 -0.418787

58 6 0 3.503835 6.484313 0.802703

59 1 0 3.290726 6.881808 1.799296

60 1 0 3.281328 7.244930 0.049133

61 1 0 4.555824 6.211966 0.741680

62 6 0 6.580568 3.505537 -0.441942

63 1 0 7.148084 3.309942 -1.356287

64 1 0 7.198122 3.273187 0.430486

65 1 0 6.295621 4.555440 -0.413161

66 6 0 6.580799 -3.504951 -0.444268

67 1 0 7.198434 -3.273163 0.428251

68 1 0 7.148208 -3.308710 -1.358542

69 1 0 6.295913 -4.554890 -0.416170

70 6 0 -3.503160 6.484471 0.805115

71 1 0 -3.281154 7.245112 0.051421

72 1 0 -3.289324 6.881913 1.801574

73 1 0 -4.555205 6.212177 0.744829

74 6 0 -6.580960 3.505457 -0.440886

75 1 0 -7.198439 3.273200 0.431620

76 1 0 -7.148550 3.309767 -1.355164

77 1 0 -6.296011 4.555364 -0.412240

78 6 0 -6.581055 -3.505087 -0.443167

79 1 0 -7.148550 -3.308783 -1.357374

80 1 0 -7.198620 -3.273402 0.429430

81 1 0 -6.296128 -4.555017 -0.415191

82 6 0 -3.503094 -6.484830 0.803625

83 1 0 -3.289222 -6.882534 1.799972

84 1 0 -3.281131 -7.245279 0.049724

85 1 0 -4.555136 -6.212504 0.743453

86 6 0 3.503953 -6.484594 0.801217

87 1 0 3.281509 -7.245025 0.047441

88 1 0 3.290817 -6.882356 1.797698

89 1 0 4.555933 -6.212190 0.740309

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0448405 0.0437828 0.0225351

Leave Link 202 at Sat Jul 6 02:02:09 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8039.3996340209 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= 89 NActive= 89 NUniq= 89 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= -0.2278496854 Hartrees.

Nuclear repulsion after empirical dispersion term = 8039.1717843355 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6436

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.14D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 430

GePol: Fraction of low-weight points (<1% of avg) = 6.68%

GePol: Cavity surface area = 704.698 Ang\*\*2

GePol: Cavity volume = 802.617 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0088992793 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8039.1628850563 Hartrees.

Leave Link 301 at Sat Jul 6 02:02:09 2019, MaxMem= 1342177280 cpu: 1.5

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44289 LenP2D= 111280.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.71D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 02:02:13 2019, MaxMem= 1342177280 cpu: 41.5

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 02:02:14 2019, MaxMem= 1342177280 cpu: 3.2

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Lowest energy guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000072 -0.000067 0.000005 Ang= -0.01 deg.

Guess basis will be translated and rotated to current coordinates.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000027 -0.000001 0.000038 Ang= -0.01 deg.

Guess basis will be translated and rotated to current coordinates.

CkInt1: FT= 7.93D-02

Max alpha theta= 8.901 degrees.

Max beta theta= 8.876 degrees.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0171 S= 1.0057

Leave Link 401 at Sat Jul 6 02:02:24 2019, MaxMem= 1342177280 cpu: 123.4

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 124266288.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.03D-14 for 1591.

Iteration 1 A\*A^-1 deviation from orthogonality is 6.31D-15 for 4985 970.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.99D-15 for 499.

Iteration 1 A^-1\*A deviation from orthogonality is 3.34D-12 for 1659 1648.

E= -2649.79501601155

DIIS: error= 4.66D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79501601155 IErMin= 1 ErrMin= 4.66D-04

ErrMax= 4.66D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.22D-04 BMatP= 2.22D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.66D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 10.369 Goal= None Shift= 0.000

Gap= 10.410 Goal= None Shift= 0.000

RMSDP=4.39D-05 MaxDP=3.07D-03 OVMax= 1.40D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.33D-05 CP: 1.00D+00

E= -2649.79507692644 Delta-E= -0.000060914888 Rises=F Damp=F

DIIS: error= 1.58D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79507692644 IErMin= 2 ErrMin= 1.58D-04

ErrMax= 1.58D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.13D-05 BMatP= 2.22D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.58D-03

Coeff-Com: 0.236D+00 0.764D+00

Coeff-En: 0.000D+00 0.100D+01

Coeff: 0.235D+00 0.765D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=5.99D-06 MaxDP=3.37D-04 DE=-6.09D-05 OVMax= 1.28D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 5.77D-06 CP: 1.00D+00 9.72D-01

E= -2649.79507781639 Delta-E= -0.000000889953 Rises=F Damp=F

DIIS: error= 1.35D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79507781639 IErMin= 3 ErrMin= 1.35D-04

ErrMax= 1.35D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.50D-05 BMatP= 5.13D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.35D-03

Coeff-Com: -0.923D-02 0.485D+00 0.524D+00

Coeff-En: 0.000D+00 0.475D+00 0.525D+00

Coeff: -0.921D-02 0.485D+00 0.524D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=3.32D-06 MaxDP=2.50D-04 DE=-8.90D-07 OVMax= 8.32D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.34D-06 CP: 1.00D+00 9.96D-01 5.16D-01

E= -2649.79508484542 Delta-E= -0.000007029026 Rises=F Damp=F

DIIS: error= 2.28D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79508484542 IErMin= 4 ErrMin= 2.28D-05

ErrMax= 2.28D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.52D-06 BMatP= 4.50D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.104D-01 0.241D+00 0.288D+00 0.481D+00

Coeff: -0.104D-01 0.241D+00 0.288D+00 0.481D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=6.52D-07 MaxDP=4.78D-05 DE=-7.03D-06 OVMax= 1.29D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.08D-07 CP: 1.00D+00 9.97D-01 5.56D-01 6.66D-01

E= -2649.79508513070 Delta-E= -0.000000285279 Rises=F Damp=F

DIIS: error= 5.73D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79508513070 IErMin= 5 ErrMin= 5.73D-06

ErrMax= 5.73D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.96D-08 BMatP= 1.52D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.408D-02 0.645D-01 0.826D-01 0.244D+00 0.613D+00

Coeff: -0.408D-02 0.645D-01 0.826D-01 0.244D+00 0.613D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.71D-07 MaxDP=1.13D-05 DE=-2.85D-07 OVMax= 3.78D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.34D-07 CP: 1.00D+00 9.97D-01 5.53D-01 7.13D-01 8.06D-01

E= -2649.79508514861 Delta-E= -0.000000017915 Rises=F Damp=F

DIIS: error= 2.60D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79508514861 IErMin= 6 ErrMin= 2.60D-06

ErrMax= 2.60D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.27D-08 BMatP= 9.96D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.154D-02 0.208D-01 0.276D-01 0.108D+00 0.353D+00 0.492D+00

Coeff: -0.154D-02 0.208D-01 0.276D-01 0.108D+00 0.353D+00 0.492D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=7.15D-08 MaxDP=5.81D-06 DE=-1.79D-08 OVMax= 2.26D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.20D-08 CP: 1.00D+00 9.97D-01 5.50D-01 7.14D-01 8.39D-01

CP: 6.64D-01

E= -2649.79508515134 Delta-E= -0.000000002728 Rises=F Damp=F

DIIS: error= 9.30D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79508515134 IErMin= 7 ErrMin= 9.30D-07

ErrMax= 9.30D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.80D-09 BMatP= 1.27D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.700D-04-0.389D-02-0.442D-02 0.219D-02 0.541D-01 0.286D+00

Coeff-Com: 0.666D+00

Coeff: 0.700D-04-0.389D-02-0.442D-02 0.219D-02 0.541D-01 0.286D+00

Coeff: 0.666D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.71D-08 MaxDP=2.08D-06 DE=-2.73D-09 OVMax= 1.80D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.20D-08 CP: 1.00D+00 9.97D-01 5.51D-01 7.18D-01 8.56D-01

CP: 7.59D-01 9.89D-01

E= -2649.79508515167 Delta-E= -0.000000000333 Rises=F Damp=F

DIIS: error= 3.29D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.79508515167 IErMin= 8 ErrMin= 3.29D-07

ErrMax= 3.29D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.82D-10 BMatP= 1.80D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.170D-03-0.392D-02-0.474D-02-0.107D-01-0.136D-01 0.841D-01

Coeff-Com: 0.286D+00 0.663D+00

Coeff: 0.170D-03-0.392D-02-0.474D-02-0.107D-01-0.136D-01 0.841D-01

Coeff: 0.286D+00 0.663D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.36D-08 MaxDP=9.71D-07 DE=-3.33D-10 OVMax= 1.08D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 9.55D-09 CP: 1.00D+00 9.97D-01 5.51D-01 7.19D-01 8.62D-01

CP: 8.07D-01 1.10D+00 1.06D+00

E= -2649.79508515196 Delta-E= -0.000000000291 Rises=F Damp=F

DIIS: error= 1.70D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.79508515196 IErMin= 9 ErrMin= 1.70D-07

ErrMax= 1.70D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.74D-11 BMatP= 1.82D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.729D-04-0.503D-03-0.645D-03-0.624D-02-0.274D-01-0.614D-01

Coeff-Com: -0.120D+00 0.361D+00 0.855D+00

Coeff: 0.729D-04-0.503D-03-0.645D-03-0.624D-02-0.274D-01-0.614D-01

Coeff: -0.120D+00 0.361D+00 0.855D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.09D-08 MaxDP=8.27D-07 DE=-2.91D-10 OVMax= 1.00D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 4.46D-09 CP: 1.00D+00 9.97D-01 5.52D-01 7.20D-01 8.66D-01

CP: 8.34D-01 1.21D+00 1.38D+00 1.16D+00

E= -2649.79508515207 Delta-E= -0.000000000102 Rises=F Damp=F

DIIS: error= 8.84D-08 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -2649.79508515207 IErMin=10 ErrMin= 8.84D-08

ErrMax= 8.84D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.62D-11 BMatP= 6.74D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.193D-05 0.727D-03 0.828D-03-0.653D-03-0.111D-01-0.535D-01

Coeff-Com: -0.136D+00 0.505D-01 0.463D+00 0.687D+00

Coeff: -0.193D-05 0.727D-03 0.828D-03-0.653D-03-0.111D-01-0.535D-01

Coeff: -0.136D+00 0.505D-01 0.463D+00 0.687D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.57D-09 MaxDP=3.87D-07 DE=-1.02D-10 OVMax= 4.05D-06

Error on total polarization charges = 0.07287

SCF Done: E(UB3LYP) = -2649.79508515 A.U. after 10 cycles

NFock= 10 Conv=0.46D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0171 S= 1.0057

<L.S>= 0.000000000000E+00

KE= 2.690163785655D+03 PE=-2.235704777812D+04 EE= 8.977926022256D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.58

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0171, after 2.0002

Leave Link 502 at Sat Jul 6 02:10:23 2019, MaxMem= 1342177280 cpu: 5642.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44289 LenP2D= 111280.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 285

Leave Link 701 at Sat Jul 6 02:10:43 2019, MaxMem= 1342177280 cpu: 220.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 02:10:43 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 02:12:14 2019, MaxMem= 1342177280 cpu: 1094.9

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-1.28046177D-04 1.19784729D-03 1.60855500D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.001226176 0.001626463 -0.000323541

2 7 -0.000016451 -0.000406842 0.001769412

3 6 -0.001288120 0.001663712 -0.000327723

4 6 0.001425401 -0.000523458 -0.000081446

5 6 -0.001437309 -0.000549052 -0.000093590

6 7 0.000435643 0.000832979 -0.000299858

7 6 -0.001064140 0.000265245 0.000865059

8 7 0.001318623 -0.000044606 -0.001720128

9 6 -0.001139634 -0.000421600 0.000860820

10 6 0.001113191 0.000958268 -0.000602637

11 6 0.001140419 -0.000973030 -0.000609327

12 7 -0.000425118 0.000739126 -0.000299618

13 6 -0.001133746 -0.000954884 -0.000608281

14 6 -0.001106298 0.000939857 -0.000601662

15 6 0.001225715 -0.000553659 0.000867792

16 7 -0.001387315 -0.000046368 -0.001721688

17 6 0.001149222 0.000394910 0.000871544

18 7 -0.000461596 -0.000571742 -0.000309536

19 7 -0.000017500 0.000329278 0.001820265

20 6 0.001194837 -0.001563566 -0.000337550

21 6 -0.001453722 0.000549520 -0.000092207

22 6 0.001441509 0.000523661 -0.000080167

23 6 -0.001259000 -0.001601286 -0.000341483

24 7 0.000473440 -0.000667640 -0.000309710

25 30 0.000040196 0.000066742 0.001498768

26 6 0.001370478 0.000586141 0.000261507

27 6 -0.000580512 -0.000319556 0.000020381

28 6 -0.000577263 0.000315153 0.000021311

29 6 0.001361607 -0.000589771 0.000259769

30 6 0.000114619 0.000630996 0.000385042

31 6 -0.000032988 -0.000279657 -0.000102129

32 6 0.000030721 -0.000275406 -0.000103368

33 6 -0.000112739 0.000620657 0.000386328

34 6 -0.001364599 0.000590693 0.000263187

35 6 0.000580511 -0.000308749 0.000020607

36 6 0.000577284 0.000304308 0.000021577

37 6 -0.001355836 -0.000594398 0.000261333

38 6 -0.000120896 -0.000621722 0.000386995

39 6 0.000026718 0.000277719 -0.000103156

40 6 -0.000029019 0.000281891 -0.000101917

41 6 0.000122686 -0.000631919 0.000385757

42 1 -0.000088067 0.000182454 -0.000048838

43 1 -0.000087780 -0.000182597 -0.000048622

44 1 -0.000061010 -0.000079613 -0.000002378

45 1 0.000059992 -0.000079732 -0.000001733

46 1 0.000087473 0.000182592 -0.000048323

47 1 0.000087165 -0.000182728 -0.000048103

48 1 0.000060148 0.000079278 -0.000001443

49 1 -0.000061090 0.000079135 -0.000002081

50 8 0.000392823 -0.000315351 -0.000767445

51 8 -0.000398574 -0.000322192 -0.000764849

52 8 -0.000121506 0.000928446 0.000001420

53 8 -0.000124454 -0.000930769 0.000003096

54 8 0.000398373 0.000319211 -0.000768040

55 8 -0.000403837 0.000325702 -0.000765354

56 8 0.000130183 -0.000929120 0.000002720

57 8 0.000127672 0.000927180 0.000001191

58 6 0.000323490 -0.000514234 0.000333318

59 1 -0.000015298 0.000108124 0.000034679

60 1 0.000013178 0.000137166 -0.000047450

61 1 0.000055762 -0.000069018 -0.000003717

62 6 -0.000360256 0.000150950 -0.000032261

63 1 0.000053920 0.000015864 0.000002492

64 1 0.000148016 0.000082549 0.000008078

65 1 -0.000116180 0.000042406 0.000004061

66 6 -0.000358876 -0.000149792 -0.000031376

67 1 0.000147038 -0.000081134 0.000007946

68 1 0.000054639 -0.000016494 0.000002747

69 1 -0.000116125 -0.000042666 0.000005827

70 6 -0.000320198 -0.000512123 0.000334244

71 1 -0.000015250 0.000137542 -0.000047670

72 1 0.000016023 0.000106910 0.000033345

73 1 -0.000055999 -0.000069103 -0.000003914

74 6 0.000357110 0.000151561 -0.000032127

75 1 -0.000147934 0.000082236 0.000007450

76 1 -0.000053838 0.000015744 0.000002891

77 1 0.000116129 0.000042849 0.000005103

78 6 0.000355707 -0.000150428 -0.000031250

79 1 -0.000054540 -0.000016369 0.000003138

80 1 -0.000147000 -0.000080838 0.000007312

81 1 0.000116139 -0.000043101 0.000006831

82 6 -0.000318691 0.000509189 0.000334933

83 1 0.000015428 -0.000106747 0.000033563

84 1 -0.000015251 -0.000136996 -0.000048222

85 1 -0.000056407 0.000069501 -0.000004483

86 6 0.000322001 0.000511299 0.000334008

87 1 0.000013116 -0.000136584 -0.000048014

88 1 -0.000014739 -0.000107939 0.000034867

89 1 0.000056177 0.000069373 -0.000004298

-------------------------------------------------------------------

Cartesian Forces: Max 0.001820265 RMS 0.000583193

Leave Link 716 at Sat Jul 6 02:12:14 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001976485 RMS 0.000514064

Search for a local minimum.

Step number 16 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .51406D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 6 5 8 7 9

12 11 14 13 16

ITU= 0 -1 -1 0 -1 0 0 0 0 0 0 1 1 1 1 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.00526 0.01102 0.01309 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01316 0.01355

Eigenvalues --- 0.01442 0.01569 0.01572 0.01578 0.01583

Eigenvalues --- 0.01599 0.01617 0.01619 0.01707 0.01709

Eigenvalues --- 0.01712 0.01715 0.01793 0.01837 0.01872

Eigenvalues --- 0.01889 0.01923 0.01925 0.01926 0.01950

Eigenvalues --- 0.01978 0.02010 0.02021 0.02022 0.02023

Eigenvalues --- 0.02044 0.02052 0.02053 0.02053 0.02054

Eigenvalues --- 0.02057 0.02057 0.02057 0.02057 0.02060

Eigenvalues --- 0.02062 0.02067 0.02067 0.02067 0.02070

Eigenvalues --- 0.02070 0.02070 0.02070 0.02083 0.02083

Eigenvalues --- 0.02084 0.02132 0.02244 0.02260 0.02260

Eigenvalues --- 0.02260 0.02260 0.02260 0.02260 0.02345

Eigenvalues --- 0.02359 0.02363 0.02377 0.02743 0.03912

Eigenvalues --- 0.08709 0.09985 0.09985 0.09985 0.09991

Eigenvalues --- 0.09991 0.09991 0.10015 0.10114 0.10650

Eigenvalues --- 0.10650 0.10650 0.10655 0.10656 0.10656

Eigenvalues --- 0.10656 0.10669 0.13331 0.13453 0.14767

Eigenvalues --- 0.15955 0.15980 0.15989 0.15997 0.15999

Eigenvalues --- 0.15999 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16001 0.16008

Eigenvalues --- 0.16194 0.17031 0.18110 0.21186 0.21619

Eigenvalues --- 0.22474 0.22474 0.22475 0.22476 0.24027

Eigenvalues --- 0.24150 0.24323 0.24500 0.24504 0.24508

Eigenvalues --- 0.24513 0.24672 0.24776 0.24810 0.24864

Eigenvalues --- 0.24897 0.24917 0.24983 0.24989 0.24991

Eigenvalues --- 0.24994 0.24995 0.24995 0.24997 0.24998

Eigenvalues --- 0.24999 0.24999 0.24999 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25088 0.25333 0.27977

Eigenvalues --- 0.33175 0.33587 0.33630 0.33640 0.33671

Eigenvalues --- 0.33716 0.34062 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34063 0.34063 0.34078 0.34078

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34081

Eigenvalues --- 0.34081 0.34615 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34686 0.34687 0.34820

Eigenvalues --- 0.34939 0.34995 0.35277 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35632 0.35635

Eigenvalues --- 0.36627 0.37046 0.37136 0.37734 0.40216

Eigenvalues --- 0.41061 0.41209 0.41215 0.41215 0.41215

Eigenvalues --- 0.41215 0.41215 0.41216 0.41394 0.41396

Eigenvalues --- 0.41405 0.41407 0.41909 0.42215 0.42473

Eigenvalues --- 0.42540 0.43642 0.44499 0.44559 0.44739

Eigenvalues --- 0.44779 0.44871 0.44999 0.45000 0.45001

Eigenvalues --- 0.45002 0.45358 0.45365 0.45427 0.45899

Eigenvalues --- 0.47235 0.47354 0.48999 0.49227 0.49298

Eigenvalues --- 0.49827 0.51725 0.53554 0.53554 0.53554

Eigenvalues --- 0.53554 0.53554 0.53554 0.53993 0.54592

Eigenvalues --- 0.55000 0.56056 0.57388 0.57525 0.57556

Eigenvalues --- 0.64473

RFO step: Lambda=-8.04559727D-04 EMin= 5.25599974D-03

Quartic linear search produced a step of -0.46391.

Maximum step size ( 0.057) exceeded in Quadratic search.

-- Step size scaled by 0.858

Iteration 1 RMS(Cart)= 0.02476187 RMS(Int)= 0.00007351

Iteration 2 RMS(Cart)= 0.00025631 RMS(Int)= 0.00002008

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00002008

ITry= 1 IFail=0 DXMaxC= 8.06D-02 DCOld= 1.00D+10 DXMaxT= 5.71D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58361 -0.00047 -0.00021 -0.00237 -0.00259 2.58103

R2 2.74489 -0.00174 -0.00023 -0.00900 -0.00923 2.73566

R3 2.56016 -0.00004 0.00003 0.00405 0.00411 2.56427

R4 2.58358 -0.00046 -0.00027 -0.00164 -0.00190 2.58168

R5 3.87652 0.00020 -0.00244 0.00384 0.00134 3.87786

R6 2.74482 -0.00171 -0.00027 -0.00866 -0.00892 2.73589

R7 2.55995 0.00006 -0.00017 0.00633 0.00621 2.56617

R8 2.69307 0.00046 0.00000 0.00323 0.00325 2.69632

R9 2.66495 -0.00115 -0.00022 -0.00431 -0.00453 2.66042

R10 2.66493 -0.00115 -0.00022 -0.00426 -0.00448 2.66046

R11 2.48118 0.00046 -0.00058 0.00464 0.00411 2.48529

R12 2.59709 -0.00029 -0.00019 -0.00010 -0.00030 2.59678

R13 2.79282 0.00007 0.00003 0.00373 0.00377 2.79659

R14 2.59711 -0.00031 -0.00010 -0.00099 -0.00111 2.59600

R15 3.85030 -0.00053 -0.00300 -0.00891 -0.01199 3.83831

R16 2.79288 0.00004 0.00009 0.00334 0.00343 2.79631

R17 2.48160 0.00025 -0.00035 0.00185 0.00153 2.48313

R18 2.66562 -0.00018 -0.00009 -0.00227 -0.00234 2.66328

R19 2.64796 -0.00097 -0.00013 -0.00430 -0.00443 2.64353

R20 2.64798 -0.00098 -0.00014 -0.00431 -0.00445 2.64353

R21 2.48147 0.00030 -0.00040 0.00264 0.00227 2.48374

R22 2.66562 -0.00018 0.00001 -0.00306 -0.00304 2.66258

R23 2.79281 0.00005 0.00009 0.00336 0.00346 2.79627

R24 2.64800 -0.00099 -0.00012 -0.00443 -0.00455 2.64345

R25 2.79287 0.00002 0.00015 0.00295 0.00310 2.79597

R26 2.64799 -0.00098 -0.00012 -0.00442 -0.00454 2.64345

R27 2.59714 -0.00033 -0.00016 -0.00023 -0.00040 2.59674

R28 2.48190 0.00008 -0.00017 -0.00020 -0.00037 2.48153

R29 2.59712 -0.00031 -0.00025 0.00066 0.00041 2.59754

R30 3.84978 -0.00051 -0.00307 -0.00836 -0.01145 3.83832

R31 2.56026 -0.00010 0.00018 0.00248 0.00267 2.56292

R32 2.58369 -0.00050 -0.00028 -0.00179 -0.00207 2.58162

R33 2.58365 -0.00049 -0.00034 -0.00106 -0.00138 2.58227

R34 3.87573 0.00021 -0.00248 0.00423 0.00174 3.87746

R35 2.74488 -0.00175 -0.00019 -0.00927 -0.00946 2.73541

R36 2.69306 0.00046 0.00008 0.00259 0.00267 2.69573

R37 2.66495 -0.00115 -0.00022 -0.00429 -0.00451 2.66044

R38 2.74480 -0.00172 -0.00023 -0.00892 -0.00915 2.73565

R39 2.66497 -0.00115 -0.00022 -0.00435 -0.00456 2.66040

R40 2.56004 0.00000 -0.00001 0.00479 0.00481 2.56486

R41 2.65258 0.00125 0.00027 0.00463 0.00490 2.65747

R42 2.54831 0.00123 0.00009 0.00136 0.00145 2.54976

R43 2.62699 0.00145 0.00001 0.00282 0.00282 2.62981

R44 2.04385 0.00001 0.00000 0.00042 0.00042 2.04427

R45 2.65259 0.00124 0.00028 0.00457 0.00484 2.65743

R46 2.04384 0.00001 0.00000 0.00042 0.00042 2.04426

R47 2.54831 0.00123 0.00009 0.00138 0.00146 2.54977

R48 2.64139 0.00083 0.00034 0.00142 0.00176 2.64315

R49 2.55172 0.00080 0.00020 -0.00140 -0.00121 2.55051

R50 2.64460 0.00121 0.00017 0.00367 0.00384 2.64845

R51 2.04397 -0.00010 -0.00005 0.00038 0.00033 2.04430

R52 2.64140 0.00083 0.00035 0.00137 0.00171 2.64311

R53 2.04397 -0.00010 -0.00005 0.00038 0.00033 2.04430

R54 2.55172 0.00080 0.00019 -0.00137 -0.00118 2.55054

R55 2.65259 0.00125 0.00028 0.00461 0.00489 2.65748

R56 2.54831 0.00124 0.00010 0.00134 0.00144 2.54975

R57 2.62696 0.00146 0.00000 0.00296 0.00296 2.62991

R58 2.04385 0.00001 0.00000 0.00042 0.00042 2.04427

R59 2.65260 0.00124 0.00028 0.00456 0.00484 2.65744

R60 2.04385 0.00001 0.00000 0.00042 0.00042 2.04426

R61 2.54832 0.00124 0.00009 0.00136 0.00145 2.54977

R62 2.64141 0.00083 0.00035 0.00138 0.00173 2.64314

R63 2.55172 0.00080 0.00019 -0.00140 -0.00121 2.55052

R64 2.64458 0.00122 0.00017 0.00380 0.00397 2.64854

R65 2.04397 -0.00010 -0.00005 0.00038 0.00033 2.04430

R66 2.64140 0.00083 0.00034 0.00143 0.00177 2.64317

R67 2.04397 -0.00010 -0.00005 0.00038 0.00033 2.04430

R68 2.55173 0.00079 0.00020 -0.00143 -0.00123 2.55050

R69 2.69436 -0.00004 0.00020 -0.00108 -0.00088 2.69347

R70 2.69436 -0.00004 0.00020 -0.00108 -0.00088 2.69348

R71 2.69634 -0.00009 0.00004 -0.00118 -0.00114 2.69520

R72 2.69634 -0.00009 0.00004 -0.00117 -0.00113 2.69521

R73 2.69435 -0.00004 0.00020 -0.00106 -0.00086 2.69349

R74 2.69436 -0.00004 0.00020 -0.00105 -0.00086 2.69350

R75 2.69634 -0.00008 0.00004 -0.00114 -0.00110 2.69523

R76 2.69634 -0.00008 0.00004 -0.00115 -0.00111 2.69523

R77 2.06717 0.00007 -0.00003 -0.00005 -0.00008 2.06709

R78 2.06656 0.00013 0.00005 0.00038 0.00043 2.06699

R79 2.05675 0.00007 0.00000 -0.00040 -0.00040 2.05635

R80 2.06695 0.00002 0.00000 -0.00032 -0.00032 2.06663

R81 2.06706 0.00007 0.00002 -0.00014 -0.00012 2.06694

R82 2.05652 0.00007 0.00001 -0.00038 -0.00038 2.05615

R83 2.06706 0.00007 0.00002 -0.00014 -0.00013 2.06693

R84 2.06695 0.00002 0.00000 -0.00032 -0.00032 2.06663

R85 2.05652 0.00007 0.00001 -0.00038 -0.00038 2.05615

R86 2.06656 0.00013 0.00005 0.00038 0.00043 2.06699

R87 2.06717 0.00007 -0.00003 -0.00006 -0.00009 2.06708

R88 2.05675 0.00007 0.00000 -0.00040 -0.00040 2.05635

R89 2.06706 0.00007 0.00002 -0.00014 -0.00013 2.06693

R90 2.06695 0.00002 0.00001 -0.00033 -0.00032 2.06662

R91 2.05652 0.00007 0.00001 -0.00038 -0.00038 2.05615

R92 2.06695 0.00002 0.00001 -0.00033 -0.00033 2.06662

R93 2.06706 0.00007 0.00002 -0.00015 -0.00013 2.06693

R94 2.05652 0.00007 0.00001 -0.00038 -0.00038 2.05615

R95 2.06717 0.00007 -0.00003 -0.00006 -0.00009 2.06708

R96 2.06657 0.00013 0.00005 0.00038 0.00042 2.06699

R97 2.05674 0.00007 0.00000 -0.00040 -0.00040 2.05635

R98 2.06657 0.00013 0.00005 0.00038 0.00043 2.06699

R99 2.06717 0.00007 -0.00003 -0.00006 -0.00009 2.06708

R100 2.05675 0.00007 0.00000 -0.00040 -0.00040 2.05635

A1 1.88865 0.00036 -0.00015 0.00077 0.00059 1.88924

A2 2.21602 -0.00015 -0.00001 -0.00293 -0.00292 2.21310

A3 2.17844 -0.00021 0.00019 0.00203 0.00223 2.18067

A4 1.93092 -0.00039 0.00027 -0.00027 -0.00001 1.93091

A5 2.16933 0.00023 -0.00071 0.00295 0.00221 2.17155

A6 2.16949 0.00023 -0.00052 0.00107 0.00048 2.16998

A7 1.88868 0.00035 -0.00011 0.00045 0.00030 1.88898

A8 2.21606 -0.00017 0.00001 -0.00307 -0.00303 2.21303

A9 2.17837 -0.00018 0.00013 0.00249 0.00262 2.18100

A10 1.85818 -0.00016 0.00002 -0.00039 -0.00037 1.85781

A11 2.31843 -0.00049 -0.00024 -0.00122 -0.00146 2.31697

A12 2.10651 0.00065 0.00021 0.00165 0.00186 2.10837

A13 1.85816 -0.00015 0.00003 -0.00034 -0.00032 1.85784

A14 2.31847 -0.00050 -0.00023 -0.00132 -0.00155 2.31691

A15 2.10651 0.00065 0.00020 0.00170 0.00190 2.10841

A16 2.18790 -0.00041 -0.00016 -0.00330 -0.00341 2.18450

A17 2.22872 0.00064 0.00080 0.00494 0.00575 2.23447

A18 2.16727 -0.00011 -0.00017 -0.00124 -0.00138 2.16589

A19 1.88648 -0.00053 -0.00045 -0.00388 -0.00435 1.88213

A20 1.92842 0.00075 0.00063 0.00491 0.00558 1.93400

A21 2.16302 -0.00036 0.00015 -0.00253 -0.00244 2.16058

A22 2.16271 -0.00035 -0.00003 -0.00070 -0.00074 2.16197

A23 1.88646 -0.00051 -0.00050 -0.00352 -0.00403 1.88244

A24 2.22872 0.00067 0.00076 0.00515 0.00591 2.23463

A25 2.16730 -0.00015 -0.00008 -0.00182 -0.00187 2.16543

A26 1.86166 0.00014 0.00014 0.00127 0.00141 1.86307

A27 2.30788 -0.00107 -0.00029 -0.00578 -0.00608 2.30180

A28 2.11357 0.00092 0.00018 0.00440 0.00459 2.11815

A29 1.86169 0.00014 0.00014 0.00120 0.00134 1.86302

A30 2.30787 -0.00106 -0.00033 -0.00555 -0.00589 2.30198

A31 2.11356 0.00092 0.00022 0.00425 0.00447 2.11803

A32 2.18793 -0.00042 -0.00001 -0.00457 -0.00454 2.18339

A33 1.86169 0.00014 0.00015 0.00123 0.00138 1.86306

A34 2.11356 0.00092 0.00021 0.00431 0.00452 2.11808

A35 2.30787 -0.00106 -0.00033 -0.00564 -0.00598 2.30189

A36 1.86166 0.00014 0.00015 0.00131 0.00145 1.86311

A37 2.11357 0.00092 0.00017 0.00447 0.00465 2.11822

A38 2.30788 -0.00107 -0.00029 -0.00588 -0.00618 2.30170

A39 1.88648 -0.00051 -0.00059 -0.00285 -0.00344 1.88304

A40 2.16739 -0.00018 0.00010 -0.00331 -0.00320 2.16419

A41 2.22862 0.00070 0.00068 0.00597 0.00666 2.23528

A42 1.92839 0.00076 0.00082 0.00351 0.00433 1.93272

A43 2.16269 -0.00035 -0.00011 -0.00006 -0.00016 2.16253

A44 2.16302 -0.00036 0.00007 -0.00192 -0.00189 2.16112

A45 2.16737 -0.00014 0.00001 -0.00272 -0.00270 2.16467

A46 2.22862 0.00068 0.00072 0.00575 0.00649 2.23511

A47 1.88649 -0.00053 -0.00055 -0.00322 -0.00377 1.88272

A48 2.18796 -0.00041 0.00014 -0.00570 -0.00554 2.18242

A49 1.93092 -0.00037 0.00044 -0.00157 -0.00118 1.92974

A50 2.16931 0.00022 -0.00080 0.00367 0.00286 2.17217

A51 2.16948 0.00022 -0.00060 0.00176 0.00109 2.17058

A52 2.21595 -0.00013 -0.00007 -0.00236 -0.00240 2.21354

A53 2.17854 -0.00023 0.00034 0.00076 0.00108 2.17962

A54 1.88863 0.00036 -0.00024 0.00146 0.00120 1.88983

A55 1.85818 -0.00016 0.00004 -0.00038 -0.00035 1.85783

A56 2.31844 -0.00050 -0.00023 -0.00133 -0.00155 2.31688

A57 2.10651 0.00065 0.00019 0.00175 0.00194 2.10845

A58 1.85821 -0.00016 0.00003 -0.00042 -0.00040 1.85781

A59 2.10651 0.00065 0.00021 0.00168 0.00189 2.10840

A60 2.31841 -0.00048 -0.00024 -0.00122 -0.00146 2.31695

A61 1.88866 0.00035 -0.00020 0.00113 0.00091 1.88956

A62 2.21598 -0.00015 -0.00005 -0.00249 -0.00251 2.21348

A63 2.17848 -0.00019 0.00028 0.00123 0.00149 2.17997

A64 2.18793 -0.00041 -0.00001 -0.00441 -0.00438 2.18355

A65 1.55689 0.00009 0.00152 0.00216 0.00384 1.56073

A66 1.55711 0.00004 0.00176 -0.00013 0.00174 1.55885

A67 1.55724 0.00004 0.00175 -0.00011 0.00176 1.55900

A68 1.55748 -0.00001 0.00200 -0.00246 -0.00040 1.55708

A69 2.04858 -0.00097 -0.00029 -0.00540 -0.00569 2.04289

A70 2.07366 -0.00068 -0.00011 -0.00130 -0.00141 2.07225

A71 2.16094 0.00165 0.00039 0.00671 0.00710 2.16804

A72 2.12104 0.00005 0.00009 0.00106 0.00115 2.12219

A73 2.10115 -0.00023 -0.00010 -0.00252 -0.00261 2.09854

A74 2.06098 0.00018 0.00000 0.00147 0.00147 2.06246

A75 2.12104 0.00005 0.00010 0.00100 0.00109 2.12213

A76 2.06098 0.00018 -0.00001 0.00151 0.00150 2.06249

A77 2.10115 -0.00023 -0.00010 -0.00249 -0.00259 2.09856

A78 2.04858 -0.00097 -0.00028 -0.00543 -0.00571 2.04286

A79 2.07365 -0.00068 -0.00009 -0.00136 -0.00145 2.07220

A80 2.16095 0.00165 0.00036 0.00681 0.00717 2.16812

A81 2.05406 -0.00069 -0.00027 -0.00185 -0.00212 2.05194

A82 2.06923 -0.00128 -0.00087 -0.00612 -0.00699 2.06224

A83 2.15986 0.00197 0.00113 0.00799 0.00912 2.16898

A84 2.12255 0.00004 0.00005 0.00021 0.00025 2.12280

A85 2.10117 0.00000 0.00000 -0.00033 -0.00033 2.10084

A86 2.05944 -0.00004 -0.00007 0.00015 0.00009 2.05953

A87 2.12255 0.00004 0.00005 0.00019 0.00024 2.12280

A88 2.05944 -0.00004 -0.00007 0.00017 0.00010 2.05954

A89 2.10117 0.00000 0.00000 -0.00033 -0.00033 2.10083

A90 2.05406 -0.00069 -0.00027 -0.00187 -0.00214 2.05192

A91 2.06924 -0.00129 -0.00087 -0.00614 -0.00700 2.06224

A92 2.15985 0.00198 0.00112 0.00803 0.00915 2.16900

A93 2.04859 -0.00097 -0.00029 -0.00544 -0.00573 2.04285

A94 2.07366 -0.00068 -0.00014 -0.00112 -0.00126 2.07240

A95 2.16094 0.00165 0.00042 0.00657 0.00699 2.16793

A96 2.12104 0.00005 0.00008 0.00117 0.00124 2.12228

A97 2.10115 -0.00023 -0.00009 -0.00259 -0.00267 2.09848

A98 2.06099 0.00018 0.00000 0.00143 0.00143 2.06242

A99 2.12104 0.00005 0.00009 0.00111 0.00119 2.12223

A100 2.06099 0.00018 -0.00001 0.00147 0.00147 2.06246

A101 2.10115 -0.00023 -0.00009 -0.00256 -0.00265 2.09850

A102 2.04858 -0.00097 -0.00029 -0.00547 -0.00576 2.04283

A103 2.07365 -0.00068 -0.00012 -0.00117 -0.00130 2.07236

A104 2.16094 0.00165 0.00040 0.00666 0.00706 2.16800

A105 2.05406 -0.00069 -0.00026 -0.00192 -0.00218 2.05188

A106 2.06925 -0.00129 -0.00088 -0.00607 -0.00694 2.06231

A107 2.15984 0.00197 0.00113 0.00800 0.00913 2.16897

A108 2.12256 0.00004 0.00004 0.00028 0.00032 2.12287

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D3 -3.13600 -0.00054 -0.00033 -0.02231 -0.02263 3.12456

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D5 -0.01059 0.00036 0.00256 0.00660 0.00915 -0.00143

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D8 0.01322 0.00027 -0.00081 0.01351 0.01271 0.02594

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D53 -3.10164 -0.00013 0.00682 -0.01209 -0.00526 -3.10690

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D197 -3.11017 -0.00042 0.00492 -0.01752 -0.01260 -3.12277

D198 0.04022 -0.00040 0.00646 -0.02017 -0.01372 0.02650

D199 -0.00004 0.00000 0.00002 -0.00010 -0.00008 -0.00012

D200 -3.13376 -0.00002 0.00218 -0.00429 -0.00211 -3.13587

D201 3.13371 0.00001 -0.00216 0.00414 0.00199 3.13570

D202 -0.00001 0.00000 0.00001 -0.00005 -0.00004 -0.00005

D203 0.01181 -0.00005 0.00168 -0.00509 -0.00341 0.00840

D204 -3.12110 -0.00003 0.00323 -0.00784 -0.00462 -3.12573

D205 -3.13784 -0.00003 -0.00054 -0.00080 -0.00133 -3.13917

D206 0.01243 -0.00001 0.00102 -0.00355 -0.00254 0.00989

D207 3.11013 0.00042 -0.00489 0.01741 0.01252 3.12264

D208 -0.04021 0.00040 -0.00645 0.02021 0.01375 -0.02646

D209 1.09606 -0.00003 0.00013 -0.00460 -0.00447 1.09159

D210 -1.04692 -0.00005 0.00001 -0.00425 -0.00424 -1.05116

D211 -3.11833 -0.00003 0.00018 -0.00397 -0.00379 -3.12212

D212 1.04693 0.00005 -0.00001 0.00433 0.00432 1.05125

D213 -1.09605 0.00003 -0.00014 0.00469 0.00455 -1.09150

D214 3.11835 0.00003 -0.00019 0.00407 0.00387 3.12223

D215 1.09738 0.00005 0.00019 -0.00070 -0.00051 1.09687

D216 -1.04677 -0.00005 0.00031 -0.00050 -0.00019 -1.04696

D217 -3.11613 -0.00003 0.00018 -0.00076 -0.00058 -3.11670

D218 1.04680 0.00005 -0.00033 0.00052 0.00019 1.04699

D219 -1.09736 -0.00005 -0.00020 0.00072 0.00052 -1.09684

D220 3.11615 0.00003 -0.00020 0.00078 0.00058 3.11674

D221 1.04693 0.00005 -0.00001 0.00425 0.00424 1.05117

D222 -1.09604 0.00003 -0.00014 0.00460 0.00447 -1.09157

D223 3.11835 0.00003 -0.00019 0.00398 0.00378 3.12214

D224 1.09602 -0.00003 0.00015 -0.00470 -0.00455 1.09147

D225 -1.04695 -0.00005 0.00002 -0.00433 -0.00431 -1.05126

D226 -3.11837 -0.00003 0.00021 -0.00408 -0.00387 -3.12224

D227 1.09734 0.00005 0.00021 -0.00074 -0.00053 1.09681

D228 -1.04682 -0.00005 0.00034 -0.00054 -0.00020 -1.04702

D229 -3.11618 -0.00003 0.00021 -0.00081 -0.00060 -3.11677

D230 1.04680 0.00005 -0.00033 0.00052 0.00019 1.04699

D231 -1.09736 -0.00005 -0.00020 0.00073 0.00053 -1.09683

D232 3.11615 0.00003 -0.00019 0.00078 0.00059 3.11674

Item Value Threshold Converged?

Maximum Force 0.001976 0.000450 NO

RMS Force 0.000514 0.000300 NO

Maximum Displacement 0.080599 0.001800 NO

RMS Displacement 0.024828 0.001200 NO

Predicted change in Energy=-4.498144D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 02:12:16 2019, MaxMem= 1342177280 cpu: 14.5

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=0 Diff= 4.84D-04

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 -1.123377 2.800627 -0.021807

2 7 0 -0.000282 2.043016 -0.195444

3 6 0 1.123155 2.800782 -0.021996

4 6 0 0.713159 4.155117 0.284146

5 6 0 -0.713671 4.154886 0.284492

6 7 0 2.410690 2.384496 -0.136040

7 6 0 2.796332 1.130078 -0.221846

8 7 0 2.018151 -0.000845 -0.160521

9 6 0 2.795329 -1.131955 -0.221774

10 6 0 4.206396 -0.706330 -0.353607

11 6 0 4.207142 0.703016 -0.353440

12 7 0 -2.410019 2.384872 -0.135889

13 6 0 -4.204970 0.704297 -0.353719

14 6 0 -4.204716 -0.704680 -0.353913

15 6 0 -2.794041 -1.130811 -0.221543

16 7 0 -2.015535 -0.000152 -0.159998

17 6 0 -2.794244 1.130876 -0.221599

18 7 0 -2.410447 -2.383755 -0.135529

19 7 0 -0.001023 -2.040241 -0.194865

20 6 0 -1.124188 -2.798293 -0.021138

21 6 0 -0.715009 -4.152511 0.285417

22 6 0 0.711512 -4.153251 0.285061

23 6 0 1.121953 -2.799240 -0.021323

24 7 0 2.409411 -2.385066 -0.135662

25 30 0 0.001280 0.001252 -0.400901

26 6 0 -5.396149 1.432013 -0.444896

27 6 0 -6.590253 0.695067 -0.537829

28 6 0 -6.589947 -0.696567 -0.538221

29 6 0 -5.395509 -1.432966 -0.445576

30 6 0 1.431890 -5.331245 0.559578

31 6 0 0.697868 -6.492930 0.820431

32 6 0 -0.703631 -6.492131 0.821028

33 6 0 -1.436534 -5.329654 0.560654

34 6 0 5.398703 1.430276 -0.443895

35 6 0 6.592529 0.692807 -0.536265

36 6 0 6.591743 -0.698882 -0.536622

37 6 0 5.397076 -1.434980 -0.444510

38 6 0 -1.434738 5.332338 0.559659

39 6 0 -0.701322 6.494507 0.820029

40 6 0 0.700227 6.494800 0.819453

41 6 0 1.433926 5.332894 0.558618

42 1 0 7.543531 1.202956 -0.611043

43 1 0 7.542148 -1.210095 -0.611696

44 1 0 1.208007 7.425694 1.033646

45 1 0 -1.209325 7.425172 1.034687

46 1 0 -7.541019 1.205576 -0.613138

47 1 0 -7.540468 -1.207482 -0.613852

48 1 0 -1.211993 -7.422601 1.035682

49 1 0 1.205340 -7.423997 1.034603

50 8 0 2.782053 5.268571 0.561715

51 8 0 -2.782842 5.267390 0.563995

52 8 0 5.337979 2.778174 -0.440049

53 8 0 5.334664 -2.782811 -0.441419

54 8 0 2.780044 -5.267274 0.562650

55 8 0 -2.784620 -5.264073 0.565008

56 8 0 -5.333242 -2.780808 -0.442772

57 8 0 -5.334659 2.779880 -0.441265

58 6 0 3.516850 6.463170 0.815799

59 1 0 3.311019 6.855841 1.815780

60 1 0 3.300469 7.232490 0.068982

61 1 0 4.565497 6.180206 0.749561

62 6 0 6.557057 3.517883 -0.468986

63 1 0 7.119133 3.331308 -1.388361

64 1 0 7.184846 3.288477 0.396808

65 1 0 6.262456 4.564715 -0.433761

66 6 0 6.552825 -3.524007 -0.471062

67 1 0 7.181084 -3.295894 0.394730

68 1 0 7.114926 -3.337574 -1.390449

69 1 0 6.256944 -4.570497 -0.436405

70 6 0 -3.517917 6.461639 0.818940

71 1 0 -3.302629 7.231129 0.071983

72 1 0 -3.311241 6.854295 1.818751

73 1 0 -4.566509 6.178225 0.753746

74 6 0 -6.553322 3.520271 -0.470961

75 1 0 -7.181659 3.291387 0.394571

76 1 0 -7.115037 3.333809 -1.390576

77 1 0 -6.258172 4.566950 -0.435813

78 6 0 -6.551487 -3.521862 -0.473214

79 1 0 -7.113100 -3.335114 -1.392831

80 1 0 -7.180139 -3.293893 0.392328

81 1 0 -6.255761 -4.568400 -0.438689

82 6 0 -3.520236 -6.458037 0.819785

83 1 0 -3.313709 -6.850943 1.819524

84 1 0 -3.305302 -7.227495 0.072694

85 1 0 -4.568706 -6.174157 0.754664

86 6 0 3.514520 -6.462125 0.816533

87 1 0 3.297909 -7.231253 0.069587

88 1 0 3.308589 -6.854902 1.816449

89 1 0 4.563250 -6.179457 0.750332

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0448816 0.0439260 0.0226006

Leave Link 202 at Sat Jul 6 02:12:17 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8045.9578937855 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= 89 NActive= 89 NUniq= 89 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= -0.2280310288 Hartrees.

Nuclear repulsion after empirical dispersion term = 8045.7298627567 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6429

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.22D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 420

GePol: Fraction of low-weight points (<1% of avg) = 6.53%

GePol: Cavity surface area = 703.026 Ang\*\*2

GePol: Cavity volume = 801.212 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0089269469 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8045.7209358099 Hartrees.

Leave Link 301 at Sat Jul 6 02:12:17 2019, MaxMem= 1342177280 cpu: 1.3

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44368 LenP2D= 111395.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.61D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 02:12:21 2019, MaxMem= 1342177280 cpu: 42.0

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 02:12:21 2019, MaxMem= 1342177280 cpu: 3.0

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000104 0.000106 0.000092 Ang= 0.02 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>= 2.0171 S= 1.0057

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2650.02715890222

Leave Link 401 at Sat Jul 6 02:12:39 2019, MaxMem= 1342177280 cpu: 204.7

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 123996123.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.66D-15 for 6399.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.63D-15 for 6409 6024.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.88D-15 for 6399.

Iteration 1 A^-1\*A deviation from orthogonality is 9.76D-12 for 1764 1736.

E= -2649.79307299071

DIIS: error= 8.32D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79307299071 IErMin= 1 ErrMin= 8.32D-04

ErrMax= 8.32D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.38D-03 BMatP= 5.38D-03

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.32D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.687 Goal= None Shift= 0.000

Gap= 0.745 Goal= None Shift= 0.000

RMSDP=7.10D-05 MaxDP=2.26D-03 OVMax= 6.22D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 7.10D-05 CP: 1.00D+00

E= -2649.79521122585 Delta-E= -0.002138235137 Rises=F Damp=F

DIIS: error= 1.79D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79521122585 IErMin= 2 ErrMin= 1.79D-04

ErrMax= 1.79D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.53D-04 BMatP= 5.38D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.79D-03

Coeff-Com: -0.255D-01 0.103D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.254D-01 0.103D+01

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.22D-05 MaxDP=8.79D-04 DE=-2.14D-03 OVMax= 2.62D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.18D-05 CP: 1.00D+00 1.04D+00

E= -2649.79519355189 Delta-E= 0.000017673961 Rises=F Damp=F

DIIS: error= 3.49D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -2649.79521122585 IErMin= 2 ErrMin= 1.79D-04

ErrMax= 3.49D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.06D-04 BMatP= 1.53D-04

IDIUse=3 WtCom= 3.49D-01 WtEn= 6.51D-01

Coeff-Com: -0.391D-01 0.627D+00 0.412D+00

Coeff-En: 0.000D+00 0.595D+00 0.405D+00

Coeff: -0.136D-01 0.606D+00 0.408D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=7.73D-06 MaxDP=6.93D-04 DE= 1.77D-05 OVMax= 1.54D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.28D-06 CP: 1.00D+00 1.05D+00 4.58D-01

E= -2649.79525442161 Delta-E= -0.000060869725 Rises=F Damp=F

DIIS: error= 8.19D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79525442161 IErMin= 4 ErrMin= 8.19D-05

ErrMax= 8.19D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-05 BMatP= 1.53D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.133D-01 0.170D+00 0.196D+00 0.648D+00

Coeff: -0.133D-01 0.170D+00 0.196D+00 0.648D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.96D-06 MaxDP=1.60D-04 DE=-6.09D-05 OVMax= 4.97D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.57D-06 CP: 1.00D+00 1.05D+00 5.29D-01 8.29D-01

E= -2649.79525634225 Delta-E= -0.000001920635 Rises=F Damp=F

DIIS: error= 3.01D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79525634225 IErMin= 5 ErrMin= 3.01D-05

ErrMax= 3.01D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.27D-06 BMatP= 1.04D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.343D-02 0.280D-01 0.702D-01 0.397D+00 0.508D+00

Coeff: -0.343D-02 0.280D-01 0.702D-01 0.397D+00 0.508D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=7.82D-07 MaxDP=5.25D-05 DE=-1.92D-06 OVMax= 2.11D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 5.56D-07 CP: 1.00D+00 1.05D+00 5.29D-01 8.96D-01 7.10D-01

E= -2649.79525680668 Delta-E= -0.000000464435 Rises=F Damp=F

DIIS: error= 8.97D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79525680668 IErMin= 6 ErrMin= 8.97D-06

ErrMax= 8.97D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.42D-07 BMatP= 2.27D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.571D-04-0.105D-01 0.740D-02 0.106D+00 0.245D+00 0.652D+00

Coeff: 0.571D-04-0.105D-01 0.740D-02 0.106D+00 0.245D+00 0.652D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.69D-07 MaxDP=1.40D-05 DE=-4.64D-07 OVMax= 1.54D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.03D-07 CP: 1.00D+00 1.05D+00 5.33D-01 9.20D-01 7.70D-01

CP: 8.19D-01

E= -2649.79525684466 Delta-E= -0.000000037977 Rises=F Damp=F

DIIS: error= 4.15D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79525684466 IErMin= 7 ErrMin= 4.15D-06

ErrMax= 4.15D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.21D-08 BMatP= 1.42D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.553D-03-0.114D-01-0.538D-02 0.121D-01 0.857D-01 0.413D+00

Coeff-Com: 0.506D+00

Coeff: 0.553D-03-0.114D-01-0.538D-02 0.121D-01 0.857D-01 0.413D+00

Coeff: 0.506D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.12D-07 MaxDP=5.76D-06 DE=-3.80D-08 OVMax= 3.44D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 9.40D-08 CP: 1.00D+00 1.05D+00 5.35D-01 9.27D-01 7.70D-01

CP: 9.01D-01 9.76D-01

E= -2649.79525685648 Delta-E= -0.000000011818 Rises=F Damp=F

DIIS: error= 1.60D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.79525685648 IErMin= 8 ErrMin= 1.60D-06

ErrMax= 1.60D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.71D-09 BMatP= 4.21D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.130D-03-0.101D-02-0.245D-02-0.157D-01-0.206D-01-0.368D-03

Coeff-Com: 0.971D-01 0.943D+00

Coeff: 0.130D-03-0.101D-02-0.245D-02-0.157D-01-0.206D-01-0.368D-03

Coeff: 0.971D-01 0.943D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=7.24D-08 MaxDP=3.77D-06 DE=-1.18D-08 OVMax= 7.07D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 3.54D-08 CP: 1.00D+00 1.05D+00 5.35D-01 9.32D-01 7.81D-01

CP: 9.52D-01 1.21D+00 1.16D+00

E= -2649.79525685835 Delta-E= -0.000000001875 Rises=F Damp=F

DIIS: error= 7.47D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.79525685835 IErMin= 9 ErrMin= 7.47D-07

ErrMax= 7.47D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.51D-09 BMatP= 1.71D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.304D-04 0.168D-02-0.341D-03-0.116D-01-0.286D-01-0.775D-01

Coeff-Com: -0.564D-01 0.593D+00 0.580D+00

Coeff: -0.304D-04 0.168D-02-0.341D-03-0.116D-01-0.286D-01-0.775D-01

Coeff: -0.564D-01 0.593D+00 0.580D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=3.26D-08 MaxDP=2.62D-06 DE=-1.88D-09 OVMax= 2.08D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.96D-08 CP: 1.00D+00 1.05D+00 5.36D-01 9.33D-01 7.86D-01

CP: 9.70D-01 1.28D+00 1.33D+00 9.10D-01

E= -2649.79525685887 Delta-E= -0.000000000515 Rises=F Damp=F

DIIS: error= 3.48D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -2649.79525685887 IErMin=10 ErrMin= 3.48D-07

ErrMax= 3.48D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.29D-10 BMatP= 1.51D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.498D-04 0.120D-02 0.491D-03-0.222D-02-0.100D-01-0.405D-01

Coeff-Com: -0.675D-01 0.950D-01 0.307D+00 0.717D+00

Coeff: -0.498D-04 0.120D-02 0.491D-03-0.222D-02-0.100D-01-0.405D-01

Coeff: -0.675D-01 0.950D-01 0.307D+00 0.717D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.64D-08 MaxDP=1.44D-06 DE=-5.15D-10 OVMax= 1.41D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 8.24D-09 CP: 1.00D+00 1.05D+00 5.36D-01 9.34D-01 7.86D-01

CP: 9.76D-01 1.32D+00 1.41D+00 1.08D+00 9.88D-01

E= -2649.79525685896 Delta-E= -0.000000000098 Rises=F Damp=F

DIIS: error= 1.69D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -2649.79525685896 IErMin=11 ErrMin= 1.69D-07

ErrMax= 1.69D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.23D-11 BMatP= 2.29D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.158D-04 0.196D-03 0.300D-03 0.125D-02 0.122D-02-0.225D-02

Coeff-Com: -0.239D-01-0.682D-01 0.245D-01 0.367D+00 0.700D+00

Coeff: -0.158D-04 0.196D-03 0.300D-03 0.125D-02 0.122D-02-0.225D-02

Coeff: -0.239D-01-0.682D-01 0.245D-01 0.367D+00 0.700D+00

Gap= 0.046 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=6.47D-09 MaxDP=6.39D-07 DE=-9.82D-11 OVMax= 6.16D-06

Error on total polarization charges = 0.07302

SCF Done: E(UB3LYP) = -2649.79525686 A.U. after 11 cycles

NFock= 11 Conv=0.65D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0170 S= 1.0056

<L.S>= 0.000000000000E+00

KE= 2.690166490052D+03 PE=-2.237018485014D+04 EE= 8.984502167419D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.60

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0170, after 2.0002

Leave Link 502 at Sat Jul 6 02:21:34 2019, MaxMem= 1342177280 cpu: 6319.2

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44368 LenP2D= 111395.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 285

Leave Link 701 at Sat Jul 6 02:21:54 2019, MaxMem= 1342177280 cpu: 220.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 02:21:54 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 02:23:29 2019, MaxMem= 1342177280 cpu: 1143.5

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-1.33748071D-03-6.44353121D-03 1.94687631D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.001089415 -0.001022401 -0.000735606

2 7 0.000275068 -0.001447718 -0.000109032

3 6 0.001631333 -0.001481358 -0.000832149

4 6 -0.000683994 0.000360282 -0.000199206

5 6 0.000796148 0.000463092 -0.000190703

6 7 -0.001234324 -0.001383196 0.000239302

7 6 0.000175684 0.000948700 0.000687126

8 7 -0.000374231 0.000392767 -0.000199971

9 6 0.000806584 -0.000201261 0.000582887

10 6 -0.001256365 -0.000294238 -0.000193192

11 6 -0.001334824 0.000408985 -0.000185900

12 7 0.001012461 -0.001069065 0.000243637

13 6 0.001290273 0.000423620 -0.000200068

14 6 0.001211596 -0.000304410 -0.000206507

15 6 -0.001138625 0.000536096 0.000512730

16 7 -0.000202800 0.000401009 -0.000234646

17 6 -0.000492441 0.000234467 0.000615990

18 7 0.001076213 0.000338962 0.000265470

19 7 0.000266336 0.000818920 -0.000044426

20 6 -0.000640110 0.000784862 -0.000721405

21 6 0.000798612 -0.000495369 -0.000180143

22 6 -0.000681738 -0.000392581 -0.000188327

23 6 0.001198580 0.001247606 -0.000818641

24 7 -0.001303968 0.000669271 0.000262610

25 30 -0.000026221 0.000008126 0.000283915

26 6 -0.000993889 -0.000278829 0.000123099

27 6 0.000200555 0.000481263 0.000097105

28 6 0.000197818 -0.000474009 0.000097774

29 6 -0.000966689 0.000288355 0.000125200

30 6 -0.000295657 0.000072079 0.000435912

31 6 -0.000217455 -0.000296754 -0.000081881

32 6 0.000221036 -0.000312581 -0.000080820

33 6 0.000296810 0.000109079 0.000426887

34 6 0.000975564 -0.000340414 0.000123673

35 6 -0.000186631 0.000412252 0.000098111

36 6 -0.000185047 -0.000405448 0.000098008

37 6 0.000949028 0.000352305 0.000125690

38 6 0.000363482 -0.000109564 0.000430671

39 6 0.000263920 0.000318943 -0.000079113

40 6 -0.000258950 0.000302553 -0.000080064

41 6 -0.000360819 -0.000072221 0.000439769

42 1 0.000077686 0.000009054 -0.000072041

43 1 0.000084427 -0.000008728 -0.000071638

44 1 -0.000039077 -0.000031926 0.000050725

45 1 0.000040337 -0.000030532 0.000052103

46 1 -0.000078865 0.000015252 -0.000070893

47 1 -0.000083561 -0.000014163 -0.000070856

48 1 0.000037103 0.000032311 0.000052927

49 1 -0.000034906 0.000034343 0.000050724

50 8 0.000326851 0.000730884 -0.000182706

51 8 -0.000293434 0.000757424 -0.000188448

52 8 0.000259359 -0.000358207 -0.000033658

53 8 0.000315178 0.000394120 -0.000030016

54 8 0.000306929 -0.000781044 -0.000175687

55 8 -0.000272798 -0.000807286 -0.000182154

56 8 -0.000408268 0.000395812 -0.000022162

57 8 -0.000354206 -0.000364273 -0.000027355

58 6 0.000062496 0.000040874 0.000019318

59 1 -0.000207580 -0.000006195 0.000126527

60 1 0.000062341 0.000109917 0.000014397

61 1 0.000191424 -0.000025395 -0.000021150

62 6 0.000129251 -0.000283759 -0.000093183

63 1 0.000101574 -0.000052953 -0.000178090

64 1 0.000082464 -0.000063187 0.000165774

65 1 -0.000090266 0.000167337 0.000006224

66 6 0.000121568 0.000281698 -0.000087447

67 1 0.000082365 0.000066776 0.000166619

68 1 0.000103930 0.000054924 -0.000179225

69 1 -0.000086314 -0.000162730 0.000007546

70 6 -0.000057514 0.000037288 0.000018670

71 1 -0.000066849 0.000111693 0.000013222

72 1 0.000209042 -0.000005548 0.000125941

73 1 -0.000188225 -0.000025536 -0.000023948

74 6 -0.000110748 -0.000293930 -0.000089710

75 1 -0.000085373 -0.000065726 0.000167648

76 1 -0.000106441 -0.000053860 -0.000180808

77 1 0.000090575 0.000164081 0.000008556

78 6 -0.000102540 0.000294664 -0.000084848

79 1 -0.000109218 0.000054923 -0.000181818

80 1 -0.000085857 0.000067594 0.000168821

81 1 0.000088067 -0.000159516 0.000009843

82 6 -0.000047948 -0.000024411 0.000015305

83 1 0.000209136 0.000002468 0.000129224

84 1 -0.000067680 -0.000114911 0.000012421

85 1 -0.000185153 0.000028134 -0.000026249

86 6 0.000055655 -0.000029113 0.000016761

87 1 0.000061109 -0.000111714 0.000014337

88 1 -0.000207679 0.000003813 0.000129222

89 1 0.000188726 0.000027084 -0.000022529

-------------------------------------------------------------------

Cartesian Forces: Max 0.001631333 RMS 0.000449933

Leave Link 716 at Sat Jul 6 02:23:29 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001645617 RMS 0.000399198

Search for a local minimum.

Step number 17 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .39920D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 4 6 5 8 7

10 9 11 14 13

16 17

DE= -1.72D-04 DEPred=-4.50D-04 R= 3.82D-01

Trust test= 3.82D-01 RLast= 1.25D-01 DXMaxT set to 5.71D-02

ITU= 0 0 -1 -1 0 -1 0 0 0 0 0 0 1 1 1 1 0

Eigenvalues --- 0.00487 0.01172 0.01260 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01316 0.01344

Eigenvalues --- 0.01395 0.01570 0.01571 0.01583 0.01599

Eigenvalues --- 0.01609 0.01617 0.01620 0.01707 0.01709

Eigenvalues --- 0.01713 0.01716 0.01813 0.01836 0.01870

Eigenvalues --- 0.01883 0.01923 0.01925 0.01949 0.01951

Eigenvalues --- 0.01972 0.01999 0.02020 0.02022 0.02037

Eigenvalues --- 0.02052 0.02053 0.02053 0.02053 0.02053

Eigenvalues --- 0.02057 0.02057 0.02057 0.02057 0.02057

Eigenvalues --- 0.02066 0.02067 0.02067 0.02070 0.02070

Eigenvalues --- 0.02070 0.02071 0.02076 0.02083 0.02083

Eigenvalues --- 0.02131 0.02195 0.02243 0.02260 0.02260

Eigenvalues --- 0.02260 0.02260 0.02260 0.02260 0.02343

Eigenvalues --- 0.02352 0.02358 0.02365 0.02609 0.04001

Eigenvalues --- 0.09920 0.09978 0.09978 0.09978 0.09985

Eigenvalues --- 0.09985 0.09985 0.10023 0.10644 0.10648

Eigenvalues --- 0.10648 0.10648 0.10652 0.10653 0.10653

Eigenvalues --- 0.10653 0.12389 0.13404 0.13458 0.14364

Eigenvalues --- 0.15960 0.15982 0.15993 0.15998 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16003 0.16051

Eigenvalues --- 0.16154 0.16799 0.19106 0.21215 0.21652

Eigenvalues --- 0.22473 0.22474 0.22476 0.22477 0.24207

Eigenvalues --- 0.24258 0.24388 0.24507 0.24514 0.24563

Eigenvalues --- 0.24571 0.24653 0.24782 0.24830 0.24866

Eigenvalues --- 0.24900 0.24923 0.24979 0.24980 0.24993

Eigenvalues --- 0.24994 0.24997 0.24997 0.24998 0.24998

Eigenvalues --- 0.24999 0.24999 0.24999 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25001 0.25144 0.26640 0.28856

Eigenvalues --- 0.33425 0.33609 0.33631 0.33674 0.33715

Eigenvalues --- 0.34054 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34063 0.34065 0.34078 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34081

Eigenvalues --- 0.34180 0.34623 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34686 0.34687 0.34855

Eigenvalues --- 0.34941 0.35150 0.35574 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35632 0.35895

Eigenvalues --- 0.36574 0.37061 0.37132 0.37954 0.40738

Eigenvalues --- 0.40834 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41215 0.41216 0.41413 0.41416 0.41417

Eigenvalues --- 0.41419 0.41533 0.41767 0.42298 0.42462

Eigenvalues --- 0.42817 0.44447 0.44559 0.44706 0.44774

Eigenvalues --- 0.44874 0.44998 0.44999 0.45001 0.45002

Eigenvalues --- 0.45092 0.45365 0.45367 0.45890 0.46141

Eigenvalues --- 0.46763 0.47261 0.47980 0.49264 0.49315

Eigenvalues --- 0.49835 0.53038 0.53554 0.53554 0.53554

Eigenvalues --- 0.53554 0.53554 0.53557 0.54766 0.55009

Eigenvalues --- 0.56062 0.56831 0.57400 0.57553 0.58747

Eigenvalues --- 0.61331

En-DIIS/RFO-DIIS IScMMF= 0 using points: 17 16

RFO step: Lambda=-1.38505546D-04.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 1.72D-04 SmlDif= 1.00D-05

RMS Error= 0.7491060273D-03 NUsed= 2 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.63481 0.36519

Iteration 1 RMS(Cart)= 0.01405260 RMS(Int)= 0.00004935

Iteration 2 RMS(Cart)= 0.00010236 RMS(Int)= 0.00000633

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000633

ITry= 1 IFail=0 DXMaxC= 4.29D-02 DCOld= 1.00D+10 DXMaxT= 5.71D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58103 0.00033 0.00094 0.00041 0.00133 2.58236

R2 2.73566 0.00155 0.00337 0.00162 0.00500 2.74066

R3 2.56427 -0.00052 -0.00150 -0.00241 -0.00390 2.56037

R4 2.58168 0.00023 0.00069 0.00007 0.00075 2.58243

R5 3.87786 -0.00105 -0.00049 -0.00583 -0.00636 3.87151

R6 2.73589 0.00136 0.00326 0.00143 0.00470 2.74059

R7 2.56617 -0.00142 -0.00227 -0.00353 -0.00578 2.56038

R8 2.69632 0.00001 -0.00119 -0.00125 -0.00242 2.69390

R9 2.66042 0.00125 0.00165 0.00025 0.00190 2.66233

R10 2.66046 0.00124 0.00164 0.00024 0.00188 2.66233

R11 2.48529 -0.00163 -0.00150 -0.00146 -0.00294 2.48235

R12 2.59678 -0.00010 0.00011 -0.00063 -0.00051 2.59627

R13 2.79659 -0.00013 -0.00138 -0.00148 -0.00285 2.79374

R14 2.59600 0.00014 0.00041 -0.00018 0.00022 2.59622

R15 3.83831 0.00033 0.00438 0.00061 0.00497 3.84329

R16 2.79631 0.00012 -0.00125 -0.00121 -0.00246 2.79385

R17 2.48313 -0.00037 -0.00056 -0.00018 -0.00072 2.48240

R18 2.66328 0.00018 0.00085 0.00112 0.00198 2.66526

R19 2.64353 0.00125 0.00162 0.00035 0.00196 2.64549

R20 2.64353 0.00121 0.00162 0.00031 0.00193 2.64546

R21 2.48374 -0.00065 -0.00083 -0.00052 -0.00133 2.48241

R22 2.66258 0.00040 0.00111 0.00159 0.00270 2.66528

R23 2.79627 0.00004 -0.00126 -0.00124 -0.00250 2.79377

R24 2.64345 0.00132 0.00166 0.00040 0.00206 2.64551

R25 2.79597 0.00028 -0.00113 -0.00099 -0.00212 2.79385

R26 2.64345 0.00135 0.00166 0.00043 0.00209 2.64554

R27 2.59674 0.00008 0.00015 -0.00056 -0.00041 2.59633

R28 2.48153 0.00062 0.00013 0.00077 0.00092 2.48245

R29 2.59754 -0.00016 -0.00015 -0.00100 -0.00115 2.59638

R30 3.83832 0.00070 0.00418 0.00108 0.00525 3.84357

R31 2.56292 0.00019 -0.00097 -0.00158 -0.00254 2.56038

R32 2.58162 0.00031 0.00075 0.00007 0.00081 2.58243

R33 2.58227 0.00022 0.00050 -0.00025 0.00023 2.58251

R34 3.87746 -0.00061 -0.00063 -0.00523 -0.00590 3.87157

R35 2.73541 0.00165 0.00346 0.00180 0.00526 2.74067

R36 2.69573 0.00017 -0.00098 -0.00085 -0.00181 2.69393

R37 2.66044 0.00128 0.00165 0.00028 0.00193 2.66236

R38 2.73565 0.00146 0.00334 0.00161 0.00495 2.74061

R39 2.66040 0.00129 0.00167 0.00029 0.00196 2.66236

R40 2.56486 -0.00072 -0.00176 -0.00270 -0.00445 2.56041

R41 2.65747 -0.00071 -0.00179 -0.00044 -0.00223 2.65524

R42 2.54976 -0.00064 -0.00053 0.00076 0.00023 2.54999

R43 2.62981 -0.00062 -0.00103 0.00051 -0.00052 2.62928

R44 2.04427 0.00008 -0.00015 -0.00010 -0.00026 2.04401

R45 2.65743 -0.00066 -0.00177 -0.00041 -0.00218 2.65526

R46 2.04426 0.00009 -0.00015 -0.00010 -0.00025 2.04401

R47 2.54977 -0.00068 -0.00053 0.00073 0.00020 2.54997

R48 2.64315 -0.00007 -0.00064 0.00039 -0.00025 2.64290

R49 2.55051 0.00036 0.00044 0.00178 0.00222 2.55273

R50 2.64845 -0.00078 -0.00140 0.00014 -0.00127 2.64718

R51 2.04430 -0.00004 -0.00012 -0.00031 -0.00043 2.04387

R52 2.64311 -0.00004 -0.00063 0.00042 -0.00021 2.64290

R53 2.04430 -0.00003 -0.00012 -0.00031 -0.00043 2.04387

R54 2.55054 0.00032 0.00043 0.00175 0.00218 2.55272

R55 2.65748 -0.00069 -0.00178 -0.00043 -0.00221 2.65527

R56 2.54975 -0.00061 -0.00053 0.00078 0.00026 2.55001

R57 2.62991 -0.00067 -0.00108 0.00047 -0.00061 2.62930

R58 2.04427 0.00008 -0.00015 -0.00011 -0.00026 2.04401

R59 2.65744 -0.00064 -0.00177 -0.00039 -0.00215 2.65528

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R61 2.54977 -0.00066 -0.00053 0.00075 0.00022 2.54999

R62 2.64314 -0.00003 -0.00063 0.00042 -0.00021 2.64293

R63 2.55052 0.00035 0.00044 0.00177 0.00221 2.55273

R64 2.64854 -0.00082 -0.00145 0.00009 -0.00136 2.64719

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R67 2.04430 -0.00004 -0.00012 -0.00031 -0.00043 2.04387

R68 2.55050 0.00039 0.00045 0.00180 0.00225 2.55274

R69 2.69347 0.00018 0.00032 0.00022 0.00054 2.69401

R70 2.69348 0.00018 0.00032 0.00021 0.00054 2.69402

R71 2.69520 0.00007 0.00042 0.00033 0.00074 2.69594

R72 2.69521 0.00007 0.00041 0.00032 0.00074 2.69594

R73 2.69349 0.00017 0.00031 0.00021 0.00052 2.69401

R74 2.69350 0.00016 0.00031 0.00020 0.00051 2.69401

R75 2.69523 0.00005 0.00040 0.00031 0.00071 2.69595

R76 2.69523 0.00005 0.00040 0.00031 0.00072 2.69595

R77 2.06709 0.00015 0.00003 0.00008 0.00011 2.06720

R78 2.06699 0.00006 -0.00016 -0.00006 -0.00021 2.06678

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R80 2.06663 0.00021 0.00012 0.00002 0.00014 2.06677

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R82 2.05615 0.00019 0.00014 0.00018 0.00032 2.05646

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A5 2.17155 -0.00002 -0.00081 0.00048 -0.00033 2.17122

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A11 2.31697 0.00043 0.00053 -0.00037 0.00014 2.31712

A12 2.10837 -0.00037 -0.00068 0.00024 -0.00044 2.10793

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A15 2.10841 -0.00042 -0.00069 0.00015 -0.00055 2.10785

A16 2.18450 0.00049 0.00124 0.00076 0.00200 2.18649

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A18 2.16589 0.00003 0.00050 0.00108 0.00159 2.16749

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A91 2.06224 0.00104 0.00256 0.00060 0.00315 2.06539

A92 2.16900 -0.00136 -0.00334 -0.00055 -0.00390 2.16511

A93 2.04285 0.00075 0.00209 0.00068 0.00277 2.04562

A94 2.07240 0.00063 0.00046 -0.00036 0.00010 2.07250

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A96 2.12228 -0.00008 -0.00045 -0.00023 -0.00068 2.12160

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A98 2.06242 0.00001 -0.00052 0.00024 -0.00028 2.06214

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A130 1.90919 -0.00004 0.00004 -0.00005 -0.00001 1.90918

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A146 1.91183 -0.00003 0.00037 -0.00058 -0.00021 1.91162

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D3 3.12456 0.00027 0.00826 -0.00392 0.00435 3.12891

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D6 -3.13496 0.00014 -0.00199 0.00727 0.00528 -3.12968

D7 -3.12373 -0.00025 -0.00599 0.00315 -0.00286 -3.12658

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D9 0.20364 -0.00017 -0.00071 -0.00586 -0.00657 0.19706

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D13 -2.99310 0.00002 0.00100 -0.00837 -0.00738 -3.00049

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D44 -0.02580 0.00012 -0.00170 0.00197 0.00028 -0.02552

D45 -0.00840 -0.00003 0.00081 -0.00095 -0.00014 -0.00854

D46 -3.13038 -0.00004 -0.00144 0.00242 0.00099 -3.12940

D47 -0.01460 -0.00003 0.00146 -0.00104 0.00042 -0.01418

D48 3.08791 0.00017 0.00133 -0.00150 -0.00016 3.08775

D49 2.88869 0.00002 -0.00220 0.00743 0.00523 2.89391

D50 -0.29199 0.00021 -0.00233 0.00697 0.00464 -0.28735

D51 -0.23405 0.00014 -0.00262 0.00462 0.00200 -0.23205

D52 3.10724 -0.00009 -0.00205 0.00480 0.00277 3.11000

D53 -3.10690 0.00015 0.00192 -0.00488 -0.00298 -3.10988

D54 0.23438 -0.00008 0.00249 -0.00470 -0.00221 0.23217

D55 0.00882 0.00001 -0.00089 0.00040 -0.00049 0.00833

D56 3.13079 0.00002 0.00136 -0.00290 -0.00155 3.12925

D57 -3.09561 -0.00015 -0.00068 0.00090 0.00022 -3.09539

D58 0.02636 -0.00014 0.00157 -0.00240 -0.00084 0.02552

D59 0.05126 -0.00008 0.00114 -0.00135 -0.00021 0.05105

D60 -3.13524 0.00014 0.00099 -0.00193 -0.00094 -3.13618

D61 -0.00025 0.00001 0.00005 0.00033 0.00038 0.00012

D62 3.12425 0.00004 0.00204 -0.00260 -0.00054 3.12370

D63 -3.12474 -0.00002 -0.00195 0.00319 0.00123 -3.12351

D64 -0.00024 0.00001 0.00004 0.00026 0.00030 0.00007

D65 -3.12049 -0.00003 -0.00143 0.00171 0.00028 -3.12021

D66 0.02323 0.00004 -0.00088 0.00067 -0.00021 0.02302

D67 -0.00091 -0.00001 0.00111 -0.00198 -0.00087 -0.00178

D68 -3.14037 0.00007 0.00166 -0.00302 -0.00136 3.14145

D69 3.12081 0.00003 0.00137 -0.00211 -0.00074 3.12007

D70 -0.02282 -0.00006 0.00081 -0.00121 -0.00040 -0.02322

D71 0.00120 0.00000 -0.00116 0.00166 0.00050 0.00170

D72 3.14076 -0.00008 -0.00173 0.00257 0.00084 -3.14158

D73 -3.13479 0.00018 0.00085 -0.00197 -0.00113 -3.13592

D74 0.05135 -0.00004 0.00111 -0.00124 -0.00013 0.05121

D75 0.00027 -0.00001 -0.00005 -0.00033 -0.00039 -0.00012

D76 3.12499 0.00002 0.00189 -0.00335 -0.00145 3.12354

D77 -3.12447 -0.00004 -0.00199 0.00276 0.00076 -3.12372

D78 0.00025 -0.00001 -0.00005 -0.00026 -0.00031 -0.00006

D79 -3.09629 -0.00015 -0.00052 0.00150 0.00098 -3.09531

D80 0.00846 0.00001 -0.00083 0.00087 0.00005 0.00851

D81 0.02598 -0.00013 0.00166 -0.00207 -0.00041 0.02557

D82 3.13073 0.00003 0.00136 -0.00269 -0.00134 3.12939

D83 -0.00104 0.00000 0.00112 -0.00179 -0.00067 -0.00171

D84 -3.14051 0.00007 0.00167 -0.00284 -0.00117 3.14151

D85 -3.12096 -0.00003 -0.00134 0.00220 0.00086 -3.12010

D86 0.02276 0.00005 -0.00079 0.00115 0.00036 0.02312

D87 -0.00892 0.00001 0.00092 -0.00031 0.00061 -0.00831

D88 3.09567 0.00016 0.00067 -0.00098 -0.00031 3.09536

D89 -3.13116 -0.00001 -0.00127 0.00317 0.00191 -3.12925

D90 -0.02657 0.00015 -0.00152 0.00250 0.00099 -0.02558

D91 0.00073 0.00001 -0.00106 0.00210 0.00104 0.00177

D92 3.14009 -0.00006 -0.00159 0.00328 0.00169 -3.14140

D93 3.12063 0.00004 0.00141 -0.00180 -0.00039 3.12023

D94 -0.02320 -0.00003 0.00088 -0.00062 0.00026 -0.02294

D95 0.01473 0.00000 -0.00150 0.00091 -0.00059 0.01414

D96 -2.88782 -0.00004 0.00198 -0.00781 -0.00582 -2.89365

D97 -3.08790 -0.00020 -0.00135 0.00151 0.00016 -3.08773

D98 0.29274 -0.00025 0.00213 -0.00721 -0.00507 0.28767

D99 3.13491 -0.00015 -0.00091 0.00206 0.00115 3.13606

D100 -0.05141 0.00006 -0.00111 0.00129 0.00018 -0.05123

D101 3.08825 0.00019 0.00125 -0.00169 -0.00045 3.08780

D102 -0.01456 -0.00001 0.00147 -0.00112 0.00035 -0.01421

D103 -0.29215 0.00022 -0.00234 0.00691 0.00458 -0.28758

D104 2.88822 0.00002 -0.00211 0.00749 0.00537 2.89360

D105 3.10614 -0.00008 -0.00168 0.00522 0.00354 3.10968

D106 -0.23470 0.00006 -0.00244 0.00480 0.00237 -0.23233

D107 0.23435 -0.00012 0.00257 -0.00472 -0.00215 0.23219

D108 -3.10649 0.00002 0.00181 -0.00514 -0.00333 -3.10981

D109 -0.20378 0.00018 0.00073 0.00606 0.00679 -0.19699

D110 2.96108 -0.00010 -0.00253 0.00887 0.00635 2.96743

D111 -3.12388 -0.00034 -0.00854 0.00359 -0.00494 -3.12882

D112 -0.00239 -0.00009 -0.00572 0.00116 -0.00456 -0.00695

D113 0.16883 -0.00024 -0.00182 -0.00639 -0.00820 0.16063

D114 -2.99287 0.00000 0.00099 -0.00881 -0.00782 -3.00069

D115 0.00258 0.00008 0.00568 -0.00134 0.00434 0.00691

D116 3.12428 0.00032 0.00845 -0.00373 0.00471 3.12899

D117 2.99322 -0.00002 -0.00110 0.00855 0.00746 3.00068

D118 -0.16827 0.00022 0.00167 0.00617 0.00784 -0.16043

D119 2.93769 -0.00015 -0.00960 0.01033 0.00071 2.93840

D120 0.03224 0.00003 0.00207 0.00096 0.00302 0.03527

D121 -0.03231 -0.00006 -0.00205 -0.00097 -0.00302 -0.03533

D122 -2.93776 0.00012 0.00962 -0.01034 -0.00071 -2.93847

D123 3.12320 0.00029 0.00620 -0.00288 0.00332 3.12653

D124 -0.02629 0.00010 0.00477 -0.00953 -0.00475 -0.03104

D125 0.00123 0.00006 0.00344 -0.00051 0.00293 0.00416

D126 3.13492 -0.00014 0.00202 -0.00716 -0.00515 3.12977

D127 0.00030 -0.00001 -0.00007 -0.00028 -0.00035 -0.00005

D128 3.13515 -0.00017 -0.00128 -0.00588 -0.00716 3.12799

D129 -3.13454 0.00015 0.00114 0.00541 0.00655 -3.12799

D130 0.00031 -0.00001 -0.00008 -0.00018 -0.00026 0.00005

D131 -3.14133 0.00020 0.00040 0.00927 0.00967 -3.13166

D132 -0.00687 0.00018 -0.00001 0.01024 0.01023 0.00336

D133 -0.00856 -0.00002 -0.00118 0.00184 0.00066 -0.00790

D134 3.12590 -0.00004 -0.00159 0.00280 0.00122 3.12712

D135 -0.00172 -0.00004 -0.00333 0.00098 -0.00234 -0.00407

D136 -3.12390 -0.00028 -0.00604 0.00330 -0.00274 -3.12664

D137 -3.13543 0.00015 -0.00189 0.00752 0.00563 -3.12980

D138 0.02558 -0.00008 -0.00461 0.00984 0.00523 0.03081

D139 0.00817 0.00003 0.00128 -0.00161 -0.00033 0.00783

D140 -3.12646 0.00006 0.00173 -0.00254 -0.00080 -3.12726

D141 3.14096 -0.00019 -0.00031 -0.00892 -0.00923 3.13173

D142 0.00633 -0.00016 0.00014 -0.00984 -0.00970 -0.00337

D143 0.20344 -0.00016 -0.00065 -0.00588 -0.00653 0.19691

D144 -2.96120 0.00012 0.00256 -0.00864 -0.00609 -2.96728

D145 0.00087 0.00001 -0.00109 0.00199 0.00089 0.00177

D146 -3.13897 0.00007 -0.00039 0.00156 0.00117 -3.13780

D147 3.14021 -0.00007 -0.00167 0.00310 0.00143 -3.14154

D148 0.00037 -0.00001 -0.00097 0.00268 0.00171 0.00208

D149 -3.09091 -0.00012 -0.00016 -0.00122 -0.00138 -3.09230

D150 0.05297 -0.00004 0.00042 -0.00235 -0.00193 0.05104

D151 0.00010 0.00000 -0.00002 -0.00013 -0.00015 -0.00005

D152 -3.13984 0.00005 0.00068 -0.00045 0.00023 -3.13961

D153 3.13998 -0.00006 -0.00070 0.00028 -0.00042 3.13956

D154 0.00004 0.00000 -0.00001 -0.00003 -0.00004 0.00000

D155 -0.00091 -0.00001 0.00110 -0.00191 -0.00082 -0.00173

D156 -3.14013 0.00006 0.00165 -0.00317 -0.00151 3.14154

D157 3.13900 -0.00007 0.00038 -0.00159 -0.00121 3.13779

D158 -0.00022 0.00000 0.00094 -0.00284 -0.00191 -0.00213

D159 3.09112 0.00011 0.00012 0.00093 0.00105 3.09217

D160 -0.05288 0.00003 -0.00044 0.00220 0.00176 -0.05112

D161 -0.00845 -0.00002 -0.00124 0.00177 0.00053 -0.00793

D162 3.13911 0.00003 -0.00047 0.00050 0.00003 3.13914

D163 3.12570 -0.00005 -0.00169 0.00275 0.00106 3.12676

D164 -0.00992 0.00001 -0.00093 0.00149 0.00056 -0.00936

D165 -3.12245 -0.00030 0.00452 -0.02036 -0.01584 -3.13829

D166 0.02662 -0.00028 0.00498 -0.02135 -0.01637 0.01025

D167 0.00013 0.00000 -0.00003 -0.00009 -0.00012 0.00000

D168 -3.13570 0.00005 0.00073 -0.00123 -0.00050 -3.13620

D169 3.13589 -0.00006 -0.00078 0.00115 0.00036 3.13625

D170 0.00005 0.00000 -0.00002 0.00001 -0.00001 0.00004

D171 0.00842 0.00003 0.00125 -0.00172 -0.00047 0.00795

D172 -3.12557 0.00004 0.00166 -0.00276 -0.00110 -3.12666

D173 -3.13907 -0.00003 0.00047 -0.00055 -0.00009 -3.13916

D174 0.01013 -0.00002 0.00087 -0.00159 -0.00071 0.00942

D175 3.12257 0.00029 -0.00455 0.02017 0.01562 3.13819

D176 -0.02667 0.00027 -0.00496 0.02120 0.01624 -0.01043

D177 -0.00104 -0.00001 0.00114 -0.00186 -0.00073 -0.00177

D178 3.13892 -0.00007 0.00041 -0.00159 -0.00118 3.13774

D179 -3.14048 0.00008 0.00173 -0.00282 -0.00109 -3.14157

D180 -0.00052 0.00002 0.00100 -0.00255 -0.00154 -0.00206

D181 3.09089 0.00013 0.00015 0.00135 0.00150 3.09239

D182 -0.05289 0.00004 -0.00045 0.00232 0.00187 -0.05102

D183 -0.00010 0.00000 0.00002 0.00014 0.00015 0.00005

D184 3.13996 -0.00006 -0.00071 0.00031 -0.00040 3.13956

D185 -3.14010 0.00006 0.00073 -0.00013 0.00060 -3.13950

D186 -0.00004 0.00000 0.00001 0.00004 0.00004 0.00001

D187 0.00107 0.00000 -0.00114 0.00179 0.00065 0.00172

D188 3.14041 -0.00007 -0.00172 0.00289 0.00118 3.14158

D189 -3.13895 0.00007 -0.00040 0.00161 0.00122 -3.13774

D190 0.00038 -0.00001 -0.00097 0.00272 0.00174 0.00212

D191 -3.09110 -0.00011 -0.00012 -0.00104 -0.00116 -3.09225

D192 0.05279 -0.00003 0.00046 -0.00216 -0.00170 0.05110

D193 -0.00837 -0.00002 -0.00125 0.00168 0.00042 -0.00794

D194 3.13913 0.00003 -0.00048 0.00052 0.00004 3.13918

D195 3.12559 -0.00004 -0.00165 0.00271 0.00105 3.12665

D196 -0.01009 0.00002 -0.00088 0.00155 0.00067 -0.00942

D197 -3.12277 -0.00029 0.00460 -0.02016 -0.01556 -3.13832

D198 0.02650 -0.00027 0.00501 -0.02119 -0.01618 0.01032

D199 -0.00012 0.00000 0.00003 0.00008 0.00011 -0.00001

D200 -3.13587 0.00006 0.00077 -0.00114 -0.00036 -3.13624

D201 3.13570 -0.00005 -0.00073 0.00122 0.00049 3.13619

D202 -0.00005 0.00000 0.00001 0.00000 0.00001 -0.00004

D203 0.00840 0.00002 0.00125 -0.00172 -0.00048 0.00793

D204 -3.12573 0.00004 0.00169 -0.00272 -0.00103 -3.12675

D205 -3.13917 -0.00003 0.00049 -0.00048 0.00001 -3.13916

D206 0.00989 -0.00001 0.00093 -0.00147 -0.00054 0.00935

D207 3.12264 0.00030 -0.00457 0.02031 0.01574 3.13838

D208 -0.02646 0.00027 -0.00502 0.02130 0.01628 -0.01018

D209 1.09159 -0.00010 0.00163 -0.00341 -0.00178 1.08981

D210 -1.05116 0.00001 0.00155 -0.00250 -0.00095 -1.05210

D211 -3.12212 -0.00009 0.00138 -0.00326 -0.00187 -3.12400

D212 1.05125 -0.00001 -0.00158 0.00260 0.00102 1.05227

D213 -1.09150 0.00010 -0.00166 0.00350 0.00184 -1.08966

D214 3.12223 0.00009 -0.00142 0.00334 0.00193 3.12415

D215 1.09687 -0.00001 0.00019 -0.00083 -0.00064 1.09623

D216 -1.04696 -0.00001 0.00007 -0.00111 -0.00104 -1.04800

D217 -3.11670 0.00000 0.00021 -0.00086 -0.00065 -3.11735

D218 1.04699 0.00001 -0.00007 0.00103 0.00096 1.04795

D219 -1.09684 0.00001 -0.00019 0.00077 0.00058 -1.09626

D220 3.11674 0.00000 -0.00021 0.00078 0.00056 3.11730

D221 1.05117 -0.00001 -0.00155 0.00246 0.00091 1.05208

D222 -1.09157 0.00010 -0.00163 0.00337 0.00174 -1.08984

D223 3.12214 0.00009 -0.00138 0.00322 0.00184 3.12397

D224 1.09147 -0.00010 0.00166 -0.00347 -0.00181 1.08967

D225 -1.05126 0.00001 0.00157 -0.00259 -0.00101 -1.05227

D226 -3.12224 -0.00009 0.00141 -0.00332 -0.00191 -3.12415

D227 1.09681 -0.00001 0.00019 -0.00072 -0.00053 1.09628

D228 -1.04702 -0.00001 0.00007 -0.00098 -0.00091 -1.04793

D229 -3.11677 0.00000 0.00022 -0.00072 -0.00050 -3.11728

D230 1.04699 0.00001 -0.00007 0.00104 0.00097 1.04796

D231 -1.09683 0.00001 -0.00019 0.00076 0.00057 -1.09627

D232 3.11674 0.00000 -0.00021 0.00078 0.00057 3.11730

Item Value Threshold Converged?

Maximum Force 0.001646 0.000450 NO

RMS Force 0.000399 0.000300 NO

Maximum Displacement 0.042876 0.001800 NO

RMS Displacement 0.014041 0.001200 NO

Predicted change in Energy=-1.426368D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 02:23:31 2019, MaxMem= 1342177280 cpu: 13.6

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=3 Diff= 4.09D-04

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 -1.123243 2.796962 -0.030145

2 7 0 0.000189 2.038275 -0.202446

3 6 0 1.124059 2.796491 -0.030632

4 6 0 0.713565 4.155048 0.267805

5 6 0 -0.711984 4.155373 0.268091

6 7 0 2.409392 2.381809 -0.138809

7 6 0 2.798059 1.129886 -0.223548

8 7 0 2.019204 -0.000456 -0.166307

9 6 0 2.797746 -1.130966 -0.223876

10 6 0 4.208326 -0.705879 -0.347793

11 6 0 4.208472 0.704514 -0.347695

12 7 0 -2.408744 2.382737 -0.137992

13 6 0 -4.208436 0.706008 -0.346660

14 6 0 -4.208776 -0.704400 -0.346774

15 6 0 -2.798335 -1.130003 -0.223063

16 7 0 -2.019333 0.000265 -0.165565

17 6 0 -2.797851 1.130917 -0.222721

18 7 0 -2.409648 -2.381997 -0.138629

19 7 0 -0.000546 -2.038327 -0.202836

20 6 0 -1.124288 -2.796689 -0.030839

21 6 0 -0.713484 -4.155349 0.266915

22 6 0 0.712081 -4.155529 0.266665

23 6 0 1.123097 -2.797016 -0.031299

24 7 0 2.408595 -2.382786 -0.139408

25 30 0 -0.000033 0.000010 -0.409084

26 6 0 -5.402375 1.432250 -0.429878

27 6 0 -6.596796 0.697172 -0.515366

28 6 0 -6.597167 -0.694185 -0.515418

29 6 0 -5.403151 -1.429947 -0.430046

30 6 0 1.432838 -5.334384 0.541797

31 6 0 0.699580 -6.496248 0.803290

32 6 0 -0.701248 -6.496082 0.803569

33 6 0 -1.434362 -5.334058 0.542367

34 6 0 5.402604 1.430369 -0.431076

35 6 0 6.596784 0.694893 -0.516705

36 6 0 6.596685 -0.696472 -0.516734

37 6 0 5.402417 -1.431834 -0.431201

38 6 0 -1.432440 5.334192 0.544083

39 6 0 -0.698905 6.495855 0.805783

40 6 0 0.701925 6.495525 0.805456

41 6 0 1.434760 5.333500 0.543423

42 1 0 7.547921 1.205156 -0.586828

43 1 0 7.547763 -1.206847 -0.586873

44 1 0 1.209862 7.425917 1.020314

45 1 0 -1.206299 7.426480 1.020916

46 1 0 -7.547777 1.207756 -0.585307

47 1 0 -7.548430 -1.204238 -0.585397

48 1 0 -1.208976 -7.426628 1.018258

49 1 0 1.207181 -7.426919 1.017734

50 8 0 2.784269 5.273342 0.546648

51 8 0 -2.781970 5.274734 0.548070

52 8 0 5.344218 2.778506 -0.426881

53 8 0 5.344027 -2.779958 -0.427063

54 8 0 2.782367 -5.274802 0.545105

55 8 0 -2.783869 -5.274208 0.546338

56 8 0 -5.345338 -2.778089 -0.425876

57 8 0 -5.343695 2.780364 -0.425596

58 6 0 3.516026 6.465575 0.821384

59 1 0 3.305886 6.840365 1.827378

60 1 0 3.299697 7.247101 0.087503

61 1 0 4.565802 6.186553 0.753236

62 6 0 6.565459 3.515593 -0.450419

63 1 0 7.131105 3.327450 -1.367370

64 1 0 7.188263 3.284769 0.418654

65 1 0 6.272854 4.563206 -0.416633

66 6 0 6.565315 -3.516972 -0.450458

67 1 0 7.187987 -3.286090 0.418693

68 1 0 7.131066 -3.328781 -1.367334

69 1 0 6.272796 -4.564608 -0.416706

70 6 0 -3.512924 6.467387 0.823126

71 1 0 -3.296719 7.248693 0.088972

72 1 0 -3.301886 6.842217 1.828914

73 1 0 -4.562890 6.188896 0.755755

74 6 0 -6.564813 3.517666 -0.448853

75 1 0 -7.187505 3.286844 0.420301

76 1 0 -7.130647 3.329716 -1.365728

77 1 0 -6.272031 4.565226 -0.415000

78 6 0 -6.566964 -3.514549 -0.449028

79 1 0 -7.132787 -3.326152 -1.365820

80 1 0 -7.189382 -3.283334 0.420218

81 1 0 -6.274916 -4.562313 -0.415267

82 6 0 -3.515159 -6.466814 0.820693

83 1 0 -3.304267 -6.842278 1.826276

84 1 0 -3.299146 -7.247761 0.086099

85 1 0 -4.565043 -6.187990 0.753440

86 6 0 3.513577 -6.467506 0.819248

87 1 0 3.296905 -7.248552 0.084955

88 1 0 3.303248 -6.842722 1.825044

89 1 0 4.563480 -6.188927 0.751266

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0448762 0.0438624 0.0225686

Leave Link 202 at Sat Jul 6 02:23:32 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8043.2378705985 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= 89 NActive= 89 NUniq= 89 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= -0.2279562075 Hartrees.

Nuclear repulsion after empirical dispersion term = 8043.0099143911 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6405

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.19D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 395

GePol: Fraction of low-weight points (<1% of avg) = 6.17%

GePol: Cavity surface area = 704.065 Ang\*\*2

GePol: Cavity volume = 801.852 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0089731404 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8043.0009412507 Hartrees.

Leave Link 301 at Sat Jul 6 02:23:32 2019, MaxMem= 1342177280 cpu: 1.4

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44351 LenP2D= 111374.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.58D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 02:23:36 2019, MaxMem= 1342177280 cpu: 41.8

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 02:23:36 2019, MaxMem= 1342177280 cpu: 2.5

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000105 -0.000104 0.000000 Ang= -0.02 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>= 2.0170 S= 1.0056

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2650.02714899864

Leave Link 401 at Sat Jul 6 02:23:54 2019, MaxMem= 1342177280 cpu: 204.2

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 123072075.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.04D-14 for 6392.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.78D-15 for 2388 409.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.99D-15 for 6392.

Iteration 1 A^-1\*A deviation from orthogonality is 8.17D-07 for 5015 4964.

Iteration 2 A\*A^-1 deviation from unit magnitude is 4.55D-15 for 1745.

Iteration 2 A\*A^-1 deviation from orthogonality is 5.36D-15 for 4964 977.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.33D-15 for 723.

Iteration 2 A^-1\*A deviation from orthogonality is 1.05D-15 for 6371 91.

E= -2649.79442996585

DIIS: error= 8.88D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79442996585 IErMin= 1 ErrMin= 8.88D-04

ErrMax= 8.88D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.26D-03 BMatP= 2.26D-03

IDIUse=3 WtCom= 9.91D-01 WtEn= 8.88D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.686 Goal= None Shift= 0.000

Gap= 0.745 Goal= None Shift= 0.000

RMSDP=4.12D-05 MaxDP=1.67D-03 OVMax= 5.80D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.12D-05 CP: 1.00D+00

E= -2649.79538918293 Delta-E= -0.000959217077 Rises=F Damp=F

DIIS: error= 1.23D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79538918293 IErMin= 2 ErrMin= 1.23D-04

ErrMax= 1.23D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.11D-05 BMatP= 2.26D-03

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.23D-03

Coeff-Com: -0.339D-01 0.103D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.339D-01 0.103D+01

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=8.05D-06 MaxDP=6.70D-04 DE=-9.59D-04 OVMax= 1.72D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 7.85D-06 CP: 1.00D+00 1.04D+00

E= -2649.79537977105 Delta-E= 0.000009411873 Rises=F Damp=F

DIIS: error= 2.40D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -2649.79538918293 IErMin= 2 ErrMin= 1.23D-04

ErrMax= 2.40D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.34D-04 BMatP= 6.11D-05

IDIUse=3 WtCom= 3.92D-01 WtEn= 6.08D-01

Coeff-Com: -0.431D-01 0.646D+00 0.397D+00

Coeff-En: 0.000D+00 0.614D+00 0.386D+00

Coeff: -0.169D-01 0.626D+00 0.390D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=5.55D-06 MaxDP=4.50D-04 DE= 9.41D-06 OVMax= 1.16D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.50D-06 CP: 1.00D+00 1.05D+00 3.72D-01

E= -2649.79540753535 Delta-E= -0.000027764296 Rises=F Damp=F

DIIS: error= 4.70D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79540753535 IErMin= 4 ErrMin= 4.70D-05

ErrMax= 4.70D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.87D-06 BMatP= 6.11D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.131D-01 0.152D+00 0.180D+00 0.681D+00

Coeff: -0.131D-01 0.152D+00 0.180D+00 0.681D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.21D-06 MaxDP=1.07D-04 DE=-2.78D-05 OVMax= 3.76D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 9.90D-07 CP: 1.00D+00 1.05D+00 4.54D-01 9.19D-01

E= -2649.79540821169 Delta-E= -0.000000676346 Rises=F Damp=F

DIIS: error= 2.12D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79540821169 IErMin= 5 ErrMin= 2.12D-05

ErrMax= 2.12D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.76D-07 BMatP= 3.87D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.379D-02 0.304D-01 0.739D-01 0.430D+00 0.469D+00

Coeff: -0.379D-02 0.304D-01 0.739D-01 0.430D+00 0.469D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=5.05D-07 MaxDP=3.78D-05 DE=-6.76D-07 OVMax= 1.20D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.32D-07 CP: 1.00D+00 1.05D+00 4.62D-01 9.62D-01 6.39D-01

E= -2649.79540845490 Delta-E= -0.000000243203 Rises=F Damp=F

DIIS: error= 5.33D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79540845490 IErMin= 6 ErrMin= 5.33D-06

ErrMax= 5.33D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.32D-08 BMatP= 9.76D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.166D-03-0.101D-01 0.597D-02 0.919D-01 0.205D+00 0.707D+00

Coeff: 0.166D-03-0.101D-01 0.597D-02 0.919D-01 0.205D+00 0.707D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.62D-07 MaxDP=8.11D-06 DE=-2.43D-07 OVMax= 1.33D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.27D-07 CP: 1.00D+00 1.05D+00 4.64D-01 9.87D-01 7.05D-01

CP: 8.82D-01

E= -2649.79540846944 Delta-E= -0.000000014543 Rises=F Damp=F

DIIS: error= 2.52D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79540846944 IErMin= 7 ErrMin= 2.52D-06

ErrMax= 2.52D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.15D-08 BMatP= 4.32D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.503D-03-0.941D-02-0.464D-02 0.729D-02 0.664D-01 0.410D+00

Coeff-Com: 0.530D+00

Coeff: 0.503D-03-0.941D-02-0.464D-02 0.729D-02 0.664D-01 0.410D+00

Coeff: 0.530D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=6.36D-08 MaxDP=4.32D-06 DE=-1.45D-08 OVMax= 3.40D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 5.30D-08 CP: 1.00D+00 1.05D+00 4.65D-01 9.94D-01 7.14D-01

CP: 9.63D-01 1.07D+00

E= -2649.79540847385 Delta-E= -0.000000004411 Rises=F Damp=F

DIIS: error= 1.16D-06 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.79540847385 IErMin= 8 ErrMin= 1.16D-06

ErrMax= 1.16D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.55D-10 BMatP= 1.15D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.125D-03-0.485D-03-0.300D-02-0.204D-01-0.313D-01-0.317D-01

Coeff-Com: 0.136D+00 0.951D+00

Coeff: 0.125D-03-0.485D-03-0.300D-02-0.204D-01-0.313D-01-0.317D-01

Coeff: 0.136D+00 0.951D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=5.51D-08 MaxDP=2.81D-06 DE=-4.41D-09 OVMax= 6.31D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.38D-08 CP: 1.00D+00 1.05D+00 4.66D-01 1.00D+00 7.28D-01

CP: 1.03D+00 1.37D+00 1.16D+00

E= -2649.79540847506 Delta-E= -0.000000001208 Rises=F Damp=F

DIIS: error= 5.14D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.79540847506 IErMin= 9 ErrMin= 5.14D-07

ErrMax= 5.14D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.45D-10 BMatP= 9.55D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.432D-04 0.188D-02-0.543D-03-0.121D-01-0.322D-01-0.104D+00

Coeff-Com: -0.660D-01 0.524D+00 0.689D+00

Coeff: -0.432D-04 0.188D-02-0.543D-03-0.121D-01-0.322D-01-0.104D+00

Coeff: -0.660D-01 0.524D+00 0.689D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.69D-08 MaxDP=1.41D-06 DE=-1.21D-09 OVMax= 2.29D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.26D-08 CP: 1.00D+00 1.05D+00 4.66D-01 1.00D+00 7.35D-01

CP: 1.06D+00 1.49D+00 1.42D+00 1.01D+00

E= -2649.79540847531 Delta-E= -0.000000000247 Rises=F Damp=F

DIIS: error= 2.30D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -2649.79540847531 IErMin=10 ErrMin= 2.30D-07

ErrMax= 2.30D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.31D-10 BMatP= 5.45D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.591D-04 0.121D-02 0.566D-03-0.918D-03-0.974D-02-0.487D-01

Coeff-Com: -0.835D-01 0.542D-01 0.407D+00 0.680D+00

Coeff: -0.591D-04 0.121D-02 0.566D-03-0.918D-03-0.974D-02-0.487D-01

Coeff: -0.835D-01 0.542D-01 0.407D+00 0.680D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.19D-08 MaxDP=8.36D-07 DE=-2.47D-10 OVMax= 1.08D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.68D-09 CP: 1.00D+00 1.05D+00 4.66D-01 1.00D+00 7.35D-01

CP: 1.07D+00 1.54D+00 1.49D+00 1.20D+00 9.10D-01

E= -2649.79540847549 Delta-E= -0.000000000186 Rises=F Damp=F

DIIS: error= 8.74D-08 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -2649.79540847549 IErMin=11 ErrMin= 8.74D-08

ErrMax= 8.74D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.02D-11 BMatP= 1.31D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.185D-04 0.198D-03 0.355D-03 0.183D-02 0.123D-02-0.336D-02

Coeff-Com: -0.283D-01-0.649D-01 0.741D-01 0.324D+00 0.694D+00

Coeff: -0.185D-04 0.198D-03 0.355D-03 0.183D-02 0.123D-02-0.336D-02

Coeff: -0.283D-01-0.649D-01 0.741D-01 0.324D+00 0.694D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=3.90D-09 MaxDP=3.97D-07 DE=-1.86D-10 OVMax= 2.88D-06

Error on total polarization charges = 0.07297

SCF Done: E(UB3LYP) = -2649.79540848 A.U. after 11 cycles

NFock= 11 Conv=0.39D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0171 S= 1.0057

<L.S>= 0.000000000000E+00

KE= 2.690156958173D+03 PE=-2.236473486999D+04 EE= 8.981781562087D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.63

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0171, after 2.0002

Leave Link 502 at Sat Jul 6 02:32:53 2019, MaxMem= 1342177280 cpu: 6373.8

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44351 LenP2D= 111374.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 279

Leave Link 701 at Sat Jul 6 02:33:12 2019, MaxMem= 1342177280 cpu: 219.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 02:33:12 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 02:34:44 2019, MaxMem= 1342177280 cpu: 1095.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 9.02069662D-04 1.46555693D-03 2.52252484D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000466187 0.000542391 -0.000711629

2 7 0.000037011 -0.000316525 0.000412989

3 6 -0.000462293 0.000533369 -0.000701920

4 6 0.000545298 -0.000252826 -0.000007369

5 6 -0.000558274 -0.000247338 0.000008763

6 7 0.000427934 -0.000150122 0.000058346

7 6 -0.000255205 -0.000051403 0.000745764

8 7 -0.000055891 0.000018584 -0.000475305

9 6 -0.000262862 0.000035308 0.000770824

10 6 0.000157081 0.000461853 -0.000293824

11 6 0.000147798 -0.000475991 -0.000279929

12 7 -0.000452576 -0.000166575 0.000057848

13 6 -0.000155967 -0.000469167 -0.000284977

14 6 -0.000164096 0.000457067 -0.000298110

15 6 0.000285761 0.000058059 0.000783802

16 7 0.000023105 0.000022563 -0.000508834

17 6 0.000281932 -0.000071799 0.000757486

18 7 -0.000476645 0.000176345 0.000055711

19 7 0.000030193 0.000299142 0.000422995

20 6 0.000499514 -0.000531328 -0.000715944

21 6 -0.000560930 0.000241041 0.000009034

22 6 0.000549078 0.000246670 -0.000009146

23 6 -0.000491064 -0.000523655 -0.000704006

24 7 0.000451800 0.000163923 0.000057266

25 30 -0.000032582 -0.000009576 0.000450118

26 6 0.000052109 0.000444606 0.000217371

27 6 -0.000150427 -0.000203576 0.000028060

28 6 -0.000150259 0.000209276 0.000025410

29 6 0.000055052 -0.000436497 0.000219912

30 6 0.000402319 -0.000050215 0.000372113

31 6 -0.000164038 0.000004627 -0.000132490

32 6 0.000165726 0.000004520 -0.000131078

33 6 -0.000398248 -0.000046923 0.000376349

34 6 -0.000044481 0.000455599 0.000210960

35 6 0.000144286 -0.000194629 0.000027587

36 6 0.000143644 0.000200828 0.000024438

37 6 -0.000047249 -0.000444592 0.000214198

38 6 -0.000405222 0.000053891 0.000378199

39 6 0.000157355 -0.000010966 -0.000132431

40 6 -0.000154445 -0.000011714 -0.000133684

41 6 0.000410143 0.000057288 0.000374025

42 1 0.000062410 0.000093156 -0.000041348

43 1 0.000059456 -0.000091115 -0.000041105

44 1 0.000068432 0.000031992 0.000089733

45 1 -0.000068317 0.000031158 0.000087694

46 1 -0.000060787 0.000090914 -0.000042583

47 1 -0.000057149 -0.000088924 -0.000042511

48 1 -0.000066060 -0.000030490 0.000088171

49 1 0.000066804 -0.000030859 0.000089836

50 8 -0.000148131 0.000114777 -0.000375608

51 8 0.000136245 0.000108919 -0.000376241

52 8 0.000028441 -0.000126227 -0.000080418

53 8 0.000006277 0.000106595 -0.000087041

54 8 -0.000135142 -0.000101250 -0.000376417

55 8 0.000123773 -0.000095439 -0.000379374

56 8 0.000010557 0.000095742 -0.000089550

57 8 -0.000010391 -0.000116268 -0.000086263

58 6 -0.000172220 -0.000195341 0.000099313

59 1 -0.000150995 0.000100976 0.000064038

60 1 0.000079215 0.000137334 -0.000046966

61 1 0.000037643 -0.000071483 -0.000010615

62 6 -0.000156067 -0.000221593 -0.000055139

63 1 0.000091268 -0.000026184 -0.000089755

64 1 0.000110027 -0.000019879 0.000080019

65 1 -0.000064677 0.000059349 -0.000011693

66 6 -0.000154953 0.000217281 -0.000055351

67 1 0.000110877 0.000017772 0.000079668

68 1 0.000090096 0.000024351 -0.000089239

69 1 -0.000067131 -0.000061639 -0.000012377

70 6 0.000167053 -0.000193946 0.000101225

71 1 -0.000076975 0.000135015 -0.000047177

72 1 0.000149008 0.000100309 0.000064165

73 1 -0.000039335 -0.000071887 -0.000009769

74 6 0.000156236 -0.000216978 -0.000055021

75 1 -0.000110191 -0.000018330 0.000079177

76 1 -0.000090071 -0.000025694 -0.000088980

77 1 0.000065899 0.000061188 -0.000011189

78 6 0.000155737 0.000215329 -0.000056197

79 1 -0.000089293 0.000023640 -0.000088432

80 1 -0.000111299 0.000015688 0.000079119

81 1 0.000068554 -0.000063511 -0.000012015

82 6 0.000164394 0.000193488 0.000102165

83 1 0.000147972 -0.000099374 0.000064048

84 1 -0.000077723 -0.000133596 -0.000047369

85 1 -0.000040610 0.000072664 -0.000009261

86 6 -0.000168219 0.000193633 0.000100083

87 1 0.000079781 -0.000135460 -0.000046348

88 1 -0.000150046 -0.000099578 0.000063787

89 1 0.000039054 0.000072239 -0.000009782

-------------------------------------------------------------------

Cartesian Forces: Max 0.000783802 RMS 0.000246575

Leave Link 716 at Sat Jul 6 02:34:44 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.000500406 RMS 0.000125273

Search for a local minimum.

Step number 18 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .12527D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 4 6 5 8 7

9 11 14 13 16

17 18

DE= -1.52D-04 DEPred=-1.43D-04 R= 1.06D+00

TightC=F SS= 1.41D+00 RLast= 7.42D-02 DXNew= 9.6039D-02 2.2254D-01

Trust test= 1.06D+00 RLast= 7.42D-02 DXMaxT set to 9.60D-02

ITU= 1 0 0 -1 -1 0 -1 0 0 0 0 0 0 1 1 1 1 0

Eigenvalues --- 0.00606 0.00856 0.01266 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01316 0.01370

Eigenvalues --- 0.01397 0.01569 0.01571 0.01583 0.01598

Eigenvalues --- 0.01599 0.01618 0.01621 0.01707 0.01710

Eigenvalues --- 0.01713 0.01716 0.01758 0.01836 0.01869

Eigenvalues --- 0.01880 0.01922 0.01924 0.01946 0.01949

Eigenvalues --- 0.01984 0.01999 0.02020 0.02022 0.02034

Eigenvalues --- 0.02052 0.02053 0.02053 0.02053 0.02054

Eigenvalues --- 0.02057 0.02057 0.02057 0.02057 0.02059

Eigenvalues --- 0.02067 0.02067 0.02068 0.02070 0.02070

Eigenvalues --- 0.02070 0.02070 0.02075 0.02083 0.02083

Eigenvalues --- 0.02144 0.02160 0.02252 0.02260 0.02260

Eigenvalues --- 0.02260 0.02260 0.02260 0.02260 0.02344

Eigenvalues --- 0.02358 0.02363 0.02390 0.02858 0.04518

Eigenvalues --- 0.09919 0.09981 0.09981 0.09981 0.09990

Eigenvalues --- 0.09990 0.09990 0.10037 0.10646 0.10646

Eigenvalues --- 0.10646 0.10647 0.10657 0.10657 0.10657

Eigenvalues --- 0.10661 0.12665 0.13368 0.13461 0.15197

Eigenvalues --- 0.15843 0.15975 0.15996 0.15999 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16006 0.16034

Eigenvalues --- 0.16279 0.16937 0.19200 0.20868 0.21653

Eigenvalues --- 0.22473 0.22475 0.22476 0.22476 0.24189

Eigenvalues --- 0.24240 0.24452 0.24474 0.24506 0.24513

Eigenvalues --- 0.24593 0.24727 0.24791 0.24843 0.24875

Eigenvalues --- 0.24904 0.24948 0.24978 0.24979 0.24988

Eigenvalues --- 0.24989 0.24993 0.24995 0.24998 0.24998

Eigenvalues --- 0.24999 0.24999 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25025 0.25157 0.26221 0.30216

Eigenvalues --- 0.32668 0.33631 0.33633 0.33675 0.33716

Eigenvalues --- 0.34059 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34063 0.34064 0.34078 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34081

Eigenvalues --- 0.34154 0.34610 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34686 0.34687 0.34883

Eigenvalues --- 0.34946 0.35260 0.35603 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35632 0.35956

Eigenvalues --- 0.36611 0.37050 0.37132 0.38019 0.40240

Eigenvalues --- 0.41215 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41215 0.41236 0.41403 0.41408 0.41412

Eigenvalues --- 0.41415 0.41480 0.41921 0.42219 0.42468

Eigenvalues --- 0.43190 0.44480 0.44560 0.44712 0.44758

Eigenvalues --- 0.44851 0.44942 0.44998 0.45000 0.45001

Eigenvalues --- 0.45003 0.45365 0.45365 0.45442 0.45862

Eigenvalues --- 0.47165 0.47262 0.48505 0.49271 0.49321

Eigenvalues --- 0.49836 0.50250 0.53554 0.53554 0.53554

Eigenvalues --- 0.53554 0.53554 0.53559 0.54040 0.54971

Eigenvalues --- 0.55407 0.56063 0.57400 0.57557 0.57590

Eigenvalues --- 0.66865

En-DIIS/RFO-DIIS IScMMF= 0 using points: 18 17 16

RFO step: Lambda=-2.29117128D-05.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=F DC= 1.72D-04 SmlDif= 1.00D-05

RMS Error= 0.4681553492D-03 NUsed= 3 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.85779 0.02610 0.11611

Iteration 1 RMS(Cart)= 0.00860574 RMS(Int)= 0.00003233

Iteration 2 RMS(Cart)= 0.00008391 RMS(Int)= 0.00000483

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000483

ITry= 1 IFail=0 DXMaxC= 3.57D-02 DCOld= 1.00D+10 DXMaxT= 9.60D-02 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58236 0.00016 0.00011 0.00010 0.00020 2.58256

R2 2.74066 -0.00013 0.00036 -0.00156 -0.00120 2.73946

R3 2.56037 0.00044 0.00008 0.00173 0.00182 2.56219

R4 2.58243 0.00015 0.00011 0.00005 0.00015 2.58258

R5 3.87151 0.00011 0.00075 0.00157 0.00228 3.87379

R6 2.74059 -0.00009 0.00037 -0.00155 -0.00118 2.73941

R7 2.56038 0.00045 0.00010 0.00157 0.00168 2.56206

R8 2.69390 0.00050 -0.00003 0.00203 0.00201 2.69591

R9 2.66233 0.00018 0.00026 0.00056 0.00081 2.66314

R10 2.66233 0.00017 0.00025 0.00054 0.00079 2.66312

R11 2.48235 0.00006 -0.00006 -0.00030 -0.00034 2.48201

R12 2.59627 0.00003 0.00011 0.00040 0.00051 2.59678

R13 2.79374 0.00036 -0.00003 0.00196 0.00193 2.79567

R14 2.59622 0.00002 0.00010 0.00045 0.00055 2.59677

R15 3.84329 0.00009 0.00068 0.00152 0.00219 3.84547

R16 2.79385 0.00029 -0.00005 0.00192 0.00187 2.79572

R17 2.48240 0.00001 -0.00007 -0.00021 -0.00027 2.48214

R18 2.66526 -0.00031 -0.00001 -0.00113 -0.00113 2.66412

R19 2.64549 0.00018 0.00024 0.00016 0.00040 2.64589

R20 2.64546 0.00021 0.00024 0.00020 0.00044 2.64590

R21 2.48241 0.00002 -0.00007 -0.00025 -0.00030 2.48211

R22 2.66528 -0.00034 -0.00003 -0.00108 -0.00111 2.66418

R23 2.79377 0.00034 -0.00005 0.00198 0.00194 2.79570

R24 2.64551 0.00018 0.00024 0.00018 0.00042 2.64593

R25 2.79385 0.00027 -0.00006 0.00193 0.00187 2.79572

R26 2.64554 0.00015 0.00023 0.00015 0.00038 2.64592

R27 2.59633 -0.00002 0.00010 0.00034 0.00045 2.59678

R28 2.48245 -0.00003 -0.00009 -0.00014 -0.00021 2.48224

R29 2.59638 -0.00002 0.00012 0.00027 0.00039 2.59678

R30 3.84357 0.00008 0.00058 0.00202 0.00259 3.84616

R31 2.56038 0.00041 0.00005 0.00182 0.00188 2.56226

R32 2.58243 0.00013 0.00013 0.00000 0.00012 2.58254

R33 2.58251 0.00012 0.00013 -0.00003 0.00008 2.58259

R34 3.87157 0.00012 0.00064 0.00226 0.00286 3.87443

R35 2.74067 -0.00014 0.00035 -0.00155 -0.00120 2.73947

R36 2.69393 0.00047 -0.00005 0.00205 0.00201 2.69594

R37 2.66236 0.00016 0.00025 0.00052 0.00077 2.66313

R38 2.74061 -0.00010 0.00036 -0.00155 -0.00119 2.73942

R39 2.66236 0.00016 0.00025 0.00054 0.00079 2.66315

R40 2.56041 0.00041 0.00007 0.00164 0.00173 2.56214

R41 2.65524 0.00020 -0.00025 0.00125 0.00100 2.65624

R42 2.54999 -0.00032 -0.00020 -0.00029 -0.00049 2.54950

R43 2.62928 -0.00008 -0.00025 0.00016 -0.00009 2.62919

R44 2.04401 0.00010 -0.00001 0.00029 0.00028 2.04429

R45 2.65526 0.00019 -0.00025 0.00125 0.00099 2.65625

R46 2.04401 0.00009 -0.00001 0.00029 0.00027 2.04428

R47 2.54997 -0.00029 -0.00020 -0.00025 -0.00045 2.54952

R48 2.64290 0.00002 -0.00017 0.00048 0.00032 2.64321

R49 2.55273 -0.00034 -0.00018 -0.00023 -0.00041 2.55232

R50 2.64718 -0.00008 -0.00027 0.00005 -0.00022 2.64696

R51 2.04387 0.00008 0.00002 0.00003 0.00005 2.04392

R52 2.64290 0.00002 -0.00017 0.00048 0.00031 2.64322

R53 2.04387 0.00007 0.00002 0.00003 0.00005 2.04392

R54 2.55272 -0.00032 -0.00017 -0.00022 -0.00039 2.55233

R55 2.65527 0.00018 -0.00025 0.00123 0.00098 2.65624

R56 2.55001 -0.00034 -0.00020 -0.00031 -0.00051 2.54950

R57 2.62930 -0.00010 -0.00026 0.00013 -0.00012 2.62917

R58 2.04401 0.00010 -0.00001 0.00030 0.00029 2.04429

R59 2.65528 0.00018 -0.00026 0.00123 0.00097 2.65626

R60 2.04401 0.00010 -0.00001 0.00029 0.00028 2.04429

R61 2.54999 -0.00030 -0.00020 -0.00027 -0.00047 2.54951

R62 2.64293 0.00000 -0.00017 0.00046 0.00029 2.64322

R63 2.55273 -0.00034 -0.00017 -0.00024 -0.00041 2.55231

R64 2.64719 -0.00009 -0.00027 0.00002 -0.00025 2.64693

R65 2.04387 0.00008 0.00002 0.00003 0.00006 2.04393

R66 2.64292 0.00001 -0.00017 0.00046 0.00029 2.64321

R67 2.04387 0.00008 0.00002 0.00003 0.00006 2.04393

R68 2.55274 -0.00036 -0.00018 -0.00026 -0.00044 2.55231

R69 2.69401 -0.00011 0.00003 -0.00029 -0.00026 2.69375

R70 2.69402 -0.00011 0.00003 -0.00028 -0.00026 2.69376

R71 2.69594 -0.00012 0.00003 -0.00037 -0.00035 2.69560

R72 2.69594 -0.00012 0.00003 -0.00037 -0.00034 2.69560

R73 2.69401 -0.00011 0.00003 -0.00029 -0.00026 2.69375

R74 2.69401 -0.00011 0.00003 -0.00029 -0.00026 2.69375

R75 2.69595 -0.00012 0.00003 -0.00037 -0.00034 2.69560

R76 2.69595 -0.00012 0.00003 -0.00037 -0.00035 2.69560

R77 2.06720 0.00012 -0.00001 0.00041 0.00040 2.06760

R78 2.06678 0.00011 -0.00002 0.00035 0.00033 2.06711

R79 2.05670 0.00006 0.00000 0.00027 0.00027 2.05697

R80 2.06677 0.00013 0.00002 0.00041 0.00043 2.06720

R81 2.06703 0.00013 0.00000 0.00044 0.00044 2.06747

R82 2.05646 0.00007 0.00000 0.00031 0.00031 2.05677

R83 2.06703 0.00013 0.00000 0.00044 0.00044 2.06747

R84 2.06677 0.00013 0.00002 0.00041 0.00043 2.06720

R85 2.05646 0.00008 0.00000 0.00031 0.00031 2.05677

R86 2.06678 0.00011 -0.00002 0.00034 0.00032 2.06710

R87 2.06720 0.00012 -0.00001 0.00041 0.00040 2.06760

R88 2.05670 0.00006 0.00000 0.00027 0.00027 2.05697

R89 2.06703 0.00013 0.00000 0.00044 0.00044 2.06747

R90 2.06677 0.00013 0.00002 0.00041 0.00043 2.06720

R91 2.05646 0.00008 0.00000 0.00031 0.00031 2.05677

R92 2.06677 0.00012 0.00002 0.00041 0.00042 2.06720

R93 2.06703 0.00013 0.00000 0.00044 0.00044 2.06747

R94 2.05645 0.00008 0.00000 0.00032 0.00032 2.05677

R95 2.06720 0.00012 -0.00001 0.00041 0.00040 2.06760

R96 2.06678 0.00011 -0.00002 0.00034 0.00032 2.06711

R97 2.05670 0.00006 0.00000 0.00027 0.00027 2.05697

R98 2.06678 0.00011 -0.00002 0.00034 0.00032 2.06710

R99 2.06720 0.00012 -0.00001 0.00041 0.00040 2.06760

R100 2.05670 0.00006 0.00000 0.00027 0.00027 2.05697

A1 1.88896 0.00008 -0.00003 0.00144 0.00140 1.89036

A2 2.21459 -0.00006 0.00013 -0.00099 -0.00088 2.21371

A3 2.17946 -0.00001 -0.00009 -0.00036 -0.00044 2.17902

A4 1.93073 -0.00005 0.00003 -0.00159 -0.00154 1.92919

A5 2.17122 0.00001 -0.00021 0.00117 0.00096 2.17218

A6 2.17096 0.00004 -0.00020 0.00122 0.00102 2.17197

A7 1.88898 0.00006 -0.00004 0.00144 0.00140 1.89038

A8 2.21471 -0.00008 0.00011 -0.00099 -0.00089 2.21382

A9 2.17932 0.00003 -0.00007 -0.00037 -0.00042 2.17890

A10 1.85803 -0.00004 0.00001 -0.00064 -0.00063 1.85741

A11 2.31712 0.00015 0.00015 0.00065 0.00080 2.31791

A12 2.10793 -0.00010 -0.00015 -0.00008 -0.00024 2.10769

A13 1.85804 -0.00005 0.00001 -0.00064 -0.00064 1.85741

A14 2.31718 0.00012 0.00014 0.00061 0.00074 2.31792

A15 2.10785 -0.00008 -0.00014 -0.00003 -0.00017 2.10768

A16 2.18649 -0.00003 0.00011 0.00058 0.00069 2.18718

A17 2.23151 0.00004 -0.00025 0.00114 0.00089 2.23240

A18 2.16749 -0.00006 -0.00007 -0.00052 -0.00059 2.16690

A19 1.88348 0.00003 0.00031 -0.00033 -0.00003 1.88345

A20 1.93265 -0.00010 -0.00046 0.00024 -0.00019 1.93245

A21 2.16239 0.00007 0.00003 -0.00036 -0.00034 2.16205

A22 2.16255 0.00004 0.00000 -0.00034 -0.00035 2.16220

A23 1.88345 0.00006 0.00032 -0.00033 -0.00002 1.88343

A24 2.23139 0.00008 -0.00023 0.00117 0.00093 2.23232

A25 2.16763 -0.00013 -0.00010 -0.00053 -0.00064 2.16699

A26 1.86253 0.00001 -0.00009 0.00021 0.00013 1.86266

A27 2.30461 -0.00003 0.00031 -0.00080 -0.00050 2.30411

A28 2.11587 0.00002 -0.00021 0.00058 0.00037 2.11624

A29 1.86255 0.00000 -0.00009 0.00019 0.00011 1.86266

A30 2.30446 0.00003 0.00033 -0.00071 -0.00038 2.30408

A31 2.11599 -0.00003 -0.00023 0.00051 0.00028 2.11627

A32 2.18647 -0.00003 0.00009 0.00074 0.00083 2.18730

A33 1.86257 -0.00001 -0.00009 0.00017 0.00009 1.86266

A34 2.11596 -0.00002 -0.00022 0.00052 0.00030 2.11625

A35 2.30448 0.00003 0.00032 -0.00071 -0.00039 2.30410

A36 1.86255 0.00000 -0.00009 0.00019 0.00011 1.86266

A37 2.11586 0.00004 -0.00020 0.00061 0.00040 2.11627

A38 2.30459 -0.00003 0.00031 -0.00082 -0.00051 2.30408

A39 1.88346 0.00007 0.00034 -0.00036 -0.00003 1.88343

A40 2.16761 -0.00014 -0.00012 -0.00042 -0.00054 2.16707

A41 2.23140 0.00008 -0.00022 0.00108 0.00085 2.23224

A42 1.93261 -0.00011 -0.00049 0.00034 -0.00013 1.93248

A43 2.16253 0.00004 0.00002 -0.00035 -0.00033 2.16220

A44 2.16238 0.00007 0.00004 -0.00035 -0.00032 2.16206

A45 2.16749 -0.00008 -0.00009 -0.00040 -0.00049 2.16700

A46 2.23150 0.00004 -0.00024 0.00104 0.00079 2.23230

A47 1.88347 0.00005 0.00033 -0.00036 -0.00004 1.88344

A48 2.18648 -0.00004 0.00007 0.00086 0.00093 2.18740

A49 1.93076 -0.00007 -0.00001 -0.00153 -0.00151 1.92925

A50 2.17123 0.00002 -0.00020 0.00115 0.00095 2.17218

A51 2.17096 0.00005 -0.00018 0.00118 0.00100 2.17195

A52 2.21461 -0.00007 0.00013 -0.00107 -0.00095 2.21365

A53 2.17947 -0.00003 -0.00010 -0.00026 -0.00035 2.17912

A54 1.88893 0.00010 -0.00001 0.00142 0.00140 1.89032

A55 1.85807 -0.00006 0.00001 -0.00065 -0.00065 1.85742

A56 2.31717 0.00012 0.00014 0.00059 0.00072 2.31789

A57 2.10785 -0.00006 -0.00014 0.00000 -0.00015 2.10770

A58 1.85806 -0.00006 0.00001 -0.00065 -0.00064 1.85741

A59 2.10791 -0.00009 -0.00015 -0.00006 -0.00021 2.10770

A60 2.31711 0.00015 0.00015 0.00064 0.00078 2.31790

A61 1.88894 0.00008 -0.00002 0.00142 0.00140 1.89034

A62 2.21474 -0.00009 0.00011 -0.00106 -0.00096 2.21377

A63 2.17933 0.00001 -0.00008 -0.00028 -0.00035 2.17898

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D3 3.12891 0.00009 0.00201 0.00409 0.00610 3.13501

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D7 -3.12658 -0.00014 -0.00150 -0.00424 -0.00574 -3.13233

D8 0.03108 -0.00007 -0.00221 0.00095 -0.00126 0.02982

D9 0.19706 -0.00015 0.00071 -0.00318 -0.00247 0.19459

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D13 -3.00049 0.00009 0.00137 -0.00498 -0.00362 -3.00410

D14 0.16056 -0.00014 0.00054 -0.00983 -0.00929 0.15127

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D153 3.13956 -0.00008 -0.00016 -0.00178 -0.00195 3.13761

D154 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D155 -0.00173 0.00002 0.00047 -0.00117 -0.00070 -0.00243

D156 3.14154 0.00015 0.00074 0.00175 0.00249 -3.13916

D157 3.13779 -0.00006 0.00029 -0.00299 -0.00269 3.13510

D158 -0.00213 0.00007 0.00057 -0.00007 0.00050 -0.00163

D159 3.09217 0.00017 -0.00011 0.00589 0.00578 3.09795

D160 -0.05112 0.00003 -0.00039 0.00293 0.00254 -0.04858

D161 -0.00793 0.00001 -0.00047 0.00223 0.00176 -0.00617

D162 3.13914 0.00006 -0.00015 0.00185 0.00169 3.14083

D163 3.12676 0.00000 -0.00069 0.00381 0.00312 3.12988

D164 -0.00936 0.00004 -0.00037 0.00342 0.00304 -0.00632

D165 -3.13829 -0.00014 0.00369 -0.01803 -0.01434 3.13056

D166 0.01025 -0.00012 0.00391 -0.01961 -0.01570 -0.00544

D167 0.00000 0.00000 0.00001 -0.00002 -0.00001 -0.00001

D168 -3.13620 0.00004 0.00030 -0.00041 -0.00011 -3.13631

D169 3.13625 -0.00004 -0.00030 0.00036 0.00006 3.13631

D170 0.00004 0.00000 0.00000 -0.00003 -0.00004 0.00001

D171 0.00795 -0.00001 0.00046 -0.00223 -0.00176 0.00618

D172 -3.12666 0.00000 0.00068 -0.00389 -0.00321 -3.12987

D173 -3.13916 -0.00006 0.00016 -0.00183 -0.00166 -3.14082

D174 0.00942 -0.00004 0.00038 -0.00349 -0.00311 0.00630

D175 3.13819 0.00014 -0.00367 0.01793 0.01426 -3.13073

D176 -0.01043 0.00012 -0.00389 0.01961 0.01572 0.00529

D177 -0.00177 0.00002 0.00047 -0.00105 -0.00058 -0.00235

D178 3.13774 -0.00006 0.00030 -0.00297 -0.00267 3.13507

D179 -3.14157 0.00015 0.00071 0.00192 0.00262 -3.13895

D180 -0.00206 0.00007 0.00054 -0.00001 0.00053 -0.00153

D181 3.09239 0.00016 -0.00016 0.00600 0.00584 3.09823

D182 -0.05102 0.00003 -0.00041 0.00300 0.00259 -0.04843

D183 0.00005 0.00000 -0.00002 -0.00004 -0.00006 -0.00001

D184 3.13956 -0.00008 -0.00017 -0.00188 -0.00205 3.13751

D185 -3.13950 0.00007 0.00015 0.00184 0.00199 -3.13751

D186 0.00001 0.00000 0.00000 0.00001 0.00000 0.00001

D187 0.00172 -0.00002 -0.00046 0.00108 0.00063 0.00235

D188 3.14158 -0.00015 -0.00071 -0.00190 -0.00261 3.13897

D189 -3.13774 0.00006 -0.00030 0.00295 0.00265 -3.13509

D190 0.00212 -0.00007 -0.00056 -0.00003 -0.00058 0.00154

D191 -3.09225 -0.00017 0.00013 -0.00598 -0.00586 -3.09811

D192 0.05110 -0.00004 0.00039 -0.00296 -0.00257 0.04853

D193 -0.00794 0.00001 -0.00046 0.00222 0.00176 -0.00618

D194 3.13918 0.00005 -0.00016 0.00178 0.00162 3.14079

D195 3.12665 0.00000 -0.00068 0.00393 0.00326 3.12990

D196 -0.00942 0.00004 -0.00037 0.00349 0.00311 -0.00631

D197 -3.13832 -0.00014 0.00368 -0.01789 -0.01421 3.13065

D198 0.01032 -0.00012 0.00389 -0.01961 -0.01572 -0.00540

D199 -0.00001 0.00000 -0.00001 -0.00001 -0.00002 -0.00003

D200 -3.13624 0.00004 0.00030 -0.00041 -0.00011 -3.13635

D201 3.13619 -0.00004 -0.00030 0.00042 0.00012 3.13631

D202 -0.00004 0.00000 0.00000 0.00003 0.00003 -0.00001

D203 0.00793 -0.00001 0.00046 -0.00222 -0.00176 0.00617

D204 -3.12675 0.00000 0.00068 -0.00388 -0.00320 -3.12995

D205 -3.13916 -0.00006 0.00015 -0.00181 -0.00166 -3.14082

D206 0.00935 -0.00004 0.00037 -0.00347 -0.00310 0.00625

D207 3.13838 0.00013 -0.00369 0.01788 0.01419 -3.13062

D208 -0.01018 0.00012 -0.00391 0.01955 0.01564 0.00546

D209 1.08981 -0.00014 0.00077 -0.00945 -0.00868 1.08113

D210 -1.05210 -0.00012 0.00063 -0.00902 -0.00839 -1.06050

D211 -3.12400 -0.00012 0.00071 -0.00932 -0.00861 -3.13261

D212 1.05227 0.00011 -0.00065 0.00900 0.00836 1.06062

D213 -1.08966 0.00014 -0.00079 0.00943 0.00864 -1.08102

D214 3.12415 0.00011 -0.00072 0.00929 0.00857 3.13272

D215 1.09623 0.00000 0.00015 -0.00076 -0.00061 1.09562

D216 -1.04800 -0.00001 0.00017 -0.00114 -0.00097 -1.04898

D217 -3.11735 -0.00002 0.00016 -0.00107 -0.00091 -3.11826

D218 1.04795 0.00001 -0.00016 0.00112 0.00096 1.04891

D219 -1.09626 0.00000 -0.00014 0.00072 0.00058 -1.09568

D220 3.11730 0.00002 -0.00015 0.00104 0.00089 3.11820

D221 1.05208 0.00012 -0.00062 0.00900 0.00838 1.06046

D222 -1.08984 0.00014 -0.00077 0.00942 0.00866 -1.08118

D223 3.12397 0.00012 -0.00070 0.00930 0.00860 3.13257

D224 1.08967 -0.00014 0.00079 -0.00942 -0.00863 1.08103

D225 -1.05227 -0.00012 0.00064 -0.00902 -0.00837 -1.06064

D226 -3.12415 -0.00012 0.00072 -0.00930 -0.00858 -3.13273

D227 1.09628 0.00000 0.00014 -0.00069 -0.00055 1.09573

D228 -1.04793 -0.00001 0.00015 -0.00111 -0.00096 -1.04889

D229 -3.11728 -0.00002 0.00014 -0.00101 -0.00087 -3.11815

D230 1.04796 0.00001 -0.00016 0.00109 0.00093 1.04889

D231 -1.09627 0.00000 -0.00014 0.00070 0.00056 -1.09571

D232 3.11730 0.00002 -0.00015 0.00101 0.00086 3.11816

Item Value Threshold Converged?

Maximum Force 0.000500 0.000450 NO

RMS Force 0.000125 0.000300 YES

Maximum Displacement 0.035735 0.001800 NO

RMS Displacement 0.008604 0.001200 NO

Predicted change in Energy=-5.522703D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 02:34:45 2019, MaxMem= 1342177280 cpu: 14.9

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=3 Diff= 1.00D-04

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 -1.122434 2.799994 -0.038835

2 7 0 0.000452 2.039749 -0.208630

3 6 0 1.123819 2.799371 -0.039140

4 6 0 0.714436 4.158753 0.253988

5 6 0 -0.712177 4.159144 0.254277

6 7 0 2.409962 2.382334 -0.139483

7 6 0 2.798375 1.129919 -0.214833

8 7 0 2.019021 -0.000497 -0.159430

9 6 0 2.797875 -1.131243 -0.215066

10 6 0 4.209636 -0.705840 -0.336229

11 6 0 4.209936 0.703954 -0.336032

12 7 0 -2.408855 2.383558 -0.139024

13 6 0 -4.209844 0.706069 -0.335483

14 6 0 -4.210236 -0.703753 -0.335652

15 6 0 -2.798657 -1.129847 -0.214811

16 7 0 -2.019246 0.000525 -0.159297

17 6 0 -2.798032 1.131340 -0.214564

18 7 0 -2.410073 -2.382346 -0.139624

19 7 0 -0.000581 -2.039857 -0.209007

20 6 0 -1.123864 -2.799586 -0.039573

21 6 0 -0.714272 -4.159054 0.253031

22 6 0 0.712358 -4.159352 0.252878

23 6 0 1.122435 -2.800073 -0.039785

24 7 0 2.408792 -2.383535 -0.139987

25 30 0 0.000063 0.000135 -0.413940

26 6 0 -5.403920 1.432828 -0.415915

27 6 0 -6.598931 0.697488 -0.499589

28 6 0 -6.599308 -0.693821 -0.499750

29 6 0 -5.404699 -1.429841 -0.416251

30 6 0 1.432959 -5.338724 0.528342

31 6 0 0.698971 -6.499839 0.792001

32 6 0 -0.701741 -6.499541 0.792159

33 6 0 -1.435297 -5.338112 0.528673

34 6 0 5.404316 1.430138 -0.416887

35 6 0 6.598966 0.694254 -0.500934

36 6 0 6.598672 -0.697045 -0.501143

37 6 0 5.403719 -1.432475 -0.417308

38 6 0 -1.432580 5.338441 0.530497

39 6 0 -0.698455 6.499428 0.794348

40 6 0 0.702241 6.499063 0.793988

41 6 0 1.435616 5.337685 0.529790

42 1 0 7.549971 1.205014 -0.571567

43 1 0 7.549470 -1.208167 -0.571921

44 1 0 1.209946 7.429225 1.010537

45 1 0 -1.205569 7.429849 1.011167

46 1 0 -7.549725 1.208689 -0.569860

47 1 0 -7.550381 -1.204478 -0.570139

48 1 0 -1.209311 -7.429808 1.008560

49 1 0 1.206197 -7.430322 1.008280

50 8 0 2.784975 5.279285 0.529612

51 8 0 -2.781972 5.280733 0.531057

52 8 0 5.347054 2.778058 -0.415606

53 8 0 5.345894 -2.780379 -0.416406

54 8 0 2.782353 -5.280943 0.528456

55 8 0 -2.784667 -5.279736 0.529091

56 8 0 -5.347560 -2.777779 -0.415113

57 8 0 -5.346087 2.780726 -0.414485

58 6 0 3.516942 6.467101 0.821653

59 1 0 3.301582 6.830194 1.831059

60 1 0 3.306243 7.258393 0.096391

61 1 0 4.566669 6.186852 0.755573

62 6 0 6.568537 3.514220 -0.443896

63 1 0 7.132293 3.323248 -1.361696

64 1 0 7.193514 3.286043 0.424611

65 1 0 6.275870 4.562065 -0.412674

66 6 0 6.567051 -3.517084 -0.444770

67 1 0 7.192062 -3.289375 0.423835

68 1 0 7.130965 -3.326165 -1.362484

69 1 0 6.273922 -4.564806 -0.413802

70 6 0 -3.513198 6.468916 0.823478

71 1 0 -3.302597 7.260051 0.098018

72 1 0 -3.297026 6.831972 1.832720

73 1 0 -4.563100 6.189158 0.758091

74 6 0 -6.567247 3.517452 -0.442099

75 1 0 -7.191954 3.289377 0.426630

76 1 0 -7.131487 3.326934 -1.359695

77 1 0 -6.274087 4.565156 -0.410776

78 6 0 -6.569068 -3.513928 -0.442780

79 1 0 -7.133298 -3.322983 -1.360293

80 1 0 -7.193601 -3.285750 0.426046

81 1 0 -6.276383 -4.561771 -0.411691

82 6 0 -3.516562 -6.467673 0.820824

83 1 0 -3.300738 -6.831351 1.829918

84 1 0 -3.306299 -7.258556 0.094990

85 1 0 -4.566301 -6.187306 0.755431

86 6 0 3.513756 -6.469174 0.820219

87 1 0 3.302828 -7.260125 0.094654

88 1 0 3.298087 -6.832509 1.829472

89 1 0 4.563615 -6.189354 0.754403

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0448510 0.0438576 0.0225496

Leave Link 202 at Sat Jul 6 02:34:46 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8041.6178112059 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= 89 NActive= 89 NUniq= 89 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= -0.2279144078 Hartrees.

Nuclear repulsion after empirical dispersion term = 8041.3898967981 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6394

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.11D-10

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 387

GePol: Fraction of low-weight points (<1% of avg) = 6.05%

GePol: Cavity surface area = 704.276 Ang\*\*2

GePol: Cavity volume = 801.909 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0089455490 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8041.3809512491 Hartrees.

Leave Link 301 at Sat Jul 6 02:34:47 2019, MaxMem= 1342177280 cpu: 1.5

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44341 LenP2D= 111344.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.65D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 02:34:50 2019, MaxMem= 1342177280 cpu: 41.8

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 02:34:51 2019, MaxMem= 1342177280 cpu: 3.3

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000001 0.000006 0.000036 Ang= 0.00 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>= 2.0171 S= 1.0057

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2650.02646240588

Leave Link 401 at Sat Jul 6 02:35:09 2019, MaxMem= 1342177280 cpu: 209.9

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 122649708.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.35D-14 for 508.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.18D-15 for 6375 6005.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.88D-15 for 2619.

Iteration 1 A^-1\*A deviation from orthogonality is 1.32D-09 for 5193 5141.

Iteration 2 A\*A^-1 deviation from unit magnitude is 1.38D-14 for 1017.

Iteration 2 A\*A^-1 deviation from orthogonality is 1.47D-14 for 4058 518.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.44D-15 for 1574.

Iteration 2 A^-1\*A deviation from orthogonality is 4.60D-16 for 6380 100.

E= -2649.79479949062

DIIS: error= 8.25D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79479949062 IErMin= 1 ErrMin= 8.25D-04

ErrMax= 8.25D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.43D-03 BMatP= 1.43D-03

IDIUse=3 WtCom= 9.92D-01 WtEn= 8.25D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.685 Goal= None Shift= 0.000

Gap= 0.744 Goal= None Shift= 0.000

RMSDP=4.16D-05 MaxDP=2.06D-03 OVMax= 5.18D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.16D-05 CP: 1.00D+00

E= -2649.79544104325 Delta-E= -0.000641552628 Rises=F Damp=F

DIIS: error= 9.06D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79544104325 IErMin= 2 ErrMin= 9.06D-05

ErrMax= 9.06D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.22D-05 BMatP= 1.43D-03

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.646D-01 0.106D+01

Coeff: -0.646D-01 0.106D+01

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.32D-06 MaxDP=1.46D-04 DE=-6.42D-04 OVMax= 5.10D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.80D-06 CP: 1.00D+00 1.05D+00

E= -2649.79544654993 Delta-E= -0.000005506678 Rises=F Damp=F

DIIS: error= 9.25D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79544654993 IErMin= 2 ErrMin= 9.06D-05

ErrMax= 9.25D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.62D-05 BMatP= 2.22D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.390D-01 0.530D+00 0.509D+00

Coeff: -0.390D-01 0.530D+00 0.509D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.31D-06 MaxDP=1.36D-04 DE=-5.51D-06 OVMax= 4.41D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.75D-06 CP: 1.00D+00 1.05D+00 6.15D-01

E= -2649.79544884109 Delta-E= -0.000002291168 Rises=F Damp=F

DIIS: error= 2.79D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79544884109 IErMin= 4 ErrMin= 2.79D-05

ErrMax= 2.79D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.11D-06 BMatP= 1.62D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.919D-02 0.113D+00 0.279D+00 0.617D+00

Coeff: -0.919D-02 0.113D+00 0.279D+00 0.617D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=7.81D-07 MaxDP=5.63D-05 DE=-2.29D-06 OVMax= 9.67D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.97D-07 CP: 1.00D+00 1.05D+00 7.12D-01 7.33D-01

E= -2649.79544919841 Delta-E= -0.000000357313 Rises=F Damp=F

DIIS: error= 1.12D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79544919841 IErMin= 5 ErrMin= 1.12D-05

ErrMax= 1.12D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.65D-07 BMatP= 2.11D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.260D-02 0.273D-01 0.118D+00 0.327D+00 0.530D+00

Coeff: -0.260D-02 0.273D-01 0.118D+00 0.327D+00 0.530D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.15D-07 MaxDP=1.96D-05 DE=-3.57D-07 OVMax= 4.43D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.38D-07 CP: 1.00D+00 1.05D+00 7.22D-01 7.84D-01 7.33D-01

E= -2649.79544922480 Delta-E= -0.000000026392 Rises=F Damp=F

DIIS: error= 3.25D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79544922480 IErMin= 6 ErrMin= 3.25D-06

ErrMax= 3.25D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.71D-08 BMatP= 1.65D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.294D-03-0.761D-02 0.111D-01 0.586D-01 0.266D+00 0.672D+00

Coeff: 0.294D-03-0.761D-02 0.111D-01 0.586D-01 0.266D+00 0.672D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=7.22D-08 MaxDP=7.11D-06 DE=-2.64D-08 OVMax= 3.11D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 5.72D-08 CP: 1.00D+00 1.05D+00 7.26D-01 7.91D-01 7.77D-01

CP: 7.69D-01

E= -2649.79544922811 Delta-E= -0.000000003309 Rises=F Damp=F

DIIS: error= 1.11D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79544922811 IErMin= 7 ErrMin= 1.11D-06

ErrMax= 1.11D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.70D-09 BMatP= 1.71D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.351D-03-0.630D-02-0.241D-02 0.871D-02 0.109D+00 0.380D+00

Coeff-Com: 0.511D+00

Coeff: 0.351D-03-0.630D-02-0.241D-02 0.871D-02 0.109D+00 0.380D+00

Coeff: 0.511D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=3.18D-08 MaxDP=2.55D-06 DE=-3.31D-09 OVMax= 2.03D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 2.85D-08 CP: 1.00D+00 1.05D+00 7.27D-01 7.92D-01 7.89D-01

CP: 8.33D-01 8.49D-01

E= -2649.79544922899 Delta-E= -0.000000000886 Rises=F Damp=F

DIIS: error= 3.84D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.79544922899 IErMin= 8 ErrMin= 3.84D-07

ErrMax= 3.84D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.14D-10 BMatP= 2.70D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.993D-04-0.123D-02-0.376D-02-0.982D-02-0.944D-02 0.306D-01

Coeff-Com: 0.275D+00 0.719D+00

Coeff: 0.993D-04-0.123D-02-0.376D-02-0.982D-02-0.944D-02 0.306D-01

Coeff: 0.275D+00 0.719D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.69D-08 MaxDP=7.67D-07 DE=-8.86D-10 OVMax= 1.45D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 9.55D-09 CP: 1.00D+00 1.05D+00 7.27D-01 7.94D-01 7.97D-01

CP: 8.65D-01 1.06D+00 1.03D+00

E= -2649.79544922901 Delta-E= -0.000000000011 Rises=F Damp=F

DIIS: error= 2.02D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.79544922901 IErMin= 9 ErrMin= 2.02D-07

ErrMax= 2.02D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.39D-11 BMatP= 4.14D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.283D-04 0.813D-03-0.105D-02-0.638D-02-0.274D-01-0.652D-01

Coeff-Com: 0.299D-01 0.321D+00 0.749D+00

Coeff: -0.283D-04 0.813D-03-0.105D-02-0.638D-02-0.274D-01-0.652D-01

Coeff: 0.299D-01 0.321D+00 0.749D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=9.88D-09 MaxDP=4.63D-07 DE=-1.09D-11 OVMax= 1.02D-05

Error on total polarization charges = 0.07300

SCF Done: E(UB3LYP) = -2649.79544923 A.U. after 9 cycles

NFock= 9 Conv=0.99D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0171 S= 1.0057

<L.S>= 0.000000000000E+00

KE= 2.690124559130D+03 PE=-2.236146537729D+04 EE= 8.980164417683D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.61

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0171, after 2.0002

Leave Link 502 at Sat Jul 6 02:42:59 2019, MaxMem= 1342177280 cpu: 5542.2

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44341 LenP2D= 111344.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 276

Leave Link 701 at Sat Jul 6 02:43:18 2019, MaxMem= 1342177280 cpu: 224.5

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 02:43:19 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 02:44:53 2019, MaxMem= 1342177280 cpu: 1129.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 8.83133011D-04 1.14261048D-03 2.80344695D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000513141 -0.000296390 -0.000464999

2 7 0.000018336 0.000157650 0.000524009

3 6 0.000466200 -0.000253610 -0.000464343

4 6 -0.000072478 0.000128746 0.000068810

5 6 0.000057155 0.000118312 0.000063495

6 7 0.000037954 0.000125896 0.000281367

7 6 -0.000046296 -0.000297785 -0.000082106

8 7 0.000022229 0.000001505 -0.000530911

9 6 -0.000094212 0.000243460 -0.000091389

10 6 -0.000169240 -0.000153659 0.000118986

11 6 -0.000163122 0.000144676 0.000113121

12 7 -0.000037105 0.000132587 0.000275494

13 6 0.000159965 0.000148316 0.000110615

14 6 0.000168209 -0.000157852 0.000115045

15 6 0.000151545 0.000213454 -0.000059202

16 7 0.000023256 -0.000000201 -0.000557228

17 6 0.000100771 -0.000274451 -0.000055574

18 7 -0.000056036 -0.000098047 0.000275238

19 7 0.000012384 -0.000100336 0.000520287

20 6 -0.000519060 0.000340744 -0.000464220

21 6 0.000048987 -0.000120679 0.000062277

22 6 -0.000065592 -0.000130677 0.000062065

23 6 0.000471749 0.000294704 -0.000456249

24 7 0.000057441 -0.000093344 0.000281581

25 30 -0.000064443 -0.000055587 0.001048449

26 6 -0.000274870 -0.000067200 -0.000119044

27 6 0.000125345 0.000002105 0.000013896

28 6 0.000125404 -0.000008052 0.000013620

29 6 -0.000280523 0.000058772 -0.000116686

30 6 0.000111681 -0.000002867 0.000211380

31 6 -0.000067006 0.000088295 -0.000075415

32 6 0.000063587 0.000089569 -0.000074542

33 6 -0.000117622 -0.000008294 0.000207903

34 6 0.000276306 -0.000056991 -0.000124885

35 6 -0.000127408 0.000009880 0.000012328

36 6 -0.000127678 -0.000016493 0.000011803

37 6 0.000282530 0.000050696 -0.000120944

38 6 -0.000126290 0.000010320 0.000203796

39 6 0.000059090 -0.000091047 -0.000074658

40 6 -0.000061851 -0.000090246 -0.000075008

41 6 0.000120688 0.000004901 0.000206692

42 1 -0.000009691 -0.000017568 0.000020755

43 1 -0.000007685 0.000013960 0.000020520

44 1 0.000096792 0.000017554 0.000050706

45 1 -0.000098545 0.000018068 0.000050782

46 1 0.000007543 -0.000016087 0.000019093

47 1 0.000006084 0.000012763 0.000018791

48 1 -0.000099105 -0.000020573 0.000051274

49 1 0.000098176 -0.000019584 0.000051324

50 8 0.000003493 -0.000195476 -0.000335482

51 8 -0.000004856 -0.000197471 -0.000331544

52 8 -0.000258668 0.000020781 0.000000570

53 8 -0.000261845 -0.000020041 -0.000003340

54 8 -0.000001658 0.000200640 -0.000339103

55 8 -0.000003856 0.000204276 -0.000336162

56 8 0.000277343 -0.000018143 -0.000009548

57 8 0.000273056 0.000015651 -0.000007579

58 6 -0.000149175 -0.000029079 0.000180205

59 1 -0.000076024 0.000066394 -0.000054708

60 1 0.000031148 0.000013335 -0.000044805

61 1 -0.000050966 0.000001770 0.000030240

62 6 -0.000036733 -0.000036462 -0.000031139

63 1 0.000007028 -0.000011912 0.000023160

64 1 -0.000008757 -0.000006916 -0.000022202

65 1 0.000037180 -0.000019562 -0.000009745

66 6 -0.000036003 0.000040562 -0.000030518

67 1 -0.000008711 0.000008662 -0.000022338

68 1 0.000007014 0.000013180 0.000022707

69 1 0.000036478 0.000018927 -0.000009076

70 6 0.000151435 -0.000027966 0.000179094

71 1 -0.000029643 0.000013477 -0.000044370

72 1 0.000076021 0.000066685 -0.000053435

73 1 0.000051020 0.000001351 0.000030600

74 6 0.000035797 -0.000037520 -0.000031165

75 1 0.000008471 -0.000007822 -0.000023081

76 1 -0.000006120 -0.000013511 0.000023174

77 1 -0.000037727 -0.000019228 -0.000010133

78 6 0.000035915 0.000042787 -0.000032086

79 1 -0.000006214 0.000014873 0.000022746

80 1 0.000008186 0.000009001 -0.000022949

81 1 -0.000036996 0.000018407 -0.000010286

82 6 0.000154862 0.000028408 0.000180763

83 1 0.000076533 -0.000067047 -0.000054188

84 1 -0.000029195 -0.000013633 -0.000044329

85 1 0.000050690 -0.000001856 0.000030777

86 6 -0.000152477 0.000027117 0.000180247

87 1 0.000031618 -0.000013651 -0.000044286

88 1 -0.000077310 -0.000066013 -0.000054911

89 1 -0.000050762 -0.000002289 0.000030126

-------------------------------------------------------------------

Cartesian Forces: Max 0.001048449 RMS 0.000168134

Leave Link 716 at Sat Jul 6 02:44:53 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.000713564 RMS 0.000120056

Search for a local minimum.

Step number 19 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .12006D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 6 5 7 9 11

14 13 16 17 18

19

DE= -4.08D-05 DEPred=-5.52D-05 R= 7.38D-01

TightC=F SS= 1.41D+00 RLast= 7.85D-02 DXNew= 1.6152D-01 2.3551D-01

Trust test= 7.38D-01 RLast= 7.85D-02 DXMaxT set to 1.62D-01

ITU= 1 1 0 0 -1 -1 0 -1 0 0 0 0 0 0 1 1 1 1 0

Eigenvalues --- 0.00323 0.01143 0.01315 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01317 0.01433

Eigenvalues --- 0.01560 0.01570 0.01575 0.01583 0.01599

Eigenvalues --- 0.01618 0.01621 0.01627 0.01707 0.01710

Eigenvalues --- 0.01713 0.01716 0.01762 0.01836 0.01870

Eigenvalues --- 0.01879 0.01921 0.01923 0.01944 0.01948

Eigenvalues --- 0.01993 0.01999 0.02020 0.02022 0.02036

Eigenvalues --- 0.02052 0.02052 0.02053 0.02053 0.02053

Eigenvalues --- 0.02057 0.02057 0.02057 0.02057 0.02057

Eigenvalues --- 0.02065 0.02067 0.02067 0.02070 0.02070

Eigenvalues --- 0.02070 0.02071 0.02083 0.02083 0.02085

Eigenvalues --- 0.02130 0.02159 0.02257 0.02260 0.02260

Eigenvalues --- 0.02260 0.02260 0.02260 0.02261 0.02344

Eigenvalues --- 0.02358 0.02362 0.02814 0.03163 0.04131

Eigenvalues --- 0.09905 0.09977 0.09977 0.09977 0.09987

Eigenvalues --- 0.09987 0.09987 0.10072 0.10646 0.10646

Eigenvalues --- 0.10646 0.10653 0.10659 0.10659 0.10659

Eigenvalues --- 0.10662 0.12446 0.13299 0.13457 0.15070

Eigenvalues --- 0.15853 0.15982 0.15994 0.15998 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16009 0.16062

Eigenvalues --- 0.16397 0.16877 0.20149 0.21099 0.21652

Eigenvalues --- 0.22473 0.22475 0.22475 0.22477 0.24215

Eigenvalues --- 0.24354 0.24441 0.24505 0.24513 0.24598

Eigenvalues --- 0.24608 0.24754 0.24798 0.24850 0.24883

Eigenvalues --- 0.24911 0.24961 0.24979 0.24980 0.24981

Eigenvalues --- 0.24986 0.24995 0.24996 0.24998 0.24998

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25001 0.25066 0.25241 0.28654 0.29950

Eigenvalues --- 0.32848 0.33631 0.33657 0.33676 0.33717

Eigenvalues --- 0.34043 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34063 0.34075 0.34081 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34082

Eigenvalues --- 0.34104 0.34598 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34686 0.34689 0.34890

Eigenvalues --- 0.34950 0.35218 0.35570 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35632 0.35701

Eigenvalues --- 0.36908 0.37026 0.37133 0.37563 0.39975

Eigenvalues --- 0.41215 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41216 0.41249 0.41375 0.41408 0.41414

Eigenvalues --- 0.41417 0.41420 0.41800 0.42173 0.42470

Eigenvalues --- 0.42989 0.44380 0.44559 0.44648 0.44777

Eigenvalues --- 0.44872 0.44998 0.44999 0.45001 0.45003

Eigenvalues --- 0.45027 0.45364 0.45366 0.45825 0.46250

Eigenvalues --- 0.47258 0.47430 0.48855 0.49283 0.49337

Eigenvalues --- 0.49839 0.50230 0.53554 0.53554 0.53554

Eigenvalues --- 0.53554 0.53554 0.53560 0.54154 0.54980

Eigenvalues --- 0.55624 0.56064 0.57405 0.57557 0.57639

Eigenvalues --- 0.66588

En-DIIS/RFO-DIIS IScMMF= 0 using points: 19 18 17 16

RFO step: Lambda=-1.68918939D-05.

NNeg= 0 NP= 4 Switch= 2.50D-03 Rises=F DC= 1.72D-04 SmlDif= 1.00D-05

RMS Error= 0.3767327273D-03 NUsed= 4 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.89340 0.40482 -0.15043 -0.14779

Iteration 1 RMS(Cart)= 0.00654596 RMS(Int)= 0.00001991

Iteration 2 RMS(Cart)= 0.00006733 RMS(Int)= 0.00000672

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000672

ITry= 1 IFail=0 DXMaxC= 3.79D-02 DCOld= 1.00D+10 DXMaxT= 1.62D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58256 0.00001 -0.00001 0.00024 0.00025 2.58280

R2 2.73946 -0.00004 0.00025 0.00033 0.00058 2.74004

R3 2.56219 -0.00025 -0.00075 -0.00042 -0.00119 2.56100

R4 2.58258 0.00000 -0.00007 0.00027 0.00022 2.58279

R5 3.87379 -0.00021 -0.00194 -0.00197 -0.00387 3.86992

R6 2.73941 -0.00002 0.00021 0.00047 0.00067 2.74008

R7 2.56206 -0.00018 -0.00098 -0.00013 -0.00113 2.56093

R8 2.69591 0.00003 -0.00046 0.00032 -0.00015 2.69576

R9 2.66314 -0.00021 -0.00019 0.00007 -0.00011 2.66303

R10 2.66312 -0.00021 -0.00019 0.00007 -0.00012 2.66300

R11 2.48201 -0.00007 -0.00023 0.00097 0.00072 2.48273

R12 2.59678 -0.00024 -0.00025 -0.00036 -0.00061 2.59617

R13 2.79567 -0.00030 -0.00050 -0.00025 -0.00076 2.79491

R14 2.59677 -0.00024 -0.00016 -0.00045 -0.00061 2.59616

R15 3.84547 -0.00032 -0.00052 -0.00176 -0.00226 3.84322

R16 2.79572 -0.00033 -0.00043 -0.00045 -0.00088 2.79484

R17 2.48214 -0.00015 0.00004 0.00059 0.00061 2.48275

R18 2.66412 -0.00012 0.00037 -0.00011 0.00024 2.66437

R19 2.64589 -0.00015 -0.00011 0.00012 0.00001 2.64590

R20 2.64590 -0.00016 -0.00013 0.00016 0.00004 2.64594

R21 2.48211 -0.00013 -0.00003 0.00068 0.00063 2.48273

R22 2.66418 -0.00015 0.00047 -0.00027 0.00020 2.66437

R23 2.79570 -0.00031 -0.00044 -0.00034 -0.00079 2.79492

R24 2.64593 -0.00017 -0.00010 0.00009 -0.00002 2.64592

R25 2.79572 -0.00034 -0.00037 -0.00057 -0.00094 2.79478

R26 2.64592 -0.00017 -0.00009 0.00004 -0.00005 2.64587

R27 2.59678 -0.00026 -0.00023 -0.00046 -0.00069 2.59609

R28 2.48224 -0.00023 0.00024 0.00029 0.00051 2.48275

R29 2.59678 -0.00025 -0.00032 -0.00036 -0.00069 2.59609

R30 3.84616 -0.00038 -0.00040 -0.00194 -0.00232 3.84384

R31 2.56226 -0.00031 -0.00056 -0.00068 -0.00126 2.56100

R32 2.58254 -0.00001 -0.00008 0.00023 0.00017 2.58271

R33 2.58259 -0.00001 -0.00014 0.00028 0.00015 2.58275

R34 3.87443 -0.00027 -0.00181 -0.00204 -0.00382 3.87061

R35 2.73947 -0.00006 0.00030 0.00025 0.00055 2.74002

R36 2.69594 0.00000 -0.00036 0.00018 -0.00018 2.69576

R37 2.66313 -0.00022 -0.00017 0.00002 -0.00015 2.66298

R38 2.73942 -0.00002 0.00025 0.00041 0.00066 2.74008

R39 2.66315 -0.00022 -0.00018 0.00004 -0.00014 2.66301

R40 2.56214 -0.00023 -0.00080 -0.00038 -0.00119 2.56094

R41 2.65624 -0.00010 -0.00005 -0.00017 -0.00022 2.65603

R42 2.54950 -0.00005 0.00034 -0.00017 0.00016 2.54967

R43 2.62919 0.00000 0.00027 -0.00012 0.00015 2.62934

R44 2.04429 -0.00002 -0.00004 0.00000 -0.00005 2.04424

R45 2.65625 -0.00012 -0.00004 -0.00021 -0.00025 2.65600

R46 2.04428 -0.00001 -0.00004 -0.00001 -0.00005 2.04423

R47 2.54952 -0.00006 0.00032 -0.00014 0.00018 2.54971

R48 2.64321 -0.00010 0.00015 -0.00015 0.00000 2.64322

R49 2.55232 -0.00024 0.00053 -0.00028 0.00024 2.55257

R50 2.64696 -0.00004 0.00021 -0.00026 -0.00005 2.64691

R51 2.04392 0.00007 -0.00009 0.00011 0.00003 2.04395

R52 2.64322 -0.00010 0.00016 -0.00017 -0.00001 2.64321

R53 2.04392 0.00007 -0.00008 0.00011 0.00003 2.04395

R54 2.55233 -0.00024 0.00052 -0.00026 0.00026 2.55259

R55 2.65624 -0.00011 -0.00004 -0.00020 -0.00024 2.65600

R56 2.54950 -0.00004 0.00034 -0.00019 0.00015 2.54965

R57 2.62917 0.00001 0.00027 -0.00012 0.00014 2.62932

R58 2.04429 -0.00002 -0.00005 0.00000 -0.00005 2.04424

R59 2.65626 -0.00012 -0.00003 -0.00024 -0.00027 2.65599

R60 2.04429 -0.00001 -0.00004 0.00000 -0.00005 2.04424

R61 2.54951 -0.00005 0.00033 -0.00016 0.00017 2.54969

R62 2.64322 -0.00010 0.00016 -0.00019 -0.00003 2.64319

R63 2.55231 -0.00024 0.00053 -0.00027 0.00025 2.55256

R64 2.64693 -0.00003 0.00021 -0.00026 -0.00005 2.64688

R65 2.04393 0.00007 -0.00009 0.00011 0.00003 2.04395

R66 2.64321 -0.00010 0.00016 -0.00017 -0.00001 2.64320

R67 2.04393 0.00007 -0.00009 0.00011 0.00003 2.04395

R68 2.55231 -0.00024 0.00053 -0.00030 0.00024 2.55254

R69 2.69375 -0.00006 0.00006 -0.00019 -0.00013 2.69362

R70 2.69376 -0.00006 0.00006 -0.00018 -0.00013 2.69363

R71 2.69560 -0.00004 0.00009 -0.00010 -0.00001 2.69559

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R73 2.69375 -0.00006 0.00006 -0.00018 -0.00013 2.69362

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R75 2.69560 -0.00004 0.00009 -0.00009 -0.00001 2.69559

R76 2.69560 -0.00004 0.00009 -0.00009 -0.00001 2.69559

R77 2.06760 -0.00001 -0.00002 0.00002 0.00000 2.06760

R78 2.06711 0.00003 -0.00003 0.00008 0.00005 2.06716

R79 2.05697 -0.00005 0.00002 -0.00008 -0.00006 2.05691

R80 2.06720 -0.00001 -0.00005 0.00002 -0.00003 2.06716

R81 2.06747 -0.00002 -0.00004 -0.00001 -0.00004 2.06743

R82 2.05677 -0.00003 0.00001 -0.00002 -0.00002 2.05676

R83 2.06747 -0.00002 -0.00004 -0.00001 -0.00004 2.06743

R84 2.06720 -0.00001 -0.00005 0.00002 -0.00003 2.06716

R85 2.05677 -0.00003 0.00000 -0.00002 -0.00001 2.05676

R86 2.06710 0.00003 -0.00003 0.00008 0.00005 2.06715

R87 2.06760 -0.00001 -0.00002 0.00002 0.00000 2.06759

R88 2.05697 -0.00005 0.00002 -0.00007 -0.00006 2.05691

R89 2.06747 -0.00002 -0.00004 -0.00001 -0.00004 2.06743

R90 2.06720 -0.00001 -0.00005 0.00001 -0.00004 2.06716

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R92 2.06720 -0.00001 -0.00005 0.00001 -0.00004 2.06716

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R95 2.06760 -0.00001 -0.00002 0.00002 0.00000 2.06759

R96 2.06711 0.00003 -0.00003 0.00008 0.00005 2.06715

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R98 2.06710 0.00003 -0.00003 0.00008 0.00005 2.06715

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R100 2.05697 -0.00005 0.00002 -0.00008 -0.00006 2.05691

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A2 2.21371 0.00017 0.00011 0.00036 0.00047 2.21418

A3 2.17902 0.00005 0.00002 0.00003 0.00002 2.17904

A4 1.92919 0.00028 0.00011 0.00058 0.00065 1.92984

A5 2.17218 -0.00014 0.00013 0.00015 0.00026 2.17243

A6 2.17197 -0.00013 0.00026 0.00009 0.00033 2.17230

A7 1.89038 -0.00022 -0.00010 -0.00047 -0.00055 1.88983

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A9 2.17890 0.00008 -0.00007 0.00023 0.00014 2.17904

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A11 2.31791 -0.00008 -0.00026 -0.00002 -0.00029 2.31762

A12 2.10769 0.00000 0.00017 -0.00017 -0.00001 2.10768

A13 1.85741 0.00008 0.00008 0.00012 0.00020 1.85761

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A16 2.18718 -0.00015 0.00002 0.00004 0.00004 2.18723

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A18 2.16690 -0.00011 0.00033 -0.00014 0.00019 2.16708

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A20 1.93245 -0.00001 0.00044 -0.00012 0.00030 1.93275

A21 2.16205 0.00002 0.00021 0.00034 0.00056 2.16261

A22 2.16220 0.00001 0.00010 0.00041 0.00051 2.16271

A23 1.88343 0.00003 -0.00029 0.00021 -0.00007 1.88337

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A25 2.16699 -0.00015 0.00045 -0.00041 0.00003 2.16703

A26 1.86266 -0.00002 0.00004 -0.00009 -0.00006 1.86260

A27 2.30411 -0.00001 -0.00001 0.00014 0.00013 2.30424

A28 2.11624 0.00004 -0.00004 0.00000 -0.00005 2.11619

A29 1.86266 -0.00002 0.00005 -0.00011 -0.00006 1.86260

A30 2.30408 0.00000 -0.00009 0.00034 0.00025 2.30433

A31 2.11627 0.00002 0.00002 -0.00018 -0.00016 2.11611

A32 2.18730 -0.00018 0.00016 -0.00017 -0.00002 2.18728

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A35 2.30410 0.00000 -0.00007 0.00033 0.00026 2.30436

A36 1.86266 -0.00002 0.00004 -0.00010 -0.00007 1.86259

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A38 2.30408 -0.00002 0.00000 0.00011 0.00012 2.30419

A39 1.88343 0.00004 -0.00038 0.00032 -0.00004 1.88338

A40 2.16707 -0.00019 0.00061 -0.00065 -0.00005 2.16702

A41 2.23224 0.00015 -0.00026 0.00037 0.00010 2.23234

A42 1.93248 -0.00003 0.00062 -0.00031 0.00029 1.93277

A43 2.16220 0.00001 0.00001 0.00052 0.00053 2.16272

A44 2.16206 0.00002 0.00013 0.00047 0.00059 2.16265

A45 2.16700 -0.00015 0.00050 -0.00036 0.00013 2.16714

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A48 2.18740 -0.00020 0.00029 -0.00038 -0.00010 2.18731

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A50 2.17218 -0.00013 0.00004 0.00028 0.00029 2.17247

A51 2.17195 -0.00012 0.00017 0.00021 0.00036 2.17231

A52 2.21365 0.00018 0.00006 0.00042 0.00049 2.21414

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A56 2.31789 -0.00008 -0.00022 -0.00010 -0.00033 2.31756

A57 2.10770 0.00001 0.00012 -0.00004 0.00009 2.10779

A58 1.85741 0.00008 0.00008 0.00012 0.00020 1.85761

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A60 2.31790 -0.00007 -0.00025 -0.00001 -0.00027 2.31763

A61 1.89034 -0.00021 -0.00020 -0.00033 -0.00051 1.88983

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A63 2.17898 0.00006 0.00007 0.00004 0.00009 2.17907

A64 2.18729 -0.00017 0.00015 -0.00016 -0.00002 2.18727

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A66 1.55826 0.00003 0.00026 0.00063 0.00087 1.55913

A67 1.55830 0.00003 0.00025 0.00059 0.00083 1.55913

A68 1.55817 0.00001 0.00045 0.00038 0.00082 1.55899

A69 2.04532 -0.00002 0.00001 0.00011 0.00013 2.04544

A70 2.07368 -0.00020 -0.00022 -0.00029 -0.00051 2.07317

A71 2.16418 0.00022 0.00021 0.00017 0.00038 2.16456

A72 2.12161 -0.00001 0.00000 0.00000 0.00000 2.12160

A73 2.09887 0.00002 -0.00006 0.00013 0.00007 2.09894

A74 2.06270 0.00000 0.00006 -0.00013 -0.00007 2.06263

A75 2.12162 -0.00002 0.00002 -0.00006 -0.00005 2.12157

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A77 2.09887 0.00002 -0.00007 0.00015 0.00009 2.09896

A78 2.04531 -0.00002 0.00003 0.00007 0.00010 2.04540

A79 2.07365 -0.00020 -0.00019 -0.00038 -0.00057 2.07309

A80 2.16421 0.00022 0.00016 0.00030 0.00047 2.16468

A81 2.05242 0.00002 -0.00008 0.00008 0.00000 2.05243

A82 2.06584 0.00008 -0.00015 0.00039 0.00024 2.06609

A83 2.16491 -0.00010 0.00023 -0.00047 -0.00025 2.16466

A84 2.12304 -0.00001 -0.00007 0.00006 -0.00001 2.12303

A85 2.10104 -0.00007 0.00007 -0.00004 0.00003 2.10107

A86 2.05909 0.00008 0.00000 -0.00002 -0.00002 2.05907

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A90 2.05243 0.00001 -0.00007 0.00005 -0.00002 2.05241

A91 2.06582 0.00009 -0.00014 0.00037 0.00023 2.06605

A92 2.16492 -0.00010 0.00021 -0.00042 -0.00021 2.16471

A93 2.04534 -0.00002 0.00001 0.00012 0.00013 2.04547

A94 2.07364 -0.00019 -0.00028 -0.00015 -0.00043 2.07321

A95 2.16420 0.00021 0.00027 0.00003 0.00030 2.16450

A96 2.12158 0.00000 -0.00002 0.00002 0.00000 2.12159

A97 2.09888 0.00001 -0.00005 0.00011 0.00007 2.09895

A98 2.06272 -0.00001 0.00007 -0.00014 -0.00007 2.06264

A99 2.12160 -0.00001 0.00000 -0.00004 -0.00004 2.12156

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A102 2.04534 -0.00002 0.00002 0.00009 0.00011 2.04545

A103 2.07362 -0.00018 -0.00024 -0.00025 -0.00048 2.07314

A104 2.16421 0.00021 0.00022 0.00015 0.00037 2.16459

A105 2.05246 0.00001 -0.00007 0.00006 -0.00001 2.05245

A106 2.06582 0.00009 -0.00017 0.00045 0.00028 2.06609

A107 2.16489 -0.00010 0.00024 -0.00051 -0.00026 2.16463

A108 2.12303 -0.00001 -0.00007 0.00005 -0.00002 2.12300

A109 2.10105 -0.00007 0.00007 -0.00004 0.00003 2.10107

A110 2.05910 0.00008 0.00000 -0.00001 0.00000 2.05910

A111 2.12302 -0.00001 -0.00008 0.00007 -0.00001 2.12301

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A116 2.16488 -0.00009 0.00026 -0.00055 -0.00028 2.16460

A117 2.06798 -0.00069 0.00043 -0.00125 -0.00082 2.06716

A118 2.06800 -0.00070 0.00042 -0.00125 -0.00083 2.06718

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A126 1.94770 -0.00001 0.00013 0.00062 0.00075 1.94845

A127 1.84234 0.00001 0.00018 0.00020 0.00038 1.84273

A128 1.91103 -0.00004 -0.00015 -0.00063 -0.00078 1.91026

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A130 1.90896 -0.00001 0.00001 -0.00032 -0.00031 1.90864

A131 1.94749 -0.00001 -0.00004 -0.00020 -0.00024 1.94726

A132 1.94527 -0.00002 0.00000 -0.00027 -0.00027 1.94501

A133 1.84006 0.00006 -0.00005 0.00064 0.00058 1.84065

A134 1.91265 -0.00002 0.00005 -0.00015 -0.00010 1.91255

A135 1.90786 -0.00001 0.00006 -0.00001 0.00005 1.90791

A136 1.90882 0.00000 -0.00002 0.00002 0.00000 1.90882

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A143 1.94770 -0.00001 0.00014 0.00060 0.00074 1.94844

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A146 1.91105 -0.00004 -0.00015 -0.00062 -0.00077 1.91028

A147 1.90895 -0.00001 0.00000 -0.00030 -0.00030 1.90865

A148 1.90844 0.00004 0.00006 0.00035 0.00041 1.90885

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A163 1.84233 0.00001 0.00017 0.00022 0.00039 1.84272

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A166 1.90894 -0.00001 0.00000 -0.00030 -0.00030 1.90864

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A170 1.91105 -0.00004 -0.00015 -0.00062 -0.00077 1.91027

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D2 3.00401 -0.00007 0.00229 0.00424 0.00653 3.01054

D3 3.13501 -0.00015 -0.00270 -0.00135 -0.00405 3.13096

D4 -0.15144 -0.00005 0.00061 0.00467 0.00528 -0.14617

D5 -0.00426 0.00010 0.00055 0.00122 0.00177 -0.00248

D6 -3.12529 0.00008 0.00191 0.00378 0.00570 -3.11960

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D8 0.02982 0.00006 0.00355 0.00336 0.00691 0.03673

D9 0.19459 -0.00010 -0.00141 -0.00628 -0.00769 0.18690

D10 -2.96304 -0.00008 -0.00335 -0.00579 -0.00914 -2.97218

D11 -0.00735 0.00017 0.00107 0.00162 0.00269 -0.00466

D12 -3.13516 0.00015 0.00272 0.00122 0.00394 -3.13122

D13 -3.00410 0.00007 -0.00222 -0.00441 -0.00663 -3.01073

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D15 -2.93434 -0.00026 -0.00450 -0.00675 -0.01126 -2.94560

D16 -0.04235 0.00011 0.00076 0.00001 0.00077 -0.04158

D17 0.04259 -0.00011 -0.00076 0.00013 -0.00064 0.04195

D18 2.93458 0.00026 0.00450 0.00689 0.01140 2.94597

D19 0.00443 -0.00010 -0.00069 -0.00080 -0.00149 0.00294

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D21 3.13259 -0.00008 -0.00229 -0.00041 -0.00271 3.12988

D22 -0.02956 -0.00005 -0.00361 -0.00308 -0.00669 -0.03625

D23 -0.19468 0.00011 0.00138 0.00632 0.00770 -0.18698

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D27 -3.12415 -0.00002 0.00121 0.00202 0.00323 -3.12091

D28 -0.00011 0.00000 0.00004 -0.00017 -0.00012 -0.00023

D29 -3.12469 -0.00001 0.00189 0.00478 0.00667 -3.11802

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D31 -0.00605 0.00002 0.00042 0.00181 0.00223 -0.00382

D32 3.13039 0.00001 0.00060 0.00192 0.00252 3.13290

D33 3.12484 0.00001 -0.00200 -0.00446 -0.00646 3.11838

D34 -0.01157 0.00002 -0.00218 -0.00452 -0.00669 -0.01826

D35 0.00619 -0.00002 -0.00047 -0.00160 -0.00208 0.00411

D36 -3.13022 -0.00001 -0.00066 -0.00166 -0.00231 -3.13253

D37 -0.04591 -0.00013 -0.00003 -0.00152 -0.00155 -0.04746

D38 3.13154 -0.00019 0.00113 -0.00270 -0.00157 3.12997

D39 -3.09584 0.00003 0.00148 -0.00097 0.00051 -3.09532

D40 0.28319 -0.00001 -0.00183 -0.00382 -0.00565 0.27754

D41 0.01457 0.00008 0.00049 0.00005 0.00054 0.01511

D42 -2.88960 0.00003 -0.00282 -0.00280 -0.00562 -2.89522

D43 3.10325 0.00000 -0.00132 0.00112 -0.00020 3.10304

D44 -0.01773 -0.00006 -0.00006 -0.00189 -0.00195 -0.01968

D45 -0.00861 -0.00005 -0.00036 0.00014 -0.00022 -0.00883

D46 -3.12958 -0.00011 0.00090 -0.00287 -0.00198 -3.13156

D47 -0.01460 -0.00008 -0.00042 -0.00021 -0.00063 -0.01523

D48 3.09586 -0.00004 -0.00145 0.00086 -0.00060 3.09526

D49 2.88953 -0.00003 0.00291 0.00262 0.00554 2.89508

D50 -0.28319 0.00001 0.00188 0.00369 0.00557 -0.27761

D51 -0.23354 0.00011 0.00182 0.00365 0.00547 -0.22806

D52 3.10695 -0.00007 0.00198 -0.00046 0.00152 3.10847

D53 -3.10693 0.00006 -0.00198 0.00051 -0.00146 -3.10839

D54 0.23356 -0.00011 -0.00182 -0.00360 -0.00542 0.22814

D55 0.00870 0.00005 0.00017 0.00029 0.00047 0.00917

D56 3.12963 0.00011 -0.00105 0.00323 0.00217 3.13181

D57 -3.10321 0.00000 0.00117 -0.00074 0.00044 -3.10277

D58 0.01772 0.00006 -0.00005 0.00220 0.00214 0.01987

D59 0.04594 0.00014 0.00002 0.00155 0.00157 0.04751

D60 -3.13145 0.00019 -0.00118 0.00279 0.00161 -3.12984

D61 -0.00006 0.00000 0.00011 -0.00026 -0.00014 -0.00020

D62 3.12362 0.00005 -0.00098 0.00237 0.00138 3.12500

D63 -3.12369 -0.00005 0.00117 -0.00281 -0.00163 -3.12532

D64 -0.00002 0.00000 0.00008 -0.00018 -0.00010 -0.00012

D65 -3.12077 -0.00003 0.00072 -0.00160 -0.00088 -3.12165

D66 0.02552 0.00000 0.00003 -0.00093 -0.00091 0.02461

D67 -0.00233 0.00004 -0.00065 0.00169 0.00104 -0.00129

D68 -3.13922 0.00007 -0.00134 0.00235 0.00101 -3.13821

D69 3.12085 0.00003 -0.00086 0.00191 0.00105 3.12190

D70 -0.02547 0.00000 -0.00021 0.00137 0.00116 -0.02430

D71 0.00235 -0.00004 0.00055 -0.00147 -0.00092 0.00144

D72 3.13922 -0.00006 0.00120 -0.00201 -0.00080 3.13842

D73 -3.13162 0.00019 -0.00114 0.00287 0.00174 -3.12988

D74 0.04614 0.00013 0.00005 0.00148 0.00153 0.04766

D75 0.00002 0.00000 -0.00011 0.00028 0.00017 0.00018

D76 3.12350 0.00006 -0.00119 0.00290 0.00171 3.12520

D77 -3.12348 -0.00005 0.00101 -0.00243 -0.00142 -3.12490

D78 0.00000 0.00000 -0.00008 0.00020 0.00012 0.00012

D79 -3.10299 0.00000 0.00132 -0.00113 0.00019 -3.10280

D80 0.00861 0.00005 0.00034 0.00003 0.00036 0.00898

D81 0.01778 0.00006 0.00004 0.00197 0.00201 0.01979

D82 3.12939 0.00012 -0.00095 0.00313 0.00218 3.13157

D83 -0.00242 0.00004 -0.00058 0.00154 0.00097 -0.00145

D84 -3.13939 0.00007 -0.00127 0.00227 0.00100 -3.13840

D85 -3.12069 -0.00003 0.00086 -0.00193 -0.00107 -3.12176

D86 0.02552 0.00000 0.00017 -0.00121 -0.00104 0.02448

D87 -0.00864 -0.00005 -0.00016 -0.00049 -0.00065 -0.00929

D88 3.10305 0.00000 -0.00119 0.00075 -0.00043 3.10262

D89 -3.12939 -0.00012 0.00110 -0.00351 -0.00241 -3.13180

D90 -0.01770 -0.00007 0.00007 -0.00227 -0.00220 -0.01990

D91 0.00242 -0.00004 0.00067 -0.00178 -0.00111 0.00132

D92 3.13942 -0.00007 0.00140 -0.00263 -0.00123 3.13819

D93 3.12067 0.00003 -0.00073 0.00161 0.00087 3.12154

D94 -0.02553 0.00000 0.00000 0.00075 0.00075 -0.02478

D95 0.01454 0.00009 0.00039 0.00052 0.00091 0.01545

D96 -2.88975 0.00004 -0.00295 -0.00253 -0.00549 -2.89523

D97 -3.09570 0.00004 0.00144 -0.00076 0.00069 -3.09501

D98 0.28320 -0.00001 -0.00190 -0.00381 -0.00571 0.27749

D99 3.13157 -0.00019 0.00119 -0.00293 -0.00174 3.12983

D100 -0.04608 -0.00013 -0.00005 -0.00144 -0.00149 -0.04757

D101 3.09561 -0.00004 -0.00147 0.00086 -0.00061 3.09500

D102 -0.01453 -0.00009 -0.00046 -0.00034 -0.00080 -0.01533

D103 -0.28326 0.00001 0.00185 0.00392 0.00577 -0.27750

D104 2.88978 -0.00004 0.00287 0.00271 0.00558 2.89536

D105 3.10699 -0.00006 0.00202 -0.00046 0.00156 3.10855

D106 -0.23347 0.00012 0.00181 0.00370 0.00552 -0.22795

D107 0.23343 -0.00011 -0.00182 -0.00380 -0.00562 0.22781

D108 -3.10703 0.00007 -0.00202 0.00036 -0.00166 -3.10869

D109 -0.19443 0.00010 0.00146 0.00619 0.00764 -0.18678

D110 2.96313 0.00008 0.00337 0.00579 0.00916 2.97229

D111 -3.13505 0.00016 0.00264 0.00149 0.00413 -3.13092

D112 -0.00726 0.00018 0.00099 0.00183 0.00282 -0.00444

D113 0.15115 0.00005 -0.00070 -0.00464 -0.00534 0.14580

D114 -3.00424 0.00007 -0.00235 -0.00430 -0.00665 -3.01090

D115 0.00727 -0.00017 -0.00104 -0.00168 -0.00272 0.00455

D116 3.13511 -0.00016 -0.00267 -0.00144 -0.00411 3.13100

D117 3.00428 -0.00007 0.00229 0.00446 0.00675 3.01102

D118 -0.15107 -0.00005 0.00066 0.00469 0.00536 -0.14571

D119 2.93454 0.00026 0.00451 0.00688 0.01140 2.94593

D120 0.04253 -0.00011 -0.00071 0.00006 -0.00065 0.04188

D121 -0.04268 0.00011 0.00071 -0.00011 0.00061 -0.04207

D122 -2.93469 -0.00026 -0.00451 -0.00692 -0.01143 -2.94612

D123 3.13243 -0.00009 -0.00215 -0.00090 -0.00305 3.12938

D124 -0.02968 -0.00006 -0.00350 -0.00347 -0.00696 -0.03664

D125 0.00430 -0.00011 -0.00053 -0.00124 -0.00178 0.00252

D126 3.12537 -0.00008 -0.00188 -0.00381 -0.00569 3.11968

D127 0.00002 0.00000 -0.00009 0.00024 0.00016 0.00017

D128 3.12409 0.00002 -0.00120 -0.00206 -0.00326 3.12083

D129 -3.12405 -0.00002 0.00107 0.00243 0.00350 -3.12055

D130 0.00002 0.00000 -0.00004 0.00013 0.00008 0.00011

D131 -3.12482 -0.00001 0.00199 0.00448 0.00647 -3.11835

D132 0.01156 -0.00002 0.00218 0.00454 0.00672 0.01828

D133 -0.00613 0.00002 0.00049 0.00161 0.00210 -0.00404

D134 3.13025 0.00001 0.00067 0.00168 0.00235 3.13260

D135 -0.00433 0.00010 0.00068 0.00084 0.00152 -0.00281

D136 -3.13251 0.00008 0.00225 0.00061 0.00287 -3.12964

D137 -3.12540 0.00008 0.00198 0.00354 0.00552 -3.11989

D138 0.02960 0.00006 0.00355 0.00331 0.00687 0.03647

D139 0.00610 -0.00002 -0.00043 -0.00177 -0.00220 0.00390

D140 -3.13026 -0.00002 -0.00062 -0.00186 -0.00248 -3.13274

D141 3.12479 0.00001 -0.00189 -0.00478 -0.00666 3.11812

D142 -0.01158 0.00002 -0.00207 -0.00487 -0.00694 -0.01852

D143 0.19452 -0.00011 -0.00143 -0.00624 -0.00767 0.18685

D144 -2.96299 -0.00008 -0.00331 -0.00597 -0.00928 -2.97227

D145 0.00243 -0.00004 0.00064 -0.00170 -0.00107 0.00136

D146 -3.13510 -0.00001 0.00022 -0.00050 -0.00028 -3.13538

D147 3.13914 -0.00007 0.00137 -0.00247 -0.00110 3.13804

D148 0.00161 -0.00004 0.00095 -0.00126 -0.00031 0.00130

D149 -3.09804 -0.00005 0.00026 -0.00316 -0.00289 -3.10093

D150 0.04851 -0.00002 -0.00048 -0.00238 -0.00286 0.04565

D151 0.00000 0.00000 -0.00004 0.00012 0.00008 0.00007

D152 -3.13761 0.00003 -0.00042 0.00121 0.00079 -3.13682

D153 3.13761 -0.00003 0.00037 -0.00106 -0.00069 3.13692

D154 0.00000 0.00000 -0.00001 0.00003 0.00002 0.00002

D155 -0.00243 0.00004 -0.00061 0.00163 0.00101 -0.00141

D156 -3.13916 0.00008 -0.00139 0.00253 0.00115 -3.13801

D157 3.13510 0.00001 -0.00023 0.00051 0.00028 3.13538

D158 -0.00163 0.00005 -0.00100 0.00142 0.00042 -0.00121

D159 3.09795 0.00005 -0.00035 0.00342 0.00307 3.10102

D160 -0.04858 0.00002 0.00043 0.00250 0.00293 -0.04565

D161 -0.00617 0.00002 0.00047 0.00168 0.00216 -0.00401

D162 3.14083 0.00004 0.00002 0.00214 0.00216 -3.14020

D163 3.12988 0.00001 0.00067 0.00178 0.00245 3.13233

D164 -0.00632 0.00003 0.00022 0.00224 0.00246 -0.00386

D165 3.13056 -0.00001 -0.00502 -0.00844 -0.01346 3.11710

D166 -0.00544 0.00000 -0.00522 -0.00854 -0.01376 -0.01920

D167 -0.00001 0.00000 -0.00002 0.00007 0.00005 0.00004

D168 -3.13631 0.00002 -0.00043 0.00043 0.00000 -3.13631

D169 3.13631 -0.00001 0.00042 -0.00038 0.00004 3.13635

D170 0.00001 0.00000 0.00001 -0.00001 -0.00001 0.00000

D171 0.00618 -0.00002 -0.00046 -0.00173 -0.00218 0.00400

D172 -3.12987 -0.00001 -0.00066 -0.00180 -0.00245 -3.13232

D173 -3.14082 -0.00004 -0.00004 -0.00210 -0.00214 3.14023

D174 0.00630 -0.00003 -0.00023 -0.00217 -0.00240 0.00390

D175 -3.13073 0.00001 0.00498 0.00857 0.01355 -3.11718

D176 0.00529 0.00001 0.00518 0.00864 0.01382 0.01911

D177 -0.00235 0.00004 -0.00062 0.00162 0.00100 -0.00135

D178 3.13507 0.00002 -0.00023 0.00058 0.00035 3.13542

D179 -3.13895 0.00007 -0.00131 0.00219 0.00088 -3.13807

D180 -0.00153 0.00004 -0.00092 0.00115 0.00023 -0.00130

D181 3.09823 0.00005 -0.00024 0.00306 0.00282 3.10106

D182 -0.04843 0.00002 0.00046 0.00248 0.00295 -0.04548

D183 -0.00001 0.00000 0.00004 -0.00011 -0.00006 -0.00007

D184 3.13751 -0.00003 0.00039 -0.00104 -0.00066 3.13686

D185 -3.13751 0.00002 -0.00033 0.00091 0.00058 -3.13694

D186 0.00001 0.00000 0.00001 -0.00003 -0.00002 -0.00001

D187 0.00235 -0.00004 0.00059 -0.00155 -0.00096 0.00139

D188 3.13897 -0.00007 0.00132 -0.00225 -0.00093 3.13804

D189 -3.13509 -0.00002 0.00024 -0.00060 -0.00035 -3.13544

D190 0.00154 -0.00004 0.00098 -0.00130 -0.00032 0.00121

D191 -3.09811 -0.00005 0.00033 -0.00324 -0.00291 -3.10102

D192 0.04853 -0.00002 -0.00042 -0.00253 -0.00295 0.04558

D193 -0.00618 0.00002 0.00045 0.00174 0.00219 -0.00399

D194 3.14079 0.00004 0.00003 0.00210 0.00213 -3.14026

D195 3.12990 0.00001 0.00064 0.00180 0.00244 3.13234

D196 -0.00631 0.00003 0.00022 0.00216 0.00238 -0.00392

D197 3.13065 -0.00002 -0.00499 -0.00857 -0.01355 3.11710

D198 -0.00540 0.00000 -0.00518 -0.00863 -0.01380 -0.01920

D199 -0.00003 0.00000 0.00002 -0.00008 -0.00006 -0.00009

D200 -3.13635 0.00001 -0.00041 0.00035 -0.00006 -3.13640

D201 3.13631 -0.00002 0.00043 -0.00043 0.00000 3.13630

D202 -0.00001 0.00000 -0.00001 0.00001 0.00000 -0.00001

D203 0.00617 -0.00002 -0.00046 -0.00170 -0.00216 0.00401

D204 -3.12995 -0.00001 -0.00065 -0.00182 -0.00247 -3.13241

D205 -3.14082 -0.00004 -0.00002 -0.00215 -0.00217 3.14020

D206 0.00625 -0.00003 -0.00021 -0.00227 -0.00247 0.00378

D207 -3.13062 0.00001 0.00503 0.00838 0.01341 -3.11720

D208 0.00546 0.00000 0.00522 0.00850 0.01372 0.01918

D209 1.08113 -0.00016 -0.00027 -0.01114 -0.01141 1.06972

D210 -1.06050 -0.00011 -0.00001 -0.01063 -0.01065 -1.07114

D211 -3.13261 -0.00010 -0.00020 -0.01070 -0.01090 3.13967

D212 1.06062 0.00011 0.00005 0.01054 0.01059 1.07121

D213 -1.08102 0.00016 0.00030 0.01106 0.01136 -1.06966

D214 3.13272 0.00010 0.00023 0.01063 0.01086 -3.13960

D215 1.09562 -0.00003 -0.00020 -0.00170 -0.00190 1.09371

D216 -1.04898 0.00001 -0.00023 -0.00117 -0.00141 -1.05039

D217 -3.11826 -0.00001 -0.00018 -0.00143 -0.00161 -3.11987

D218 1.04891 -0.00001 0.00021 0.00116 0.00137 1.05029

D219 -1.09568 0.00003 0.00019 0.00168 0.00187 -1.09381

D220 3.11820 0.00001 0.00016 0.00143 0.00159 3.11978

D221 1.06046 0.00011 0.00000 0.01066 0.01067 1.07113

D222 -1.08118 0.00016 0.00026 0.01118 0.01143 -1.06975

D223 3.13257 0.00010 0.00019 0.01074 0.01093 -3.13968

D224 1.08103 -0.00016 -0.00029 -0.01110 -0.01139 1.06964

D225 -1.06064 -0.00011 -0.00005 -0.01058 -0.01062 -1.07127

D226 -3.13273 -0.00010 -0.00023 -0.01067 -0.01089 3.13957

D227 1.09573 -0.00004 -0.00018 -0.00174 -0.00192 1.09382

D228 -1.04889 0.00001 -0.00020 -0.00123 -0.00142 -1.05031

D229 -3.11815 -0.00001 -0.00015 -0.00150 -0.00164 -3.11979

D230 1.04889 -0.00001 0.00022 0.00117 0.00139 1.05028

D231 -1.09571 0.00004 0.00019 0.00170 0.00189 -1.09382

D232 3.11816 0.00001 0.00016 0.00144 0.00160 3.11976

Item Value Threshold Converged?

Maximum Force 0.000714 0.000450 NO

RMS Force 0.000120 0.000300 YES

Maximum Displacement 0.037932 0.001800 NO

RMS Displacement 0.006539 0.001200 NO

Predicted change in Energy=-3.539608D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 02:44:55 2019, MaxMem= 1342177280 cpu: 15.3

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=0 Diff= 5.43D-04

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 -1.121840 2.800195 -0.033345

2 7 0 0.001199 2.038258 -0.195437

3 6 0 1.125118 2.798919 -0.033517

4 6 0 0.715677 4.160758 0.249711

5 6 0 -0.710859 4.161512 0.250057

6 7 0 2.410589 2.381727 -0.133741

7 6 0 2.798797 1.128892 -0.209756

8 7 0 2.019415 -0.001073 -0.153555

9 6 0 2.797447 -1.131973 -0.209597

10 6 0 4.208785 -0.707383 -0.332815

11 6 0 4.209667 0.702539 -0.332740

12 7 0 -2.407818 2.384468 -0.133657

13 6 0 -4.208862 0.707396 -0.333192

14 6 0 -4.209582 -0.702529 -0.333298

15 6 0 -2.798768 -1.128701 -0.209934

16 7 0 -2.019462 0.001275 -0.153936

17 6 0 -2.797512 1.132112 -0.210019

18 7 0 -2.410540 -2.381519 -0.133500

19 7 0 -0.001183 -2.038140 -0.194966

20 6 0 -1.125070 -2.798777 -0.033069

21 6 0 -0.715709 -4.160584 0.250269

22 6 0 0.710823 -4.161461 0.250141

23 6 0 1.121835 -2.800086 -0.033038

24 7 0 2.407779 -2.384352 -0.133343

25 30 0 0.000166 0.000219 -0.395910

26 6 0 -5.402607 1.434242 -0.417507

27 6 0 -6.597483 0.699203 -0.503777

28 6 0 -6.598130 -0.692185 -0.503987

29 6 0 -5.403929 -1.428313 -0.417850

30 6 0 1.430893 -5.342049 0.521378

31 6 0 0.696413 -6.503199 0.783520

32 6 0 -0.704272 -6.502289 0.783723

33 6 0 -1.437282 -5.340182 0.521741

34 6 0 5.404245 1.428041 -0.417059

35 6 0 6.598301 0.691688 -0.503283

36 6 0 6.597387 -0.699685 -0.503466

37 6 0 5.402361 -1.434463 -0.417350

38 6 0 -1.430993 5.341939 0.521800

39 6 0 -0.696617 6.503186 0.783726

40 6 0 0.704052 6.502509 0.783211

41 6 0 1.437128 5.340535 0.520846

42 1 0 7.549369 1.201942 -0.576284

43 1 0 7.547779 -1.211176 -0.576608

44 1 0 1.211975 7.432935 0.998177

45 1 0 -1.203503 7.434088 0.999074

46 1 0 -7.547982 1.210511 -0.576816

47 1 0 -7.549089 -1.202603 -0.577198

48 1 0 -1.212245 -7.432635 0.998909

49 1 0 1.203227 -7.434211 0.998559

50 8 0 2.786638 5.282817 0.518007

51 8 0 -2.780569 5.285457 0.520015

52 8 0 5.347110 2.776049 -0.416650

53 8 0 5.343308 -2.782405 -0.417307

54 8 0 2.780478 -5.285785 0.518924

55 8 0 -2.786800 -5.282055 0.519655

56 8 0 -5.346262 -2.776326 -0.417861

57 8 0 -5.343899 2.782189 -0.417095

58 6 0 3.517425 6.468319 0.821835

59 1 0 3.293908 6.826354 1.831273

60 1 0 3.313443 7.264156 0.099592

61 1 0 4.567443 6.187757 0.762560

62 6 0 6.568606 3.511877 -0.451991

63 1 0 7.128210 3.318330 -1.371770

64 1 0 7.197236 3.285185 0.414237

65 1 0 6.276912 4.560017 -0.421863

66 6 0 6.563727 -3.520018 -0.452826

67 1 0 7.192716 -3.294407 0.413423

68 1 0 7.123583 -3.327120 -1.372586

69 1 0 6.270500 -4.567736 -0.422890

70 6 0 -3.510051 6.471577 0.824586

71 1 0 -3.305957 7.267299 0.102251

72 1 0 -3.285370 6.829292 1.833876

73 1 0 -4.560371 6.191963 0.766170

74 6 0 -6.564506 3.519501 -0.452274

75 1 0 -7.193349 3.293485 0.413975

76 1 0 -7.124408 3.326718 -1.372030

77 1 0 -6.271542 4.567285 -0.422059

78 6 0 -6.567393 -3.512756 -0.453383

79 1 0 -7.127085 -3.319294 -1.373123

80 1 0 -7.196155 -3.286604 0.412890

81 1 0 -6.275150 -4.560753 -0.423500

82 6 0 -3.517838 -6.467312 0.823839

83 1 0 -3.293844 -6.825517 1.833108

84 1 0 -3.314610 -7.263142 0.101379

85 1 0 -4.567789 -6.186344 0.765252

86 6 0 3.509937 -6.472048 0.822979

87 1 0 3.305307 -7.267683 0.100702

88 1 0 3.285782 -6.829811 1.832370

89 1 0 4.560267 -6.192590 0.763979

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0448273 0.0438844 0.0225459

Leave Link 202 at Sat Jul 6 02:44:56 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8041.8186141492 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= 89 NActive= 89 NUniq= 89 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= -0.2279214949 Hartrees.

Nuclear repulsion after empirical dispersion term = 8041.5906926543 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6375

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.18D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 347

GePol: Fraction of low-weight points (<1% of avg) = 5.44%

GePol: Cavity surface area = 704.009 Ang\*\*2

GePol: Cavity volume = 801.720 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0089973383 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8041.5816953160 Hartrees.

Leave Link 301 at Sat Jul 6 02:44:56 2019, MaxMem= 1342177280 cpu: 1.3

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44336 LenP2D= 111337.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.59D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 02:44:59 2019, MaxMem= 1342177280 cpu: 42.7

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 02:45:00 2019, MaxMem= 1342177280 cpu: 2.5

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000078 0.000063 0.000165 Ang= 0.02 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>= 2.0171 S= 1.0057

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2650.02665155392

Leave Link 401 at Sat Jul 6 02:45:21 2019, MaxMem= 1342177280 cpu: 229.0

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 121921875.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.22D-15 for 6367.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.70D-15 for 3175 887.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.44D-15 for 6367.

Iteration 1 A^-1\*A deviation from orthogonality is 1.30D-09 for 5174 5122.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.89D-15 for 272.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.90D-15 for 6361 115.

Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 1250.

Iteration 2 A^-1\*A deviation from orthogonality is 9.94D-16 for 6374 752.

E= -2649.79503790931

DIIS: error= 6.51D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79503790931 IErMin= 1 ErrMin= 6.51D-04

ErrMax= 6.51D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.92D-04 BMatP= 9.92D-04

IDIUse=3 WtCom= 9.93D-01 WtEn= 6.51D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.685 Goal= None Shift= 0.000

Gap= 0.744 Goal= None Shift= 0.000

RMSDP=3.03D-05 MaxDP=1.42D-03 OVMax= 3.63D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.02D-05 CP: 1.00D+00

E= -2649.79548214074 Delta-E= -0.000444231424 Rises=F Damp=F

DIIS: error= 8.67D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79548214074 IErMin= 2 ErrMin= 8.67D-05

ErrMax= 8.67D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.73D-05 BMatP= 9.92D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.581D-01 0.106D+01

Coeff: -0.581D-01 0.106D+01

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.13D-06 MaxDP=1.57D-04 DE=-4.44D-04 OVMax= 1.11D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.84D-06 CP: 1.00D+00 1.05D+00

E= -2649.79548615781 Delta-E= -0.000004017074 Rises=F Damp=F

DIIS: error= 1.25D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79548615781 IErMin= 2 ErrMin= 8.67D-05

ErrMax= 1.25D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.55D-05 BMatP= 1.73D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.25D-03

Coeff-Com: -0.387D-01 0.547D+00 0.492D+00

Coeff-En: 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.386D-01 0.546D+00 0.492D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.18D-06 MaxDP=1.41D-04 DE=-4.02D-06 OVMax= 6.52D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.50D-06 CP: 1.00D+00 1.06D+00 5.97D-01

E= -2649.79548841785 Delta-E= -0.000002260045 Rises=F Damp=F

DIIS: error= 2.44D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79548841785 IErMin= 4 ErrMin= 2.44D-05

ErrMax= 2.44D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.52D-06 BMatP= 1.55D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.970D-02 0.122D+00 0.254D+00 0.634D+00

Coeff: -0.970D-02 0.122D+00 0.254D+00 0.634D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=6.54D-07 MaxDP=5.00D-05 DE=-2.26D-06 OVMax= 1.99D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.72D-07 CP: 1.00D+00 1.06D+00 6.91D-01 8.23D-01

E= -2649.79548870260 Delta-E= -0.000000284741 Rises=F Damp=F

DIIS: error= 1.17D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79548870260 IErMin= 5 ErrMin= 1.17D-05

ErrMax= 1.17D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.46D-07 BMatP= 1.52D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.250D-02 0.247D-01 0.109D+00 0.375D+00 0.494D+00

Coeff: -0.250D-02 0.247D-01 0.109D+00 0.375D+00 0.494D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.66D-07 MaxDP=1.63D-05 DE=-2.85D-07 OVMax= 6.91D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.01D-07 CP: 1.00D+00 1.06D+00 7.00D-01 8.89D-01 7.15D-01

E= -2649.79548874802 Delta-E= -0.000000045426 Rises=F Damp=F

DIIS: error= 3.73D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79548874802 IErMin= 6 ErrMin= 3.73D-06

ErrMax= 3.73D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.88D-08 BMatP= 2.46D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.529D-03-0.123D-01 0.593D-02 0.645D-01 0.236D+00 0.706D+00

Coeff: 0.529D-03-0.123D-01 0.593D-02 0.645D-01 0.236D+00 0.706D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.06D-07 MaxDP=6.30D-06 DE=-4.54D-08 OVMax= 6.43D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 7.83D-08 CP: 1.00D+00 1.06D+00 7.06D-01 9.14D-01 8.05D-01

CP: 8.35D-01

E= -2649.79548875313 Delta-E= -0.000000005108 Rises=F Damp=F

DIIS: error= 1.71D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79548875313 IErMin= 7 ErrMin= 1.71D-06

ErrMax= 1.71D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.19D-09 BMatP= 1.88D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.580D-03-0.992D-02-0.831D-02-0.396D-02 0.812D-01 0.404D+00

Coeff-Com: 0.536D+00

Coeff: 0.580D-03-0.992D-02-0.831D-02-0.396D-02 0.812D-01 0.404D+00

Coeff: 0.536D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.79D-08 MaxDP=2.88D-06 DE=-5.11D-09 OVMax= 1.80D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 3.55D-08 CP: 1.00D+00 1.06D+00 7.10D-01 9.19D-01 8.24D-01

CP: 9.57D-01 9.44D-01

E= -2649.79548875456 Delta-E= -0.000000001428 Rises=F Damp=F

DIIS: error= 5.53D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.79548875456 IErMin= 8 ErrMin= 5.53D-07

ErrMax= 5.53D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.82D-10 BMatP= 4.19D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.726D-04-0.131D-03-0.456D-02-0.201D-01-0.357D-01-0.367D-01

Coeff-Com: 0.223D+00 0.874D+00

Coeff: 0.726D-04-0.131D-03-0.456D-02-0.201D-01-0.357D-01-0.367D-01

Coeff: 0.223D+00 0.874D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.77D-08 MaxDP=1.03D-06 DE=-1.43D-09 OVMax= 1.79D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.20D-08 CP: 1.00D+00 1.06D+00 7.11D-01 9.25D-01 8.41D-01

CP: 1.01D+00 1.17D+00 1.05D+00

E= -2649.79548875463 Delta-E= -0.000000000075 Rises=F Damp=F

DIIS: error= 2.65D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2649.79548875463 IErMin= 9 ErrMin= 2.65D-07

ErrMax= 2.65D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.18D-10 BMatP= 4.82D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.423D-04 0.131D-02-0.107D-02-0.943D-02-0.281D-01-0.720D-01

Coeff-Com: 0.395D-01 0.442D+00 0.628D+00

Coeff: -0.423D-04 0.131D-02-0.107D-02-0.943D-02-0.281D-01-0.720D-01

Coeff: 0.395D-01 0.442D+00 0.628D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.01D-08 MaxDP=6.25D-07 DE=-7.46D-11 OVMax= 6.47D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 6.93D-09 CP: 1.00D+00 1.06D+00 7.12D-01 9.26D-01 8.45D-01

CP: 1.03D+00 1.23D+00 1.16D+00 8.84D-01

E= -2649.79548875457 Delta-E= 0.000000000060 Rises=F Damp=F

DIIS: error= 1.62D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin= 9 EnMin= -2649.79548875463 IErMin=10 ErrMin= 1.62D-07

ErrMax= 1.62D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.10D-11 BMatP= 1.18D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.479D-04 0.906D-03 0.628D-03-0.403D-03-0.799D-02-0.384D-01

Coeff-Com: -0.401D-01 0.398D-01 0.440D+00 0.605D+00

Coeff: -0.479D-04 0.906D-03 0.628D-03-0.403D-03-0.799D-02-0.384D-01

Coeff: -0.401D-01 0.398D-01 0.440D+00 0.605D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=5.09D-09 MaxDP=3.04D-07 DE= 6.00D-11 OVMax= 3.21D-06

Error on total polarization charges = 0.07300

SCF Done: E(UB3LYP) = -2649.79548875 A.U. after 10 cycles

NFock= 10 Conv=0.51D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0171 S= 1.0057

<L.S>= 0.000000000000E+00

KE= 2.690133546778D+03 PE=-2.236186754680D+04 EE= 8.980356815949D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.65

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0171, after 2.0002

Leave Link 502 at Sat Jul 6 02:53:53 2019, MaxMem= 1342177280 cpu: 6041.1

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44336 LenP2D= 111337.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 274

Leave Link 701 at Sat Jul 6 02:54:13 2019, MaxMem= 1342177280 cpu: 225.6

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 02:54:13 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 02:55:54 2019, MaxMem= 1342177280 cpu: 1200.0

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 4.28125422D-04-2.42136315D-04 2.92798927D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000035971 0.000010903 -0.000379940

2 7 0.000014963 0.000446012 0.000305511

3 6 -0.000075380 0.000049640 -0.000392999

4 6 0.000016800 -0.000022870 0.000128719

5 6 -0.000011710 -0.000034973 0.000107986

6 7 0.000436537 -0.000227947 0.000205729

7 6 -0.000105871 0.000087292 0.000020515

8 7 -0.000066057 0.000000456 -0.000117613

9 6 -0.000134339 -0.000116424 -0.000003526

10 6 0.000032952 -0.000022192 0.000089222

11 6 0.000045102 0.000035428 0.000074523

12 7 -0.000422097 -0.000210726 0.000201879

13 6 -0.000049805 0.000030153 0.000082149

14 6 -0.000035694 -0.000016093 0.000097602

15 6 0.000148930 -0.000141054 -0.000002928

16 7 0.000142977 0.000004958 -0.000098006

17 6 0.000124550 0.000108265 0.000015270

18 7 -0.000410813 0.000211873 0.000200034

19 7 -0.000006515 -0.000369844 0.000270298

20 6 0.000014713 0.000008230 -0.000379859

21 6 -0.000010115 0.000032402 0.000108790

22 6 0.000018403 0.000020615 0.000126376

23 6 -0.000049879 -0.000039545 -0.000390435

24 7 0.000427962 0.000232377 0.000211057

25 30 -0.000054636 -0.000060420 0.000196333

26 6 -0.000112806 0.000091434 -0.000075142

27 6 0.000049491 -0.000077282 -0.000035564

28 6 0.000046199 0.000070117 -0.000031875

29 6 -0.000116835 -0.000108953 -0.000078256

30 6 0.000149504 -0.000041162 0.000126500

31 6 -0.000068037 0.000079497 -0.000040269

32 6 0.000063090 0.000079997 -0.000041145

33 6 -0.000160184 -0.000047423 0.000121874

34 6 0.000107121 0.000094108 -0.000070968

35 6 -0.000046559 -0.000080634 -0.000034447

36 6 -0.000044710 0.000071736 -0.000032577

37 6 0.000112638 -0.000107790 -0.000071783

38 6 -0.000160926 0.000045260 0.000118036

39 6 0.000066715 -0.000077061 -0.000040606

40 6 -0.000068697 -0.000078203 -0.000039328

41 6 0.000152538 0.000040122 0.000121636

42 1 0.000003233 -0.000012083 0.000028328

43 1 0.000009377 0.000007817 0.000028422

44 1 0.000080917 0.000008745 0.000007595

45 1 -0.000082398 0.000008994 0.000008821

46 1 -0.000008097 -0.000008528 0.000029245

47 1 -0.000010796 0.000006310 0.000028784

48 1 -0.000083163 -0.000011867 0.000009719

49 1 0.000084154 -0.000009972 0.000007175

50 8 -0.000035228 -0.000240009 -0.000227093

51 8 0.000051980 -0.000230915 -0.000226283

52 8 -0.000254516 0.000023080 -0.000022819

53 8 -0.000233498 0.000003416 -0.000019094

54 8 -0.000055335 0.000226853 -0.000231652

55 8 0.000067263 0.000221600 -0.000229255

56 8 0.000220222 0.000014972 -0.000010287

57 8 0.000242338 0.000003662 -0.000019664

58 6 -0.000119495 0.000095094 0.000173982

59 1 -0.000006760 0.000030532 -0.000029523

60 1 -0.000001238 -0.000028557 -0.000108496

61 1 -0.000042061 -0.000024576 0.000031386

62 6 0.000026789 -0.000109286 -0.000006868

63 1 0.000022833 0.000015646 0.000010617

64 1 0.000007991 0.000011813 -0.000004242

65 1 -0.000019035 -0.000033660 -0.000000656

66 6 0.000026679 0.000113086 -0.000003467

67 1 0.000007184 -0.000007897 -0.000004314

68 1 0.000023476 -0.000012418 0.000009587

69 1 -0.000016695 0.000035100 0.000001112

70 6 0.000122630 0.000097617 0.000169607

71 1 0.000000669 -0.000027370 -0.000107239

72 1 0.000008167 0.000030585 -0.000028169

73 1 0.000043343 -0.000023868 0.000030342

74 6 -0.000027892 -0.000111315 -0.000004760

75 1 -0.000007288 0.000008070 -0.000004224

76 1 -0.000023266 0.000014053 0.000009492

77 1 0.000016418 -0.000034698 -0.000000150

78 6 -0.000027056 0.000118828 -0.000005408

79 1 -0.000024551 -0.000011949 0.000008649

80 1 -0.000007130 -0.000007058 -0.000003628

81 1 0.000015932 0.000035889 0.000001216

82 6 0.000127553 -0.000095402 0.000170618

83 1 0.000010076 -0.000032102 -0.000028573

84 1 0.000000399 0.000025213 -0.000108058

85 1 0.000044725 0.000023463 0.000028560

86 6 -0.000120495 -0.000096754 0.000173110

87 1 -0.000002693 0.000027799 -0.000107528

88 1 -0.000008495 -0.000030534 -0.000028933

89 1 -0.000042659 0.000022298 0.000031244

-------------------------------------------------------------------

Cartesian Forces: Max 0.000446012 RMS 0.000121072

Leave Link 716 at Sat Jul 6 02:55:54 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000516293 RMS 0.000086139

Search for a local minimum.

Step number 20 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .86139D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 6 5 7 9 11

14 13 16 17 18

19 20

DE= -3.95D-05 DEPred=-3.54D-05 R= 1.12D+00

TightC=F SS= 1.41D+00 RLast= 7.83D-02 DXNew= 2.7164D-01 2.3485D-01

Trust test= 1.12D+00 RLast= 7.83D-02 DXMaxT set to 2.35D-01

ITU= 1 1 1 0 0 -1 -1 0 -1 0 0 0 0 0 0 1 1 1 1 0

Eigenvalues --- 0.00303 0.01119 0.01316 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01322 0.01469

Eigenvalues --- 0.01529 0.01570 0.01574 0.01583 0.01598

Eigenvalues --- 0.01618 0.01623 0.01693 0.01708 0.01710

Eigenvalues --- 0.01712 0.01716 0.01786 0.01835 0.01869

Eigenvalues --- 0.01875 0.01920 0.01921 0.01938 0.01946

Eigenvalues --- 0.01996 0.02004 0.02020 0.02021 0.02031

Eigenvalues --- 0.02040 0.02052 0.02053 0.02053 0.02053

Eigenvalues --- 0.02057 0.02057 0.02057 0.02057 0.02060

Eigenvalues --- 0.02067 0.02067 0.02067 0.02070 0.02070

Eigenvalues --- 0.02070 0.02071 0.02083 0.02083 0.02088

Eigenvalues --- 0.02148 0.02256 0.02259 0.02260 0.02260

Eigenvalues --- 0.02260 0.02260 0.02261 0.02298 0.02344

Eigenvalues --- 0.02357 0.02361 0.02899 0.03352 0.04182

Eigenvalues --- 0.09894 0.09980 0.09980 0.09980 0.09987

Eigenvalues --- 0.09987 0.09987 0.10136 0.10642 0.10642

Eigenvalues --- 0.10642 0.10653 0.10657 0.10657 0.10657

Eigenvalues --- 0.10666 0.12372 0.13271 0.13463 0.15207

Eigenvalues --- 0.15985 0.15988 0.15996 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16007 0.16042 0.16193

Eigenvalues --- 0.16457 0.16848 0.20440 0.21238 0.21682

Eigenvalues --- 0.22473 0.22475 0.22476 0.22478 0.24253

Eigenvalues --- 0.24327 0.24478 0.24504 0.24514 0.24611

Eigenvalues --- 0.24639 0.24731 0.24810 0.24869 0.24891

Eigenvalues --- 0.24917 0.24972 0.24973 0.24982 0.24985

Eigenvalues --- 0.24990 0.24995 0.24996 0.24997 0.24998

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25004 0.25105 0.25246 0.28120 0.30427

Eigenvalues --- 0.33285 0.33634 0.33678 0.33716 0.33755

Eigenvalues --- 0.34053 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34063 0.34076 0.34081 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34085

Eigenvalues --- 0.34213 0.34598 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34686 0.34689 0.34897

Eigenvalues --- 0.34954 0.35189 0.35609 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35632 0.36223

Eigenvalues --- 0.36612 0.37037 0.37133 0.37470 0.40347

Eigenvalues --- 0.41215 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41216 0.41243 0.41408 0.41410 0.41415

Eigenvalues --- 0.41416 0.41521 0.41696 0.42288 0.42472

Eigenvalues --- 0.43207 0.44453 0.44560 0.44688 0.44818

Eigenvalues --- 0.44878 0.44998 0.45000 0.45002 0.45003

Eigenvalues --- 0.45140 0.45365 0.45366 0.45962 0.46293

Eigenvalues --- 0.47267 0.47636 0.49011 0.49296 0.49360

Eigenvalues --- 0.49844 0.50593 0.53554 0.53554 0.53554

Eigenvalues --- 0.53554 0.53554 0.53568 0.54128 0.54988

Eigenvalues --- 0.55792 0.56069 0.57410 0.57559 0.57675

Eigenvalues --- 0.65353

En-DIIS/RFO-DIIS IScMMF= 0 using points: 20 19 18 17 16

RFO step: Lambda=-7.68680370D-06.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 1.72D-04 SmlDif= 1.00D-05

RMS Error= 0.2366238088D-03 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.37394 -0.31140 -0.28518 0.14819 0.07445

Iteration 1 RMS(Cart)= 0.01316177 RMS(Int)= 0.00002192

Iteration 2 RMS(Cart)= 0.00007224 RMS(Int)= 0.00000169

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000169

ITry= 1 IFail=0 DXMaxC= 5.95D-02 DCOld= 1.00D+10 DXMaxT= 2.35D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58280 -0.00006 0.00000 -0.00019 -0.00019 2.58261

R2 2.74004 -0.00015 -0.00028 -0.00017 -0.00045 2.73959

R3 2.56100 0.00018 0.00023 -0.00009 0.00014 2.56114

R4 2.58279 -0.00007 0.00006 -0.00027 -0.00020 2.58259

R5 3.86992 0.00005 0.00001 -0.00067 -0.00066 3.86927

R6 2.74008 -0.00019 -0.00020 -0.00044 -0.00064 2.73944

R7 2.56093 0.00019 0.00051 -0.00039 0.00011 2.56104

R8 2.69576 0.00002 0.00037 -0.00007 0.00030 2.69606

R9 2.66303 -0.00021 -0.00008 -0.00035 -0.00043 2.66260

R10 2.66300 -0.00019 -0.00008 -0.00031 -0.00039 2.66262

R11 2.48273 -0.00027 0.00060 -0.00095 -0.00036 2.48237

R12 2.59617 -0.00005 -0.00006 -0.00024 -0.00030 2.59587

R13 2.79491 -0.00014 0.00019 -0.00061 -0.00042 2.79450

R14 2.59616 -0.00004 -0.00016 -0.00011 -0.00027 2.59589

R15 3.84322 -0.00009 -0.00092 0.00010 -0.00081 3.84240

R16 2.79484 -0.00007 0.00008 -0.00017 -0.00009 2.79475

R17 2.48275 -0.00026 0.00026 -0.00049 -0.00023 2.48252

R18 2.66437 -0.00011 -0.00025 0.00009 -0.00016 2.66421

R19 2.64590 -0.00013 -0.00008 -0.00013 -0.00021 2.64569

R20 2.64594 -0.00016 -0.00006 -0.00025 -0.00031 2.64563

R21 2.48273 -0.00025 0.00034 -0.00057 -0.00023 2.48251

R22 2.66437 -0.00010 -0.00037 0.00026 -0.00011 2.66426

R23 2.79492 -0.00011 0.00013 -0.00039 -0.00026 2.79466

R24 2.64592 -0.00014 -0.00010 -0.00013 -0.00023 2.64569

R25 2.79478 -0.00006 0.00001 -0.00001 -0.00001 2.79477

R26 2.64587 -0.00011 -0.00012 -0.00001 -0.00013 2.64574

R27 2.59609 -0.00001 -0.00011 -0.00006 -0.00017 2.59592

R28 2.48275 -0.00026 0.00000 -0.00012 -0.00012 2.48263

R29 2.59609 -0.00002 -0.00001 -0.00020 -0.00021 2.59588

R30 3.84384 -0.00015 -0.00102 0.00023 -0.00079 3.84305

R31 2.56100 0.00019 0.00001 0.00019 0.00020 2.56120

R32 2.58271 -0.00004 0.00004 -0.00017 -0.00012 2.58259

R33 2.58275 -0.00002 0.00011 -0.00019 -0.00008 2.58267

R34 3.87061 -0.00001 -0.00006 -0.00061 -0.00068 3.86994

R35 2.74002 -0.00014 -0.00034 -0.00005 -0.00039 2.73963

R36 2.69576 0.00003 0.00026 0.00007 0.00033 2.69608

R37 2.66298 -0.00018 -0.00010 -0.00024 -0.00034 2.66264

R38 2.74008 -0.00017 -0.00025 -0.00029 -0.00054 2.73954

R39 2.66301 -0.00020 -0.00010 -0.00028 -0.00037 2.66264

R40 2.56094 0.00022 0.00029 -0.00008 0.00021 2.56116

R41 2.65603 -0.00002 0.00011 0.00006 0.00017 2.65620

R42 2.54967 -0.00011 -0.00013 0.00011 -0.00002 2.54965

R43 2.62934 -0.00005 -0.00004 0.00021 0.00017 2.62951

R44 2.04424 0.00000 0.00003 0.00000 0.00002 2.04426

R45 2.65600 -0.00001 0.00009 0.00010 0.00020 2.65620

R46 2.04423 0.00000 0.00002 0.00001 0.00003 2.04427

R47 2.54971 -0.00014 -0.00011 0.00002 -0.00009 2.54961

R48 2.64322 -0.00008 -0.00005 0.00013 0.00008 2.64330

R49 2.55257 -0.00022 -0.00034 0.00023 -0.00010 2.55246

R50 2.64691 0.00000 -0.00004 0.00014 0.00010 2.64701

R51 2.04395 0.00005 0.00008 0.00000 0.00009 2.04404

R52 2.64321 -0.00007 -0.00007 0.00016 0.00009 2.64330

R53 2.04395 0.00005 0.00008 0.00001 0.00009 2.04405

R54 2.55259 -0.00024 -0.00032 0.00017 -0.00016 2.55243

R55 2.65600 -0.00001 0.00010 0.00011 0.00021 2.65622

R56 2.54965 -0.00008 -0.00014 0.00019 0.00005 2.54970

R57 2.62932 -0.00003 -0.00004 0.00027 0.00023 2.62954

R58 2.04424 0.00000 0.00003 -0.00003 0.00000 2.04424

R59 2.65599 0.00000 0.00008 0.00016 0.00024 2.65623

R60 2.04424 0.00000 0.00003 0.00000 0.00003 2.04427

R61 2.54969 -0.00012 -0.00012 0.00008 -0.00004 2.54964

R62 2.64319 -0.00006 -0.00007 0.00021 0.00014 2.64333

R63 2.55256 -0.00022 -0.00033 0.00024 -0.00010 2.55247

R64 2.64688 0.00002 -0.00003 0.00018 0.00016 2.64704

R65 2.04395 0.00005 0.00008 0.00000 0.00008 2.04404

R66 2.64320 -0.00006 -0.00006 0.00018 0.00012 2.64331

R67 2.04395 0.00005 0.00008 -0.00001 0.00008 2.04403

R68 2.55254 -0.00020 -0.00035 0.00030 -0.00004 2.55250

R69 2.69362 -0.00001 -0.00012 0.00012 0.00000 2.69362

R70 2.69363 -0.00001 -0.00012 0.00012 0.00000 2.69363

R71 2.69559 -0.00003 -0.00011 0.00005 -0.00006 2.69553

R72 2.69560 -0.00003 -0.00010 0.00003 -0.00007 2.69552

R73 2.69362 -0.00001 -0.00012 0.00012 0.00000 2.69363

R74 2.69362 -0.00001 -0.00011 0.00010 -0.00001 2.69361

R75 2.69559 -0.00003 -0.00010 0.00002 -0.00009 2.69551

R76 2.69559 -0.00003 -0.00010 0.00003 -0.00007 2.69552

R77 2.06760 -0.00002 0.00001 0.00001 0.00001 2.06761

R78 2.06716 0.00005 0.00005 0.00018 0.00023 2.06739

R79 2.05691 -0.00004 -0.00006 0.00004 -0.00002 2.05689

R80 2.06716 0.00000 0.00001 0.00006 0.00006 2.06723

R81 2.06743 0.00000 0.00000 0.00007 0.00007 2.06750

R82 2.05676 -0.00003 -0.00003 0.00005 0.00002 2.05677

R83 2.06743 0.00000 0.00000 0.00007 0.00007 2.06750

R84 2.06716 0.00000 0.00001 0.00006 0.00007 2.06723

R85 2.05676 -0.00003 -0.00003 0.00003 0.00001 2.05677

R86 2.06715 0.00005 0.00005 0.00018 0.00024 2.06739

R87 2.06759 -0.00001 0.00001 0.00001 0.00001 2.06761

R88 2.05691 -0.00004 -0.00005 0.00003 -0.00002 2.05689

R89 2.06743 0.00000 0.00000 0.00007 0.00007 2.06750

R90 2.06716 0.00000 0.00000 0.00007 0.00007 2.06723

R91 2.05676 -0.00003 -0.00003 0.00004 0.00001 2.05677

R92 2.06716 0.00000 0.00000 0.00007 0.00008 2.06724

R93 2.06743 0.00000 0.00000 0.00008 0.00008 2.06751

R94 2.05676 -0.00003 -0.00002 0.00003 0.00001 2.05677

R95 2.06759 -0.00001 0.00000 0.00002 0.00002 2.06761

R96 2.06715 0.00005 0.00005 0.00019 0.00024 2.06740

R97 2.05691 -0.00004 -0.00005 0.00003 -0.00003 2.05689

R98 2.06715 0.00005 0.00005 0.00018 0.00023 2.06738

R99 2.06760 -0.00001 0.00000 0.00001 0.00002 2.06761

R100 2.05691 -0.00004 -0.00005 0.00003 -0.00002 2.05689

A1 1.88986 -0.00017 -0.00008 -0.00040 -0.00048 1.88937

A2 2.21418 0.00011 0.00001 0.00029 0.00029 2.21447

A3 2.17904 0.00006 0.00008 0.00011 0.00020 2.17924

A4 1.92984 0.00021 0.00019 0.00044 0.00063 1.93047

A5 2.17243 -0.00010 0.00006 0.00009 0.00015 2.17258

A6 2.17230 -0.00010 -0.00007 0.00012 0.00005 2.17235

A7 1.88983 -0.00015 -0.00014 -0.00024 -0.00038 1.88945

A8 2.21421 0.00011 -0.00006 0.00046 0.00039 2.21460

A9 2.17904 0.00004 0.00021 -0.00021 0.00000 2.17904

A10 1.85763 0.00005 0.00002 0.00009 0.00011 1.85774

A11 2.31762 -0.00010 0.00002 -0.00038 -0.00035 2.31727

A12 2.10768 0.00004 -0.00006 0.00031 0.00026 2.10794

A13 1.85761 0.00005 0.00001 0.00011 0.00013 1.85773

A14 2.31759 -0.00006 -0.00002 -0.00017 -0.00018 2.31741

A15 2.10774 0.00001 -0.00001 0.00007 0.00007 2.10781

A16 2.18723 -0.00012 -0.00013 0.00012 -0.00002 2.18721

A17 2.23233 0.00010 0.00026 0.00055 0.00081 2.23313

A18 2.16708 -0.00015 -0.00022 -0.00039 -0.00061 2.16647

A19 1.88333 0.00005 -0.00002 -0.00011 -0.00013 1.88320

A20 1.93275 -0.00007 -0.00001 0.00032 0.00031 1.93306

A21 2.16261 0.00002 -0.00003 0.00002 -0.00001 2.16260

A22 2.16271 0.00004 0.00009 0.00013 0.00023 2.16294

A23 1.88337 0.00002 0.00005 -0.00032 -0.00028 1.88309

A24 2.23235 0.00007 0.00035 0.00021 0.00056 2.23291

A25 2.16703 -0.00009 -0.00038 0.00015 -0.00023 2.16680

A26 1.86260 0.00000 0.00000 0.00004 0.00004 1.86264

A27 2.30424 -0.00001 -0.00015 0.00000 -0.00016 2.30409

A28 2.11619 0.00002 0.00017 -0.00003 0.00014 2.11633

A29 1.86260 0.00000 -0.00001 0.00008 0.00006 1.86266

A30 2.30433 -0.00008 -0.00004 -0.00045 -0.00050 2.30383

A31 2.11611 0.00007 0.00008 0.00038 0.00046 2.11656

A32 2.18728 -0.00013 -0.00030 0.00035 0.00004 2.18732

A33 1.86258 0.00001 -0.00002 0.00010 0.00008 1.86266

A34 2.11610 0.00005 0.00010 0.00025 0.00035 2.11645

A35 2.30436 -0.00006 -0.00006 -0.00035 -0.00041 2.30395

A36 1.86259 0.00000 0.00000 0.00007 0.00006 1.86265

A37 2.11625 0.00001 0.00020 -0.00009 0.00011 2.11636

A38 2.30419 -0.00001 -0.00017 0.00003 -0.00014 2.30405

A39 1.88338 0.00001 0.00014 -0.00044 -0.00029 1.88309

A40 2.16702 -0.00010 -0.00058 0.00035 -0.00023 2.16679

A41 2.23234 0.00008 0.00046 0.00012 0.00058 2.23292

A42 1.93277 -0.00006 -0.00020 0.00054 0.00034 1.93312

A43 2.16272 0.00004 0.00019 -0.00003 0.00016 2.16289

A44 2.16265 0.00002 0.00006 -0.00010 -0.00003 2.16262

A45 2.16714 -0.00014 -0.00041 -0.00012 -0.00054 2.16660

A46 2.23228 0.00010 0.00036 0.00043 0.00078 2.23306

A47 1.88333 0.00004 0.00007 -0.00026 -0.00019 1.88314

A48 2.18731 -0.00014 -0.00047 0.00057 0.00009 2.18740

A49 1.92985 0.00021 -0.00001 0.00069 0.00068 1.93053

A50 2.17247 -0.00010 0.00016 -0.00006 0.00011 2.17258

A51 2.17231 -0.00011 0.00003 -0.00004 -0.00001 2.17230

A52 2.21414 0.00012 0.00006 0.00030 0.00036 2.21450

A53 2.17907 0.00005 -0.00009 0.00027 0.00018 2.17924

A54 1.88988 -0.00018 0.00003 -0.00056 -0.00053 1.88935

A55 1.85760 0.00006 0.00000 0.00017 0.00017 1.85776

A56 2.31756 -0.00006 -0.00003 -0.00018 -0.00020 2.31736

A57 2.10779 0.00000 0.00001 0.00003 0.00004 2.10782

A58 1.85761 0.00006 0.00001 0.00012 0.00013 1.85774

A59 2.10770 0.00002 -0.00005 0.00021 0.00017 2.10786

A60 2.31763 -0.00008 0.00002 -0.00031 -0.00028 2.31735

A61 1.88983 -0.00016 -0.00003 -0.00042 -0.00045 1.88938

A62 2.21418 0.00012 0.00000 0.00046 0.00045 2.21463

A63 2.17907 0.00004 0.00004 -0.00004 0.00001 2.17908

A64 2.18727 -0.00012 -0.00029 0.00037 0.00007 2.18734

A65 1.55926 0.00001 0.00042 0.00010 0.00051 1.55977

A66 1.55913 0.00001 0.00020 0.00032 0.00051 1.55965

A67 1.55913 0.00001 0.00019 0.00034 0.00052 1.55965

A68 1.55899 0.00001 -0.00003 0.00055 0.00051 1.55950

A69 2.04544 -0.00003 -0.00016 -0.00018 -0.00034 2.04510

A70 2.07317 -0.00012 -0.00009 -0.00021 -0.00031 2.07287

A71 2.16456 0.00014 0.00025 0.00040 0.00065 2.16521

A72 2.12160 -0.00001 0.00004 0.00001 0.00005 2.12166

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A85 2.10107 -0.00007 -0.00005 -0.00034 -0.00039 2.10068

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A115 2.06611 -0.00001 -0.00002 -0.00005 -0.00007 2.06604

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A118 2.06718 -0.00050 -0.00056 -0.00074 -0.00130 2.06587

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D3 3.13096 0.00001 -0.00042 0.00058 0.00016 3.13112

D4 -0.14617 0.00006 0.00118 0.00567 0.00686 -0.13931

D5 -0.00248 0.00001 0.00058 -0.00080 -0.00022 -0.00270

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D8 0.03673 -0.00007 0.00041 -0.00153 -0.00112 0.03561

D9 0.18690 -0.00009 -0.00171 -0.00530 -0.00701 0.17989

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D33 3.11838 0.00006 -0.00078 0.00058 -0.00020 3.11818

D34 -0.01826 0.00002 -0.00075 -0.00221 -0.00295 -0.02122

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D36 -3.13253 -0.00003 -0.00048 -0.00300 -0.00348 -3.13601

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D45 -0.00883 -0.00002 0.00011 -0.00059 -0.00048 -0.00931

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D52 3.10847 -0.00007 -0.00066 -0.00054 -0.00120 3.10727

D53 -3.10839 0.00007 0.00069 0.00018 0.00088 -3.10751

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D99 3.12983 -0.00011 -0.00137 -0.00166 -0.00303 3.12680

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D163 3.13233 0.00003 0.00053 0.00307 0.00360 3.13593

D164 -0.00386 0.00003 0.00080 0.00183 0.00262 -0.00123

D165 3.11710 0.00011 -0.00148 -0.00254 -0.00403 3.11307

D166 -0.01920 0.00006 -0.00147 -0.00552 -0.00699 -0.02620

D167 0.00004 0.00000 0.00004 -0.00021 -0.00017 -0.00013

D168 -3.13631 -0.00001 0.00025 -0.00118 -0.00093 -3.13724

D169 3.13635 0.00000 -0.00022 0.00101 0.00079 3.13714

D170 0.00000 0.00000 -0.00001 0.00003 0.00003 0.00003

D171 0.00400 0.00001 -0.00057 -0.00001 -0.00058 0.00342

D172 -3.13232 -0.00003 -0.00054 -0.00304 -0.00357 -3.13590

D173 3.14023 0.00001 -0.00079 0.00099 0.00020 3.14043

D174 0.00390 -0.00003 -0.00076 -0.00204 -0.00280 0.00110

D175 -3.11718 -0.00012 0.00155 0.00199 0.00354 -3.11364

D176 0.01911 -0.00007 0.00152 0.00504 0.00656 0.02567

D177 -0.00135 0.00003 0.00073 0.00034 0.00107 -0.00027

D178 3.13542 0.00003 0.00031 0.00116 0.00147 3.13689

D179 -3.13807 0.00003 0.00109 -0.00095 0.00014 -3.13793

D180 -0.00130 0.00003 0.00067 -0.00013 0.00053 -0.00077

D181 3.10106 -0.00002 0.00112 -0.00151 -0.00039 3.10066

D182 -0.04548 -0.00002 0.00076 -0.00020 0.00056 -0.04492

D183 -0.00007 0.00000 -0.00006 0.00033 0.00027 0.00020

D184 3.13686 0.00000 -0.00043 0.00087 0.00044 3.13730

D185 -3.13694 0.00000 0.00036 -0.00047 -0.00011 -3.13705

D186 -0.00001 0.00000 -0.00001 0.00007 0.00006 0.00005

D187 0.00139 -0.00003 -0.00070 -0.00054 -0.00124 0.00015

D188 3.13804 -0.00003 -0.00112 0.00106 -0.00006 3.13798

D189 -3.13544 -0.00003 -0.00032 -0.00110 -0.00142 -3.13686

D190 0.00121 -0.00002 -0.00074 0.00051 -0.00024 0.00097

D191 -3.10102 0.00003 -0.00122 0.00216 0.00094 -3.10009

D192 0.04558 0.00002 -0.00079 0.00053 -0.00026 0.04532

D193 -0.00399 -0.00001 0.00058 -0.00008 0.00050 -0.00350

D194 -3.14026 -0.00001 0.00079 -0.00102 -0.00023 -3.14049

D195 3.13234 0.00003 0.00054 0.00287 0.00342 3.13576

D196 -0.00392 0.00003 0.00076 0.00193 0.00269 -0.00123

D197 3.11710 0.00011 -0.00155 -0.00204 -0.00359 3.11350

D198 -0.01920 0.00007 -0.00152 -0.00501 -0.00654 -0.02574

D199 -0.00009 0.00000 -0.00004 0.00021 0.00017 0.00008

D200 -3.13640 0.00000 0.00021 -0.00093 -0.00072 -3.13712

D201 3.13630 0.00000 -0.00025 0.00112 0.00087 3.13718

D202 -0.00001 0.00000 0.00000 -0.00001 -0.00001 -0.00002

D203 0.00401 0.00001 -0.00056 -0.00003 -0.00059 0.00342

D204 -3.13241 -0.00003 -0.00055 -0.00291 -0.00346 -3.13587

D205 3.14020 0.00001 -0.00082 0.00114 0.00032 3.14052

D206 0.00378 -0.00003 -0.00081 -0.00174 -0.00255 0.00123

D207 -3.11720 -0.00011 0.00147 0.00237 0.00383 -3.11337

D208 0.01918 -0.00007 0.00146 0.00527 0.00673 0.02591

D209 1.06972 -0.00009 -0.00408 -0.00738 -0.01147 1.05826

D210 -1.07114 -0.00012 -0.00398 -0.00745 -0.01143 -1.08258

D211 3.13967 -0.00006 -0.00392 -0.00711 -0.01103 3.12865

D212 1.07121 0.00012 0.00393 0.00742 0.01135 1.08257

D213 -1.06966 0.00009 0.00404 0.00735 0.01139 -1.05827

D214 -3.13960 0.00006 0.00388 0.00706 0.01094 -3.12866

D215 1.09371 0.00001 -0.00057 -0.00036 -0.00093 1.09278

D216 -1.05039 -0.00002 -0.00034 -0.00088 -0.00122 -1.05160

D217 -3.11987 0.00000 -0.00047 -0.00049 -0.00096 -3.12083

D218 1.05029 0.00002 0.00035 0.00066 0.00101 1.05130

D219 -1.09381 0.00000 0.00057 0.00024 0.00081 -1.09300

D220 3.11978 0.00000 0.00048 0.00029 0.00077 3.12055

D221 1.07113 0.00012 0.00399 0.00730 0.01129 1.08242

D222 -1.06975 0.00009 0.00410 0.00727 0.01137 -1.05838

D223 -3.13968 0.00006 0.00394 0.00699 0.01092 -3.12876

D224 1.06964 -0.00009 -0.00406 -0.00736 -0.01142 1.05822

D225 -1.07127 -0.00012 -0.00395 -0.00742 -0.01137 -1.08264

D226 3.13957 -0.00006 -0.00390 -0.00705 -0.01095 3.12861

D227 1.09382 0.00000 -0.00059 -0.00020 -0.00079 1.09302

D228 -1.05031 -0.00002 -0.00038 -0.00061 -0.00099 -1.05130

D229 -3.11979 0.00000 -0.00051 -0.00024 -0.00075 -3.12054

D230 1.05028 0.00002 0.00035 0.00066 0.00101 1.05129

D231 -1.09382 -0.00001 0.00058 0.00021 0.00079 -1.09303

D232 3.11976 0.00000 0.00048 0.00031 0.00079 3.12055

Item Value Threshold Converged?

Maximum Force 0.000516 0.000450 NO

RMS Force 0.000086 0.000300 YES

Maximum Displacement 0.059489 0.001800 NO

RMS Displacement 0.013152 0.001200 NO

Predicted change in Energy=-1.372082D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 02:55:55 2019, MaxMem= 1342177280 cpu: 13.9

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=3 Diff= 1.13D-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 -1.119800 2.801902 -0.028326

2 7 0 0.002743 2.038163 -0.184401

3 6 0 1.127475 2.798690 -0.028509

4 6 0 0.719210 4.162522 0.244910

5 6 0 -0.707481 4.164667 0.244764

6 7 0 2.412674 2.379719 -0.125529

7 6 0 2.799350 1.126478 -0.199333

8 7 0 2.019463 -0.002929 -0.142812

9 6 0 2.796424 -1.134377 -0.199168

10 6 0 4.207966 -0.710612 -0.322326

11 6 0 4.209665 0.699226 -0.322897

12 7 0 -2.406199 2.386423 -0.125217

13 6 0 -4.208027 0.710776 -0.322483

14 6 0 -4.210142 -0.699087 -0.322045

15 6 0 -2.799728 -1.126695 -0.199126

16 7 0 -2.019689 0.002651 -0.142758

17 6 0 -2.796458 1.134221 -0.199096

18 7 0 -2.412853 -2.380034 -0.125535

19 7 0 -0.002916 -2.038505 -0.184666

20 6 0 -1.127583 -2.799153 -0.028906

21 6 0 -0.719041 -4.163151 0.243818

22 6 0 0.707664 -4.164942 0.244286

23 6 0 1.119765 -2.802122 -0.028723

24 7 0 2.406177 -2.386591 -0.125329

25 30 0 0.000056 0.000019 -0.380187

26 6 0 -5.400558 1.439127 -0.408979

27 6 0 -6.596226 0.705204 -0.495239

28 6 0 -6.598370 -0.686271 -0.494522

29 6 0 -5.404969 -1.423816 -0.407710

30 6 0 1.426967 -5.347817 0.506412

31 6 0 0.691602 -6.510455 0.759543

32 6 0 -0.709136 -6.508759 0.758878

33 6 0 -1.441437 -5.344304 0.505200

34 6 0 5.404037 1.424462 -0.409701

35 6 0 6.597746 0.687338 -0.495986

36 6 0 6.596173 -0.704156 -0.495101

37 6 0 5.400812 -1.438533 -0.408121

38 6 0 -1.426533 5.347718 0.506727

39 6 0 -0.690901 6.510081 0.760441

40 6 0 0.709851 6.507914 0.760670

41 6 0 1.441917 5.343281 0.507098

42 1 0 7.549016 1.197141 -0.569507

43 1 0 7.546316 -1.216186 -0.567924

44 1 0 1.218985 7.439388 0.968318

45 1 0 -1.197227 7.443118 0.967943

46 1 0 -7.546152 1.217563 -0.568543

47 1 0 -7.549876 -1.195770 -0.567288

48 1 0 -1.218097 -7.440451 0.966002

49 1 0 1.198122 -7.443373 0.967117

50 8 0 2.791352 5.284574 0.501526

51 8 0 -2.776132 5.293363 0.500886

52 8 0 5.346387 2.772474 -0.410368

53 8 0 5.340471 -2.786394 -0.407051

54 8 0 2.776552 -5.293073 0.501253

55 8 0 -2.790866 -5.286316 0.498812

56 8 0 -5.348375 -2.771826 -0.406674

57 8 0 -5.339604 2.786965 -0.409330

58 6 0 3.522142 6.471117 0.801254

59 1 0 3.291757 6.838092 1.805933

60 1 0 3.324946 7.261168 0.070635

61 1 0 4.572013 6.188124 0.751935

62 6 0 6.567766 3.508335 -0.447748

63 1 0 7.127053 3.313547 -1.367498

64 1 0 7.196995 3.283433 0.418559

65 1 0 6.275598 4.556396 -0.419172

66 6 0 6.560527 -3.524525 -0.442697

67 1 0 7.189710 -3.299358 0.423577

68 1 0 7.120624 -3.332117 -1.362457

69 1 0 6.266506 -4.572022 -0.412638

70 6 0 -3.503079 6.482362 0.800247

71 1 0 -3.303138 7.271623 0.069522

72 1 0 -3.271680 6.848744 1.804908

73 1 0 -4.553867 6.202827 0.750771

74 6 0 -6.559277 3.525669 -0.446215

75 1 0 -7.188911 3.301755 0.420054

76 1 0 -7.119117 3.332569 -1.365987

77 1 0 -6.264734 4.573049 -0.417169

78 6 0 -6.570503 -3.506499 -0.442444

79 1 0 -7.129978 -3.312503 -1.362253

80 1 0 -7.199136 -3.279596 0.423777

81 1 0 -6.279425 -4.554818 -0.412383

82 6 0 -3.521047 -6.473506 0.797433

83 1 0 -3.290994 -6.840915 1.802031

84 1 0 -3.322945 -7.263004 0.066458

85 1 0 -4.571069 -6.191159 0.747676

86 6 0 3.503650 -6.481801 0.801311

87 1 0 3.304183 -7.271350 0.070772

88 1 0 3.271894 -6.847909 1.805993

89 1 0 4.554400 -6.202054 0.752209

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0447945 0.0439353 0.0225314

Leave Link 202 at Sat Jul 6 02:55:56 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8042.1118270788 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= 89 NActive= 89 NUniq= 89 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= -0.2279664879 Hartrees.

Nuclear repulsion after empirical dispersion term = 8041.8838605908 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6378

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.61D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 348

GePol: Fraction of low-weight points (<1% of avg) = 5.46%

GePol: Cavity surface area = 703.650 Ang\*\*2

GePol: Cavity volume = 801.582 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0089894338 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8041.8748711570 Hartrees.

Leave Link 301 at Sat Jul 6 02:55:56 2019, MaxMem= 1342177280 cpu: 1.3

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44315 LenP2D= 111304.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.57D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 02:56:00 2019, MaxMem= 1342177280 cpu: 42.8

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 02:56:01 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000011 -0.000009 0.000399 Ang= -0.05 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>= 2.0171 S= 1.0057

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2650.02666731477

Leave Link 401 at Sat Jul 6 02:56:18 2019, MaxMem= 1342177280 cpu: 209.4

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 122036652.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.44D-15 for 6357.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.84D-15 for 5773 4475.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.99D-15 for 6357.

Iteration 1 A^-1\*A deviation from orthogonality is 2.23D-10 for 6378 5843.

Iteration 2 A\*A^-1 deviation from unit magnitude is 4.44D-15 for 961.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.72D-15 for 3726 137.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 1863.

Iteration 2 A^-1\*A deviation from orthogonality is 4.34D-16 for 3718 1392.

E= -2649.79500560222

DIIS: error= 5.36D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79500560222 IErMin= 1 ErrMin= 5.36D-04

ErrMax= 5.36D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D-03 BMatP= 1.09D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.36D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.685 Goal= None Shift= 0.000

Gap= 0.744 Goal= None Shift= 0.000

RMSDP=2.39D-05 MaxDP=8.22D-04 OVMax= 3.09D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.38D-05 CP: 1.00D+00

E= -2649.79550010347 Delta-E= -0.000494501248 Rises=F Damp=F

DIIS: error= 6.68D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79550010347 IErMin= 2 ErrMin= 6.68D-05

ErrMax= 6.68D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.14D-05 BMatP= 1.09D-03

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.647D-01 0.106D+01

Coeff: -0.647D-01 0.106D+01

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=3.32D-06 MaxDP=1.39D-04 DE=-4.95D-04 OVMax= 6.82D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.90D-06 CP: 1.00D+00 1.07D+00

E= -2649.79550610721 Delta-E= -0.000006003746 Rises=F Damp=F

DIIS: error= 4.87D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79550610721 IErMin= 3 ErrMin= 4.87D-05

ErrMax= 4.87D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.02D-06 BMatP= 1.14D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.300D-01 0.428D+00 0.602D+00

Coeff: -0.300D-01 0.428D+00 0.602D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.47D-06 MaxDP=1.04D-04 DE=-6.00D-06 OVMax= 6.05D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.24D-06 CP: 1.00D+00 1.08D+00 7.42D-01

E= -2649.79550661714 Delta-E= -0.000000509923 Rises=F Damp=F

DIIS: error= 3.04D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79550661714 IErMin= 4 ErrMin= 3.04D-05

ErrMax= 3.04D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.64D-06 BMatP= 4.02D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.708D-02 0.774D-01 0.385D+00 0.544D+00

Coeff: -0.708D-02 0.774D-01 0.385D+00 0.544D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=6.15D-07 MaxDP=5.42D-05 DE=-5.10D-07 OVMax= 1.69D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 3.61D-07 CP: 1.00D+00 1.08D+00 8.45D-01 6.80D-01

E= -2649.79550696689 Delta-E= -0.000000349748 Rises=F Damp=F

DIIS: error= 8.48D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79550696689 IErMin= 5 ErrMin= 8.48D-06

ErrMax= 8.48D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.16D-07 BMatP= 1.64D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.646D-03-0.558D-02 0.142D+00 0.286D+00 0.578D+00

Coeff: -0.646D-03-0.558D-02 0.142D+00 0.286D+00 0.578D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.10D-07 MaxDP=1.31D-05 DE=-3.50D-07 OVMax= 4.38D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.67D-07 CP: 1.00D+00 1.08D+00 8.59D-01 7.20D-01 7.10D-01

E= -2649.79550698656 Delta-E= -0.000000019671 Rises=F Damp=F

DIIS: error= 3.29D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79550698656 IErMin= 6 ErrMin= 3.29D-06

ErrMax= 3.29D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.20D-08 BMatP= 1.16D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.645D-03-0.153D-01 0.273D-01 0.893D-01 0.349D+00 0.549D+00

Coeff: 0.645D-03-0.153D-01 0.273D-01 0.893D-01 0.349D+00 0.549D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=8.44D-08 MaxDP=5.17D-06 DE=-1.97D-08 OVMax= 3.53D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 4.69D-08 CP: 1.00D+00 1.08D+00 8.63D-01 7.34D-01 7.75D-01

CP: 6.32D-01

E= -2649.79550699131 Delta-E= -0.000000004758 Rises=F Damp=F

DIIS: error= 6.93D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79550699131 IErMin= 7 ErrMin= 6.93D-07

ErrMax= 6.93D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.11D-09 BMatP= 2.20D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.356D-03-0.716D-02 0.473D-02 0.257D-01 0.135D+00 0.271D+00

Coeff-Com: 0.570D+00

Coeff: 0.356D-03-0.716D-02 0.473D-02 0.257D-01 0.135D+00 0.271D+00

Coeff: 0.570D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.40D-08 MaxDP=1.17D-06 DE=-4.76D-09 OVMax= 8.16D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.91D-08 CP: 1.00D+00 1.08D+00 8.65D-01 7.34D-01 7.81D-01

CP: 7.06D-01 9.38D-01

E= -2649.79550699165 Delta-E= -0.000000000331 Rises=F Damp=F

DIIS: error= 3.41D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2649.79550699165 IErMin= 8 ErrMin= 3.41D-07

ErrMax= 3.41D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.26D-10 BMatP= 1.11D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.124D-04 0.475D-03-0.501D-02-0.116D-01-0.257D-01-0.211D-02

Coeff-Com: 0.310D+00 0.734D+00

Coeff: 0.124D-04 0.475D-03-0.501D-02-0.116D-01-0.257D-01-0.211D-02

Coeff: 0.310D+00 0.734D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.30D-08 MaxDP=6.75D-07 DE=-3.31D-10 OVMax= 1.06D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 7.37D-09 CP: 1.00D+00 1.08D+00 8.66D-01 7.36D-01 7.88D-01

CP: 7.28D-01 1.13D+00 9.65D-01

E= -2649.79550699161 Delta-E= 0.000000000036 Rises=F Damp=F

DIIS: error= 1.45D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 8 EnMin= -2649.79550699165 IErMin= 9 ErrMin= 1.45D-07

ErrMax= 1.45D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.01D-11 BMatP= 2.26D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.345D-04 0.107D-02-0.302D-02-0.896D-02-0.286D-01-0.305D-01

Coeff-Com: 0.893D-01 0.384D+00 0.597D+00

Coeff: -0.345D-04 0.107D-02-0.302D-02-0.896D-02-0.286D-01-0.305D-01

Coeff: 0.893D-01 0.384D+00 0.597D+00

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.93D-09 MaxDP=3.80D-07 DE= 3.64D-11 OVMax= 3.06D-06

Error on total polarization charges = 0.07299

SCF Done: E(UB3LYP) = -2649.79550699 A.U. after 9 cycles

NFock= 9 Conv=0.49D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0171 S= 1.0057

<L.S>= 0.000000000000E+00

KE= 2.690141678451D+03 PE=-2.236245463104D+04 EE= 8.980642574445D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0171, after 2.0002

Leave Link 502 at Sat Jul 6 03:04:07 2019, MaxMem= 1342177280 cpu: 5520.8

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44315 LenP2D= 111304.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 273

Leave Link 701 at Sat Jul 6 03:04:27 2019, MaxMem= 1342177280 cpu: 225.5

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 03:04:28 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 03:06:02 2019, MaxMem= 1342177280 cpu: 1130.4

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.24874976D-03 2.36466867D-03 2.73928493D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000055364 -0.000016074 -0.000284075

2 7 0.000043431 0.000131722 0.000256386

3 6 -0.000080885 -0.000018176 -0.000232721

4 6 -0.000125994 0.000028499 0.000148245

5 6 0.000091934 0.000016657 0.000189228

6 7 0.000197714 -0.000063746 0.000185183

7 6 0.000057552 -0.000017796 -0.000137542

8 7 -0.000307557 -0.000010121 0.000102336

9 6 0.000005784 -0.000008413 -0.000076737

10 6 0.000033408 -0.000026344 0.000048443

11 6 0.000027806 -0.000012927 0.000080745

12 7 -0.000221145 -0.000086346 0.000212074

13 6 -0.000026192 -0.000000580 0.000079467

14 6 -0.000027178 -0.000034010 0.000049516

15 6 0.000013518 -0.000031619 -0.000063374

16 7 0.000347749 0.000000027 0.000090462

17 6 -0.000023143 0.000004535 -0.000137664

18 7 -0.000264026 0.000118742 0.000185280

19 7 -0.000008632 -0.000078243 0.000265401

20 6 0.000066954 0.000043449 -0.000281466

21 6 0.000088979 -0.000015154 0.000188845

22 6 -0.000110747 -0.000022531 0.000148186

23 6 -0.000076528 0.000023505 -0.000237797

24 7 0.000250460 0.000109786 0.000192371

25 30 -0.000060161 -0.000059806 -0.000301408

26 6 -0.000110133 -0.000019750 0.000050656

27 6 0.000055165 -0.000037165 -0.000044087

28 6 0.000052670 0.000055145 -0.000047351

29 6 -0.000101162 0.000031432 0.000046739

30 6 0.000031684 -0.000095385 -0.000150417

31 6 -0.000074453 0.000034064 0.000029390

32 6 0.000077158 0.000037406 0.000032874

33 6 -0.000026457 -0.000093762 -0.000143071

34 6 0.000118034 -0.000000798 0.000047405

35 6 -0.000061165 -0.000025482 -0.000042991

36 6 -0.000060785 0.000042651 -0.000051041

37 6 0.000111159 0.000024173 0.000049383

38 6 -0.000032409 0.000099984 -0.000140755

39 6 0.000069759 -0.000043094 0.000031423

40 6 -0.000057903 -0.000043287 0.000028614

41 6 0.000044559 0.000103685 -0.000149748

42 1 0.000021483 -0.000022471 0.000011871

43 1 0.000015886 0.000028645 0.000012941

44 1 0.000000925 0.000005612 -0.000011291

45 1 0.000000870 0.000000837 -0.000017138

46 1 -0.000018798 -0.000027080 0.000012060

47 1 -0.000006291 0.000035486 0.000011684

48 1 0.000007742 0.000001788 -0.000016865

49 1 -0.000002181 0.000001793 -0.000013802

50 8 -0.000047962 -0.000155655 -0.000007099

51 8 0.000029493 -0.000165220 -0.000020032

52 8 -0.000098728 -0.000043016 -0.000080338

53 8 -0.000143381 0.000008961 -0.000100931

54 8 -0.000019898 0.000181033 -0.000009009

55 8 -0.000002258 0.000193472 -0.000001731

56 8 0.000169209 -0.000023813 -0.000104294

57 8 0.000135611 -0.000018640 -0.000094627

58 6 -0.000072381 0.000135656 0.000112160

59 1 0.000064708 -0.000014664 -0.000044795

60 1 0.000018324 -0.000056143 -0.000055363

61 1 -0.000032731 -0.000002377 0.000033109

62 6 0.000035964 -0.000020863 0.000011373

63 1 -0.000009319 0.000002420 0.000020185

64 1 -0.000013432 -0.000010029 -0.000018801

65 1 0.000018747 -0.000026703 -0.000009622

66 6 0.000036780 0.000002630 0.000010574

67 1 -0.000011454 0.000004871 -0.000020673

68 1 -0.000013219 -0.000005281 0.000021818

69 1 0.000018241 0.000024514 -0.000014712

70 6 0.000052709 0.000135325 0.000114979

71 1 -0.000009910 -0.000060950 -0.000049524

72 1 -0.000068852 -0.000015885 -0.000045072

73 1 0.000028209 -0.000000709 0.000038787

74 6 -0.000037890 -0.000005861 0.000014984

75 1 0.000014432 -0.000007995 -0.000019720

76 1 0.000011633 0.000003845 0.000021588

77 1 -0.000019266 -0.000025465 -0.000011352

78 6 -0.000036633 0.000000127 0.000005997

79 1 0.000013789 -0.000008437 0.000023416

80 1 0.000011063 -0.000002879 -0.000019760

81 1 -0.000015161 0.000023076 -0.000017018

82 6 0.000047330 -0.000130850 0.000117201

83 1 -0.000070202 0.000015376 -0.000046776

84 1 -0.000014254 0.000060394 -0.000052099

85 1 0.000027956 0.000002391 0.000039371

86 6 -0.000054479 -0.000140028 0.000111108

87 1 0.000016862 0.000059404 -0.000051554

88 1 0.000066511 0.000016740 -0.000045908

89 1 -0.000029982 0.000001764 0.000038293

-------------------------------------------------------------------

Cartesian Forces: Max 0.000347749 RMS 0.000089675

Leave Link 716 at Sat Jul 6 03:06:02 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000215934 RMS 0.000050721

Search for a local minimum.

Step number 21 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .50721D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 6 5 7 9 11

14 13 16 17 18

19 20 21

DE= -1.82D-05 DEPred=-1.37D-05 R= 1.33D+00

TightC=F SS= 1.41D+00 RLast= 5.66D-02 DXNew= 3.9497D-01 1.6980D-01

Trust test= 1.33D+00 RLast= 5.66D-02 DXMaxT set to 2.35D-01

ITU= 1 1 1 1 0 0 -1 -1 0 -1 0 0 0 0 0 0 1 1 1 1

ITU= 0

Eigenvalues --- 0.00269 0.01100 0.01315 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01320 0.01434

Eigenvalues --- 0.01562 0.01569 0.01582 0.01598 0.01600

Eigenvalues --- 0.01618 0.01665 0.01704 0.01708 0.01712

Eigenvalues --- 0.01714 0.01716 0.01835 0.01864 0.01871

Eigenvalues --- 0.01892 0.01919 0.01922 0.01945 0.01982

Eigenvalues --- 0.01994 0.02016 0.02020 0.02021 0.02029

Eigenvalues --- 0.02044 0.02052 0.02053 0.02053 0.02056

Eigenvalues --- 0.02057 0.02057 0.02057 0.02057 0.02058

Eigenvalues --- 0.02066 0.02067 0.02067 0.02070 0.02070

Eigenvalues --- 0.02070 0.02076 0.02083 0.02083 0.02149

Eigenvalues --- 0.02181 0.02249 0.02260 0.02260 0.02260

Eigenvalues --- 0.02260 0.02260 0.02263 0.02341 0.02355

Eigenvalues --- 0.02356 0.02500 0.02764 0.03376 0.03975

Eigenvalues --- 0.09975 0.09978 0.09978 0.09987 0.09988

Eigenvalues --- 0.09988 0.10010 0.10174 0.10640 0.10643

Eigenvalues --- 0.10643 0.10643 0.10658 0.10658 0.10658

Eigenvalues --- 0.10671 0.12411 0.13295 0.13465 0.15311

Eigenvalues --- 0.15982 0.15988 0.15998 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16003 0.16007 0.16045 0.16148

Eigenvalues --- 0.16551 0.16807 0.20579 0.21418 0.21708

Eigenvalues --- 0.22474 0.22476 0.22476 0.22482 0.23835

Eigenvalues --- 0.24269 0.24500 0.24507 0.24522 0.24587

Eigenvalues --- 0.24667 0.24767 0.24818 0.24882 0.24901

Eigenvalues --- 0.24922 0.24973 0.24974 0.24985 0.24987

Eigenvalues --- 0.24995 0.24996 0.24997 0.24998 0.24999

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25002

Eigenvalues --- 0.25027 0.25096 0.25899 0.27442 0.30583

Eigenvalues --- 0.33002 0.33634 0.33679 0.33717 0.33772

Eigenvalues --- 0.34017 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34063 0.34066 0.34077 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34081

Eigenvalues --- 0.34240 0.34617 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34687 0.34689 0.34898

Eigenvalues --- 0.34959 0.35053 0.35595 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35635 0.35761

Eigenvalues --- 0.36804 0.37025 0.37132 0.37432 0.40355

Eigenvalues --- 0.41215 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41217 0.41240 0.41378 0.41410 0.41414

Eigenvalues --- 0.41417 0.41434 0.41941 0.42208 0.42471

Eigenvalues --- 0.43270 0.44440 0.44560 0.44678 0.44773

Eigenvalues --- 0.44878 0.44998 0.45002 0.45003 0.45006

Eigenvalues --- 0.45273 0.45365 0.45367 0.45872 0.46113

Eigenvalues --- 0.47051 0.47275 0.48852 0.49315 0.49374

Eigenvalues --- 0.49848 0.50290 0.53554 0.53554 0.53554

Eigenvalues --- 0.53554 0.53554 0.53632 0.54202 0.54995

Eigenvalues --- 0.55878 0.56073 0.57412 0.57560 0.57692

Eigenvalues --- 0.64368

En-DIIS/RFO-DIIS IScMMF= 0 using points: 21 20 19 18 17

RFO step: Lambda=-3.99168255D-06.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 1.52D-04 SmlDif= 1.00D-05

RMS Error= 0.2041166562D-03 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.97677 0.25517 -0.20740 -0.11614 0.09159

Iteration 1 RMS(Cart)= 0.00653131 RMS(Int)= 0.00001271

Iteration 2 RMS(Cart)= 0.00002624 RMS(Int)= 0.00000302

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000302

ITry= 1 IFail=0 DXMaxC= 2.94D-02 DCOld= 1.00D+10 DXMaxT= 2.35D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58261 0.00000 -0.00006 0.00007 0.00002 2.58264

R2 2.73959 -0.00002 -0.00034 0.00034 0.00000 2.73959

R3 2.56114 0.00015 0.00012 0.00009 0.00021 2.56135

R4 2.58259 -0.00002 -0.00001 0.00000 0.00000 2.58259

R5 3.86927 0.00000 -0.00024 -0.00044 -0.00067 3.86860

R6 2.73944 0.00006 -0.00029 0.00033 0.00004 2.73948

R7 2.56104 0.00021 0.00031 -0.00001 0.00029 2.56133

R8 2.69606 -0.00007 0.00023 -0.00037 -0.00015 2.69591

R9 2.66260 -0.00006 -0.00017 0.00009 -0.00008 2.66252

R10 2.66262 -0.00007 -0.00017 0.00008 -0.00009 2.66253

R11 2.48237 0.00001 0.00044 -0.00041 0.00001 2.48238

R12 2.59587 0.00006 -0.00008 0.00018 0.00010 2.59597

R13 2.79450 0.00007 0.00014 -0.00019 -0.00005 2.79445

R14 2.59589 0.00003 -0.00014 0.00018 0.00004 2.59594

R15 3.84240 -0.00010 -0.00091 -0.00043 -0.00132 3.84108

R16 2.79475 -0.00006 0.00007 -0.00019 -0.00013 2.79462

R17 2.48252 -0.00011 0.00021 -0.00031 -0.00011 2.48241

R18 2.66421 -0.00007 -0.00015 -0.00004 -0.00019 2.66402

R19 2.64569 -0.00006 -0.00016 0.00018 0.00002 2.64571

R20 2.64563 0.00000 -0.00015 0.00021 0.00006 2.64569

R21 2.48251 -0.00009 0.00027 -0.00032 -0.00007 2.48244

R22 2.66426 -0.00010 -0.00023 0.00000 -0.00023 2.66403

R23 2.79466 0.00002 0.00010 -0.00015 -0.00005 2.79461

R24 2.64569 -0.00005 -0.00018 0.00020 0.00003 2.64572

R25 2.79477 -0.00012 0.00002 -0.00021 -0.00019 2.79457

R26 2.64574 -0.00010 -0.00019 0.00019 0.00000 2.64574

R27 2.59592 0.00000 -0.00011 0.00019 0.00008 2.59600

R28 2.48263 -0.00022 0.00003 -0.00022 -0.00019 2.48244

R29 2.59588 0.00002 -0.00004 0.00015 0.00011 2.59599

R30 3.84305 -0.00015 -0.00094 -0.00061 -0.00154 3.84151

R31 2.56120 0.00005 -0.00002 0.00012 0.00010 2.56130

R32 2.58259 -0.00006 -0.00003 0.00001 -0.00001 2.58258

R33 2.58267 -0.00005 0.00002 0.00003 0.00005 2.58272

R34 3.86994 -0.00005 -0.00026 -0.00063 -0.00087 3.86906

R35 2.73963 -0.00006 -0.00037 0.00033 -0.00005 2.73958

R36 2.69608 -0.00010 0.00016 -0.00035 -0.00019 2.69589

R37 2.66264 -0.00011 -0.00018 0.00007 -0.00011 2.66252

R38 2.73954 0.00001 -0.00032 0.00033 0.00001 2.73955

R39 2.66264 -0.00009 -0.00018 0.00008 -0.00010 2.66254

R40 2.56116 0.00013 0.00017 0.00005 0.00022 2.56137

R41 2.65620 -0.00003 0.00017 -0.00024 -0.00007 2.65613

R42 2.54965 -0.00005 0.00000 -0.00017 -0.00016 2.54949

R43 2.62951 -0.00007 0.00008 -0.00021 -0.00014 2.62937

R44 2.04426 0.00000 0.00002 0.00000 0.00002 2.04428

R45 2.65620 -0.00003 0.00016 -0.00023 -0.00007 2.65613

R46 2.04427 -0.00001 0.00002 -0.00002 -0.00001 2.04426

R47 2.54961 0.00002 0.00002 -0.00013 -0.00011 2.54950

R48 2.64330 0.00001 0.00003 -0.00003 0.00000 2.64330

R49 2.55246 -0.00002 -0.00015 0.00004 -0.00011 2.55235

R50 2.64701 -0.00002 0.00010 -0.00017 -0.00007 2.64694

R51 2.04404 -0.00001 0.00004 -0.00002 0.00003 2.04406

R52 2.64330 0.00000 0.00002 -0.00002 0.00000 2.64330

R53 2.04405 -0.00001 0.00004 -0.00002 0.00002 2.04407

R54 2.55243 0.00002 -0.00014 0.00005 -0.00010 2.55233

R55 2.65622 -0.00005 0.00017 -0.00025 -0.00009 2.65613

R56 2.54970 -0.00009 0.00000 -0.00018 -0.00019 2.54952

R57 2.62954 -0.00010 0.00008 -0.00024 -0.00016 2.62939

R58 2.04424 0.00001 0.00002 0.00000 0.00002 2.04426

R59 2.65623 -0.00006 0.00015 -0.00024 -0.00008 2.65615

R60 2.04427 0.00000 0.00002 0.00000 0.00001 2.04428

R61 2.54964 -0.00003 0.00001 -0.00016 -0.00015 2.54949

R62 2.64333 -0.00002 0.00002 -0.00003 -0.00001 2.64331

R63 2.55247 -0.00003 -0.00015 0.00003 -0.00013 2.55234

R64 2.64704 -0.00004 0.00010 -0.00019 -0.00009 2.64695

R65 2.04404 0.00000 0.00004 -0.00002 0.00003 2.04406

R66 2.64331 -0.00002 0.00002 -0.00005 -0.00002 2.64329

R67 2.04403 0.00000 0.00004 -0.00001 0.00004 2.04407

R68 2.55250 -0.00007 -0.00016 0.00001 -0.00015 2.55235

R69 2.69362 0.00005 -0.00009 0.00016 0.00007 2.69369

R70 2.69363 0.00006 -0.00008 0.00017 0.00009 2.69372

R71 2.69553 0.00000 -0.00008 0.00005 -0.00003 2.69550

R72 2.69552 0.00001 -0.00008 0.00006 -0.00001 2.69551

R73 2.69363 0.00006 -0.00008 0.00018 0.00009 2.69372

R74 2.69361 0.00006 -0.00008 0.00017 0.00008 2.69369

R75 2.69551 0.00002 -0.00007 0.00006 -0.00001 2.69550

R76 2.69552 0.00001 -0.00007 0.00006 -0.00002 2.69551

R77 2.06761 -0.00006 0.00000 -0.00013 -0.00014 2.06748

R78 2.06739 -0.00001 0.00003 0.00004 0.00007 2.06746

R79 2.05689 -0.00003 -0.00004 -0.00004 -0.00008 2.05681

R80 2.06723 -0.00002 -0.00001 -0.00001 -0.00002 2.06721

R81 2.06750 -0.00002 -0.00001 -0.00002 -0.00003 2.06747

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R84 2.06723 -0.00003 -0.00001 -0.00002 -0.00003 2.06721

R85 2.05677 -0.00003 -0.00002 -0.00005 -0.00007 2.05670

R86 2.06739 -0.00001 0.00003 0.00002 0.00006 2.06745

R87 2.06761 -0.00006 0.00000 -0.00014 -0.00014 2.06747

R88 2.05689 -0.00003 -0.00004 -0.00004 -0.00008 2.05681

R89 2.06750 -0.00002 -0.00001 -0.00002 -0.00003 2.06747

R90 2.06723 -0.00003 -0.00001 -0.00001 -0.00003 2.06721

R91 2.05677 -0.00003 -0.00002 -0.00005 -0.00007 2.05670

R92 2.06724 -0.00003 -0.00001 -0.00001 -0.00003 2.06721

R93 2.06751 -0.00002 -0.00001 -0.00002 -0.00003 2.06747

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R98 2.06738 -0.00001 0.00003 0.00003 0.00006 2.06745

R99 2.06761 -0.00006 0.00000 -0.00014 -0.00014 2.06748

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A2 2.21447 0.00007 -0.00006 0.00031 0.00026 2.21473

A3 2.17924 -0.00001 0.00010 -0.00019 -0.00010 2.17914

A4 1.93047 0.00008 0.00011 0.00007 0.00017 1.93064

A5 2.17258 -0.00006 0.00011 0.00009 0.00019 2.17277

A6 2.17235 -0.00001 0.00001 0.00024 0.00024 2.17260

A7 1.88945 -0.00009 -0.00008 -0.00009 -0.00017 1.88928

A8 2.21460 0.00003 -0.00009 0.00030 0.00020 2.21481

A9 2.17904 0.00006 0.00018 -0.00020 -0.00003 2.17901

A10 1.85774 0.00003 0.00001 0.00007 0.00008 1.85783

A11 2.31727 -0.00003 -0.00005 -0.00007 -0.00012 2.31715

A12 2.10794 -0.00001 0.00003 0.00003 0.00006 2.10800

A13 1.85773 0.00003 0.00001 0.00006 0.00007 1.85781

A14 2.31741 -0.00006 -0.00008 -0.00005 -0.00013 2.31728

A15 2.10781 0.00004 0.00006 0.00002 0.00008 2.10789

A16 2.18721 -0.00005 -0.00016 -0.00023 -0.00039 2.18682

A17 2.23313 -0.00005 0.00026 -0.00017 0.00009 2.23322

A18 2.16647 0.00003 -0.00010 -0.00025 -0.00036 2.16611

A19 1.88320 0.00002 -0.00015 0.00045 0.00031 1.88350

A20 1.93306 -0.00010 0.00018 -0.00070 -0.00053 1.93253

A21 2.16260 0.00007 -0.00004 0.00030 0.00026 2.16286

A22 2.16294 0.00002 0.00005 0.00016 0.00021 2.16315

A23 1.88309 0.00007 -0.00010 0.00044 0.00034 1.88343

A24 2.23291 0.00002 0.00031 -0.00017 0.00015 2.23306

A25 2.16680 -0.00010 -0.00020 -0.00024 -0.00045 2.16635

A26 1.86264 0.00001 0.00004 -0.00010 -0.00007 1.86257

A27 2.30409 -0.00004 -0.00023 0.00028 0.00004 2.30413

A28 2.11633 0.00003 0.00020 -0.00014 0.00007 2.11640

A29 1.86266 -0.00001 0.00003 -0.00011 -0.00009 1.86257

A30 2.30383 0.00007 -0.00017 0.00031 0.00014 2.30397

A31 2.11656 -0.00006 0.00015 -0.00015 -0.00001 2.11656

A32 2.18732 -0.00007 -0.00027 -0.00016 -0.00043 2.18689

A33 1.86266 -0.00001 0.00003 -0.00011 -0.00008 1.86258

A34 2.11645 -0.00004 0.00016 -0.00017 -0.00001 2.11644

A35 2.30395 0.00005 -0.00018 0.00032 0.00014 2.30409

A36 1.86265 0.00000 0.00004 -0.00011 -0.00008 1.86257

A37 2.11636 0.00006 0.00022 -0.00009 0.00013 2.11649

A38 2.30405 -0.00006 -0.00025 0.00024 -0.00001 2.30404

A39 1.88309 0.00010 -0.00004 0.00043 0.00039 1.88348

A40 2.16679 -0.00014 -0.00033 -0.00020 -0.00054 2.16625

A41 2.23292 0.00005 0.00039 -0.00019 0.00019 2.23311

A42 1.93312 -0.00012 0.00007 -0.00065 -0.00059 1.93253

A43 2.16289 0.00003 0.00011 0.00012 0.00023 2.16312

A44 2.16262 0.00008 0.00002 0.00028 0.00029 2.16292

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A46 2.23306 -0.00003 0.00033 -0.00023 0.00010 2.23316

A47 1.88314 0.00004 -0.00009 0.00041 0.00032 1.88346

A48 2.18740 -0.00009 -0.00037 -0.00017 -0.00054 2.18686

A49 1.93053 0.00005 -0.00001 0.00011 0.00009 1.93062

A50 2.17258 -0.00004 0.00017 0.00009 0.00026 2.17283

A51 2.17230 -0.00001 0.00007 0.00018 0.00025 2.17255

A52 2.21450 0.00007 -0.00002 0.00027 0.00026 2.21475

A53 2.17924 -0.00004 -0.00001 -0.00013 -0.00015 2.17909

A54 1.88935 -0.00003 0.00003 -0.00013 -0.00010 1.88925

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A56 2.31736 -0.00009 -0.00008 -0.00011 -0.00019 2.31717

A57 2.10782 0.00006 0.00007 0.00006 0.00013 2.10796

A58 1.85774 0.00002 0.00000 0.00006 0.00006 1.85780

A59 2.10786 0.00002 0.00003 0.00003 0.00006 2.10793

A60 2.31735 -0.00003 -0.00005 -0.00006 -0.00011 2.31724

A61 1.88938 -0.00006 -0.00002 -0.00012 -0.00013 1.88925

A62 2.21463 0.00003 -0.00006 0.00027 0.00022 2.21485

A63 2.17908 0.00003 0.00007 -0.00014 -0.00008 2.17900

A64 2.18734 -0.00007 -0.00026 -0.00019 -0.00045 2.18689

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A68 1.55950 -0.00002 0.00003 -0.00009 -0.00007 1.55943

A69 2.04510 0.00000 -0.00022 0.00013 -0.00009 2.04501

A70 2.07287 -0.00005 -0.00012 0.00006 -0.00006 2.07280

A71 2.16521 0.00004 0.00034 -0.00019 0.00015 2.16536

A72 2.12166 0.00001 0.00005 0.00002 0.00007 2.12172

A73 2.09882 0.00003 -0.00008 0.00025 0.00017 2.09899

A74 2.06270 -0.00004 0.00002 -0.00026 -0.00024 2.06246

A75 2.12168 -0.00001 0.00003 0.00002 0.00005 2.12173

A76 2.06270 -0.00003 0.00004 -0.00027 -0.00024 2.06246

A77 2.09880 0.00004 -0.00007 0.00025 0.00019 2.09898

A78 2.04512 -0.00002 -0.00024 0.00009 -0.00014 2.04498

A79 2.07298 -0.00012 -0.00015 -0.00001 -0.00015 2.07282

A80 2.16508 0.00014 0.00038 -0.00009 0.00029 2.16537

A81 2.05225 -0.00003 -0.00007 -0.00007 -0.00014 2.05211

A82 2.06615 -0.00010 -0.00022 0.00003 -0.00019 2.06597

A83 2.16478 0.00013 0.00029 0.00004 0.00032 2.16510

A84 2.12308 0.00000 0.00003 0.00004 0.00006 2.12314

A85 2.10068 0.00000 -0.00002 -0.00004 -0.00006 2.10062

A86 2.05943 0.00000 -0.00001 0.00000 0.00000 2.05942

A87 2.12307 -0.00001 0.00002 0.00002 0.00004 2.12311

A88 2.05941 0.00000 0.00000 -0.00002 -0.00002 2.05939

A89 2.10070 0.00001 -0.00001 0.00000 -0.00002 2.10068

A90 2.05227 -0.00005 -0.00008 -0.00008 -0.00016 2.05212

A91 2.06616 -0.00013 -0.00023 -0.00002 -0.00025 2.06591

A92 2.16475 0.00018 0.00030 0.00010 0.00041 2.16515

A93 2.04503 0.00002 -0.00022 0.00015 -0.00007 2.04495

A94 2.07274 0.00001 -0.00007 0.00007 0.00000 2.07274

A95 2.16542 -0.00003 0.00029 -0.00022 0.00007 2.16548

A96 2.12165 0.00001 0.00006 0.00000 0.00006 2.12171

A97 2.09882 0.00003 -0.00008 0.00025 0.00017 2.09899

A98 2.06270 -0.00003 0.00002 -0.00025 -0.00023 2.06247

A99 2.12170 -0.00001 0.00004 0.00000 0.00004 2.12174

A100 2.06268 -0.00003 0.00003 -0.00026 -0.00023 2.06245

A101 2.09880 0.00004 -0.00008 0.00026 0.00019 2.09899

A102 2.04509 0.00001 -0.00023 0.00014 -0.00009 2.04501

A103 2.07288 -0.00007 -0.00010 0.00000 -0.00010 2.07278

A104 2.16520 0.00006 0.00033 -0.00014 0.00019 2.16539

A105 2.05224 -0.00002 -0.00007 -0.00004 -0.00012 2.05212

A106 2.06612 -0.00009 -0.00020 0.00003 -0.00018 2.06594

A107 2.16482 0.00011 0.00028 0.00002 0.00029 2.16511

A108 2.12310 0.00000 0.00002 0.00002 0.00005 2.12315

A109 2.10066 0.00000 -0.00002 -0.00002 -0.00005 2.10062

A110 2.05941 0.00000 0.00000 0.00000 0.00000 2.05941

A111 2.12306 0.00000 0.00003 0.00000 0.00004 2.12310

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A114 2.05221 -0.00001 -0.00006 -0.00004 -0.00010 2.05210

A115 2.06604 -0.00006 -0.00020 0.00004 -0.00015 2.06589

A116 2.16494 0.00007 0.00026 -0.00001 0.00026 2.16519

A117 2.06593 -0.00009 -0.00020 -0.00039 -0.00059 2.06535

A118 2.06587 -0.00005 -0.00020 -0.00033 -0.00053 2.06534

A119 2.07013 -0.00021 0.00003 -0.00085 -0.00082 2.06931

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A132 1.94514 -0.00002 0.00000 -0.00012 -0.00013 1.94501

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A135 1.90793 -0.00001 -0.00001 -0.00002 -0.00002 1.90790

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A137 1.94508 -0.00001 0.00000 -0.00010 -0.00010 1.94497

A138 1.94758 -0.00001 -0.00004 0.00006 0.00002 1.94759

A139 1.84033 0.00002 0.00014 0.00005 0.00019 1.84052

A140 1.91248 0.00000 -0.00009 0.00002 -0.00007 1.91241

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A142 1.90796 -0.00001 -0.00001 -0.00003 -0.00004 1.90792

A143 1.94798 -0.00008 0.00012 -0.00056 -0.00044 1.94753

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A145 1.84271 -0.00002 0.00002 -0.00004 -0.00001 1.84269

A146 1.91036 0.00005 -0.00018 0.00048 0.00031 1.91067

A147 1.90853 0.00001 -0.00007 -0.00009 -0.00016 1.90838

A148 1.90912 -0.00005 0.00007 -0.00030 -0.00023 1.90889

A149 1.94510 -0.00002 0.00000 -0.00014 -0.00014 1.94496

A150 1.94757 0.00000 -0.00004 0.00008 0.00004 1.94761

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A153 1.90875 0.00001 0.00000 0.00001 0.00001 1.90876

A154 1.90795 -0.00001 -0.00001 -0.00002 -0.00003 1.90792

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A158 1.91248 0.00000 -0.00009 0.00003 -0.00006 1.91242

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A163 1.84268 -0.00002 0.00003 -0.00007 -0.00004 1.84264

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A174 3.11914 -0.00002 0.00021 -0.00030 -0.00009 3.11905

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D2 3.01696 0.00002 0.00074 0.00345 0.00420 3.02116

D3 3.13112 -0.00001 -0.00119 0.00084 -0.00036 3.13077

D4 -0.13931 0.00003 0.00058 0.00415 0.00473 -0.13458

D5 -0.00270 0.00002 0.00066 -0.00003 0.00064 -0.00206

D6 -3.12028 -0.00002 0.00096 -0.00163 -0.00067 -3.12095

D7 -3.12999 0.00001 0.00083 -0.00071 0.00012 -3.12987

D8 0.03561 -0.00003 0.00113 -0.00231 -0.00118 0.03443

D9 0.17989 -0.00004 -0.00108 -0.00327 -0.00435 0.17555

D10 -2.97868 -0.00003 -0.00127 -0.00246 -0.00374 -2.98242

D11 -0.00400 0.00002 0.00097 -0.00020 0.00078 -0.00323

D12 -3.13116 0.00001 0.00114 -0.00069 0.00046 -3.13070

D13 -3.01678 -0.00002 -0.00081 -0.00349 -0.00430 -3.02108

D14 0.13925 -0.00003 -0.00064 -0.00398 -0.00461 0.13464

D15 -2.95183 -0.00003 -0.00229 -0.00093 -0.00322 -2.95505

D16 -0.04322 -0.00003 0.00030 -0.00287 -0.00257 -0.04578

D17 0.04337 0.00002 -0.00027 0.00282 0.00255 0.04593

D18 2.95199 0.00003 0.00233 0.00087 0.00320 2.95519

D19 0.00217 0.00000 -0.00052 0.00017 -0.00035 0.00182

D20 3.12003 0.00003 -0.00085 0.00164 0.00079 3.12082

D21 3.12970 0.00000 -0.00069 0.00065 -0.00004 3.12965

D22 -0.03563 0.00003 -0.00102 0.00212 0.00109 -0.03454

D23 -0.17996 0.00004 0.00110 0.00303 0.00413 -0.17583

D24 2.97834 0.00003 0.00130 0.00247 0.00377 2.98211

D25 0.00031 -0.00001 -0.00009 -0.00009 -0.00017 0.00014

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D27 -3.12100 -0.00004 0.00020 -0.00134 -0.00114 -3.12214

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D29 -3.11857 -0.00003 0.00089 -0.00198 -0.00108 -3.11965

D30 0.02086 -0.00007 0.00089 -0.00221 -0.00132 0.01954

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D34 -0.02122 0.00008 -0.00076 0.00223 0.00147 -0.01975

D35 0.00338 0.00000 -0.00045 0.00029 -0.00016 0.00322

D36 -3.13601 0.00004 -0.00043 0.00044 0.00001 -3.13599

D37 -0.04827 -0.00004 -0.00023 -0.00148 -0.00171 -0.04998

D38 3.12661 -0.00007 -0.00048 -0.00279 -0.00327 3.12334

D39 -3.09753 0.00001 -0.00007 0.00022 0.00015 -3.09738

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D41 0.01510 0.00004 0.00015 0.00135 0.00150 0.01660

D42 -2.89767 0.00008 -0.00070 0.00242 0.00172 -2.89595

D43 3.10470 0.00001 0.00019 0.00061 0.00079 3.10549

D44 -0.01950 -0.00004 -0.00029 -0.00232 -0.00261 -0.02211

D45 -0.00931 -0.00001 -0.00003 -0.00047 -0.00050 -0.00981

D46 -3.13351 -0.00006 -0.00051 -0.00340 -0.00390 -3.13741

D47 -0.01476 -0.00006 -0.00021 -0.00167 -0.00188 -0.01664

D48 3.09771 -0.00003 0.00002 -0.00037 -0.00035 3.09736

D49 2.89796 -0.00009 0.00063 -0.00272 -0.00209 2.89587

D50 -0.27276 -0.00006 0.00086 -0.00142 -0.00056 -0.27332

D51 -0.22442 -0.00005 0.00096 -0.00162 -0.00065 -0.22508

D52 3.10727 -0.00002 0.00005 0.00035 0.00039 3.10767

D53 -3.10751 0.00001 -0.00001 -0.00030 -0.00031 -3.10782

D54 0.22418 0.00004 -0.00093 0.00167 0.00074 0.22492

D55 0.00840 0.00005 0.00018 0.00133 0.00151 0.00991

D56 3.13280 0.00009 0.00063 0.00406 0.00469 3.13749

D57 -3.10544 0.00002 -0.00005 0.00009 0.00004 -3.10540

D58 0.01896 0.00006 0.00040 0.00281 0.00322 0.02218

D59 0.04851 0.00004 0.00024 0.00159 0.00182 0.05033

D60 -3.12658 0.00008 0.00050 0.00310 0.00359 -3.12298

D61 0.00054 -0.00002 -0.00009 -0.00051 -0.00060 -0.00006

D62 3.12701 0.00002 0.00032 0.00204 0.00236 3.12937

D63 -3.12611 -0.00006 -0.00048 -0.00289 -0.00336 -3.12947

D64 0.00036 -0.00001 -0.00007 -0.00034 -0.00040 -0.00004

D65 -3.12275 -0.00003 -0.00022 -0.00183 -0.00205 -3.12480

D66 0.02240 0.00003 -0.00008 -0.00065 -0.00073 0.02166

D67 -0.00043 0.00002 0.00029 0.00123 0.00151 0.00109

D68 -3.13846 0.00008 0.00043 0.00240 0.00283 -3.13564

D69 3.12210 0.00006 0.00033 0.00246 0.00278 3.12488

D70 -0.02322 0.00001 0.00023 0.00141 0.00164 -0.02158

D71 0.00000 0.00000 -0.00021 -0.00082 -0.00103 -0.00103

D72 3.13787 -0.00005 -0.00031 -0.00187 -0.00217 3.13569

D73 -3.12664 0.00008 0.00054 0.00297 0.00351 -3.12313

D74 0.04830 0.00005 0.00023 0.00168 0.00190 0.05020

D75 -0.00052 0.00002 0.00009 0.00056 0.00065 0.00013

D76 3.12610 0.00006 0.00051 0.00303 0.00354 3.12964

D77 -3.12694 -0.00002 -0.00034 -0.00207 -0.00242 -3.12936

D78 -0.00032 0.00002 0.00007 0.00040 0.00047 0.00015

D79 -3.10469 -0.00001 -0.00019 -0.00063 -0.00082 -3.10551

D80 0.00927 0.00001 0.00008 0.00043 0.00051 0.00978

D81 0.01945 0.00004 0.00032 0.00239 0.00271 0.02216

D82 3.13341 0.00007 0.00059 0.00345 0.00404 3.13744

D83 -0.00012 0.00001 0.00024 0.00085 0.00109 0.00097

D84 -3.13806 0.00005 0.00039 0.00188 0.00227 -3.13579

D85 -3.12216 -0.00005 -0.00033 -0.00253 -0.00286 -3.12502

D86 0.02309 -0.00001 -0.00018 -0.00150 -0.00168 0.02141

D87 -0.00839 -0.00006 -0.00023 -0.00136 -0.00160 -0.00999

D88 3.10551 -0.00002 0.00005 -0.00010 -0.00005 3.10546

D89 -3.13276 -0.00010 -0.00072 -0.00421 -0.00492 -3.13768

D90 -0.01886 -0.00007 -0.00043 -0.00294 -0.00337 -0.02223

D91 0.00051 -0.00002 -0.00032 -0.00134 -0.00165 -0.00115

D92 3.13856 -0.00008 -0.00051 -0.00255 -0.00306 3.13550

D93 3.12280 0.00003 0.00022 0.00185 0.00207 3.12487

D94 -0.02234 -0.00003 0.00003 0.00064 0.00067 -0.02167

D95 0.01472 0.00007 0.00029 0.00168 0.00197 0.01669

D96 -2.89812 0.00009 -0.00058 0.00282 0.00224 -2.89588

D97 -3.09781 0.00003 0.00001 0.00035 0.00036 -3.09745

D98 0.27253 0.00006 -0.00085 0.00149 0.00063 0.27316

D99 3.12680 -0.00009 -0.00055 -0.00310 -0.00365 3.12315

D100 -0.04821 -0.00005 -0.00022 -0.00156 -0.00178 -0.04999

D101 3.09754 -0.00002 0.00003 -0.00021 -0.00018 3.09736

D102 -0.01505 -0.00005 -0.00023 -0.00133 -0.00157 -0.01661

D103 -0.27276 -0.00006 0.00091 -0.00137 -0.00046 -0.27322

D104 2.89784 -0.00009 0.00065 -0.00249 -0.00184 2.89599

D105 3.10749 -0.00001 0.00000 0.00024 0.00023 3.10773

D106 -0.22417 -0.00004 0.00095 -0.00176 -0.00081 -0.22498

D107 0.22425 0.00005 -0.00099 0.00164 0.00065 0.22490

D108 -3.10741 0.00002 -0.00004 -0.00035 -0.00039 -3.10780

D109 -0.17959 0.00002 0.00105 0.00289 0.00394 -0.17565

D110 2.97872 0.00001 0.00129 0.00184 0.00312 2.98185

D111 -3.13150 0.00003 0.00127 -0.00066 0.00061 -3.13089

D112 -0.00436 0.00004 0.00106 0.00025 0.00132 -0.00304

D113 0.13890 -0.00002 -0.00056 -0.00383 -0.00439 0.13451

D114 -3.01714 -0.00001 -0.00077 -0.00292 -0.00369 -3.02083

D115 0.00410 -0.00003 -0.00101 -0.00005 -0.00106 0.00304

D116 3.13130 -0.00003 -0.00124 0.00070 -0.00054 3.13076

D117 3.01690 0.00002 0.00083 0.00312 0.00395 3.02085

D118 -0.13908 0.00002 0.00060 0.00387 0.00447 -0.13462

D119 2.95202 0.00004 0.00234 0.00084 0.00318 2.95520

D120 0.04338 0.00003 -0.00028 0.00281 0.00252 0.04591

D121 -0.04322 -0.00003 0.00026 -0.00276 -0.00250 -0.04572

D122 -2.95186 -0.00003 -0.00236 -0.00079 -0.00316 -2.95501

D123 3.13036 -0.00003 -0.00089 0.00053 -0.00035 3.13001

D124 -0.03522 0.00001 -0.00118 0.00194 0.00076 -0.03446

D125 0.00285 -0.00004 -0.00069 -0.00036 -0.00104 0.00181

D126 3.12046 0.00000 -0.00097 0.00105 0.00007 3.12053

D127 -0.00041 0.00002 0.00008 0.00032 0.00041 -0.00001

D128 3.12086 0.00004 -0.00020 0.00134 0.00115 3.12201

D129 -3.12151 -0.00002 0.00033 -0.00088 -0.00054 -3.12205

D130 -0.00023 0.00001 0.00005 0.00015 0.00020 -0.00004

D131 -3.11803 -0.00005 0.00077 -0.00211 -0.00134 -3.11936

D132 0.02143 -0.00009 0.00075 -0.00244 -0.00169 0.01974

D133 -0.00321 -0.00001 0.00045 -0.00054 -0.00009 -0.00331

D134 3.13624 -0.00005 0.00043 -0.00087 -0.00044 3.13579

D135 -0.00217 0.00001 0.00055 -0.00018 0.00037 -0.00180

D136 -3.12973 0.00000 0.00077 -0.00091 -0.00014 -3.12987

D137 -3.11998 -0.00002 0.00087 -0.00138 -0.00050 -3.12048

D138 0.03564 -0.00003 0.00110 -0.00211 -0.00101 0.03463

D139 0.00350 0.00000 -0.00051 0.00036 -0.00015 0.00335

D140 -3.13592 0.00003 -0.00050 0.00070 0.00020 -3.13573

D141 3.11854 0.00003 -0.00088 0.00170 0.00082 3.11936

D142 -0.02088 0.00007 -0.00087 0.00203 0.00117 -0.01971

D143 0.17953 -0.00003 -0.00107 -0.00299 -0.00406 0.17547

D144 -2.97872 -0.00002 -0.00134 -0.00212 -0.00346 -2.98218

D145 0.00036 -0.00002 -0.00029 -0.00115 -0.00144 -0.00108

D146 -3.13687 0.00001 -0.00007 -0.00061 -0.00068 -3.13755

D147 3.13809 -0.00007 -0.00045 -0.00224 -0.00269 3.13539

D148 0.00086 -0.00004 -0.00023 -0.00170 -0.00193 -0.00107

D149 -3.10051 -0.00001 -0.00070 0.00010 -0.00059 -3.10111

D150 0.04500 0.00004 -0.00053 0.00121 0.00068 0.04568

D151 -0.00017 0.00001 0.00004 0.00021 0.00025 0.00008

D152 -3.13733 0.00003 0.00022 0.00059 0.00081 -3.13652

D153 3.13715 -0.00001 -0.00018 -0.00033 -0.00050 3.13665

D154 -0.00001 0.00000 0.00001 0.00006 0.00006 0.00005

D155 -0.00027 0.00001 0.00027 0.00104 0.00131 0.00104

D156 -3.13811 0.00008 0.00047 0.00232 0.00279 -3.13532

D157 3.13680 -0.00001 0.00008 0.00065 0.00073 3.13753

D158 -0.00104 0.00006 0.00028 0.00193 0.00221 0.00117

D159 3.10029 0.00004 0.00077 0.00044 0.00121 3.10150

D160 -0.04511 -0.00003 0.00057 -0.00087 -0.00030 -0.04540

D161 -0.00335 -0.00001 0.00048 -0.00048 0.00000 -0.00335

D162 -3.14052 0.00000 0.00055 -0.00044 0.00011 -3.14041

D163 3.13593 -0.00004 0.00046 -0.00083 -0.00036 3.13557

D164 -0.00123 -0.00003 0.00053 -0.00079 -0.00026 -0.00149

D165 3.11307 0.00003 -0.00193 -0.00022 -0.00215 3.11092

D166 -0.02620 0.00007 -0.00192 0.00014 -0.00178 -0.02797

D167 -0.00013 0.00001 0.00003 0.00008 0.00010 -0.00003

D168 -3.13724 0.00001 0.00006 0.00003 0.00009 -3.13714

D169 3.13714 0.00000 -0.00004 0.00004 0.00000 3.13714

D170 0.00003 0.00000 0.00000 -0.00001 -0.00001 0.00002

D171 0.00342 0.00000 -0.00049 0.00044 -0.00006 0.00337

D172 -3.13590 0.00004 -0.00046 0.00079 0.00032 -3.13558

D173 3.14043 0.00000 -0.00053 0.00049 -0.00005 3.14038

D174 0.00110 0.00004 -0.00050 0.00083 0.00033 0.00144

D175 -3.11364 -0.00002 0.00198 0.00018 0.00216 -3.11148

D176 0.02567 -0.00006 0.00195 -0.00017 0.00178 0.02744

D177 -0.00027 0.00001 0.00026 0.00108 0.00134 0.00106

D178 3.13689 -0.00001 0.00009 0.00057 0.00066 3.13755

D179 -3.13793 0.00006 0.00037 0.00218 0.00255 -3.13538

D180 -0.00077 0.00004 0.00019 0.00167 0.00187 0.00110

D181 3.10066 0.00002 0.00067 0.00007 0.00074 3.10140

D182 -0.04492 -0.00003 0.00056 -0.00105 -0.00049 -0.04541

D183 0.00020 -0.00001 -0.00004 -0.00018 -0.00022 -0.00001

D184 3.13730 -0.00002 -0.00018 -0.00051 -0.00068 3.13662

D185 -3.13705 0.00001 0.00013 0.00032 0.00045 -3.13660

D186 0.00005 0.00000 -0.00001 -0.00001 -0.00002 0.00003

D187 0.00015 -0.00001 -0.00024 -0.00098 -0.00121 -0.00106

D188 3.13798 -0.00007 -0.00039 -0.00222 -0.00261 3.13538

D189 -3.13686 0.00001 -0.00010 -0.00064 -0.00074 -3.13759

D190 0.00097 -0.00005 -0.00024 -0.00189 -0.00213 -0.00116

D191 -3.10009 -0.00004 -0.00074 -0.00028 -0.00102 -3.10111

D192 0.04532 0.00003 -0.00059 0.00098 0.00039 0.04572

D193 -0.00350 0.00000 0.00050 -0.00031 0.00020 -0.00330

D194 -3.14049 0.00000 0.00054 -0.00049 0.00004 -3.14045

D195 3.13576 -0.00003 0.00047 -0.00046 0.00001 3.13577

D196 -0.00123 -0.00003 0.00051 -0.00065 -0.00014 -0.00138

D197 3.11350 0.00002 -0.00198 -0.00029 -0.00227 3.11123

D198 -0.02574 0.00005 -0.00195 -0.00013 -0.00208 -0.02782

D199 0.00008 0.00000 -0.00003 -0.00001 -0.00004 0.00004

D200 -3.13712 0.00000 0.00003 -0.00011 -0.00008 -3.13720

D201 3.13718 0.00000 -0.00006 0.00017 0.00011 3.13729

D202 -0.00002 0.00000 0.00000 0.00007 0.00007 0.00005

D203 0.00342 0.00000 -0.00049 0.00034 -0.00015 0.00327

D204 -3.13587 0.00004 -0.00048 0.00058 0.00011 -3.13577

D205 3.14052 0.00000 -0.00055 0.00044 -0.00011 3.14041

D206 0.00123 0.00003 -0.00054 0.00069 0.00015 0.00137

D207 -3.11337 -0.00004 0.00193 -0.00012 0.00181 -3.11156

D208 0.02591 -0.00007 0.00192 -0.00037 0.00155 0.02746

D209 1.05826 0.00000 -0.00243 -0.00482 -0.00726 1.05100

D210 -1.08258 -0.00008 -0.00232 -0.00543 -0.00775 -1.09033

D211 3.12865 -0.00003 -0.00231 -0.00495 -0.00726 3.12138

D212 1.08257 0.00007 0.00230 0.00516 0.00746 1.09003

D213 -1.05827 0.00000 0.00241 0.00460 0.00701 -1.05126

D214 -3.12866 0.00003 0.00230 0.00473 0.00703 -3.12163

D215 1.09278 -0.00001 -0.00038 -0.00045 -0.00083 1.09196

D216 -1.05160 0.00001 -0.00023 -0.00045 -0.00068 -1.05228

D217 -3.12083 0.00000 -0.00032 -0.00041 -0.00073 -3.12156

D218 1.05130 -0.00001 0.00023 0.00049 0.00072 1.05202

D219 -1.09300 0.00001 0.00038 0.00051 0.00088 -1.09212

D220 3.12055 0.00001 0.00032 0.00048 0.00080 3.12136

D221 1.08242 0.00008 0.00233 0.00536 0.00770 1.09012

D222 -1.05838 0.00000 0.00244 0.00479 0.00723 -1.05115

D223 -3.12876 0.00003 0.00232 0.00493 0.00725 -3.12151

D224 1.05822 0.00000 -0.00242 -0.00478 -0.00720 1.05102

D225 -1.08264 -0.00008 -0.00231 -0.00537 -0.00768 -1.09032

D226 3.12861 -0.00003 -0.00231 -0.00491 -0.00722 3.12140

D227 1.09302 -0.00001 -0.00039 -0.00067 -0.00107 1.09196

D228 -1.05130 0.00000 -0.00025 -0.00073 -0.00098 -1.05227

D229 -3.12054 -0.00002 -0.00034 -0.00069 -0.00103 -3.12157

D230 1.05129 -0.00001 0.00023 0.00041 0.00064 1.05193

D231 -1.09303 0.00001 0.00038 0.00043 0.00081 -1.09221

D232 3.12055 0.00001 0.00032 0.00038 0.00070 3.12125

Item Value Threshold Converged?

Maximum Force 0.000216 0.000450 YES

RMS Force 0.000051 0.000300 YES

Maximum Displacement 0.029430 0.001800 NO

RMS Displacement 0.006532 0.001200 NO

Predicted change in Energy=-1.016755D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 03:06:04 2019, MaxMem= 1342177280 cpu: 14.7

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=3 Diff= 5.94D-04

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 -1.118695 2.802408 -0.021770

2 7 0 0.003621 2.037746 -0.175045

3 6 0 1.128720 2.798300 -0.021968

4 6 0 0.720869 4.163064 0.247509

5 6 0 -0.705740 4.165736 0.247518

6 7 0 2.413944 2.378674 -0.117938

7 6 0 2.799563 1.125125 -0.192126

8 7 0 2.018864 -0.003770 -0.135271

9 6 0 2.795594 -1.135382 -0.192094

10 6 0 4.207012 -0.712406 -0.318536

11 6 0 4.209438 0.697328 -0.318498

12 7 0 -2.405437 2.387352 -0.117465

13 6 0 -4.207079 0.712361 -0.318135

14 6 0 -4.209628 -0.697379 -0.318409

15 6 0 -2.799732 -1.125345 -0.192071

16 7 0 -2.018935 0.003500 -0.135173

17 6 0 -2.795612 1.135189 -0.191811

18 7 0 -2.414048 -2.378922 -0.118099

19 7 0 -0.003796 -2.037902 -0.175369

20 6 0 -1.128827 -2.798564 -0.022385

21 6 0 -0.720815 -4.163323 0.247164

22 6 0 0.705787 -4.165843 0.247287

23 6 0 1.118609 -2.802535 -0.022199

24 7 0 2.405380 -2.387520 -0.117829

25 30 0 0.000074 0.000061 -0.371886

26 6 0 -5.398962 1.441116 -0.410230

27 6 0 -6.594407 0.707502 -0.501467

28 6 0 -6.596900 -0.683901 -0.501865

29 6 0 -5.404099 -1.421852 -0.410960

30 6 0 1.424597 -5.349879 0.505209

31 6 0 0.688608 -6.512901 0.754735

32 6 0 -0.712093 -6.510432 0.754577

33 6 0 -1.443886 -5.344792 0.504910

34 6 0 5.403785 1.421991 -0.410742

35 6 0 6.596682 0.684218 -0.501809

36 6 0 6.594339 -0.707192 -0.501882

37 6 0 5.398974 -1.440990 -0.410875

38 6 0 -1.424396 5.349962 0.504976

39 6 0 -0.688263 6.512947 0.754303

40 6 0 0.712441 6.510281 0.754340

41 6 0 1.444092 5.344488 0.505003

42 1 0 7.548038 1.193332 -0.579027

43 1 0 7.544002 -1.219481 -0.579124

44 1 0 1.221942 7.442366 0.958419

45 1 0 -1.194233 7.446965 0.958309

46 1 0 -7.544002 1.219935 -0.578579

47 1 0 -7.548313 -1.192876 -0.579320

48 1 0 -1.221479 -7.442527 0.958883

49 1 0 1.194691 -7.446772 0.959133

50 8 0 2.793413 5.284969 0.499509

51 8 0 -2.773936 5.295746 0.499445

52 8 0 5.346656 2.769926 -0.413106

53 8 0 5.337465 -2.788716 -0.413396

54 8 0 2.774134 -5.295432 0.500072

55 8 0 -2.793208 -5.285481 0.499436

56 8 0 -5.347275 -2.769792 -0.413860

57 8 0 -5.337333 2.788836 -0.412278

58 6 0 3.524222 6.472156 0.796811

59 1 0 3.288626 6.845759 1.797753

60 1 0 3.332851 7.257804 0.059867

61 1 0 4.573874 6.187226 0.755596

62 6 0 6.568729 3.504243 -0.456983

63 1 0 7.124129 3.306818 -1.378509

64 1 0 7.201119 3.280285 0.407247

65 1 0 6.278116 4.552726 -0.429428

66 6 0 6.557218 -3.526905 -0.457003

67 1 0 7.190153 -3.304822 0.407310

68 1 0 7.113385 -3.331241 -1.378443

69 1 0 6.263361 -4.574478 -0.429436

70 6 0 -3.500079 6.485715 0.797123

71 1 0 -3.305353 7.270921 0.060600

72 1 0 -3.263201 6.857888 1.798293

73 1 0 -4.550867 6.205047 0.755568

74 6 0 -6.557027 3.527135 -0.455635

75 1 0 -7.190015 3.304720 0.408552

76 1 0 -7.113165 3.331916 -1.377188

77 1 0 -6.263093 4.574675 -0.427591

78 6 0 -6.569520 -3.503791 -0.458173

79 1 0 -7.124754 -3.305852 -1.379692

80 1 0 -7.201975 -3.280038 0.406062

81 1 0 -6.279174 -4.552355 -0.431021

82 6 0 -3.523821 -6.472700 0.797092

83 1 0 -3.288157 -6.845978 1.798139

84 1 0 -3.332337 -7.258533 0.060374

85 1 0 -4.573520 -6.187957 0.755813

86 6 0 3.500356 -6.485139 0.798600

87 1 0 3.306065 -7.270734 0.062376

88 1 0 3.263111 -6.856878 1.799847

89 1 0 4.551117 -6.204326 0.757360

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0447786 0.0439532 0.0225315

Leave Link 202 at Sat Jul 6 03:06:05 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8042.3075542528 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= 89 NActive= 89 NUniq= 89 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= -0.2279659791 Hartrees.

Nuclear repulsion after empirical dispersion term = 8042.0795882737 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6386

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.90D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 373

GePol: Fraction of low-weight points (<1% of avg) = 5.84%

GePol: Cavity surface area = 703.294 Ang\*\*2

GePol: Cavity volume = 801.503 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0090003684 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8042.0705879053 Hartrees.

Leave Link 301 at Sat Jul 6 03:06:05 2019, MaxMem= 1342177280 cpu: 1.3

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44309 LenP2D= 111298.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.56D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 03:06:08 2019, MaxMem= 1342177280 cpu: 42.7

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 03:06:09 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000008 0.000004 0.000210 Ang= 0.02 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>= 2.0171 S= 1.0057

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2650.02679962966

Leave Link 401 at Sat Jul 6 03:06:27 2019, MaxMem= 1342177280 cpu: 209.3

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 122342988.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.99D-15 for 1040.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.97D-15 for 4004 531.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.55D-15 for 6379.

Iteration 1 A^-1\*A deviation from orthogonality is 1.99D-09 for 1761 1732.

Iteration 2 A\*A^-1 deviation from unit magnitude is 1.24D-14 for 2086.

Iteration 2 A\*A^-1 deviation from orthogonality is 9.61D-15 for 2544 481.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.55D-15 for 1552.

Iteration 2 A^-1\*A deviation from orthogonality is 5.41D-16 for 4710 1551.

E= -2649.79524350857

DIIS: error= 4.22D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79524350857 IErMin= 1 ErrMin= 4.22D-04

ErrMax= 4.22D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.79D-04 BMatP= 5.79D-04

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.22D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.685 Goal= None Shift= 0.000

Gap= 0.744 Goal= None Shift= 0.000

RMSDP=1.69D-05 MaxDP=8.46D-04 OVMax= 2.08D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.69D-05 CP: 1.00D+00

E= -2649.79551146767 Delta-E= -0.000267959094 Rises=F Damp=F

DIIS: error= 4.61D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79551146767 IErMin= 2 ErrMin= 4.61D-05

ErrMax= 4.61D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.73D-06 BMatP= 5.79D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.697D-01 0.107D+01

Coeff: -0.697D-01 0.107D+01

Gap= 0.045 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.11D-06 MaxDP=8.10D-05 DE=-2.68D-04 OVMax= 3.37D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.81D-06 CP: 1.00D+00 1.06D+00

E= -2649.79551454509 Delta-E= -0.000003077423 Rises=F Damp=F

DIIS: error= 3.24D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79551454509 IErMin= 3 ErrMin= 3.24D-05

ErrMax= 3.24D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.74D-06 BMatP= 5.73D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.307D-01 0.422D+00 0.609D+00

Coeff: -0.307D-01 0.422D+00 0.609D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=9.67D-07 MaxDP=8.86D-05 DE=-3.08D-06 OVMax= 2.60D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 8.63D-07 CP: 1.00D+00 1.07D+00 7.89D-01

E= -2649.79551468320 Delta-E= -0.000000138107 Rises=F Damp=F

DIIS: error= 2.81D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79551468320 IErMin= 4 ErrMin= 2.81D-05

ErrMax= 2.81D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D-06 BMatP= 1.74D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.698D-02 0.741D-01 0.431D+00 0.501D+00

Coeff: -0.698D-02 0.741D-01 0.431D+00 0.501D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.76D-07 MaxDP=4.43D-05 DE=-1.38D-07 OVMax= 1.27D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.27D-07 CP: 1.00D+00 1.07D+00 9.00D-01 5.84D-01

E= -2649.79551491101 Delta-E= -0.000000227810 Rises=F Damp=F

DIIS: error= 4.68D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79551491101 IErMin= 5 ErrMin= 4.68D-06

ErrMax= 4.68D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.12D-08 BMatP= 1.09D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.421D-03-0.587D-02 0.137D+00 0.221D+00 0.649D+00

Coeff: -0.421D-03-0.587D-02 0.137D+00 0.221D+00 0.649D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.05D-07 MaxDP=4.10D-06 DE=-2.28D-07 OVMax= 2.38D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.70D-08 CP: 1.00D+00 1.07D+00 9.12D-01 6.42D-01 7.43D-01

E= -2649.79551491646 Delta-E= -0.000000005450 Rises=F Damp=F

DIIS: error= 2.83D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79551491646 IErMin= 6 ErrMin= 2.83D-06

ErrMax= 2.83D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.71D-09 BMatP= 3.12D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.538D-03-0.122D-01 0.304D-01 0.714D-01 0.374D+00 0.536D+00

Coeff: 0.538D-03-0.122D-01 0.304D-01 0.714D-01 0.374D+00 0.536D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=3.63D-08 MaxDP=2.09D-06 DE=-5.45D-09 OVMax= 1.22D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.49D-08 CP: 1.00D+00 1.07D+00 9.16D-01 6.41D-01 7.86D-01

CP: 6.49D-01

E= -2649.79551491763 Delta-E= -0.000000001171 Rises=F Damp=F

DIIS: error= 4.34D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79551491763 IErMin= 7 ErrMin= 4.34D-07

ErrMax= 4.34D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.21D-10 BMatP= 6.71D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.281D-03-0.554D-02 0.706D-02 0.222D-01 0.143D+00 0.260D+00

Coeff-Com: 0.572D+00

Coeff: 0.281D-03-0.554D-02 0.706D-02 0.222D-01 0.143D+00 0.260D+00

Coeff: 0.572D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.23D-08 MaxDP=8.86D-07 DE=-1.17D-09 OVMax= 4.80D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.13D-08 CP: 1.00D+00 1.07D+00 9.17D-01 6.42D-01 7.92D-01

CP: 7.01D-01 9.03D-01

E= -2649.79551491753 Delta-E= 0.000000000098 Rises=F Damp=F

DIIS: error= 1.97D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 7 EnMin= -2649.79551491763 IErMin= 8 ErrMin= 1.97D-07

ErrMax= 1.97D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.87D-11 BMatP= 3.21D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.285D-04-0.107D-03-0.396D-02-0.572D-02-0.123D-01 0.183D-01

Coeff-Com: 0.367D+00 0.637D+00

Coeff: 0.285D-04-0.107D-03-0.396D-02-0.572D-02-0.123D-01 0.183D-01

Coeff: 0.367D+00 0.637D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=7.28D-09 MaxDP=4.28D-07 DE= 9.82D-11 OVMax= 5.27D-06

Error on total polarization charges = 0.07299

SCF Done: E(UB3LYP) = -2649.79551492 A.U. after 8 cycles

NFock= 8 Conv=0.73D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0171 S= 1.0057

<L.S>= 0.000000000000E+00

KE= 2.690148735824D+03 PE=-2.236285432152D+04 EE= 8.980839482873D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.65

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0171, after 2.0002

Leave Link 502 at Sat Jul 6 03:13:32 2019, MaxMem= 1342177280 cpu: 4994.8

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44309 LenP2D= 111298.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 274

Leave Link 701 at Sat Jul 6 03:13:52 2019, MaxMem= 1342177280 cpu: 225.2

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 03:13:52 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 03:15:31 2019, MaxMem= 1342177280 cpu: 1187.7

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 7.34138544D-04 1.56846481D-03 2.33106682D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000038619 0.000013477 -0.000111134

2 7 0.000050664 0.000149976 0.000097397

3 6 -0.000045421 -0.000002646 -0.000095890

4 6 -0.000086444 0.000013269 0.000091601

5 6 0.000066515 0.000005988 0.000108688

6 7 -0.000003536 -0.000045024 0.000097385

7 6 0.000061348 0.000083642 -0.000210680

8 7 0.000005993 0.000009953 0.000271309

9 6 0.000041956 -0.000083020 -0.000236495

10 6 0.000036905 -0.000006924 0.000076832

11 6 0.000028501 -0.000012936 0.000071142

12 7 -0.000024463 -0.000055728 0.000116696

13 6 -0.000026019 -0.000002144 0.000071378

14 6 -0.000027630 -0.000012933 0.000076658

15 6 -0.000038022 -0.000080254 -0.000237934

16 7 -0.000001750 0.000017627 0.000267512

17 6 -0.000046570 0.000078983 -0.000219647

18 7 -0.000046450 0.000060269 0.000086113

19 7 -0.000003371 -0.000145141 0.000073412

20 6 0.000072473 0.000006892 -0.000058831

21 6 0.000065836 -0.000009149 0.000091989

22 6 -0.000073584 -0.000001675 0.000094814

23 6 -0.000049749 -0.000001004 -0.000073257

24 7 0.000022612 0.000054474 0.000100953

25 30 -0.000041395 -0.000041071 -0.000286603

26 6 0.000002652 -0.000091384 0.000019041

27 6 0.000016959 0.000021385 -0.000034650

28 6 0.000019530 -0.000021599 -0.000030037

29 6 0.000003649 0.000092680 0.000012029

30 6 -0.000048880 -0.000024750 -0.000129468

31 6 -0.000000919 -0.000000068 0.000030208

32 6 -0.000003384 0.000002964 0.000030946

33 6 0.000049332 -0.000025664 -0.000133795

34 6 -0.000000886 -0.000082342 0.000014493

35 6 -0.000017912 0.000025640 -0.000031165

36 6 -0.000020979 -0.000025851 -0.000032229

37 6 0.000000836 0.000093220 0.000017040

38 6 0.000048810 0.000026558 -0.000133371

39 6 0.000000238 -0.000002473 0.000029636

40 6 0.000003934 -0.000000387 0.000029589

41 6 -0.000041980 0.000025184 -0.000137240

42 1 -0.000000758 -0.000023825 0.000008075

43 1 -0.000001058 0.000024278 0.000008871

44 1 -0.000014971 -0.000001689 -0.000029254

45 1 0.000012901 -0.000004377 -0.000030058

46 1 0.000000326 -0.000025327 0.000009343

47 1 0.000004121 0.000025908 0.000009013

48 1 0.000013701 0.000001835 -0.000030329

49 1 -0.000014290 0.000003704 -0.000031079

50 8 -0.000016959 -0.000050725 0.000080212

51 8 0.000004772 -0.000059989 0.000068937

52 8 -0.000006199 0.000020147 -0.000023528

53 8 -0.000023632 -0.000025666 -0.000026166

54 8 -0.000010230 0.000057399 0.000063973

55 8 0.000004871 0.000058443 0.000077441

56 8 0.000029411 -0.000031374 -0.000017797

57 8 0.000030998 0.000030351 -0.000032972

58 6 -0.000022430 0.000123709 0.000038473

59 1 0.000057148 -0.000043158 -0.000020404

60 1 0.000011955 -0.000043010 -0.000025648

61 1 0.000001772 -0.000006669 0.000001330

62 6 0.000054484 0.000036927 0.000028357

63 1 -0.000016796 0.000014291 0.000008150

64 1 -0.000011068 -0.000004845 -0.000005696

65 1 0.000000824 -0.000002484 0.000000398

66 6 0.000058196 -0.000042001 0.000030661

67 1 -0.000013594 0.000007689 -0.000006359

68 1 -0.000016453 -0.000016246 0.000008309

69 1 0.000000692 0.000001451 0.000001913

70 6 0.000013536 0.000127969 0.000034252

71 1 -0.000007946 -0.000044019 -0.000020347

72 1 -0.000055297 -0.000043428 -0.000019599

73 1 -0.000002551 -0.000007712 0.000005227

74 6 -0.000057429 0.000042703 0.000032393

75 1 0.000011717 -0.000005488 -0.000006306

76 1 0.000017529 0.000015304 0.000008817

77 1 -0.000000090 -0.000002224 -0.000000581

78 6 -0.000058509 -0.000040115 0.000024505

79 1 0.000017289 -0.000016141 0.000009631

80 1 0.000014281 0.000005421 -0.000005291

81 1 0.000000518 -0.000000319 0.000002486

82 6 0.000018134 -0.000125599 0.000036129

83 1 -0.000055633 0.000043870 -0.000020430

84 1 -0.000011138 0.000043438 -0.000024793

85 1 -0.000002864 0.000008112 0.000000573

86 6 -0.000014564 -0.000130652 0.000034041

87 1 0.000009502 0.000043877 -0.000021753

88 1 0.000055752 0.000043394 -0.000020199

89 1 0.000002013 0.000008845 0.000002645

-------------------------------------------------------------------

Cartesian Forces: Max 0.000286603 RMS 0.000061909

Leave Link 716 at Sat Jul 6 03:15:31 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000130262 RMS 0.000032924

Search for a local minimum.

Step number 22 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .32924D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 6 5 7 9 11

14 13 16 17 18

19 20 21 22

DE= -7.93D-06 DEPred=-1.02D-05 R= 7.80D-01

TightC=F SS= 1.41D+00 RLast= 3.80D-02 DXNew= 3.9497D-01 1.1402D-01

Trust test= 7.80D-01 RLast= 3.80D-02 DXMaxT set to 2.35D-01

ITU= 1 1 1 1 1 0 0 -1 -1 0 -1 0 0 0 0 0 0 1 1 1

ITU= 1 0

Eigenvalues --- 0.00196 0.01176 0.01315 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01342 0.01349

Eigenvalues --- 0.01507 0.01570 0.01582 0.01585 0.01598

Eigenvalues --- 0.01619 0.01654 0.01706 0.01708 0.01712

Eigenvalues --- 0.01714 0.01716 0.01826 0.01835 0.01869

Eigenvalues --- 0.01872 0.01919 0.01919 0.01943 0.01949

Eigenvalues --- 0.01990 0.01995 0.02020 0.02022 0.02029

Eigenvalues --- 0.02052 0.02053 0.02053 0.02053 0.02056

Eigenvalues --- 0.02057 0.02057 0.02057 0.02057 0.02062

Eigenvalues --- 0.02067 0.02067 0.02069 0.02070 0.02070

Eigenvalues --- 0.02071 0.02079 0.02083 0.02087 0.02119

Eigenvalues --- 0.02168 0.02227 0.02260 0.02260 0.02260

Eigenvalues --- 0.02260 0.02261 0.02261 0.02340 0.02352

Eigenvalues --- 0.02355 0.02381 0.02648 0.03500 0.05479

Eigenvalues --- 0.09963 0.09978 0.09979 0.09983 0.09986

Eigenvalues --- 0.09987 0.09988 0.10168 0.10635 0.10643

Eigenvalues --- 0.10643 0.10644 0.10657 0.10657 0.10657

Eigenvalues --- 0.10668 0.12534 0.13278 0.13466 0.15238

Eigenvalues --- 0.15854 0.15991 0.15996 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16002 0.16009 0.16030 0.16061

Eigenvalues --- 0.16552 0.17044 0.20716 0.21659 0.21775

Eigenvalues --- 0.22474 0.22476 0.22476 0.22483 0.24244

Eigenvalues --- 0.24275 0.24507 0.24515 0.24525 0.24560

Eigenvalues --- 0.24689 0.24772 0.24818 0.24893 0.24906

Eigenvalues --- 0.24925 0.24976 0.24977 0.24990 0.24991

Eigenvalues --- 0.24996 0.24997 0.24997 0.24998 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25014

Eigenvalues --- 0.25093 0.25131 0.25917 0.28329 0.30856

Eigenvalues --- 0.33037 0.33640 0.33679 0.33720 0.33857

Eigenvalues --- 0.34029 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34064 0.34065 0.34077 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34082

Eigenvalues --- 0.34340 0.34591 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34687 0.34689 0.34915

Eigenvalues --- 0.34968 0.35098 0.35608 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35635 0.35832

Eigenvalues --- 0.36791 0.37035 0.37134 0.37476 0.40508

Eigenvalues --- 0.41215 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41217 0.41267 0.41409 0.41414 0.41418

Eigenvalues --- 0.41426 0.41475 0.41966 0.42169 0.42471

Eigenvalues --- 0.43219 0.44474 0.44561 0.44696 0.44756

Eigenvalues --- 0.44876 0.44998 0.45002 0.45003 0.45004

Eigenvalues --- 0.45365 0.45366 0.45395 0.45994 0.46521

Eigenvalues --- 0.46941 0.47276 0.49256 0.49316 0.49399

Eigenvalues --- 0.49850 0.50723 0.53554 0.53554 0.53554

Eigenvalues --- 0.53554 0.53555 0.53649 0.54322 0.55001

Eigenvalues --- 0.56032 0.56076 0.57414 0.57560 0.57752

Eigenvalues --- 0.64393

En-DIIS/RFO-DIIS IScMMF= 0 using points: 22 21 20 19 18

RFO step: Lambda=-1.56677073D-06.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 4.08D-05 SmlDif= 1.00D-05

RMS Error= 0.1169233858D-03 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.98981 0.13912 -0.32574 0.12115 0.07567

Iteration 1 RMS(Cart)= 0.00742677 RMS(Int)= 0.00000651

Iteration 2 RMS(Cart)= 0.00001394 RMS(Int)= 0.00000140

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000140

ITry= 1 IFail=0 DXMaxC= 3.38D-02 DCOld= 1.00D+10 DXMaxT= 2.35D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58264 -0.00001 -0.00009 0.00007 -0.00002 2.58261

R2 2.73959 0.00000 -0.00008 0.00013 0.00005 2.73964

R3 2.56135 0.00005 0.00011 -0.00004 0.00008 2.56143

R4 2.58259 -0.00004 -0.00008 0.00005 -0.00004 2.58255

R5 3.86860 0.00010 0.00051 -0.00019 0.00031 3.86891

R6 2.73948 0.00004 -0.00013 0.00033 0.00020 2.73968

R7 2.56133 0.00006 0.00011 0.00012 0.00023 2.56156

R8 2.69591 -0.00008 -0.00008 -0.00022 -0.00030 2.69561

R9 2.66252 -0.00002 -0.00009 0.00005 -0.00005 2.66247

R10 2.66253 -0.00003 -0.00009 0.00001 -0.00007 2.66246

R11 2.48238 0.00003 -0.00016 0.00050 0.00034 2.48272

R12 2.59597 0.00007 0.00004 0.00017 0.00022 2.59619

R13 2.79445 0.00004 -0.00005 0.00010 0.00005 2.79450

R14 2.59594 0.00006 0.00004 0.00008 0.00012 2.59606

R15 3.84108 0.00008 0.00019 -0.00028 -0.00010 3.84098

R16 2.79462 0.00001 0.00002 -0.00011 -0.00009 2.79453

R17 2.48241 0.00000 -0.00013 0.00027 0.00015 2.48255

R18 2.66402 0.00002 0.00002 -0.00001 0.00001 2.66403

R19 2.64571 -0.00002 -0.00006 0.00003 -0.00003 2.64568

R20 2.64569 0.00000 -0.00008 0.00012 0.00004 2.64573

R21 2.48244 -0.00001 -0.00013 0.00029 0.00016 2.48260

R22 2.66403 0.00001 0.00003 -0.00011 -0.00007 2.66395

R23 2.79461 0.00001 -0.00003 -0.00003 -0.00006 2.79455

R24 2.64572 -0.00003 -0.00006 0.00002 -0.00004 2.64568

R25 2.79457 -0.00001 0.00004 -0.00023 -0.00018 2.79439

R26 2.64574 -0.00004 -0.00004 -0.00003 -0.00007 2.64568

R27 2.59600 0.00005 0.00008 0.00008 0.00016 2.59616

R28 2.48244 -0.00003 -0.00010 0.00008 -0.00001 2.48243

R29 2.59599 0.00004 0.00008 0.00012 0.00020 2.59619

R30 3.84151 0.00006 0.00018 -0.00047 -0.00030 3.84122

R31 2.56130 0.00006 0.00013 -0.00017 -0.00004 2.56126

R32 2.58258 -0.00005 -0.00006 0.00000 -0.00006 2.58252

R33 2.58272 -0.00004 -0.00005 0.00007 0.00002 2.58274

R34 3.86906 0.00007 0.00046 -0.00031 0.00014 3.86920

R35 2.73958 0.00000 -0.00007 0.00009 0.00003 2.73961

R36 2.69589 -0.00008 -0.00007 -0.00029 -0.00036 2.69554

R37 2.66252 -0.00003 -0.00007 -0.00001 -0.00008 2.66244

R38 2.73955 0.00002 -0.00011 0.00022 0.00011 2.73967

R39 2.66254 -0.00003 -0.00008 0.00001 -0.00007 2.66246

R40 2.56137 0.00006 0.00013 -0.00001 0.00012 2.56149

R41 2.65613 -0.00001 -0.00001 -0.00007 -0.00008 2.65605

R42 2.54949 0.00008 0.00000 0.00004 0.00005 2.54953

R43 2.62937 0.00000 0.00000 -0.00005 -0.00005 2.62932

R44 2.04428 -0.00001 -0.00001 -0.00002 -0.00003 2.04426

R45 2.65613 -0.00002 0.00000 -0.00009 -0.00009 2.65604

R46 2.04426 -0.00002 -0.00001 -0.00004 -0.00004 2.04422

R47 2.54950 0.00008 -0.00001 0.00008 0.00007 2.54957

R48 2.64330 0.00001 -0.00001 -0.00002 -0.00004 2.64326

R49 2.55235 0.00004 -0.00003 -0.00003 -0.00006 2.55228

R50 2.64694 0.00001 0.00004 -0.00002 0.00002 2.64696

R51 2.04406 -0.00002 0.00000 -0.00001 -0.00001 2.04405

R52 2.64330 0.00000 -0.00001 -0.00005 -0.00006 2.64324

R53 2.04407 -0.00001 0.00000 -0.00001 -0.00001 2.04406

R54 2.55233 0.00005 -0.00004 -0.00001 -0.00005 2.55228

R55 2.65613 -0.00002 0.00000 -0.00010 -0.00010 2.65602

R56 2.54952 0.00006 0.00002 -0.00001 0.00001 2.54952

R57 2.62939 -0.00001 0.00001 -0.00009 -0.00008 2.62931

R58 2.04426 -0.00001 -0.00001 -0.00001 -0.00002 2.04424

R59 2.65615 -0.00002 0.00001 -0.00013 -0.00012 2.65603

R60 2.04428 -0.00001 -0.00001 -0.00002 -0.00003 2.04426

R61 2.54949 0.00007 0.00000 0.00004 0.00004 2.54953

R62 2.64331 0.00000 0.00000 -0.00007 -0.00007 2.64325

R63 2.55234 0.00005 -0.00003 -0.00003 -0.00006 2.55228

R64 2.64695 0.00000 0.00005 -0.00005 0.00000 2.64696

R65 2.04406 -0.00002 0.00000 -0.00001 -0.00001 2.04406

R66 2.64329 0.00001 0.00000 -0.00005 -0.00005 2.64324

R67 2.04407 -0.00001 0.00000 0.00000 0.00000 2.04407

R68 2.55235 0.00003 -0.00002 -0.00008 -0.00010 2.55225

R69 2.69369 0.00005 0.00004 0.00002 0.00007 2.69376

R70 2.69372 0.00005 0.00004 0.00004 0.00008 2.69380

R71 2.69550 0.00005 0.00002 0.00005 0.00007 2.69557

R72 2.69551 0.00005 0.00002 0.00007 0.00009 2.69559

R73 2.69372 0.00005 0.00004 0.00004 0.00008 2.69380

R74 2.69369 0.00005 0.00004 0.00003 0.00007 2.69377

R75 2.69550 0.00005 0.00002 0.00007 0.00009 2.69558

R76 2.69551 0.00005 0.00002 0.00007 0.00008 2.69559

R77 2.06748 -0.00005 -0.00003 -0.00015 -0.00018 2.06730

R78 2.06746 -0.00002 0.00000 -0.00005 -0.00005 2.06741

R79 2.05681 0.00000 -0.00001 -0.00002 -0.00003 2.05678

R80 2.06721 -0.00002 -0.00002 -0.00006 -0.00008 2.06712

R81 2.06747 -0.00001 -0.00002 -0.00005 -0.00006 2.06741

R82 2.05671 0.00000 -0.00002 -0.00003 -0.00005 2.05666

R83 2.06747 -0.00001 -0.00002 -0.00005 -0.00007 2.06740

R84 2.06721 -0.00002 -0.00002 -0.00007 -0.00008 2.06712

R85 2.05670 0.00000 -0.00002 -0.00003 -0.00005 2.05665

R86 2.06745 -0.00002 0.00000 -0.00006 -0.00007 2.06738

R87 2.06747 -0.00004 -0.00003 -0.00015 -0.00017 2.06730

R88 2.05681 0.00000 -0.00001 -0.00002 -0.00003 2.05679

R89 2.06747 -0.00001 -0.00002 -0.00005 -0.00007 2.06740

R90 2.06721 -0.00002 -0.00002 -0.00007 -0.00009 2.06712

R91 2.05670 0.00000 -0.00002 -0.00003 -0.00005 2.05665

R92 2.06721 -0.00002 -0.00001 -0.00008 -0.00009 2.06712

R93 2.06747 -0.00001 -0.00001 -0.00005 -0.00007 2.06741

R94 2.05670 0.00000 -0.00002 -0.00002 -0.00004 2.05666

R95 2.06748 -0.00005 -0.00003 -0.00015 -0.00018 2.06730

R96 2.06746 -0.00002 0.00000 -0.00005 -0.00006 2.06740

R97 2.05681 0.00000 -0.00001 -0.00002 -0.00003 2.05678

R98 2.06745 -0.00002 0.00000 -0.00006 -0.00006 2.06738

R99 2.06748 -0.00005 -0.00003 -0.00015 -0.00018 2.06730

R100 2.05681 0.00000 -0.00001 -0.00002 -0.00003 2.05678

A1 1.88922 0.00000 -0.00007 -0.00003 -0.00010 1.88913

A2 2.21473 0.00002 0.00001 0.00020 0.00021 2.21494

A3 2.17914 -0.00001 0.00006 -0.00016 -0.00010 2.17904

A4 1.93064 0.00001 0.00007 0.00006 0.00014 1.93077

A5 2.17277 -0.00003 -0.00011 0.00023 0.00013 2.17290

A6 2.17260 0.00002 -0.00014 0.00030 0.00017 2.17277

A7 1.88928 -0.00002 -0.00004 -0.00013 -0.00018 1.88910

A8 2.21481 0.00000 0.00004 0.00007 0.00011 2.21491

A9 2.17901 0.00003 0.00000 0.00008 0.00008 2.17909

A10 1.85783 0.00001 0.00002 0.00007 0.00008 1.85791

A11 2.31715 -0.00001 -0.00005 0.00003 -0.00002 2.31713

A12 2.10800 0.00000 0.00005 -0.00008 -0.00003 2.10797

A13 1.85781 0.00000 0.00002 0.00004 0.00006 1.85787

A14 2.31728 -0.00003 -0.00001 -0.00008 -0.00010 2.31718

A15 2.10789 0.00002 0.00001 0.00007 0.00007 2.10796

A16 2.18682 0.00003 -0.00006 0.00009 0.00004 2.18686

A17 2.23322 -0.00004 0.00005 -0.00008 -0.00003 2.23319

A18 2.16611 0.00006 -0.00007 -0.00002 -0.00008 2.16603

A19 1.88350 -0.00002 0.00001 0.00007 0.00007 1.88357

A20 1.93253 0.00000 0.00000 -0.00019 -0.00019 1.93234

A21 2.16286 0.00001 -0.00009 0.00013 0.00004 2.16290

A22 2.16315 -0.00002 -0.00005 0.00005 0.00000 2.16316

A23 1.88343 0.00000 -0.00002 0.00018 0.00015 1.88359

A24 2.23306 -0.00002 -0.00001 0.00007 0.00006 2.23312

A25 2.16635 0.00002 0.00002 -0.00028 -0.00026 2.16609

A26 1.86257 0.00001 0.00001 0.00000 0.00000 1.86258

A27 2.30413 -0.00002 -0.00001 -0.00003 -0.00004 2.30409

A28 2.11640 0.00001 0.00000 0.00005 0.00005 2.11645

A29 1.86257 0.00001 0.00001 -0.00002 -0.00001 1.86257

A30 2.30397 0.00000 -0.00009 0.00019 0.00010 2.30408

A31 2.11656 -0.00002 0.00007 -0.00016 -0.00009 2.11647

A32 2.18689 0.00003 -0.00005 -0.00003 -0.00008 2.18682

A33 1.86258 0.00001 0.00002 -0.00002 0.00000 1.86258

A34 2.11644 0.00000 0.00005 -0.00008 -0.00002 2.11641

A35 2.30409 -0.00001 -0.00008 0.00011 0.00004 2.30412

A36 1.86257 0.00001 0.00002 -0.00002 -0.00001 1.86256

A37 2.11649 0.00001 -0.00002 0.00009 0.00008 2.11657

A38 2.30404 -0.00002 0.00000 -0.00006 -0.00006 2.30398

A39 1.88348 0.00000 -0.00003 0.00025 0.00022 1.88370

A40 2.16625 0.00001 0.00003 -0.00041 -0.00038 2.16587

A41 2.23311 -0.00001 -0.00001 0.00013 0.00012 2.23324

A42 1.93253 -0.00001 0.00000 -0.00032 -0.00032 1.93221

A43 2.16312 -0.00001 -0.00006 0.00016 0.00010 2.16322

A44 2.16292 0.00001 -0.00010 0.00018 0.00008 2.16300

A45 2.16621 0.00004 -0.00005 -0.00017 -0.00022 2.16599

A46 2.23316 -0.00003 0.00004 -0.00001 0.00004 2.23320

A47 1.88346 -0.00001 0.00000 0.00015 0.00014 1.88361

A48 2.18686 0.00002 -0.00003 -0.00018 -0.00021 2.18666

A49 1.93062 0.00001 0.00008 -0.00007 0.00002 1.93064

A50 2.17283 -0.00001 -0.00012 0.00036 0.00025 2.17308

A51 2.17255 0.00000 -0.00015 0.00031 0.00017 2.17271

A52 2.21475 0.00001 0.00002 0.00016 0.00018 2.21494

A53 2.17909 -0.00001 0.00006 -0.00021 -0.00015 2.17895

A54 1.88925 0.00000 -0.00008 0.00005 -0.00003 1.88922

A55 1.85784 0.00000 0.00003 0.00002 0.00005 1.85789

A56 2.31717 -0.00002 -0.00001 -0.00008 -0.00010 2.31707

A57 2.10796 0.00002 0.00000 0.00009 0.00009 2.10805

A58 1.85780 0.00001 0.00003 0.00004 0.00007 1.85787

A59 2.10793 0.00001 0.00004 -0.00004 0.00000 2.10793

A60 2.31724 -0.00001 -0.00004 0.00001 -0.00003 2.31721

A61 1.88925 -0.00001 -0.00006 -0.00004 -0.00010 1.88914

A62 2.21485 0.00000 0.00005 0.00010 0.00015 2.21499

A63 2.17900 0.00001 0.00001 -0.00005 -0.00004 2.17896

A64 2.18689 0.00003 -0.00004 -0.00002 -0.00006 2.18683

A65 1.55976 -0.00001 -0.00007 0.00001 -0.00005 1.55970

A66 1.55964 0.00000 -0.00007 -0.00004 -0.00011 1.55953

A67 1.55962 0.00000 -0.00006 -0.00005 -0.00010 1.55952

A68 1.55943 0.00000 -0.00006 -0.00019 -0.00025 1.55918

A69 2.04501 -0.00001 -0.00004 0.00000 -0.00004 2.04497

A70 2.07280 -0.00003 -0.00002 -0.00010 -0.00012 2.07269

A71 2.16536 0.00004 0.00007 0.00009 0.00016 2.16551

A72 2.12172 0.00000 0.00001 0.00003 0.00004 2.12176

A73 2.09899 0.00002 0.00001 0.00017 0.00018 2.09917

A74 2.06246 -0.00002 -0.00002 -0.00020 -0.00022 2.06225

A75 2.12173 0.00000 0.00003 0.00000 0.00002 2.12175

A76 2.06246 -0.00002 -0.00003 -0.00018 -0.00020 2.06226

A77 2.09898 0.00002 0.00000 0.00018 0.00018 2.09917

A78 2.04498 -0.00001 -0.00003 -0.00004 -0.00007 2.04491

A79 2.07282 -0.00004 0.00002 -0.00019 -0.00017 2.07265

A80 2.16537 0.00005 0.00001 0.00023 0.00024 2.16561

A81 2.05211 0.00000 -0.00001 0.00002 0.00001 2.05213

A82 2.06597 -0.00007 -0.00007 -0.00020 -0.00027 2.06570

A83 2.16510 0.00008 0.00008 0.00018 0.00026 2.16536

A84 2.12314 -0.00001 -0.00003 0.00000 -0.00003 2.12311

A85 2.10062 0.00001 -0.00005 0.00012 0.00007 2.10069

A86 2.05942 0.00000 0.00007 -0.00011 -0.00004 2.05938

A87 2.12311 -0.00001 -0.00002 -0.00005 -0.00006 2.12305

A88 2.05939 0.00000 0.00007 -0.00010 -0.00003 2.05936

A89 2.10068 0.00002 -0.00005 0.00014 0.00010 2.10078

A90 2.05212 0.00000 0.00001 -0.00001 -0.00001 2.05211

A91 2.06591 -0.00008 -0.00006 -0.00023 -0.00029 2.06562

A92 2.16515 0.00008 0.00005 0.00024 0.00030 2.16545

A93 2.04495 0.00000 -0.00006 0.00006 0.00000 2.04496

A94 2.07274 0.00000 -0.00006 0.00009 0.00002 2.07276

A95 2.16548 0.00001 0.00012 -0.00015 -0.00003 2.16545

A96 2.12171 0.00001 0.00001 0.00004 0.00005 2.12176

A97 2.09899 0.00002 0.00001 0.00015 0.00016 2.09915

A98 2.06247 -0.00002 -0.00002 -0.00019 -0.00021 2.06226

A99 2.12174 0.00000 0.00003 -0.00002 0.00001 2.12175

A100 2.06245 -0.00002 -0.00003 -0.00017 -0.00020 2.06225

A101 2.09899 0.00002 0.00000 0.00019 0.00019 2.09918

A102 2.04501 0.00000 -0.00004 0.00003 -0.00002 2.04499

A103 2.07278 -0.00003 -0.00002 -0.00008 -0.00009 2.07268

A104 2.16539 0.00003 0.00006 0.00005 0.00011 2.16550

A105 2.05212 0.00000 -0.00001 0.00001 0.00001 2.05213

A106 2.06594 -0.00007 -0.00009 -0.00017 -0.00025 2.06569

A107 2.16511 0.00008 0.00009 0.00015 0.00024 2.16536

A108 2.12315 -0.00001 -0.00001 -0.00004 -0.00005 2.12309

A109 2.10062 0.00001 -0.00005 0.00012 0.00007 2.10069

A110 2.05941 0.00000 0.00006 -0.00008 -0.00002 2.05939

A111 2.12310 -0.00001 -0.00002 -0.00001 -0.00004 2.12306

A112 2.05940 0.00000 0.00007 -0.00012 -0.00005 2.05935

A113 2.10068 0.00002 -0.00004 0.00013 0.00009 2.10077

A114 2.05210 0.00000 -0.00002 0.00006 0.00004 2.05214

A115 2.06589 -0.00006 -0.00010 -0.00011 -0.00022 2.06567

A116 2.16519 0.00006 0.00012 0.00005 0.00017 2.16537

A117 2.06535 0.00012 -0.00007 0.00012 0.00005 2.06540

A118 2.06534 0.00012 -0.00009 0.00015 0.00007 2.06541

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A120 2.06923 0.00007 -0.00005 0.00006 0.00000 2.06923

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A122 2.06534 0.00013 -0.00010 0.00022 0.00012 2.06546

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A129 1.90891 -0.00003 -0.00009 -0.00022 -0.00031 1.90860

A130 1.90834 0.00000 0.00007 -0.00024 -0.00018 1.90817

A131 1.94764 0.00000 0.00008 -0.00012 -0.00004 1.94761

A132 1.94501 -0.00001 0.00003 -0.00015 -0.00012 1.94489

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A142 1.90792 -0.00001 0.00000 -0.00004 -0.00005 1.90787

A143 1.94753 -0.00003 -0.00030 0.00006 -0.00025 1.94729

A144 1.94420 0.00003 0.00017 0.00020 0.00036 1.94456

A145 1.84269 -0.00002 -0.00005 -0.00011 -0.00016 1.84253

A146 1.91067 0.00005 0.00020 0.00025 0.00045 1.91112

A147 1.90838 0.00000 0.00006 -0.00018 -0.00012 1.90826

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A149 1.94496 -0.00001 0.00002 -0.00015 -0.00012 1.94483

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D2 3.02116 0.00006 -0.00077 0.00409 0.00332 3.02448

D3 3.13077 0.00003 0.00036 0.00020 0.00056 3.13133

D4 -0.13458 0.00005 -0.00091 0.00524 0.00434 -0.13025

D5 -0.00206 -0.00002 -0.00038 0.00083 0.00045 -0.00161

D6 -3.12095 -0.00005 -0.00153 -0.00010 -0.00164 -3.12258

D7 -3.12987 -0.00002 -0.00024 -0.00030 -0.00054 -3.13041

D8 0.03443 -0.00005 -0.00140 -0.00123 -0.00263 0.03180

D9 0.17555 -0.00003 0.00084 -0.00427 -0.00343 0.17212

D10 -2.98242 -0.00004 0.00068 -0.00293 -0.00225 -2.98467

D11 -0.00323 -0.00004 -0.00042 0.00070 0.00028 -0.00295

D12 -3.13070 -0.00004 -0.00031 -0.00022 -0.00053 -3.13123

D13 -3.02108 -0.00006 0.00084 -0.00434 -0.00350 -3.02458

D14 0.13464 -0.00005 0.00095 -0.00526 -0.00431 0.13033

D15 -2.95505 0.00002 0.00115 -0.00272 -0.00156 -2.95661

D16 -0.04578 -0.00004 0.00021 -0.00291 -0.00270 -0.04848

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D19 0.00182 0.00003 0.00017 -0.00015 0.00002 0.00184

D20 3.12082 0.00005 0.00140 0.00048 0.00188 3.12270

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D22 -0.03454 0.00005 0.00129 0.00138 0.00267 -0.03187

D23 -0.17583 0.00003 -0.00083 0.00406 0.00323 -0.17259

D24 2.98211 0.00004 -0.00070 0.00300 0.00230 2.98441

D25 0.00014 0.00000 0.00012 -0.00040 -0.00028 -0.00014

D26 3.12234 0.00002 0.00111 0.00039 0.00150 3.12384

D27 -3.12214 -0.00003 -0.00092 -0.00095 -0.00187 -3.12401

D28 0.00005 0.00000 0.00007 -0.00016 -0.00009 -0.00004

D29 -3.11965 -0.00004 -0.00189 -0.00042 -0.00232 -3.12197

D30 0.01954 -0.00004 -0.00170 -0.00141 -0.00311 0.01643

D31 -0.00329 -0.00001 -0.00053 0.00029 -0.00024 -0.00352

D32 3.13590 -0.00001 -0.00034 -0.00069 -0.00103 3.13487

D33 3.11947 0.00004 0.00174 0.00092 0.00266 3.12213

D34 -0.01975 0.00005 0.00154 0.00189 0.00343 -0.01632

D35 0.00322 0.00001 0.00045 -0.00012 0.00033 0.00355

D36 -3.13599 0.00001 0.00024 0.00086 0.00110 -3.13489

D37 -0.04998 -0.00001 -0.00017 -0.00080 -0.00097 -0.05095

D38 3.12334 0.00005 0.00025 0.00043 0.00068 3.12402

D39 -3.09738 -0.00002 0.00022 -0.00063 -0.00041 -3.09779

D40 0.27326 0.00001 0.00082 -0.00056 0.00026 0.27351

D41 0.01660 -0.00007 -0.00015 -0.00170 -0.00185 0.01475

D42 -2.89595 -0.00004 0.00045 -0.00163 -0.00118 -2.89713

D43 3.10549 -0.00001 -0.00035 0.00015 -0.00020 3.10528

D44 -0.02211 0.00000 -0.00015 -0.00090 -0.00105 -0.02317

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D50 -0.27332 -0.00001 -0.00078 0.00033 -0.00045 -0.27377

D51 -0.22508 -0.00002 -0.00049 -0.00043 -0.00092 -0.22600

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D63 -3.12947 0.00001 0.00027 -0.00106 -0.00079 -3.13026

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D65 -3.12480 -0.00001 0.00009 -0.00109 -0.00099 -3.12579

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D71 -0.00103 0.00001 -0.00004 0.00022 0.00018 -0.00086

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D79 -3.10551 0.00001 0.00031 0.00015 0.00046 -3.10505

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D83 0.00097 -0.00001 0.00002 -0.00007 -0.00004 0.00093

D84 -3.13579 -0.00002 -0.00035 0.00037 0.00002 -3.13577

D85 -3.12502 0.00000 0.00023 -0.00119 -0.00096 -3.12598

D86 0.02141 -0.00001 -0.00014 -0.00076 -0.00090 0.02051

D87 -0.00999 0.00005 0.00028 0.00075 0.00103 -0.00896

D88 3.10546 -0.00001 -0.00012 -0.00039 -0.00051 3.10495

D89 -3.13768 0.00005 0.00041 -0.00018 0.00023 -3.13745

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D91 -0.00115 0.00001 0.00008 0.00000 0.00008 -0.00106

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D93 3.12487 0.00000 -0.00006 0.00104 0.00098 3.12585

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D99 3.12315 0.00006 0.00033 0.00050 0.00083 3.12398

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D102 -0.01661 0.00007 0.00023 0.00149 0.00172 -0.01489

D103 -0.27322 -0.00001 -0.00085 0.00040 -0.00045 -0.27367

D104 2.89599 0.00004 -0.00047 0.00157 0.00110 2.89709

D105 3.10773 -0.00001 -0.00024 0.00043 0.00019 3.10792

D106 -0.22498 -0.00002 -0.00050 -0.00054 -0.00104 -0.22602

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D108 -3.10780 0.00001 0.00029 -0.00057 -0.00028 -3.10809

D109 -0.17565 0.00002 -0.00081 0.00377 0.00295 -0.17270

D110 2.98185 0.00005 -0.00068 0.00333 0.00265 2.98450

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D112 -0.00304 -0.00005 -0.00054 0.00067 0.00013 -0.00291

D113 0.13451 -0.00005 0.00092 -0.00486 -0.00394 0.13057

D114 -3.02083 -0.00007 0.00081 -0.00449 -0.00367 -3.02450

D115 0.00304 0.00005 0.00046 -0.00034 0.00012 0.00316

D116 3.13076 0.00003 0.00039 0.00009 0.00048 3.13123

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D136 -3.12987 -0.00002 -0.00013 -0.00054 -0.00067 -3.13054

D137 -3.12048 -0.00007 -0.00143 -0.00106 -0.00249 -3.12297

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D143 0.17547 -0.00003 0.00079 -0.00391 -0.00312 0.17235

D144 -2.98218 -0.00005 0.00071 -0.00341 -0.00270 -2.98488

D145 -0.00108 0.00001 0.00005 0.00002 0.00007 -0.00101

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D150 0.04568 0.00003 0.00066 0.00049 0.00115 0.04683

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D209 1.05100 0.00005 0.00150 -0.00210 -0.00060 1.05040

D210 -1.09033 -0.00003 0.00134 -0.00267 -0.00134 -1.09167

D211 3.12138 0.00001 0.00145 -0.00233 -0.00088 3.12050

D212 1.09003 0.00002 -0.00133 0.00253 0.00120 1.09122

D213 -1.05126 -0.00005 -0.00149 0.00202 0.00053 -1.05073

D214 -3.12163 -0.00001 -0.00145 0.00228 0.00083 -3.12080

D215 1.09196 0.00002 0.00031 0.00009 0.00040 1.09236

D216 -1.05228 0.00001 0.00020 0.00030 0.00050 -1.05178

D217 -3.12156 0.00001 0.00027 0.00016 0.00043 -3.12113

D218 1.05202 -0.00001 -0.00022 -0.00044 -0.00067 1.05136

D219 -1.09212 -0.00002 -0.00032 -0.00024 -0.00056 -1.09268

D220 3.12136 -0.00001 -0.00029 -0.00030 -0.00059 3.12076

D221 1.09012 0.00002 -0.00136 0.00262 0.00126 1.09139

D222 -1.05115 -0.00005 -0.00151 0.00207 0.00056 -1.05059

D223 -3.12151 -0.00001 -0.00147 0.00232 0.00085 -3.12066

D224 1.05102 0.00005 0.00150 -0.00207 -0.00057 1.05045

D225 -1.09032 -0.00002 0.00134 -0.00263 -0.00129 -1.09161

D226 3.12140 0.00001 0.00145 -0.00230 -0.00085 3.12055

D227 1.09196 0.00002 0.00033 0.00008 0.00041 1.09237

D228 -1.05227 0.00001 0.00024 0.00024 0.00047 -1.05180

D229 -3.12157 0.00001 0.00030 0.00013 0.00043 -3.12114

D230 1.05193 -0.00001 -0.00022 -0.00029 -0.00051 1.05142

D231 -1.09221 -0.00002 -0.00032 -0.00009 -0.00041 -1.09263

D232 3.12125 -0.00001 -0.00029 -0.00015 -0.00043 3.12082

Item Value Threshold Converged?

Maximum Force 0.000130 0.000450 YES

RMS Force 0.000033 0.000300 YES

Maximum Displacement 0.033811 0.001800 NO

RMS Displacement 0.007425 0.001200 NO

Predicted change in Energy=-3.296329D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 03:15:33 2019, MaxMem= 1342177280 cpu: 13.9

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=0 Diff= 6.40D-04

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 -1.120012 2.802379 -0.021620

2 7 0 0.002741 2.037970 -0.172827

3 6 0 1.127484 2.799410 -0.021723

4 6 0 0.718743 4.164653 0.244536

5 6 0 -0.707711 4.166510 0.244721

6 7 0 2.413062 2.380080 -0.115975

7 6 0 2.799206 1.126474 -0.189661

8 7 0 2.018786 -0.002753 -0.132808

9 6 0 2.796121 -1.134033 -0.189527

10 6 0 4.207572 -0.710566 -0.313374

11 6 0 4.209502 0.699176 -0.313307

12 7 0 -2.406642 2.386462 -0.115645

13 6 0 -4.207442 0.710373 -0.313517

14 6 0 -4.209257 -0.699328 -0.313645

15 6 0 -2.799009 -1.126506 -0.189724

16 7 0 -2.018536 0.002670 -0.132929

17 6 0 -2.796008 1.133938 -0.189674

18 7 0 -2.413050 -2.379994 -0.115775

19 7 0 -0.002903 -2.037671 -0.172569

20 6 0 -1.127591 -2.799133 -0.021322

21 6 0 -0.718958 -4.164326 0.245147

22 6 0 0.707458 -4.166357 0.244846

23 6 0 1.119845 -2.802192 -0.021280

24 7 0 2.406560 -2.386467 -0.115470

25 30 0 0.000195 0.000214 -0.370679

26 6 0 -5.399798 1.438459 -0.404480

27 6 0 -6.594866 0.704157 -0.494477

28 6 0 -6.596595 -0.687221 -0.494696

29 6 0 -5.403360 -1.424507 -0.404863

30 6 0 1.426727 -5.351239 0.497332

31 6 0 0.691231 -6.515610 0.741859

32 6 0 -0.709478 -6.513544 0.742354

33 6 0 -1.441631 -5.346995 0.498214

34 6 0 5.403783 1.424168 -0.404108

35 6 0 6.596924 0.686745 -0.493970

36 6 0 6.595017 -0.704625 -0.494115

37 6 0 5.399850 -1.438778 -0.404356

38 6 0 -1.427081 5.351238 0.497627

39 6 0 -0.691697 6.515720 0.741926

40 6 0 0.709010 6.513917 0.741695

41 6 0 1.441272 5.347511 0.497214

42 1 0 7.548331 1.195953 -0.569738

43 1 0 7.545042 -1.216420 -0.569946

44 1 0 1.217929 7.447217 0.941623

45 1 0 -1.198181 7.450317 0.941938

46 1 0 -7.544949 1.215846 -0.570318

47 1 0 -7.547920 -1.196525 -0.570748

48 1 0 -1.218471 -7.446762 0.942457

49 1 0 1.197636 -7.450320 0.941546

50 8 0 2.790557 5.288249 0.492928

51 8 0 -2.776535 5.295533 0.493671

52 8 0 5.346345 2.772092 -0.406333

53 8 0 5.338635 -2.786538 -0.406849

54 8 0 2.776192 -5.295817 0.492631

55 8 0 -2.790920 -5.287364 0.494511

56 8 0 -5.345511 -2.772440 -0.407553

57 8 0 -5.338745 2.786230 -0.406745

58 6 0 3.521002 6.477092 0.784626

59 1 0 3.284531 6.856421 1.783103

60 1 0 3.330873 7.258281 0.042680

61 1 0 4.570630 6.191722 0.746415

62 6 0 6.568404 3.506655 -0.447681

63 1 0 7.125397 3.309792 -1.368313

64 1 0 7.199250 3.282192 0.417502

65 1 0 6.277747 4.555097 -0.420061

66 6 0 6.558672 -3.524495 -0.447831

67 1 0 7.189922 -3.301580 0.417454

68 1 0 7.116403 -3.329241 -1.368359

69 1 0 6.265190 -4.572145 -0.420141

70 6 0 -3.503789 6.486036 0.786669

71 1 0 -3.311456 7.267525 0.045630

72 1 0 -3.266247 6.863579 1.785569

73 1 0 -4.554209 6.203613 0.748210

74 6 0 -6.558872 3.524043 -0.447584

75 1 0 -7.190059 3.300956 0.417703

76 1 0 -7.116618 3.328831 -1.368111

77 1 0 -6.265510 4.571723 -0.419783

78 6 0 -6.567251 -3.507514 -0.449349

79 1 0 -7.124188 -3.310585 -1.369999

80 1 0 -7.198330 -3.283650 0.415818

81 1 0 -6.276135 -4.555839 -0.422054

82 6 0 -3.521642 -6.475937 0.786629

83 1 0 -3.284915 -6.855217 1.785064

84 1 0 -3.332037 -7.257279 0.044713

85 1 0 -4.571195 -6.190236 0.748783

86 6 0 3.503364 -6.486560 0.784864

87 1 0 3.310589 -7.267748 0.043620

88 1 0 3.266193 -6.864431 1.783728

89 1 0 4.553813 -6.204298 0.746038

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0447714 0.0439687 0.0225241

Leave Link 202 at Sat Jul 6 03:15:34 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8042.3536644647 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= 89 NActive= 89 NUniq= 89 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= -0.2279823710 Hartrees.

Nuclear repulsion after empirical dispersion term = 8042.1256820937 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6395

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.17D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 398

GePol: Fraction of low-weight points (<1% of avg) = 6.22%

GePol: Cavity surface area = 703.285 Ang\*\*2

GePol: Cavity volume = 801.560 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0089840470 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8042.1166980467 Hartrees.

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(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44311 LenP2D= 111304.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.55D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

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(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 03:15:38 2019, MaxMem= 1342177280 cpu: 2.2

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000005 0.000008 -0.000226 Ang= 0.03 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>= 2.0171 S= 1.0057

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2650.02693254197

Leave Link 401 at Sat Jul 6 03:15:56 2019, MaxMem= 1342177280 cpu: 209.6

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 122688075.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.08D-14 for 1057.

Iteration 1 A\*A^-1 deviation from orthogonality is 1.09D-14 for 6376 6009.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.99D-15 for 6391.

Iteration 1 A^-1\*A deviation from orthogonality is 1.95D-10 for 1766 1737.

Iteration 2 A\*A^-1 deviation from unit magnitude is 1.71D-14 for 1597.

Iteration 2 A\*A^-1 deviation from orthogonality is 1.61D-14 for 4068 518.

Iteration 2 A^-1\*A deviation from unit magnitude is 2.00D-15 for 1578.

Iteration 2 A^-1\*A deviation from orthogonality is 1.23D-15 for 6381 116.

E= -2649.79537309952

DIIS: error= 3.00D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79537309952 IErMin= 1 ErrMin= 3.00D-04

ErrMax= 3.00D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.07D-04 BMatP= 3.07D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.00D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.685 Goal= None Shift= 0.000

Gap= 0.744 Goal= None Shift= 0.000

RMSDP=1.36D-05 MaxDP=8.36D-04 OVMax= 1.81D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.36D-05 CP: 1.00D+00

E= -2649.79551687902 Delta-E= -0.000143779504 Rises=F Damp=F

DIIS: error= 3.17D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79551687902 IErMin= 2 ErrMin= 3.17D-05

ErrMax= 3.17D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.61D-06 BMatP= 3.07D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.701D-01 0.107D+01

Coeff: -0.701D-01 0.107D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.57D-06 MaxDP=9.59D-05 DE=-1.44D-04 OVMax= 2.44D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.42D-06 CP: 1.00D+00 1.05D+00

E= -2649.79551861737 Delta-E= -0.000001738355 Rises=F Damp=F

DIIS: error= 1.46D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79551861737 IErMin= 3 ErrMin= 1.46D-05

ErrMax= 1.46D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.87D-07 BMatP= 3.61D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.265D-01 0.355D+00 0.672D+00

Coeff: -0.265D-01 0.355D+00 0.672D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=7.29D-07 MaxDP=5.26D-05 DE=-1.74D-06 OVMax= 9.39D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.74D-07 CP: 1.00D+00 1.06D+00 8.39D-01

E= -2649.79551867525 Delta-E= -0.000000057878 Rises=F Damp=F

DIIS: error= 1.34D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79551867525 IErMin= 4 ErrMin= 1.34D-05

ErrMax= 1.34D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.21D-07 BMatP= 7.87D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.737D-02 0.829D-01 0.443D+00 0.481D+00

Coeff: -0.737D-02 0.829D-01 0.443D+00 0.481D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=3.71D-07 MaxDP=2.81D-05 DE=-5.79D-08 OVMax= 4.86D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.82D-07 CP: 1.00D+00 1.06D+00 9.35D-01 5.77D-01

E= -2649.79551876886 Delta-E= -0.000000093605 Rises=F Damp=F

DIIS: error= 1.59D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79551876886 IErMin= 5 ErrMin= 1.59D-06

ErrMax= 1.59D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.10D-09 BMatP= 5.21D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.743D-04-0.790D-02 0.857D-01 0.160D+00 0.762D+00

Coeff: -0.743D-04-0.790D-02 0.857D-01 0.160D+00 0.762D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=6.95D-08 MaxDP=3.90D-06 DE=-9.36D-08 OVMax= 1.88D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.69D-08 CP: 1.00D+00 1.06D+00 9.48D-01 6.28D-01 8.30D-01

E= -2649.79551877048 Delta-E= -0.000000001624 Rises=F Damp=F

DIIS: error= 1.68D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79551877048 IErMin= 5 ErrMin= 1.59D-06

ErrMax= 1.68D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.00D-09 BMatP= 9.10D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.555D-03-0.121D-01 0.163D-01 0.596D-01 0.478D+00 0.458D+00

Coeff: 0.555D-03-0.121D-01 0.163D-01 0.596D-01 0.478D+00 0.458D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.82D-08 MaxDP=2.78D-06 DE=-1.62D-09 OVMax= 8.03D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.98D-08 CP: 1.00D+00 1.06D+00 9.51D-01 6.29D-01 8.58D-01

CP: 6.04D-01

E= -2649.79551877118 Delta-E= -0.000000000702 Rises=F Damp=F

DIIS: error= 3.43D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79551877118 IErMin= 7 ErrMin= 3.43D-07

ErrMax= 3.43D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.20D-10 BMatP= 4.00D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.298D-03-0.566D-02 0.988D-03 0.175D-01 0.188D+00 0.242D+00

Coeff-Com: 0.557D+00

Coeff: 0.298D-03-0.566D-02 0.988D-03 0.175D-01 0.188D+00 0.242D+00

Coeff: 0.557D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=9.67D-09 MaxDP=8.07D-07 DE=-7.02D-10 OVMax= 4.85D-06

Error on total polarization charges = 0.07299

SCF Done: E(UB3LYP) = -2649.79551877 A.U. after 7 cycles

NFock= 7 Conv=0.97D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0171 S= 1.0057

<L.S>= 0.000000000000E+00

KE= 2.690150024105D+03 PE=-2.236295252245D+04 EE= 8.980890281526D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0171, after 2.0002

Leave Link 502 at Sat Jul 6 03:22:20 2019, MaxMem= 1342177280 cpu: 4503.4

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44311 LenP2D= 111304.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 274

Leave Link 701 at Sat Jul 6 03:22:40 2019, MaxMem= 1342177280 cpu: 225.8

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 03:22:40 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 03:24:14 2019, MaxMem= 1342177280 cpu: 1126.6

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 7.46063847D-05-3.90832106D-04 2.18089903D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000023416 -0.000000433 0.000045330

2 7 0.000035641 0.000074830 -0.000012276

3 6 0.000000479 -0.000021057 0.000013852

4 6 0.000013549 -0.000006873 0.000000963

5 6 0.000006454 -0.000010201 -0.000017879

6 7 -0.000029421 -0.000135289 0.000012496

7 6 -0.000027068 0.000181357 0.000037448

8 7 0.000108030 0.000050482 0.000022423

9 6 0.000014680 -0.000133954 0.000020443

10 6 -0.000003547 0.000035486 -0.000015380

11 6 -0.000002531 -0.000018542 -0.000027390

12 7 0.000015023 -0.000111096 0.000004361

13 6 0.000002186 -0.000017742 -0.000022541

14 6 0.000007500 0.000032646 -0.000021900

15 6 -0.000030734 -0.000087004 0.000014347

16 7 -0.000144569 0.000037660 0.000029909

17 6 0.000000180 0.000133161 0.000029182

18 7 0.000007694 0.000065967 0.000013084

19 7 0.000033253 -0.000110907 0.000003977

20 6 0.000072798 -0.000020229 0.000024200

21 6 -0.000000073 0.000004789 -0.000014204

22 6 0.000013891 0.000017783 0.000020269

23 6 -0.000018225 0.000003510 -0.000019691

24 7 -0.000039812 0.000079750 0.000019171

25 30 -0.000023547 -0.000029986 -0.000119287

26 6 0.000030424 -0.000031502 0.000016665

27 6 -0.000014957 0.000034236 -0.000000979

28 6 -0.000012574 -0.000040768 0.000000495

29 6 0.000026900 0.000025427 0.000014454

30 6 -0.000033547 0.000017931 -0.000034629

31 6 0.000012832 -0.000019809 0.000009096

32 6 -0.000015068 -0.000023038 0.000007641

33 6 0.000029615 0.000019919 -0.000042461

34 6 -0.000038286 -0.000042739 0.000012016

35 6 0.000018260 0.000023936 0.000000658

36 6 0.000019291 -0.000032162 0.000002024

37 6 -0.000033368 0.000032930 0.000017907

38 6 0.000035161 -0.000022494 -0.000030277

39 6 -0.000009640 0.000024321 0.000006134

40 6 0.000003830 0.000026025 0.000009743

41 6 -0.000040659 -0.000027264 -0.000030169

42 1 -0.000004593 0.000001239 -0.000005190

43 1 -0.000003360 -0.000004011 -0.000006254

44 1 -0.000003535 -0.000007191 -0.000021057

45 1 0.000003172 -0.000004856 -0.000016173

46 1 0.000003624 0.000003367 -0.000004852

47 1 -0.000003767 -0.000009016 -0.000005072

48 1 -0.000000782 0.000003830 -0.000016906

49 1 -0.000003140 0.000004248 -0.000018337

50 8 0.000051412 -0.000022706 0.000082366

51 8 -0.000043487 -0.000019271 0.000073777

52 8 -0.000039253 0.000081639 -0.000050720

53 8 -0.000026412 -0.000076892 -0.000050854

54 8 0.000043444 0.000017776 0.000074660

55 8 -0.000029883 0.000004445 0.000080569

56 8 0.000008379 -0.000049309 -0.000039790

57 8 0.000021076 0.000071305 -0.000046850

58 6 0.000019109 0.000055251 -0.000019074

59 1 0.000007702 -0.000034143 0.000014158

60 1 0.000000560 -0.000011443 -0.000012834

61 1 0.000023680 -0.000004986 -0.000004866

62 6 0.000027738 0.000004894 0.000025206

63 1 0.000000242 0.000007306 -0.000012717

64 1 0.000009154 0.000001042 0.000005918

65 1 -0.000021503 0.000006341 -0.000002595

66 6 0.000028906 0.000004716 0.000028782

67 1 0.000010418 -0.000000910 0.000006183

68 1 0.000001207 -0.000006718 -0.000013958

69 1 -0.000023584 -0.000004510 -0.000001932

70 6 -0.000009826 0.000056852 -0.000022482

71 1 -0.000006262 -0.000007598 -0.000013580

72 1 -0.000002261 -0.000031230 0.000014945

73 1 -0.000019452 -0.000007483 -0.000008110

74 6 -0.000028971 -0.000004068 0.000026173

75 1 -0.000010347 -0.000000093 0.000005886

76 1 -0.000001535 0.000007830 -0.000013565

77 1 0.000023268 0.000005323 -0.000001483

78 6 -0.000028219 0.000007214 0.000027606

79 1 -0.000001662 -0.000003375 -0.000014254

80 1 -0.000009256 0.000004321 0.000006714

81 1 0.000020591 -0.000004303 -0.000000734

82 6 -0.000005659 -0.000056192 -0.000019416

83 1 -0.000005403 0.000033143 0.000014964

84 1 -0.000003010 0.000009817 -0.000014986

85 1 -0.000020855 0.000004780 -0.000007706

86 6 0.000011445 -0.000053860 -0.000016768

87 1 0.000000491 0.000010108 -0.000013283

88 1 0.000006058 0.000030953 0.000014924

89 1 0.000020880 0.000007366 -0.000005658

-------------------------------------------------------------------

Cartesian Forces: Max 0.000181357 RMS 0.000036003

Leave Link 716 at Sat Jul 6 03:24:14 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000172018 RMS 0.000027312

Search for a local minimum.

Step number 23 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .27312D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 6 5 7 9 11

14 13 16 17 18

19 20 21 22 23

DE= -3.85D-06 DEPred=-3.30D-06 R= 1.17D+00

TightC=F SS= 1.41D+00 RLast= 2.16D-02 DXNew= 3.9497D-01 6.4691D-02

Trust test= 1.17D+00 RLast= 2.16D-02 DXMaxT set to 2.35D-01

ITU= 1 1 1 1 1 1 0 0 -1 -1 0 -1 0 0 0 0 0 0 1 1

ITU= 1 1 0

Eigenvalues --- 0.00372 0.00752 0.01193 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01316 0.01348

Eigenvalues --- 0.01495 0.01571 0.01582 0.01584 0.01598

Eigenvalues --- 0.01618 0.01661 0.01689 0.01708 0.01712

Eigenvalues --- 0.01713 0.01716 0.01761 0.01835 0.01869

Eigenvalues --- 0.01873 0.01914 0.01919 0.01937 0.01948

Eigenvalues --- 0.01992 0.02001 0.02020 0.02022 0.02029

Eigenvalues --- 0.02052 0.02053 0.02053 0.02053 0.02057

Eigenvalues --- 0.02057 0.02057 0.02057 0.02059 0.02066

Eigenvalues --- 0.02067 0.02067 0.02068 0.02070 0.02070

Eigenvalues --- 0.02071 0.02079 0.02083 0.02084 0.02166

Eigenvalues --- 0.02184 0.02238 0.02260 0.02260 0.02260

Eigenvalues --- 0.02260 0.02261 0.02321 0.02350 0.02355

Eigenvalues --- 0.02385 0.02416 0.02754 0.03652 0.05804

Eigenvalues --- 0.09893 0.09979 0.09980 0.09980 0.09984

Eigenvalues --- 0.09985 0.09985 0.10117 0.10641 0.10645

Eigenvalues --- 0.10645 0.10645 0.10656 0.10656 0.10657

Eigenvalues --- 0.10682 0.12652 0.13276 0.13467 0.15222

Eigenvalues --- 0.15897 0.15994 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16001 0.16004 0.16015 0.16064 0.16191

Eigenvalues --- 0.16644 0.16983 0.20666 0.21684 0.22004

Eigenvalues --- 0.22474 0.22476 0.22477 0.22484 0.24250

Eigenvalues --- 0.24294 0.24507 0.24517 0.24519 0.24575

Eigenvalues --- 0.24701 0.24771 0.24819 0.24905 0.24914

Eigenvalues --- 0.24926 0.24981 0.24981 0.24991 0.24992

Eigenvalues --- 0.24997 0.24998 0.24998 0.24999 0.24999

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25000 0.25006 0.25019

Eigenvalues --- 0.25091 0.25265 0.26264 0.28612 0.30888

Eigenvalues --- 0.33207 0.33651 0.33680 0.33721 0.33890

Eigenvalues --- 0.34056 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34064 0.34072 0.34081 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34081 0.34091

Eigenvalues --- 0.34454 0.34591 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34687 0.34694 0.34936

Eigenvalues --- 0.35086 0.35153 0.35611 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35632 0.35640 0.35858

Eigenvalues --- 0.36596 0.37057 0.37135 0.37479 0.40393

Eigenvalues --- 0.41215 0.41215 0.41215 0.41215 0.41215

Eigenvalues --- 0.41217 0.41281 0.41410 0.41414 0.41418

Eigenvalues --- 0.41437 0.41513 0.41918 0.42206 0.42474

Eigenvalues --- 0.43130 0.44502 0.44562 0.44695 0.44794

Eigenvalues --- 0.44878 0.44998 0.45001 0.45002 0.45004

Eigenvalues --- 0.45365 0.45366 0.45649 0.45760 0.46583

Eigenvalues --- 0.47275 0.47449 0.49312 0.49381 0.49783

Eigenvalues --- 0.49854 0.50972 0.53554 0.53554 0.53554

Eigenvalues --- 0.53554 0.53557 0.53688 0.54417 0.55006

Eigenvalues --- 0.56075 0.56773 0.57417 0.57561 0.58108

Eigenvalues --- 0.66671

En-DIIS/RFO-DIIS IScMMF= 0 using points: 23 22 21 20 19

RFO step: Lambda=-8.53838931D-07.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 3.95D-05 SmlDif= 1.00D-05

RMS Error= 0.8765882678D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.83080 0.32404 -0.19313 -0.12214 0.16042

Iteration 1 RMS(Cart)= 0.00251796 RMS(Int)= 0.00000234

Iteration 2 RMS(Cart)= 0.00000369 RMS(Int)= 0.00000194

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000194

ITry= 1 IFail=0 DXMaxC= 1.25D-02 DCOld= 1.00D+10 DXMaxT= 2.35D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58261 -0.00005 -0.00002 -0.00004 -0.00007 2.58254

R2 2.73964 -0.00001 -0.00008 0.00008 0.00000 2.73964

R3 2.56143 0.00000 0.00020 -0.00017 0.00004 2.56147

R4 2.58255 -0.00006 -0.00002 -0.00010 -0.00013 2.58242

R5 3.86891 0.00001 0.00049 0.00008 0.00055 3.86946

R6 2.73968 -0.00005 -0.00011 0.00009 -0.00002 2.73966

R7 2.56156 -0.00008 0.00018 -0.00028 -0.00009 2.56147

R8 2.69561 0.00000 0.00004 -0.00009 -0.00005 2.69556

R9 2.66247 -0.00002 0.00003 -0.00009 -0.00006 2.66241

R10 2.66246 -0.00001 0.00003 -0.00009 -0.00006 2.66241

R11 2.48272 -0.00017 -0.00016 -0.00016 -0.00031 2.48241

R12 2.59619 -0.00003 0.00009 -0.00008 0.00001 2.59619

R13 2.79450 -0.00004 0.00012 -0.00019 -0.00006 2.79444

R14 2.59606 0.00000 0.00009 -0.00003 0.00006 2.59612

R15 3.84098 0.00005 0.00020 0.00047 0.00067 3.84165

R16 2.79453 -0.00001 0.00014 -0.00018 -0.00004 2.79449

R17 2.48255 -0.00007 -0.00013 -0.00004 -0.00016 2.48239

R18 2.66403 0.00001 -0.00007 0.00005 -0.00001 2.66402

R19 2.64568 -0.00002 0.00001 -0.00005 -0.00004 2.64565

R20 2.64573 -0.00004 0.00001 -0.00006 -0.00005 2.64568

R21 2.48260 -0.00008 -0.00013 -0.00008 -0.00020 2.48240

R22 2.66395 0.00003 -0.00005 0.00009 0.00004 2.66399

R23 2.79455 -0.00003 0.00014 -0.00021 -0.00007 2.79449

R24 2.64568 -0.00001 0.00002 -0.00005 -0.00003 2.64565

R25 2.79439 0.00003 0.00015 -0.00013 0.00002 2.79441

R26 2.64568 0.00001 0.00002 -0.00004 -0.00002 2.64566

R27 2.59616 0.00000 0.00010 -0.00007 0.00003 2.59619

R28 2.48243 0.00002 -0.00011 0.00006 -0.00004 2.48239

R29 2.59619 -0.00002 0.00010 -0.00013 -0.00003 2.59616

R30 3.84122 0.00007 0.00022 0.00035 0.00056 3.84177

R31 2.56126 0.00008 0.00022 -0.00005 0.00017 2.56143

R32 2.58252 -0.00004 -0.00001 -0.00009 -0.00011 2.58241

R33 2.58274 -0.00006 -0.00002 -0.00013 -0.00015 2.58259

R34 3.86920 0.00003 0.00048 -0.00006 0.00041 3.86962

R35 2.73961 0.00001 -0.00009 0.00014 0.00006 2.73966

R36 2.69554 0.00002 0.00005 -0.00005 0.00001 2.69554

R37 2.66244 0.00001 0.00003 -0.00007 -0.00003 2.66241

R38 2.73967 -0.00004 -0.00010 0.00008 -0.00002 2.73964

R39 2.66246 -0.00001 0.00003 -0.00009 -0.00005 2.66241

R40 2.56149 -0.00002 0.00020 -0.00020 0.00000 2.56149

R41 2.65605 0.00002 0.00003 -0.00004 -0.00001 2.65604

R42 2.54953 0.00008 -0.00006 0.00019 0.00013 2.54966

R43 2.62932 0.00006 -0.00004 0.00015 0.00011 2.62943

R44 2.04426 0.00000 0.00001 -0.00002 0.00000 2.04425

R45 2.65604 0.00002 0.00004 -0.00005 -0.00001 2.65603

R46 2.04422 0.00001 0.00001 0.00000 0.00001 2.04423

R47 2.54957 0.00005 -0.00005 0.00014 0.00009 2.54966

R48 2.64326 0.00003 0.00000 0.00001 0.00002 2.64328

R49 2.55228 0.00008 -0.00004 0.00010 0.00005 2.55234

R50 2.64696 0.00005 -0.00001 0.00007 0.00006 2.64702

R51 2.04405 -0.00001 0.00000 0.00001 0.00000 2.04406

R52 2.64324 0.00003 0.00001 0.00001 0.00002 2.64326

R53 2.04406 -0.00001 0.00000 0.00001 0.00001 2.04407

R54 2.55228 0.00006 -0.00004 0.00008 0.00003 2.55232

R55 2.65602 0.00004 0.00003 -0.00002 0.00001 2.65604

R56 2.54952 0.00010 -0.00006 0.00021 0.00015 2.54967

R57 2.62931 0.00008 -0.00004 0.00016 0.00012 2.62943

R58 2.04424 0.00000 0.00001 -0.00002 0.00000 2.04423

R59 2.65603 0.00004 0.00004 -0.00004 0.00000 2.65603

R60 2.04426 0.00000 0.00001 -0.00001 0.00000 2.04425

R61 2.54953 0.00008 -0.00006 0.00019 0.00013 2.54966

R62 2.64325 0.00004 0.00001 0.00002 0.00003 2.64327

R63 2.55228 0.00008 -0.00005 0.00010 0.00006 2.55234

R64 2.64696 0.00005 -0.00001 0.00008 0.00007 2.64702

R65 2.04406 -0.00001 0.00000 0.00001 0.00000 2.04406

R66 2.64324 0.00004 0.00000 0.00003 0.00003 2.64327

R67 2.04407 -0.00001 0.00000 0.00000 0.00000 2.04407

R68 2.55225 0.00010 -0.00004 0.00011 0.00007 2.55232

R69 2.69376 0.00003 0.00002 0.00007 0.00009 2.69385

R70 2.69380 0.00002 0.00002 0.00007 0.00009 2.69389

R71 2.69557 0.00002 -0.00001 0.00009 0.00008 2.69565

R72 2.69559 0.00002 -0.00001 0.00008 0.00007 2.69567

R73 2.69380 0.00002 0.00002 0.00007 0.00009 2.69389

R74 2.69377 0.00002 0.00002 0.00006 0.00008 2.69385

R75 2.69558 0.00001 -0.00001 0.00008 0.00006 2.69564

R76 2.69559 0.00002 -0.00001 0.00009 0.00007 2.69567

R77 2.06730 0.00000 0.00001 -0.00003 -0.00003 2.06727

R78 2.06741 0.00000 0.00000 0.00000 0.00000 2.06741

R79 2.05678 0.00002 0.00000 0.00006 0.00006 2.05684

R80 2.06712 0.00001 0.00001 0.00001 0.00002 2.06715

R81 2.06741 0.00001 0.00001 0.00002 0.00003 2.06744

R82 2.05666 0.00001 0.00000 0.00004 0.00004 2.05669

R83 2.06740 0.00001 0.00001 0.00002 0.00003 2.06743

R84 2.06712 0.00001 0.00001 0.00001 0.00003 2.06715

R85 2.05665 0.00001 0.00000 0.00004 0.00004 2.05669

R86 2.06738 0.00000 0.00000 0.00000 0.00000 2.06738

R87 2.06730 0.00000 0.00001 -0.00003 -0.00002 2.06728

R88 2.05679 0.00002 0.00000 0.00005 0.00006 2.05684

R89 2.06740 0.00001 0.00001 0.00002 0.00003 2.06744

R90 2.06712 0.00001 0.00001 0.00001 0.00002 2.06715

R91 2.05665 0.00001 0.00000 0.00004 0.00004 2.05669

R92 2.06712 0.00001 0.00001 0.00001 0.00003 2.06715

R93 2.06741 0.00001 0.00001 0.00002 0.00003 2.06744

R94 2.05666 0.00001 0.00000 0.00004 0.00004 2.05670

R95 2.06730 0.00000 0.00001 -0.00003 -0.00002 2.06728

R96 2.06740 0.00000 0.00000 0.00000 0.00001 2.06741

R97 2.05678 0.00002 0.00000 0.00006 0.00006 2.05684

R98 2.06738 0.00000 0.00000 0.00000 0.00000 2.06738

R99 2.06730 0.00000 0.00001 -0.00003 -0.00002 2.06728

R100 2.05678 0.00002 0.00000 0.00006 0.00006 2.05684

A1 1.88913 0.00000 0.00009 -0.00018 -0.00009 1.88903

A2 2.21494 -0.00001 -0.00008 0.00009 0.00001 2.21495

A3 2.17904 0.00002 -0.00001 0.00008 0.00007 2.17911

A4 1.93077 0.00001 -0.00012 0.00024 0.00012 1.93090

A5 2.17290 -0.00001 -0.00004 -0.00017 -0.00020 2.17270

A6 2.17277 0.00000 -0.00005 0.00000 -0.00004 2.17273

A7 1.88910 0.00002 0.00011 -0.00016 -0.00006 1.88904

A8 2.21491 0.00000 -0.00006 0.00007 0.00001 2.21492

A9 2.17909 -0.00002 -0.00004 0.00008 0.00005 2.17914

A10 1.85791 -0.00001 -0.00004 0.00005 0.00001 1.85792

A11 2.31713 -0.00002 0.00004 -0.00007 -0.00003 2.31710

A12 2.10797 0.00004 0.00001 0.00004 0.00004 2.10801

A13 1.85787 -0.00001 -0.00004 0.00005 0.00002 1.85789

A14 2.31718 0.00000 0.00006 -0.00007 -0.00002 2.31716

A15 2.10796 0.00001 -0.00001 0.00003 0.00002 2.10798

A16 2.18686 0.00003 -0.00007 0.00013 0.00006 2.18692

A17 2.23319 0.00001 0.00000 -0.00011 -0.00011 2.23309

A18 2.16603 0.00001 -0.00005 0.00022 0.00017 2.16621

A19 1.88357 -0.00002 0.00006 -0.00012 -0.00006 1.88351

A20 1.93234 0.00004 -0.00011 0.00016 0.00006 1.93241

A21 2.16290 -0.00001 -0.00006 -0.00007 -0.00012 2.16278

A22 2.16316 -0.00003 -0.00006 -0.00022 -0.00028 2.16288

A23 1.88359 -0.00004 0.00005 -0.00012 -0.00008 1.88351

A24 2.23312 -0.00001 -0.00001 -0.00010 -0.00012 2.23301

A25 2.16609 0.00005 -0.00002 0.00022 0.00020 2.16629

A26 1.86258 0.00000 0.00000 0.00003 0.00003 1.86261

A27 2.30409 -0.00002 0.00000 -0.00004 -0.00004 2.30404

A28 2.11645 0.00002 0.00001 0.00001 0.00002 2.11647

A29 1.86257 0.00001 0.00000 0.00004 0.00004 1.86261

A30 2.30408 -0.00005 -0.00002 -0.00006 -0.00008 2.30399

A31 2.11647 0.00004 0.00002 0.00002 0.00004 2.11651

A32 2.18682 0.00005 -0.00005 0.00019 0.00014 2.18696

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D3 3.13133 -0.00002 0.00049 -0.00054 -0.00004 3.13128

D4 -0.13025 -0.00002 -0.00111 0.00005 -0.00106 -0.13131

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D6 -3.12258 -0.00002 -0.00071 -0.00085 -0.00156 -3.12415

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D10 -2.98467 -0.00001 0.00152 -0.00102 0.00050 -2.98417

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D108 -3.10809 -0.00001 0.00020 0.00041 0.00061 -3.10747

D109 -0.17270 -0.00001 -0.00139 0.00052 -0.00087 -0.17357

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D131 -3.12234 -0.00002 -0.00075 -0.00138 -0.00214 -3.12448

D132 0.01612 -0.00001 -0.00085 -0.00148 -0.00233 0.01379

D133 -0.00373 -0.00001 -0.00031 -0.00056 -0.00087 -0.00460

D134 3.13473 -0.00001 -0.00041 -0.00065 -0.00106 3.13367

D135 -0.00212 0.00001 -0.00016 0.00024 0.00008 -0.00204

D136 -3.13054 0.00002 -0.00036 0.00063 0.00027 -3.13028

D137 -3.12297 0.00000 -0.00054 -0.00079 -0.00133 -3.12430

D138 0.03179 0.00001 -0.00075 -0.00040 -0.00115 0.03065

D139 0.00342 0.00002 0.00033 0.00065 0.00098 0.00440

D140 -3.13516 0.00002 0.00045 0.00066 0.00111 -3.13404

D141 3.12185 0.00003 0.00076 0.00180 0.00256 3.12441

D142 -0.01672 0.00003 0.00088 0.00182 0.00269 -0.01403

D143 0.17235 0.00001 0.00141 -0.00061 0.00080 0.17315

D144 -2.98488 0.00000 0.00166 -0.00107 0.00058 -2.98430

D145 -0.00101 0.00000 -0.00003 0.00001 -0.00002 -0.00103

D146 -3.13795 0.00000 0.00006 -0.00002 0.00004 -3.13791

D147 3.13539 -0.00001 -0.00024 -0.00003 -0.00028 3.13512

D148 -0.00154 0.00000 -0.00015 -0.00007 -0.00022 -0.00176

D149 -3.10002 0.00000 0.00017 0.00084 0.00101 -3.09901

D150 0.04683 0.00001 0.00039 0.00088 0.00127 0.04811

D151 0.00006 0.00000 0.00004 -0.00019 -0.00015 -0.00009

D152 -3.13698 0.00000 0.00010 -0.00008 0.00002 -3.13696

D153 3.13709 -0.00001 -0.00005 -0.00015 -0.00020 3.13688

D154 0.00005 0.00000 0.00001 -0.00004 -0.00004 0.00002

D155 0.00098 0.00000 0.00001 0.00009 0.00010 0.00108

D156 -3.13538 0.00001 0.00026 -0.00008 0.00018 -3.13520

D157 3.13792 0.00000 -0.00005 -0.00002 -0.00007 3.13785

D158 0.00156 0.00000 0.00020 -0.00019 0.00001 0.00157

D159 3.10058 -0.00001 -0.00012 -0.00110 -0.00122 3.09937

D160 -0.04632 -0.00002 -0.00038 -0.00092 -0.00130 -0.04762

D161 -0.00362 -0.00002 -0.00032 -0.00058 -0.00090 -0.00452

D162 -3.14090 -0.00002 -0.00024 -0.00068 -0.00092 3.14137

D163 3.13476 -0.00001 -0.00045 -0.00059 -0.00104 3.13372

D164 -0.00251 -0.00002 -0.00036 -0.00070 -0.00106 -0.00357

D165 3.11158 0.00001 0.00187 0.00064 0.00252 3.11409

D166 -0.02679 0.00001 0.00200 0.00066 0.00266 -0.02413

D167 0.00011 0.00000 -0.00001 -0.00007 -0.00008 0.00003

D168 -3.13732 0.00000 0.00008 -0.00006 0.00002 -3.13730

D169 3.13748 0.00000 -0.00009 0.00003 -0.00006 3.13742

D170 0.00006 0.00000 -0.00001 0.00004 0.00004 0.00009

D171 0.00359 0.00002 0.00033 0.00064 0.00096 0.00456

D172 -3.13468 0.00002 0.00043 0.00074 0.00117 -3.13351

D173 3.14091 0.00001 0.00024 0.00063 0.00087 -3.14140

D174 0.00265 0.00001 0.00034 0.00073 0.00107 0.00372

D175 -3.11213 -0.00001 -0.00186 -0.00089 -0.00275 -3.11489

D176 0.02611 -0.00001 -0.00197 -0.00099 -0.00296 0.02315

D177 0.00093 0.00000 0.00003 0.00010 0.00013 0.00106

D178 3.13789 0.00000 -0.00007 0.00002 -0.00005 3.13784

D179 -3.13550 0.00002 0.00027 0.00014 0.00041 -3.13509

D180 0.00146 0.00001 0.00017 0.00006 0.00023 0.00169

D181 3.10056 -0.00001 -0.00018 -0.00080 -0.00098 3.09958

D182 -0.04627 -0.00002 -0.00042 -0.00084 -0.00126 -0.04754

D183 -0.00004 0.00000 -0.00003 0.00013 0.00010 0.00006

D184 3.13710 -0.00001 -0.00010 -0.00008 -0.00018 3.13693

D185 -3.13710 0.00001 0.00007 0.00021 0.00028 -3.13682

D186 0.00005 0.00000 0.00000 0.00001 0.00000 0.00005

D187 -0.00091 -0.00001 -0.00001 -0.00017 -0.00019 -0.00110

D188 3.13551 -0.00001 -0.00027 -0.00015 -0.00043 3.13508

D189 -3.13796 0.00001 0.00006 0.00004 0.00010 -3.13786

D190 -0.00154 0.00000 -0.00020 0.00006 -0.00014 -0.00169

D191 -3.10012 0.00001 0.00011 0.00109 0.00120 -3.09892

D192 0.04672 0.00002 0.00037 0.00107 0.00145 0.04817

D193 -0.00354 -0.00002 -0.00030 -0.00075 -0.00105 -0.00459

D194 -3.14088 -0.00002 -0.00025 -0.00062 -0.00087 3.14143

D195 3.13471 -0.00001 -0.00034 -0.00086 -0.00120 3.13351

D196 -0.00263 -0.00001 -0.00030 -0.00073 -0.00102 -0.00365

D197 3.11130 0.00002 0.00195 0.00078 0.00273 3.11403

D198 -0.02693 0.00001 0.00199 0.00089 0.00288 -0.02404

D199 -0.00005 0.00000 0.00001 0.00009 0.00011 0.00005

D200 -3.13735 0.00000 0.00005 0.00010 0.00015 -3.13721

D201 3.13738 0.00000 -0.00003 -0.00003 -0.00006 3.13732

D202 0.00008 0.00000 0.00001 -0.00003 -0.00002 0.00006

D203 0.00360 0.00002 0.00029 0.00073 0.00102 0.00462

D204 -3.13460 0.00002 0.00035 0.00089 0.00124 -3.13336

D205 3.14080 0.00002 0.00025 0.00073 0.00098 -3.14141

D206 0.00260 0.00002 0.00031 0.00089 0.00120 0.00380

D207 -3.11217 -0.00001 -0.00192 -0.00064 -0.00255 -3.11472

D208 0.02600 -0.00001 -0.00197 -0.00080 -0.00277 0.02323

D209 1.05040 0.00003 0.00125 0.00077 0.00202 1.05242

D210 -1.09167 0.00001 0.00117 0.00046 0.00163 -1.09004

D211 3.12050 0.00001 0.00120 0.00061 0.00180 3.12231

D212 1.09122 0.00000 -0.00118 -0.00024 -0.00143 1.08980

D213 -1.05073 -0.00002 -0.00126 -0.00056 -0.00182 -1.05255

D214 -3.12080 -0.00001 -0.00121 -0.00039 -0.00160 -3.12240

D215 1.09236 0.00002 0.00014 0.00074 0.00088 1.09324

D216 -1.05178 0.00000 0.00008 0.00062 0.00070 -1.05108

D217 -3.12113 0.00000 0.00011 0.00061 0.00072 -3.12041

D218 1.05136 0.00000 -0.00003 -0.00076 -0.00080 1.05056

D219 -1.09268 -0.00002 -0.00010 -0.00088 -0.00098 -1.09366

D220 3.12076 0.00000 -0.00006 -0.00077 -0.00083 3.11994

D221 1.09139 0.00000 -0.00117 -0.00040 -0.00157 1.08982

D222 -1.05059 -0.00003 -0.00124 -0.00071 -0.00196 -1.05254

D223 -3.12066 -0.00001 -0.00119 -0.00054 -0.00174 -3.12239

D224 1.05045 0.00003 0.00125 0.00073 0.00198 1.05243

D225 -1.09161 0.00000 0.00117 0.00042 0.00158 -1.09002

D226 3.12055 0.00001 0.00119 0.00058 0.00178 3.12233

D227 1.09237 0.00002 0.00010 0.00087 0.00098 1.09334

D228 -1.05180 0.00000 0.00003 0.00081 0.00084 -1.05096

D229 -3.12114 0.00000 0.00006 0.00080 0.00086 -3.12028

D230 1.05142 0.00000 -0.00008 -0.00071 -0.00079 1.05063

D231 -1.09263 -0.00002 -0.00014 -0.00083 -0.00097 -1.09359

D232 3.12082 0.00000 -0.00011 -0.00070 -0.00081 3.12002

Item Value Threshold Converged?

Maximum Force 0.000172 0.000450 YES

RMS Force 0.000027 0.000300 YES

Maximum Displacement 0.012546 0.001800 NO

RMS Displacement 0.002518 0.001200 NO

Predicted change in Energy=-1.864966D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 03:24:15 2019, MaxMem= 1342177280 cpu: 14.7

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=3 Diff= 1.21D-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 -1.122380 2.801223 -0.019808

2 7 0 0.001049 2.038039 -0.171844

3 6 0 1.125127 2.800127 -0.019683

4 6 0 0.715217 4.164715 0.248080

5 6 0 -0.711213 4.165450 0.247797

6 7 0 2.410998 2.381993 -0.114586

7 6 0 2.798251 1.128950 -0.189086

8 7 0 2.018895 -0.000987 -0.131643

9 6 0 2.797154 -1.131637 -0.189048

10 6 0 4.208047 -0.706877 -0.314581

11 6 0 4.208700 0.702861 -0.314733

12 7 0 -2.408646 2.384283 -0.114550

13 6 0 -4.207987 0.706876 -0.314815

14 6 0 -4.208694 -0.702849 -0.314545

15 6 0 -2.798238 -1.128941 -0.189125

16 7 0 -2.018833 0.000961 -0.131742

17 6 0 -2.797101 1.131626 -0.189216

18 7 0 -2.411027 -2.381985 -0.114525

19 7 0 -0.001122 -2.037966 -0.171737

20 6 0 -1.125173 -2.800076 -0.019539

21 6 0 -0.715266 -4.164715 0.247973

22 6 0 0.711154 -4.165395 0.247890

23 6 0 1.122327 -2.801145 -0.019605

24 7 0 2.408627 -2.384265 -0.114346

25 30 0 0.000070 0.000072 -0.370555

26 6 0 -5.400724 1.434050 -0.407794

27 6 0 -6.595128 0.698841 -0.499117

28 6 0 -6.595814 -0.692594 -0.498696

29 6 0 -5.402140 -1.428931 -0.407038

30 6 0 1.431542 -5.349582 0.500292

31 6 0 0.697155 -6.514972 0.743343

32 6 0 -0.703586 -6.514277 0.743525

33 6 0 -1.436819 -5.348136 0.500625

34 6 0 5.402111 1.428956 -0.407709

35 6 0 6.595805 0.692617 -0.499182

36 6 0 6.595182 -0.698817 -0.498940

37 6 0 5.400813 -1.434035 -0.407282

38 6 0 -1.431603 5.349604 0.500325

39 6 0 -0.697216 6.514926 0.743694

40 6 0 0.703527 6.514173 0.744133

41 6 0 1.436768 5.348047 0.501157

42 1 0 7.546616 1.202671 -0.576703

43 1 0 7.545550 -1.209753 -0.576241

44 1 0 1.211736 7.448001 0.943400

45 1 0 -1.204584 7.449287 0.942584

46 1 0 -7.545483 1.209779 -0.576570

47 1 0 -7.546654 -1.202651 -0.575856

48 1 0 -1.211807 -7.448170 0.942469

49 1 0 1.204519 -7.449371 0.942064

50 8 0 2.786121 5.289357 0.498896

51 8 0 -2.781031 5.292505 0.497075

52 8 0 5.343145 2.776892 -0.410657

53 8 0 5.340633 -2.781912 -0.409778

54 8 0 2.780970 -5.292471 0.497074

55 8 0 -2.786173 -5.289560 0.497971

56 8 0 -5.343243 -2.776866 -0.409233

57 8 0 -5.340473 2.781924 -0.410889

58 6 0 3.515775 6.479407 0.787878

59 1 0 3.279333 6.860602 1.785636

60 1 0 3.324985 7.258659 0.044065

61 1 0 4.565592 6.194553 0.750088

62 6 0 6.564300 3.512979 -0.452989

63 1 0 7.120721 3.317010 -1.374173

64 1 0 7.196208 3.289299 0.411643

65 1 0 6.272148 4.561017 -0.425044

66 6 0 6.561227 -3.519008 -0.451011

67 1 0 7.192897 -3.295084 0.413727

68 1 0 7.118212 -3.324132 -1.372087

69 1 0 6.268296 -4.566807 -0.422396

70 6 0 -3.509441 6.483265 0.786367

71 1 0 -3.317007 7.262868 0.043368

72 1 0 -3.273261 6.863347 1.784616

73 1 0 -4.559599 6.199801 0.747575

74 6 0 -6.561015 3.519080 -0.452515

75 1 0 -7.192727 3.295649 0.412321

76 1 0 -7.117991 3.323775 -1.373505

77 1 0 -6.268009 4.566872 -0.424436

78 6 0 -6.564473 -3.512865 -0.450810

79 1 0 -7.121086 -3.317456 -1.371997

80 1 0 -7.196151 -3.288527 0.413819

81 1 0 -6.272420 -4.560915 -0.422214

82 6 0 -3.515776 -6.479788 0.786331

83 1 0 -3.279592 -6.861282 1.784038

84 1 0 -3.324666 -7.258776 0.042324

85 1 0 -4.565614 -6.195040 0.748300

86 6 0 3.509402 -6.483268 0.786158

87 1 0 3.317003 -7.262726 0.042997

88 1 0 3.273222 -6.863557 1.784327

89 1 0 4.559552 -6.199762 0.747435

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0447690 0.0439673 0.0225260

Leave Link 202 at Sat Jul 6 03:24:16 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8042.2819170013 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= 89 NActive= 89 NUniq= 89 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= -0.2279750621 Hartrees.

Nuclear repulsion after empirical dispersion term = 8042.0539419392 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6394

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.65D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 397

GePol: Fraction of low-weight points (<1% of avg) = 6.21%

GePol: Cavity surface area = 703.234 Ang\*\*2

GePol: Cavity volume = 801.584 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0089883265 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8042.0449536127 Hartrees.

Leave Link 301 at Sat Jul 6 03:24:17 2019, MaxMem= 1342177280 cpu: 1.4

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44311 LenP2D= 111304.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.56D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 03:24:21 2019, MaxMem= 1342177280 cpu: 42.7

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 03:24:21 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000004 -0.000004 -0.000429 Ang= -0.05 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>= 2.0171 S= 1.0057

Leave Link 401 at Sat Jul 6 03:24:28 2019, MaxMem= 1342177280 cpu: 72.5

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 122649708.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.11D-14 for 6382.

Iteration 1 A\*A^-1 deviation from orthogonality is 8.86D-15 for 6374 6000.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.13D-14 for 6382.

Iteration 1 A^-1\*A deviation from orthogonality is 3.51D-09 for 5212 5180.

Iteration 2 A\*A^-1 deviation from unit magnitude is 1.63D-14 for 532.

Iteration 2 A\*A^-1 deviation from orthogonality is 1.27D-14 for 4910 2088.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.78D-15 for 513.

Iteration 2 A^-1\*A deviation from orthogonality is 4.89D-16 for 3195 885.

E= -2649.79548675483

DIIS: error= 1.36D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79548675483 IErMin= 1 ErrMin= 1.36D-04

ErrMax= 1.36D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.19D-05 BMatP= 7.19D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.36D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.685 Goal= None Shift= 0.000

Gap= 0.744 Goal= None Shift= 0.000

RMSDP=7.10D-06 MaxDP=3.24D-04 OVMax= 1.02D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 7.10D-06 CP: 1.00D+00

E= -2649.79551985054 Delta-E= -0.000033095710 Rises=F Damp=F

DIIS: error= 1.69D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79551985054 IErMin= 2 ErrMin= 1.69D-05

ErrMax= 1.69D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.11D-06 BMatP= 7.19D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.664D-01 0.107D+01

Coeff: -0.664D-01 0.107D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=9.06D-07 MaxDP=5.74D-05 DE=-3.31D-05 OVMax= 2.38D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 8.24D-07 CP: 1.00D+00 1.05D+00

E= -2649.79552017626 Delta-E= -0.000000325716 Rises=F Damp=F

DIIS: error= 1.95D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79552017626 IErMin= 2 ErrMin= 1.69D-05

ErrMax= 1.95D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.00D-07 BMatP= 1.11D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.370D-01 0.508D+00 0.529D+00

Coeff: -0.370D-01 0.508D+00 0.529D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=5.07D-07 MaxDP=6.24D-05 DE=-3.26D-07 OVMax= 1.22D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 4.24D-07 CP: 1.00D+00 1.06D+00 6.76D-01

E= -2649.79552027028 Delta-E= -0.000000094025 Rises=F Damp=F

DIIS: error= 1.22D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79552027028 IErMin= 4 ErrMin= 1.22D-05

ErrMax= 1.22D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.09D-07 BMatP= 7.00D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.967D-02 0.119D+00 0.351D+00 0.539D+00

Coeff: -0.967D-02 0.119D+00 0.351D+00 0.539D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.05D-07 MaxDP=2.45D-05 DE=-9.40D-08 OVMax= 5.73D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.22D-07 CP: 1.00D+00 1.06D+00 7.82D-01 6.76D-01

E= -2649.79552031290 Delta-E= -0.000000042619 Rises=F Damp=F

DIIS: error= 2.49D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79552031290 IErMin= 5 ErrMin= 2.49D-06

ErrMax= 2.49D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.03D-09 BMatP= 2.09D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.242D-02 0.236D-01 0.136D+00 0.263D+00 0.580D+00

Coeff: -0.242D-02 0.236D-01 0.136D+00 0.263D+00 0.580D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=5.56D-08 MaxDP=3.05D-06 DE=-4.26D-08 OVMax= 1.29D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 4.37D-08 CP: 1.00D+00 1.06D+00 7.93D-01 7.34D-01 8.19D-01

E= -2649.79552031428 Delta-E= -0.000000001379 Rises=F Damp=F

DIIS: error= 9.34D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79552031428 IErMin= 6 ErrMin= 9.34D-07

ErrMax= 9.34D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.60D-09 BMatP= 8.03D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.527D-03-0.119D-01 0.676D-02 0.432D-01 0.333D+00 0.628D+00

Coeff: 0.527D-03-0.119D-01 0.676D-02 0.432D-01 0.333D+00 0.628D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.42D-08 MaxDP=1.30D-06 DE=-1.38D-09 OVMax= 1.23D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.71D-08 CP: 1.00D+00 1.06D+00 8.02D-01 7.43D-01 8.85D-01

CP: 7.12D-01

E= -2649.79552031462 Delta-E= -0.000000000337 Rises=F Damp=F

DIIS: error= 2.77D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79552031462 IErMin= 7 ErrMin= 2.77D-07

ErrMax= 2.77D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.80D-10 BMatP= 1.60D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.460D-03-0.829D-02-0.588D-02 0.585D-02 0.145D+00 0.353D+00

Coeff-Com: 0.510D+00

Coeff: 0.460D-03-0.829D-02-0.588D-02 0.585D-02 0.145D+00 0.353D+00

Coeff: 0.510D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=8.30D-09 MaxDP=4.77D-07 DE=-3.37D-10 OVMax= 3.35D-06

Error on total polarization charges = 0.07299

SCF Done: E(UB3LYP) = -2649.79552031 A.U. after 7 cycles

NFock= 7 Conv=0.83D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0171 S= 1.0057

<L.S>= 0.000000000000E+00

KE= 2.690148840207D+03 PE=-2.236280971979D+04 EE= 8.980820405655D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0171, after 2.0002

Leave Link 502 at Sat Jul 6 03:30:48 2019, MaxMem= 1342177280 cpu: 4462.0

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44311 LenP2D= 111304.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 275

Leave Link 701 at Sat Jul 6 03:31:07 2019, MaxMem= 1342177280 cpu: 225.6

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 03:31:08 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 03:32:46 2019, MaxMem= 1342177280 cpu: 1172.7

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 2.19123321D-04 1.04392333D-04 2.02032379D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000015869 0.000014298 0.000038898

2 7 -0.000011860 -0.000076164 -0.000031457

3 6 -0.000019278 0.000020562 0.000050051

4 6 0.000026268 -0.000005210 -0.000032435

5 6 -0.000014354 -0.000014207 -0.000020723

6 7 -0.000047310 -0.000012742 -0.000001023

7 6 -0.000028705 0.000035247 -0.000020230

8 7 0.000035288 0.000026333 0.000018706

9 6 -0.000015675 -0.000036565 0.000020026

10 6 0.000011161 0.000028499 -0.000020679

11 6 0.000018802 -0.000022173 -0.000012096

12 7 0.000054789 -0.000005447 -0.000022106

13 6 -0.000016482 -0.000022508 -0.000012210

14 6 -0.000012679 0.000023920 -0.000029456

15 6 0.000029657 -0.000034257 0.000023607

16 7 -0.000043423 -0.000000348 0.000012129

17 6 0.000014135 0.000034608 -0.000001119

18 7 0.000035234 0.000011614 0.000004301

19 7 0.000039797 0.000075110 -0.000006267

20 6 0.000027213 -0.000030471 0.000002536

21 6 -0.000027203 0.000012193 -0.000014691

22 6 0.000019589 0.000009355 -0.000023075

23 6 -0.000018197 -0.000014520 0.000022647

24 7 -0.000056781 0.000001207 -0.000016140

25 30 -0.000012263 -0.000015475 0.000018652

26 6 0.000028934 0.000002503 0.000012484

27 6 -0.000013072 0.000007185 0.000005440

28 6 -0.000013732 -0.000003390 0.000000064

29 6 0.000028427 0.000003053 0.000015436

30 6 -0.000017227 0.000009781 -0.000009264

31 6 0.000007376 -0.000017451 0.000000208

32 6 0.000001643 -0.000022462 0.000001392

33 6 0.000021724 0.000015345 -0.000005024

34 6 -0.000028370 -0.000005378 0.000010973

35 6 0.000010331 0.000007007 0.000001653

36 6 0.000014492 -0.000003114 0.000001617

37 6 -0.000030813 -0.000002770 0.000011437

38 6 0.000018701 -0.000011899 0.000001327

39 6 -0.000005842 0.000017414 0.000001137

40 6 0.000002297 0.000019706 0.000002104

41 6 -0.000021723 -0.000014236 -0.000005179

42 1 0.000004316 0.000008789 -0.000003288

43 1 -0.000002029 -0.000005551 -0.000004449

44 1 -0.000009550 -0.000005558 -0.000004320

45 1 0.000015395 -0.000002177 -0.000003324

46 1 0.000002320 0.000006259 -0.000005244

47 1 -0.000003408 -0.000007155 -0.000004394

48 1 0.000013069 0.000007374 -0.000005081

49 1 -0.000013950 0.000002767 -0.000001016

50 8 0.000001244 0.000041062 0.000020783

51 8 -0.000006259 0.000038598 0.000021855

52 8 0.000027641 -0.000012672 -0.000009089

53 8 0.000029270 -0.000004536 -0.000014015

54 8 0.000008771 -0.000034657 0.000030895

55 8 -0.000006508 -0.000034482 0.000023873

56 8 -0.000024510 0.000003346 -0.000020016

57 8 -0.000033672 0.000000019 -0.000009802

58 6 0.000030199 -0.000006873 -0.000029010

59 1 -0.000004901 -0.000009375 0.000005840

60 1 0.000003261 -0.000001462 0.000013457

61 1 0.000008582 0.000008932 -0.000006473

62 6 0.000001972 0.000010702 0.000019935

63 1 -0.000002765 -0.000001896 -0.000004342

64 1 -0.000003798 -0.000006847 -0.000003301

65 1 0.000002867 0.000000885 0.000003250

66 6 -0.000000348 -0.000004203 0.000017710

67 1 0.000000251 -0.000000657 -0.000003102

68 1 -0.000002894 -0.000000251 -0.000004366

69 1 -0.000000573 -0.000000587 0.000000400

70 6 -0.000025219 -0.000014671 -0.000020949

71 1 -0.000006755 0.000000746 0.000008961

72 1 0.000004619 -0.000005705 0.000005061

73 1 -0.000006444 0.000006975 -0.000008794

74 6 -0.000000542 0.000004202 0.000016955

75 1 0.000001758 -0.000001556 -0.000003100

76 1 0.000001933 0.000000510 -0.000004465

77 1 0.000000055 0.000001031 0.000002756

78 6 0.000000178 -0.000013838 0.000020789

79 1 0.000003347 0.000001727 -0.000004164

80 1 0.000000405 0.000003006 -0.000003933

81 1 -0.000002892 0.000000606 -0.000000611

82 6 -0.000034319 0.000008513 -0.000025408

83 1 0.000001738 0.000009198 0.000005477

84 1 -0.000001861 0.000002688 0.000013433

85 1 -0.000009010 -0.000009828 -0.000003276

86 6 0.000023925 0.000014770 -0.000022839

87 1 0.000007384 -0.000000981 0.000009367

88 1 -0.000005494 0.000006451 0.000005443

89 1 0.000006459 -0.000007788 -0.000007722

-------------------------------------------------------------------

Cartesian Forces: Max 0.000076164 RMS 0.000018244

Leave Link 716 at Sat Jul 6 03:32:46 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000091333 RMS 0.000014349

Search for a local minimum.

Step number 24 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .14349D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 6 5 7 9 11

14 13 16 17 18

19 20 21 22 23

24

DE= -1.54D-06 DEPred=-1.86D-06 R= 8.28D-01

TightC=F SS= 1.41D+00 RLast= 1.68D-02 DXNew= 3.9497D-01 5.0539D-02

Trust test= 8.28D-01 RLast= 1.68D-02 DXMaxT set to 2.35D-01

ITU= 1 1 1 1 1 1 1 0 0 -1 -1 0 -1 0 0 0 0 0 0 1

ITU= 1 1 1 0

Eigenvalues --- 0.00389 0.00696 0.01204 0.01316 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01317 0.01362

Eigenvalues --- 0.01431 0.01572 0.01582 0.01588 0.01598

Eigenvalues --- 0.01621 0.01696 0.01705 0.01708 0.01712

Eigenvalues --- 0.01716 0.01720 0.01779 0.01835 0.01870

Eigenvalues --- 0.01879 0.01919 0.01938 0.01954 0.01993

Eigenvalues --- 0.02003 0.02019 0.02023 0.02029 0.02039

Eigenvalues --- 0.02052 0.02053 0.02053 0.02056 0.02057

Eigenvalues --- 0.02057 0.02057 0.02058 0.02059 0.02061

Eigenvalues --- 0.02067 0.02067 0.02070 0.02070 0.02070

Eigenvalues --- 0.02078 0.02083 0.02088 0.02146 0.02184

Eigenvalues --- 0.02224 0.02237 0.02260 0.02260 0.02260

Eigenvalues --- 0.02261 0.02277 0.02320 0.02349 0.02351

Eigenvalues --- 0.02432 0.02456 0.02834 0.03689 0.05553

Eigenvalues --- 0.09920 0.09978 0.09979 0.09982 0.09985

Eigenvalues --- 0.09985 0.09989 0.10173 0.10642 0.10647

Eigenvalues --- 0.10647 0.10649 0.10657 0.10657 0.10659

Eigenvalues --- 0.10679 0.12604 0.13293 0.13466 0.15385

Eigenvalues --- 0.15940 0.15992 0.15999 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16002 0.16012 0.16022 0.16070 0.16255

Eigenvalues --- 0.16660 0.16992 0.20738 0.21686 0.22096

Eigenvalues --- 0.22474 0.22476 0.22478 0.22485 0.24197

Eigenvalues --- 0.24259 0.24508 0.24512 0.24554 0.24610

Eigenvalues --- 0.24697 0.24780 0.24817 0.24904 0.24912

Eigenvalues --- 0.24927 0.24983 0.24984 0.24989 0.24992

Eigenvalues --- 0.24995 0.24998 0.24998 0.24999 0.24999

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25004 0.25005 0.25021

Eigenvalues --- 0.25112 0.25387 0.26273 0.29088 0.30999

Eigenvalues --- 0.33406 0.33650 0.33682 0.33720 0.33951

Eigenvalues --- 0.34062 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34067 0.34074 0.34081 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34082 0.34089

Eigenvalues --- 0.34540 0.34632 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34687 0.34700 0.34937

Eigenvalues --- 0.35109 0.35166 0.35612 0.35632 0.35632

Eigenvalues --- 0.35632 0.35632 0.35633 0.35642 0.36305

Eigenvalues --- 0.36599 0.37046 0.37134 0.37564 0.40528

Eigenvalues --- 0.41215 0.41215 0.41215 0.41215 0.41217

Eigenvalues --- 0.41220 0.41299 0.41411 0.41414 0.41418

Eigenvalues --- 0.41440 0.41659 0.41897 0.42245 0.42475

Eigenvalues --- 0.43263 0.44513 0.44562 0.44724 0.44814

Eigenvalues --- 0.44878 0.44999 0.45002 0.45004 0.45004

Eigenvalues --- 0.45365 0.45366 0.45657 0.46038 0.46884

Eigenvalues --- 0.47301 0.47433 0.49309 0.49387 0.49764

Eigenvalues --- 0.49860 0.51275 0.53553 0.53554 0.53554

Eigenvalues --- 0.53555 0.53558 0.53684 0.54732 0.55015

Eigenvalues --- 0.56082 0.56822 0.57415 0.57564 0.58181

Eigenvalues --- 0.63935

En-DIIS/RFO-DIIS IScMMF= 0 using points: 24 23 22 21 20

RFO step: Lambda=-2.37216904D-07.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 1.82D-05 SmlDif= 1.00D-05

RMS Error= 0.4289434850D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.95274 0.15301 -0.13246 0.02551 0.00120

Iteration 1 RMS(Cart)= 0.00248847 RMS(Int)= 0.00000077

Iteration 2 RMS(Cart)= 0.00000258 RMS(Int)= 0.00000005

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000005

ITry= 1 IFail=0 DXMaxC= 1.23D-02 DCOld= 1.00D+10 DXMaxT= 2.35D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58254 -0.00001 0.00000 -0.00004 -0.00004 2.58250

R2 2.73964 0.00001 0.00001 -0.00002 -0.00002 2.73962

R3 2.56147 -0.00003 0.00000 -0.00003 -0.00003 2.56143

R4 2.58242 0.00001 0.00000 -0.00003 -0.00003 2.58240

R5 3.86946 -0.00001 0.00003 -0.00011 -0.00009 3.86938

R6 2.73966 0.00001 0.00002 -0.00002 0.00000 2.73966

R7 2.56147 -0.00002 0.00002 -0.00006 -0.00004 2.56144

R8 2.69556 0.00001 -0.00003 0.00004 0.00001 2.69557

R9 2.66241 0.00003 0.00000 0.00002 0.00002 2.66243

R10 2.66241 0.00003 0.00000 0.00003 0.00002 2.66243

R11 2.48241 0.00000 0.00005 -0.00011 -0.00005 2.48235

R12 2.59619 0.00000 0.00002 -0.00001 0.00001 2.59620

R13 2.79444 0.00005 0.00001 0.00007 0.00008 2.79452

R14 2.59612 0.00001 0.00001 0.00003 0.00004 2.59616

R15 3.84165 0.00000 -0.00001 0.00007 0.00006 3.84171

R16 2.79449 0.00001 0.00000 0.00000 -0.00001 2.79449

R17 2.48239 0.00000 0.00003 -0.00007 -0.00004 2.48235

R18 2.66402 0.00000 0.00001 -0.00002 -0.00001 2.66401

R19 2.64565 0.00001 0.00000 -0.00001 -0.00001 2.64564

R20 2.64568 0.00001 0.00001 -0.00003 -0.00002 2.64565

R21 2.48240 0.00001 0.00003 -0.00007 -0.00004 2.48236

R22 2.66399 0.00001 0.00000 0.00002 0.00001 2.66401

R23 2.79449 0.00003 0.00000 0.00004 0.00004 2.79452

R24 2.64565 0.00002 0.00000 0.00000 0.00000 2.64565

R25 2.79441 0.00004 -0.00002 0.00007 0.00006 2.79447

R26 2.64566 0.00001 -0.00001 -0.00001 -0.00001 2.64565

R27 2.59619 0.00000 0.00001 -0.00002 0.00000 2.59618

R28 2.48239 0.00001 0.00001 -0.00003 -0.00002 2.48237

R29 2.59616 0.00001 0.00002 -0.00001 0.00001 2.59617

R30 3.84177 0.00001 -0.00002 0.00001 0.00000 3.84177

R31 2.56143 -0.00001 -0.00001 0.00003 0.00001 2.56144

R32 2.58241 0.00000 0.00000 -0.00003 -0.00003 2.58238

R33 2.58259 -0.00002 0.00001 -0.00010 -0.00009 2.58250

R34 3.86962 -0.00001 0.00002 -0.00020 -0.00018 3.86944

R35 2.73966 0.00001 0.00000 -0.00001 -0.00001 2.73965

R36 2.69554 0.00001 -0.00003 0.00006 0.00002 2.69557

R37 2.66241 0.00003 0.00000 0.00002 0.00002 2.66242

R38 2.73964 0.00000 0.00001 -0.00004 -0.00003 2.73962

R39 2.66241 0.00003 0.00000 0.00002 0.00001 2.66243

R40 2.56149 -0.00004 0.00001 -0.00008 -0.00007 2.56142

R41 2.65604 0.00001 -0.00001 0.00002 0.00002 2.65606

R42 2.54966 0.00000 0.00000 0.00002 0.00003 2.54969

R43 2.62943 0.00000 -0.00001 0.00004 0.00003 2.62946

R44 2.04425 0.00000 0.00000 0.00000 0.00000 2.04425

R45 2.65603 0.00001 -0.00001 0.00003 0.00003 2.65605

R46 2.04423 0.00001 0.00000 0.00002 0.00002 2.04425

R47 2.54966 0.00000 0.00001 0.00002 0.00002 2.54968

R48 2.64328 0.00002 -0.00001 0.00003 0.00002 2.64330

R49 2.55234 0.00004 -0.00001 0.00006 0.00006 2.55240

R50 2.64702 0.00000 0.00000 0.00003 0.00003 2.64705

R51 2.04406 -0.00001 0.00000 -0.00001 -0.00002 2.04404

R52 2.64326 0.00002 -0.00001 0.00005 0.00004 2.64330

R53 2.04407 -0.00001 0.00000 -0.00002 -0.00003 2.04405

R54 2.55232 0.00005 0.00000 0.00007 0.00007 2.55238

R55 2.65604 0.00001 -0.00001 0.00003 0.00002 2.65606

R56 2.54967 -0.00001 0.00000 0.00001 0.00001 2.54968

R57 2.62943 0.00000 -0.00001 0.00004 0.00003 2.62946

R58 2.04423 0.00001 0.00000 0.00002 0.00002 2.04425

R59 2.65603 0.00001 -0.00001 0.00003 0.00002 2.65605

R60 2.04425 0.00000 0.00000 0.00000 0.00000 2.04425

R61 2.54966 0.00001 0.00000 0.00004 0.00004 2.54970

R62 2.64327 0.00002 -0.00001 0.00003 0.00003 2.64330

R63 2.55234 0.00004 -0.00001 0.00006 0.00006 2.55239

R64 2.64702 0.00000 0.00000 0.00002 0.00002 2.64704

R65 2.04406 -0.00001 0.00000 -0.00002 -0.00002 2.04404

R66 2.64327 0.00002 -0.00001 0.00003 0.00002 2.64330

R67 2.04407 -0.00001 0.00000 -0.00002 -0.00002 2.04405

R68 2.55232 0.00004 -0.00001 0.00006 0.00005 2.55238

R69 2.69385 0.00001 0.00000 0.00002 0.00002 2.69387

R70 2.69389 0.00000 0.00000 0.00001 0.00001 2.69390

R71 2.69565 0.00000 0.00000 0.00001 0.00001 2.69566

R72 2.69567 0.00000 0.00001 0.00001 0.00001 2.69568

R73 2.69389 0.00000 0.00000 0.00001 0.00001 2.69390

R74 2.69385 0.00001 0.00000 0.00002 0.00002 2.69387

R75 2.69564 0.00000 0.00001 0.00001 0.00002 2.69566

R76 2.69567 0.00000 0.00001 0.00001 0.00001 2.69568

R77 2.06727 0.00000 -0.00001 0.00000 -0.00001 2.06726

R78 2.06741 -0.00001 -0.00001 -0.00002 -0.00003 2.06738

R79 2.05684 0.00001 0.00000 0.00002 0.00002 2.05686

R80 2.06715 0.00000 -0.00001 0.00001 0.00000 2.06715

R81 2.06744 0.00000 -0.00001 0.00000 -0.00001 2.06743

R82 2.05669 0.00000 -0.00001 0.00000 0.00000 2.05669

R83 2.06743 0.00000 -0.00001 0.00000 -0.00001 2.06743

R84 2.06715 0.00000 -0.00001 0.00001 0.00000 2.06715

R85 2.05669 0.00000 0.00000 0.00000 0.00000 2.05669

R86 2.06738 -0.00001 -0.00001 -0.00001 -0.00002 2.06736

R87 2.06728 0.00000 -0.00001 0.00001 -0.00001 2.06727

R88 2.05684 0.00000 0.00000 0.00002 0.00002 2.05686

R89 2.06744 0.00000 -0.00001 0.00000 -0.00001 2.06743

R90 2.06715 0.00000 -0.00001 0.00001 0.00000 2.06715

R91 2.05669 0.00000 0.00000 0.00001 0.00000 2.05669

R92 2.06715 0.00000 -0.00001 0.00001 0.00000 2.06715

R93 2.06744 0.00000 -0.00001 0.00000 -0.00001 2.06743

R94 2.05670 0.00000 0.00000 0.00000 0.00000 2.05669

R95 2.06728 0.00000 -0.00001 0.00000 -0.00001 2.06726

R96 2.06741 -0.00001 -0.00001 -0.00002 -0.00003 2.06738

R97 2.05684 0.00001 0.00000 0.00002 0.00002 2.05686

R98 2.06738 -0.00001 -0.00001 -0.00001 -0.00002 2.06736

R99 2.06728 0.00000 -0.00001 0.00001 -0.00001 2.06727

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A3 2.17911 -0.00001 -0.00001 0.00002 0.00001 2.17912

A4 1.93090 -0.00004 0.00000 -0.00003 -0.00002 1.93087

A5 2.17270 0.00002 0.00002 0.00002 0.00004 2.17274

A6 2.17273 0.00002 0.00001 0.00009 0.00010 2.17283

A7 1.88904 0.00003 -0.00001 0.00004 0.00003 1.88907

A8 2.21492 -0.00003 0.00000 -0.00006 -0.00006 2.21486

A9 2.17914 -0.00001 0.00001 0.00001 0.00001 2.17915

A10 1.85792 -0.00002 0.00001 -0.00004 -0.00003 1.85788

A11 2.31710 0.00002 0.00000 0.00004 0.00005 2.31715

A12 2.10801 -0.00001 -0.00001 0.00000 0.00000 2.10801

A13 1.85789 -0.00001 0.00000 -0.00001 0.00000 1.85788

A14 2.31716 0.00001 -0.00001 0.00000 -0.00001 2.31716

A15 2.10798 0.00000 0.00000 0.00001 0.00002 2.10800

A16 2.18692 0.00002 0.00001 0.00009 0.00010 2.18702

A17 2.23309 -0.00001 0.00000 -0.00001 -0.00001 2.23308

A18 2.16621 0.00003 -0.00001 0.00010 0.00010 2.16630

A19 1.88351 -0.00002 0.00000 -0.00009 -0.00008 1.88343

A20 1.93241 0.00002 -0.00001 0.00009 0.00008 1.93249

A21 2.16278 0.00000 0.00000 -0.00001 -0.00001 2.16277

A22 2.16288 -0.00002 0.00001 -0.00016 -0.00015 2.16273

A23 1.88351 -0.00001 0.00001 -0.00006 -0.00005 1.88346

A24 2.23301 0.00001 0.00001 0.00006 0.00007 2.23307

A25 2.16629 0.00000 -0.00002 0.00002 -0.00001 2.16628

A26 1.86261 0.00000 0.00000 0.00002 0.00002 1.86263

A27 2.30404 -0.00001 0.00000 -0.00007 -0.00007 2.30397

A28 2.11647 0.00001 0.00000 0.00005 0.00005 2.11652

A29 1.86261 0.00000 0.00000 0.00003 0.00003 1.86264

A30 2.30399 0.00001 0.00001 0.00000 0.00001 2.30401

A31 2.11651 -0.00002 -0.00001 -0.00003 -0.00004 2.11647

A32 2.18696 0.00003 0.00000 0.00011 0.00010 2.18706

A33 1.86261 0.00000 0.00000 0.00001 0.00001 1.86263

A34 2.11646 0.00000 0.00000 0.00002 0.00001 2.11648

A35 2.30404 0.00000 0.00000 -0.00003 -0.00002 2.30402

A36 1.86260 0.00001 0.00000 0.00004 0.00004 1.86264

A37 2.11652 -0.00001 0.00001 -0.00002 -0.00001 2.11651

A38 2.30399 0.00000 -0.00001 -0.00002 -0.00003 2.30397

A39 1.88355 -0.00002 0.00002 -0.00011 -0.00009 1.88346

A40 2.16618 0.00002 -0.00004 0.00012 0.00008 2.16626

A41 2.23307 0.00000 0.00001 0.00002 0.00003 2.23310

A42 1.93236 0.00003 -0.00003 0.00014 0.00012 1.93248

A43 2.16292 -0.00002 0.00002 -0.00014 -0.00013 2.16279

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A51 2.17259 0.00003 0.00002 0.00010 0.00012 2.17271

A52 2.21491 -0.00002 0.00001 -0.00006 -0.00005 2.21486

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A56 2.31711 0.00002 -0.00001 0.00004 0.00004 2.31714

A57 2.10802 0.00000 0.00001 -0.00001 0.00000 2.10802

A58 1.85790 -0.00001 0.00000 -0.00002 -0.00002 1.85788

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A63 2.17907 -0.00001 -0.00001 0.00004 0.00004 2.17910

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A68 1.55925 0.00001 -0.00003 0.00014 0.00011 1.55936

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A70 2.07258 0.00003 -0.00001 0.00005 0.00004 2.07263

A71 2.16562 -0.00004 0.00001 -0.00005 -0.00005 2.16558

A72 2.12174 0.00000 0.00000 -0.00001 -0.00001 2.12173

A73 2.09919 -0.00001 0.00001 -0.00004 -0.00003 2.09917

A74 2.06225 0.00001 -0.00002 0.00005 0.00003 2.06228

A75 2.12174 0.00000 0.00000 -0.00002 -0.00002 2.12173

A76 2.06226 0.00001 -0.00002 0.00005 0.00003 2.06229

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A78 2.04494 0.00001 0.00000 0.00002 0.00002 2.04496

A79 2.07262 0.00002 -0.00001 0.00003 0.00002 2.07264

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A81 2.05212 -0.00001 0.00001 -0.00003 -0.00002 2.05210

A82 2.06564 -0.00001 -0.00002 -0.00001 -0.00003 2.06560

A83 2.16542 0.00001 0.00002 0.00004 0.00006 2.16548

A84 2.12308 0.00000 0.00000 0.00000 0.00000 2.12308

A85 2.10062 0.00001 0.00001 0.00001 0.00002 2.10064

A86 2.05948 -0.00001 -0.00001 -0.00001 -0.00002 2.05946

A87 2.12304 0.00001 -0.00001 0.00003 0.00002 2.12306

A88 2.05945 -0.00001 -0.00001 0.00000 -0.00001 2.05944

A89 2.10069 0.00000 0.00002 -0.00002 -0.00001 2.10068

A90 2.05212 -0.00001 0.00000 -0.00003 -0.00002 2.05210

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A92 2.16543 0.00001 0.00002 0.00002 0.00005 2.16548

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A94 2.07262 0.00003 0.00001 0.00002 0.00003 2.07265

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A98 2.06225 0.00001 -0.00002 0.00004 0.00003 2.06228

A99 2.12174 0.00000 0.00000 -0.00002 -0.00002 2.12172

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A102 2.04497 0.00000 0.00000 -0.00001 -0.00001 2.04496

A103 2.07259 0.00002 0.00000 0.00002 0.00002 2.07261

A104 2.16561 -0.00003 0.00000 -0.00001 -0.00001 2.16560

A105 2.05212 0.00000 0.00000 -0.00002 -0.00001 2.05210

A106 2.06564 -0.00001 -0.00002 -0.00002 -0.00003 2.06561

A107 2.16542 0.00001 0.00001 0.00003 0.00005 2.16547

A108 2.12308 0.00000 -0.00001 0.00000 0.00000 2.12308

A109 2.10061 0.00001 0.00001 0.00002 0.00003 2.10064

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A111 2.12304 0.00001 0.00000 0.00002 0.00001 2.12306

A112 2.05944 -0.00001 -0.00001 0.00001 0.00000 2.05944

A113 2.10069 0.00000 0.00001 -0.00003 -0.00001 2.10068

A114 2.05212 0.00000 0.00001 -0.00002 -0.00001 2.05211

A115 2.06560 0.00001 -0.00002 0.00002 0.00001 2.06561

A116 2.16546 0.00000 0.00001 0.00000 0.00000 2.16546

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A118 2.06543 0.00009 0.00002 0.00017 0.00019 2.06562

A119 2.06937 -0.00001 0.00001 -0.00003 -0.00002 2.06935

A120 2.06928 0.00002 0.00002 0.00004 0.00006 2.06934

A121 2.06544 0.00008 0.00002 0.00015 0.00018 2.06562

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A126 1.94715 0.00001 -0.00001 0.00003 0.00003 1.94718

A127 1.84229 0.00002 -0.00001 0.00004 0.00003 1.84232

A128 1.91156 0.00000 0.00002 0.00007 0.00010 1.91166

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A130 1.90817 -0.00001 -0.00001 -0.00004 -0.00005 1.90812

A131 1.94765 -0.00001 -0.00001 -0.00002 -0.00002 1.94763

A132 1.94496 -0.00001 -0.00001 -0.00002 -0.00003 1.94494

A133 1.84039 0.00001 0.00002 -0.00003 -0.00001 1.84039

A134 1.91252 0.00000 0.00000 0.00001 0.00001 1.91253

A135 1.90782 0.00000 0.00000 0.00001 0.00001 1.90783

A136 1.90883 0.00000 0.00000 0.00004 0.00004 1.90887

A137 1.94489 0.00000 -0.00002 0.00007 0.00006 1.94495

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A139 1.84046 0.00000 0.00002 -0.00010 -0.00007 1.84039

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A141 1.90887 0.00000 0.00000 0.00002 0.00002 1.90889

A142 1.90784 0.00000 0.00000 -0.00001 -0.00002 1.90782

A143 1.94716 0.00001 -0.00001 0.00005 0.00004 1.94720

A144 1.94451 -0.00002 0.00003 -0.00009 -0.00007 1.94445

A145 1.84235 0.00001 -0.00001 -0.00001 -0.00002 1.84233

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A148 1.90849 0.00000 -0.00003 0.00004 0.00001 1.90850

A149 1.94491 0.00000 -0.00001 0.00003 0.00002 1.94493

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A153 1.90887 0.00000 0.00000 0.00002 0.00002 1.90889

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A155 1.94766 -0.00001 0.00000 -0.00004 -0.00004 1.94761

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A157 1.84040 0.00001 0.00002 -0.00004 -0.00002 1.84038

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A159 1.90783 0.00000 0.00000 -0.00001 -0.00001 1.90782

A160 1.90883 0.00000 0.00000 0.00004 0.00004 1.90887

A161 1.94459 -0.00002 0.00003 -0.00012 -0.00009 1.94450

A162 1.94716 0.00001 -0.00001 0.00002 0.00001 1.94717

A163 1.84228 0.00002 -0.00001 0.00005 0.00004 1.84233

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A165 1.90852 0.00000 -0.00002 0.00000 -0.00002 1.90850

A166 1.90817 -0.00001 -0.00001 -0.00003 -0.00004 1.90813

A167 1.94715 0.00002 -0.00001 0.00005 0.00004 1.94720

A168 1.94453 -0.00002 0.00003 -0.00010 -0.00008 1.94445

A169 1.84234 0.00001 -0.00001 0.00001 -0.00001 1.84233

A170 1.91152 0.00000 0.00002 0.00008 0.00010 1.91162

A171 1.90826 -0.00001 -0.00001 -0.00006 -0.00007 1.90818

A172 1.90849 0.00000 -0.00002 0.00003 0.00001 1.90849

A173 3.11868 0.00001 -0.00004 0.00018 0.00014 3.11883

A174 3.11869 0.00001 -0.00004 0.00017 0.00014 3.11883

A175 3.33469 -0.00002 0.00007 -0.00041 -0.00033 3.33435

A176 2.90717 0.00001 -0.00009 0.00044 0.00035 2.90752

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D2 3.02382 0.00002 0.00026 0.00121 0.00147 3.02529

D3 3.13128 0.00000 0.00007 -0.00036 -0.00029 3.13100

D4 -0.13131 0.00000 0.00037 0.00040 0.00077 -0.13054

D5 -0.00207 -0.00001 0.00005 -0.00017 -0.00012 -0.00219

D6 -3.12415 -0.00001 -0.00008 -0.00066 -0.00074 -3.12489

D7 -3.13047 0.00001 -0.00006 0.00062 0.00056 -3.12991

D8 0.03064 0.00001 -0.00019 0.00013 -0.00006 0.03058

D9 0.17309 0.00000 -0.00028 -0.00021 -0.00049 0.17260

D10 -2.98417 -0.00002 -0.00015 -0.00115 -0.00130 -2.98547

D11 -0.00308 -0.00002 0.00001 -0.00055 -0.00054 -0.00362

D12 -3.13100 0.00000 -0.00008 0.00035 0.00027 -3.13073

D13 -3.02367 -0.00003 -0.00029 -0.00130 -0.00159 -3.02526

D14 0.13160 -0.00001 -0.00038 -0.00040 -0.00078 0.13081

D15 -2.95566 -0.00001 -0.00012 -0.00073 -0.00084 -2.95650

D16 -0.04851 0.00000 -0.00021 -0.00027 -0.00048 -0.04899

D17 0.04845 0.00000 0.00023 0.00012 0.00035 0.04880

D18 2.95560 0.00000 0.00013 0.00058 0.00071 2.95631

D19 0.00168 0.00001 0.00002 0.00042 0.00044 0.00212

D20 3.12376 0.00002 0.00013 0.00080 0.00093 3.12469

D21 3.12994 0.00000 0.00011 -0.00045 -0.00034 3.12960

D22 -0.03115 0.00000 0.00022 -0.00007 0.00015 -0.03101

D23 -0.17354 0.00001 0.00027 0.00045 0.00072 -0.17282

D24 2.98388 0.00003 0.00016 0.00149 0.00165 2.98553

D25 0.00024 -0.00001 -0.00004 -0.00015 -0.00019 0.00004

D26 3.12515 0.00000 0.00007 0.00027 0.00034 3.12549

D27 -3.12469 -0.00001 -0.00014 -0.00047 -0.00061 -3.12530

D28 0.00023 0.00000 -0.00002 -0.00006 -0.00008 0.00015

D29 -3.12453 0.00000 -0.00009 -0.00054 -0.00063 -3.12516

D30 0.01366 0.00001 -0.00016 -0.00019 -0.00036 0.01330

D31 -0.00471 0.00000 0.00003 -0.00011 -0.00008 -0.00480

D32 3.13348 0.00001 -0.00004 0.00023 0.00019 3.13367

D33 3.12421 0.00001 0.00015 0.00073 0.00088 3.12509

D34 -0.01409 0.00000 0.00022 0.00036 0.00058 -0.01350

D35 0.00441 0.00000 0.00000 0.00018 0.00018 0.00459

D36 -3.13390 -0.00001 0.00007 -0.00018 -0.00011 -3.13401

D37 -0.05184 0.00000 -0.00001 -0.00018 -0.00020 -0.05203

D38 3.12296 0.00000 0.00021 -0.00061 -0.00039 3.12256

D39 -3.09737 -0.00002 -0.00006 -0.00044 -0.00051 -3.09787

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D41 0.01534 -0.00002 -0.00026 -0.00007 -0.00033 0.01501

D42 -2.89496 -0.00001 -0.00027 0.00029 0.00002 -2.89494

D43 3.10488 0.00001 -0.00003 0.00066 0.00064 3.10551

D44 -0.02387 0.00002 -0.00001 0.00063 0.00062 -0.02325

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D46 -3.13795 0.00002 0.00018 0.00028 0.00046 -3.13749

D47 -0.01525 0.00001 0.00026 -0.00019 0.00007 -0.01518

D48 3.09722 0.00001 0.00005 0.00041 0.00045 3.09767

D49 2.89504 0.00001 0.00026 -0.00053 -0.00027 2.89477

D50 -0.27568 0.00001 0.00005 0.00007 0.00012 -0.27556

D51 -0.22722 0.00001 -0.00003 0.00009 0.00006 -0.22716

D52 3.10749 -0.00001 0.00005 -0.00034 -0.00029 3.10720

D53 -3.10745 0.00001 -0.00003 0.00047 0.00043 -3.10702

D54 0.22726 -0.00001 0.00004 0.00004 0.00008 0.22734

D55 0.00895 0.00000 -0.00014 0.00038 0.00023 0.00919

D56 3.13776 -0.00001 -0.00017 0.00031 0.00014 3.13790

D57 -3.10489 0.00000 0.00006 -0.00019 -0.00014 -3.10503

D58 0.02391 -0.00001 0.00003 -0.00026 -0.00023 0.02369

D59 0.05217 0.00000 0.00001 0.00003 0.00004 0.05221

D60 -3.12290 0.00000 -0.00023 0.00072 0.00049 -3.12241

D61 0.00015 -0.00001 -0.00001 -0.00041 -0.00042 -0.00027

D62 3.13058 -0.00001 -0.00003 -0.00038 -0.00041 3.13017

D63 -3.13033 0.00000 0.00001 -0.00035 -0.00034 -3.13067

D64 0.00010 -0.00001 0.00000 -0.00033 -0.00033 -0.00023

D65 -3.12625 0.00001 -0.00003 0.00025 0.00023 -3.12603

D66 0.02046 0.00000 -0.00007 0.00029 0.00022 0.02068

D67 0.00101 0.00000 -0.00006 0.00018 0.00013 0.00114

D68 -3.13546 0.00000 -0.00010 0.00022 0.00012 -3.13534

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D70 -0.02066 0.00001 0.00008 0.00042 0.00050 -0.02016

D71 -0.00113 0.00001 0.00006 0.00021 0.00027 -0.00086

D72 3.13532 0.00002 0.00010 0.00039 0.00049 3.13581

D73 -3.12285 0.00000 -0.00019 0.00058 0.00039 -3.12246

D74 0.05220 0.00000 0.00004 -0.00006 -0.00001 0.05218

D75 -0.00024 0.00001 0.00000 0.00037 0.00036 0.00012

D76 3.13022 0.00000 -0.00002 0.00033 0.00031 3.13053

D77 -3.13063 0.00001 0.00002 0.00025 0.00026 -3.13037

D78 -0.00017 0.00000 0.00000 0.00022 0.00021 0.00004

D79 -3.10463 -0.00002 0.00005 -0.00072 -0.00067 -3.10529

D80 0.00924 -0.00001 -0.00014 -0.00019 -0.00033 0.00891

D81 0.02408 -0.00002 0.00003 -0.00059 -0.00055 0.02353

D82 3.13795 -0.00001 -0.00016 -0.00006 -0.00022 3.13773

D83 0.00115 0.00000 -0.00005 -0.00013 -0.00017 0.00098

D84 -3.13529 -0.00001 -0.00008 -0.00015 -0.00023 -3.13553

D85 -3.12600 0.00000 -0.00002 -0.00028 -0.00030 -3.12630

D86 0.02074 -0.00001 -0.00006 -0.00030 -0.00036 0.02037

D87 -0.00884 0.00000 0.00015 -0.00042 -0.00028 -0.00912

D88 3.10504 0.00001 -0.00006 0.00032 0.00026 3.10530

D89 -3.13763 0.00000 0.00017 -0.00038 -0.00022 -3.13784

D90 -0.02374 0.00001 -0.00004 0.00036 0.00032 -0.02343

D91 -0.00095 0.00000 0.00005 -0.00013 -0.00008 -0.00103

D92 3.13563 0.00000 0.00009 -0.00021 -0.00012 3.13551

D93 3.12630 -0.00001 0.00003 -0.00017 -0.00014 3.12615

D94 -0.02032 0.00000 0.00007 -0.00025 -0.00018 -0.02050

D95 0.01516 -0.00001 -0.00024 0.00031 0.00007 0.01522

D96 -2.89518 0.00000 -0.00026 0.00067 0.00042 -2.89476

D97 -3.09734 -0.00002 -0.00003 -0.00047 -0.00050 -3.09784

D98 0.27551 -0.00001 -0.00004 -0.00011 -0.00015 0.27536

D99 3.12322 -0.00001 0.00023 -0.00108 -0.00085 3.12236

D100 -0.05181 0.00000 -0.00002 -0.00018 -0.00021 -0.05202

D101 3.09718 0.00002 0.00004 0.00048 0.00051 3.09769

D102 -0.01531 0.00001 0.00024 -0.00008 0.00016 -0.01515

D103 -0.27565 0.00001 0.00005 0.00010 0.00015 -0.27549

D104 2.89505 0.00000 0.00026 -0.00046 -0.00020 2.89485

D105 3.10750 -0.00001 0.00003 -0.00034 -0.00030 3.10720

D106 -0.22718 0.00001 -0.00004 0.00007 0.00003 -0.22716

D107 0.22721 -0.00001 0.00002 0.00005 0.00007 0.22728

D108 -3.10747 0.00001 -0.00005 0.00045 0.00040 -3.10707

D109 -0.17357 0.00001 0.00024 0.00052 0.00076 -0.17280

D110 2.98419 0.00002 0.00020 0.00081 0.00102 2.98521

D111 -3.13098 0.00000 -0.00003 0.00030 0.00027 -3.13071

D112 -0.00336 -0.00001 0.00000 0.00005 0.00005 -0.00331

D113 0.13167 -0.00001 -0.00034 -0.00055 -0.00089 0.13078

D114 -3.02389 -0.00001 -0.00031 -0.00080 -0.00111 -3.02500

D115 0.00339 0.00001 0.00003 -0.00007 -0.00004 0.00335

D116 3.13127 0.00000 0.00006 -0.00038 -0.00032 3.13095

D117 3.02395 0.00001 0.00034 0.00077 0.00111 3.02506

D118 -0.13135 0.00000 0.00037 0.00046 0.00083 -0.13052

D119 2.95555 0.00000 0.00012 0.00067 0.00079 2.95634

D120 0.04838 0.00000 0.00021 0.00023 0.00044 0.04882

D121 -0.04851 0.00000 -0.00023 -0.00029 -0.00052 -0.04903

D122 -2.95568 -0.00001 -0.00014 -0.00073 -0.00087 -2.95655

D123 3.12995 0.00000 0.00000 -0.00026 -0.00026 3.12969

D124 -0.03110 0.00000 0.00016 -0.00007 0.00009 -0.03100

D125 0.00196 0.00000 -0.00003 -0.00001 -0.00004 0.00192

D126 3.12410 0.00000 0.00013 0.00018 0.00031 3.12441

D127 0.00005 0.00000 0.00005 -0.00003 0.00002 0.00006

D128 3.12512 0.00000 0.00017 0.00013 0.00030 3.12542

D129 -3.12493 0.00000 -0.00009 -0.00019 -0.00028 -3.12521

D130 0.00015 0.00000 0.00003 -0.00003 0.00000 0.00015

D131 -3.12448 0.00000 -0.00018 -0.00044 -0.00062 -3.12510

D132 0.01379 0.00000 -0.00023 -0.00031 -0.00054 0.01325

D133 -0.00460 0.00000 0.00000 -0.00022 -0.00022 -0.00483

D134 3.13367 0.00000 -0.00006 -0.00010 -0.00015 3.13352

D135 -0.00204 -0.00001 -0.00005 0.00006 0.00001 -0.00203

D136 -3.13028 0.00000 -0.00008 0.00036 0.00029 -3.12999

D137 -3.12430 0.00000 -0.00019 -0.00013 -0.00032 -3.12462

D138 0.03065 0.00000 -0.00022 0.00017 -0.00004 0.03060

D139 0.00440 0.00000 -0.00003 0.00026 0.00022 0.00462

D140 -3.13404 0.00000 0.00001 0.00021 0.00021 -3.13383

D141 3.12441 0.00000 0.00012 0.00047 0.00059 3.12500

D142 -0.01403 0.00000 0.00016 0.00042 0.00058 -0.01345

D143 0.17315 0.00000 -0.00025 -0.00031 -0.00056 0.17260

D144 -2.98430 -0.00001 -0.00021 -0.00067 -0.00088 -2.98518

D145 -0.00103 0.00000 0.00005 -0.00004 0.00001 -0.00102

D146 -3.13791 0.00000 -0.00002 0.00015 0.00012 -3.13778

D147 3.13512 0.00001 0.00008 -0.00001 0.00007 3.13519

D148 -0.00176 0.00001 0.00001 0.00017 0.00019 -0.00157

D149 -3.09901 0.00001 0.00008 0.00049 0.00058 -3.09844

D150 0.04811 0.00001 0.00004 0.00047 0.00051 0.04862

D151 -0.00009 0.00000 0.00000 0.00013 0.00013 0.00003

D152 -3.13696 0.00000 -0.00007 0.00018 0.00011 -3.13685

D153 3.13688 0.00000 0.00007 -0.00006 0.00001 3.13689

D154 0.00002 0.00000 0.00000 0.00000 0.00000 0.00001

D155 0.00108 0.00000 -0.00005 -0.00004 -0.00009 0.00099

D156 -3.13520 0.00000 -0.00009 0.00004 -0.00005 -3.13525

D157 3.13785 0.00000 0.00002 -0.00010 -0.00007 3.13777

D158 0.00157 0.00000 -0.00002 -0.00001 -0.00003 0.00154

D159 3.09937 -0.00001 -0.00007 -0.00036 -0.00043 3.09894

D160 -0.04762 -0.00001 -0.00003 -0.00044 -0.00047 -0.04809

D161 -0.00452 0.00000 0.00001 -0.00023 -0.00022 -0.00474

D162 3.14137 0.00000 -0.00001 -0.00020 -0.00021 3.14115

D163 3.13372 0.00000 -0.00003 -0.00018 -0.00021 3.13350

D164 -0.00357 0.00000 -0.00005 -0.00015 -0.00021 -0.00378

D165 3.11409 0.00000 0.00001 -0.00006 -0.00004 3.11405

D166 -0.02413 0.00000 0.00006 -0.00011 -0.00005 -0.02418

D167 0.00003 0.00000 0.00002 -0.00002 -0.00001 0.00002

D168 -3.13730 0.00000 -0.00002 -0.00003 -0.00005 -3.13734

D169 3.13742 0.00000 0.00004 -0.00005 -0.00001 3.13740

D170 0.00009 0.00000 0.00000 -0.00006 -0.00005 0.00004

D171 0.00456 0.00000 -0.00002 0.00025 0.00023 0.00479

D172 -3.13351 0.00000 0.00004 0.00012 0.00015 -3.13335

D173 -3.14140 0.00000 0.00002 0.00026 0.00027 -3.14113

D174 0.00372 0.00000 0.00007 0.00012 0.00020 0.00391

D175 -3.11489 0.00001 0.00000 0.00025 0.00025 -3.11464

D176 0.02315 0.00001 -0.00006 0.00038 0.00033 0.02348

D177 0.00106 0.00000 -0.00006 0.00004 -0.00002 0.00104

D178 3.13784 0.00000 0.00002 -0.00007 -0.00005 3.13779

D179 -3.13509 -0.00001 -0.00010 -0.00015 -0.00025 -3.13535

D180 0.00169 -0.00001 -0.00002 -0.00026 -0.00028 0.00140

D181 3.09958 -0.00002 -0.00006 -0.00076 -0.00082 3.09876

D182 -0.04754 -0.00001 -0.00002 -0.00057 -0.00059 -0.04812

D183 0.00006 0.00000 0.00000 -0.00018 -0.00018 -0.00012

D184 3.13693 0.00000 0.00008 -0.00018 -0.00010 3.13682

D185 -3.13682 0.00000 -0.00008 -0.00007 -0.00015 -3.13697

D186 0.00005 0.00000 0.00000 -0.00007 -0.00007 -0.00002

D187 -0.00110 0.00000 0.00006 0.00007 0.00012 -0.00097

D188 3.13508 0.00001 0.00010 0.00003 0.00013 3.13521

D189 -3.13786 0.00000 -0.00002 0.00007 0.00005 -3.13782

D190 -0.00169 0.00000 0.00002 0.00003 0.00005 -0.00164

D191 -3.09892 0.00001 0.00007 0.00033 0.00040 -3.09852

D192 0.04817 0.00000 0.00003 0.00037 0.00040 0.04856

D193 -0.00459 0.00000 0.00002 -0.00015 -0.00013 -0.00472

D194 3.14143 0.00000 -0.00001 -0.00033 -0.00033 3.14110

D195 3.13351 0.00001 -0.00006 0.00024 0.00018 3.13369

D196 -0.00365 0.00000 -0.00008 0.00006 -0.00002 -0.00367

D197 3.11403 0.00000 -0.00006 0.00023 0.00017 3.11420

D198 -0.02404 -0.00001 0.00002 -0.00017 -0.00014 -0.02419

D199 0.00005 0.00000 -0.00001 -0.00002 -0.00003 0.00002

D200 -3.13721 -0.00001 -0.00002 -0.00019 -0.00021 -3.13742

D201 3.13732 0.00000 0.00001 0.00016 0.00016 3.13748

D202 0.00006 0.00000 0.00000 -0.00002 -0.00002 0.00004

D203 0.00462 0.00000 -0.00001 0.00015 0.00014 0.00476

D204 -3.13336 -0.00001 0.00007 -0.00022 -0.00015 -3.13351

D205 -3.14141 0.00000 0.00000 0.00033 0.00032 -3.14108

D206 0.00380 0.00000 0.00007 -0.00004 0.00003 0.00383

D207 -3.11472 0.00000 0.00000 -0.00004 -0.00004 -3.11476

D208 0.02323 0.00001 -0.00007 0.00033 0.00026 0.02349

D209 1.05242 0.00001 0.00005 0.00035 0.00039 1.05281

D210 -1.09004 0.00002 0.00000 0.00032 0.00033 -1.08971

D211 3.12231 0.00001 0.00003 0.00032 0.00035 3.12266

D212 1.08980 -0.00001 -0.00002 -0.00003 -0.00005 1.08975

D213 -1.05255 -0.00001 -0.00006 -0.00010 -0.00016 -1.05271

D214 -3.12240 -0.00001 -0.00004 -0.00009 -0.00013 -3.12253

D215 1.09324 0.00000 0.00002 0.00054 0.00056 1.09380

D216 -1.05108 0.00001 0.00004 0.00055 0.00059 -1.05049

D217 -3.12041 0.00001 0.00003 0.00053 0.00056 -3.11985

D218 1.05056 0.00000 -0.00005 -0.00030 -0.00035 1.05021

D219 -1.09366 -0.00001 -0.00004 -0.00037 -0.00041 -1.09407

D220 3.11994 0.00000 -0.00005 -0.00029 -0.00033 3.11960

D221 1.08982 -0.00001 -0.00001 -0.00002 -0.00003 1.08979

D222 -1.05254 -0.00001 -0.00006 -0.00008 -0.00013 -1.05267

D223 -3.12239 -0.00001 -0.00003 -0.00006 -0.00009 -3.12249

D224 1.05243 0.00001 0.00005 0.00033 0.00038 1.05281

D225 -1.09002 0.00002 0.00001 0.00030 0.00031 -1.08971

D226 3.12233 0.00001 0.00003 0.00029 0.00033 3.12266

D227 1.09334 0.00000 0.00003 0.00037 0.00040 1.09374

D228 -1.05096 0.00001 0.00004 0.00036 0.00040 -1.05056

D229 -3.12028 0.00000 0.00003 0.00032 0.00035 -3.11993

D230 1.05063 -0.00001 -0.00004 -0.00045 -0.00048 1.05015

D231 -1.09359 -0.00001 -0.00002 -0.00050 -0.00052 -1.09412

D232 3.12002 -0.00001 -0.00003 -0.00046 -0.00048 3.11954

Item Value Threshold Converged?

Maximum Force 0.000091 0.000450 YES

RMS Force 0.000014 0.000300 YES

Maximum Displacement 0.012299 0.001800 NO

RMS Displacement 0.002488 0.001200 NO

Predicted change in Energy=-4.568768D-07

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 03:32:47 2019, MaxMem= 1342177280 cpu: 16.2

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.25D-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 -1.124832 2.800312 -0.018184

2 7 0 -0.000753 2.037973 -0.169442

3 6 0 1.122627 2.801209 -0.018007

4 6 0 0.711535 4.165848 0.247680

5 6 0 -0.714901 4.165272 0.247526

6 7 0 2.408829 2.384125 -0.112763

7 6 0 2.797230 1.131459 -0.187127

8 7 0 2.018920 0.000809 -0.129448

9 6 0 2.798085 -1.129212 -0.187415

10 6 0 4.208549 -0.703210 -0.313518

11 6 0 4.208045 0.706523 -0.313099

12 7 0 -2.410693 2.382167 -0.112856

13 6 0 -4.208598 0.703160 -0.313189

14 6 0 -4.208016 -0.706573 -0.313257

15 6 0 -2.797230 -1.131468 -0.187122

16 7 0 -2.018925 -0.000827 -0.129385

17 6 0 -2.798114 1.129193 -0.187185

18 7 0 -2.408850 -2.384160 -0.112881

19 7 0 0.000717 -2.037964 -0.169586

20 6 0 -1.122635 -2.801233 -0.018201

21 6 0 -0.711534 -4.165817 0.247724

22 6 0 0.714898 -4.165232 0.247502

23 6 0 1.124804 -2.800315 -0.018459

24 7 0 2.410661 -2.382185 -0.113167

25 30 0 0.000010 0.000028 -0.367917

26 6 0 -5.401960 1.429277 -0.406367

27 6 0 -6.595665 0.693010 -0.498457

28 6 0 -6.595075 -0.698440 -0.498568

29 6 0 -5.400751 -1.433707 -0.406553

30 6 0 1.436401 -5.349125 0.498131

31 6 0 0.703075 -6.515586 0.739317

32 6 0 -0.697684 -6.516140 0.739633

33 6 0 -1.432015 -5.350247 0.498751

34 6 0 5.400870 1.433578 -0.405923

35 6 0 6.595134 0.698235 -0.498170

36 6 0 6.595603 -0.693214 -0.498784

37 6 0 5.401829 -1.429407 -0.407043

38 6 0 -1.436384 5.349237 0.497879

39 6 0 -0.703045 6.515753 0.738756

40 6 0 0.697710 6.516300 0.739007

41 6 0 1.432023 5.350350 0.498363

42 1 0 7.545513 1.209114 -0.575661

43 1 0 7.546324 -1.203392 -0.576750

44 1 0 1.205076 7.451038 0.936088

45 1 0 -1.211225 7.450092 0.935614

46 1 0 -7.546431 1.203137 -0.576209

47 1 0 -7.545398 -1.209372 -0.576414

48 1 0 -1.205034 -7.450820 0.937026

49 1 0 1.211267 -7.449862 0.936441

50 8 0 2.781459 5.292952 0.495876

51 8 0 -2.785787 5.290847 0.494717

52 8 0 5.340943 2.781478 -0.407752

53 8 0 5.342703 -2.777350 -0.410198

54 8 0 2.785803 -5.290675 0.495096

55 8 0 -2.781454 -5.292801 0.496484

56 8 0 -5.340651 -2.781600 -0.409184

57 8 0 -5.343005 2.777224 -0.408849

58 6 0 3.510246 6.484145 0.782380

59 1 0 3.274010 6.866743 1.779643

60 1 0 3.318386 7.261943 0.037343

61 1 0 4.560309 6.200172 0.744478

62 6 0 6.561611 3.518452 -0.448906

63 1 0 7.118295 3.324072 -1.370270

64 1 0 7.193517 3.294013 0.415524

65 1 0 6.268735 4.566251 -0.419614

66 6 0 6.563834 -3.513548 -0.451768

67 1 0 7.195522 -3.289361 0.412885

68 1 0 7.120486 -3.318126 -1.372931

69 1 0 6.271598 -4.561546 -0.423312

70 6 0 -3.515574 6.481358 0.781577

71 1 0 -3.323971 7.259729 0.037086

72 1 0 -3.279967 6.863563 1.779146

73 1 0 -4.565412 6.196632 0.743151

74 6 0 -6.564243 3.513270 -0.449963

75 1 0 -7.195851 3.288502 0.414597

76 1 0 -7.120915 3.318276 -1.371205

77 1 0 -6.272165 4.561295 -0.420933

78 6 0 -6.561220 -3.518696 -0.451043

79 1 0 -7.117754 -3.323770 -1.372381

80 1 0 -7.193322 -3.294921 0.413417

81 1 0 -6.268214 -4.566477 -0.422406

82 6 0 -3.510231 -6.483880 0.783484

83 1 0 -3.273835 -6.866185 1.780821

84 1 0 -3.318524 -7.261909 0.038649

85 1 0 -4.560292 -6.199886 0.745685

86 6 0 3.515608 -6.481062 0.782418

87 1 0 3.324146 -7.259660 0.038128

88 1 0 3.279887 -6.862982 1.780067

89 1 0 4.565439 -6.196295 0.744055

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0447624 0.0439733 0.0225229

Leave Link 202 at Sat Jul 6 03:32:48 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8042.1874167698 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= 89 NActive= 89 NUniq= 89 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= -0.2279762460 Hartrees.

Nuclear repulsion after empirical dispersion term = 8041.9594405238 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

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Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6399

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.69D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 400

GePol: Fraction of low-weight points (<1% of avg) = 6.25%

GePol: Cavity surface area = 703.208 Ang\*\*2

GePol: Cavity volume = 801.599 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0089846081 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8041.9504559157 Hartrees.

Leave Link 301 at Sat Jul 6 03:32:49 2019, MaxMem= 1342177280 cpu: 1.3

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44311 LenP2D= 111304.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.55D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 03:32:52 2019, MaxMem= 1342177280 cpu: 42.7

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 03:32:53 2019, MaxMem= 1342177280 cpu: 2.3

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000003 -0.000001 -0.000441 Ang= 0.05 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>= 2.0171 S= 1.0057

Leave Link 401 at Sat Jul 6 03:32:59 2019, MaxMem= 1342177280 cpu: 72.6

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 122841603.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.10D-15 for 6382.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.59D-15 for 6379 6005.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.77D-15 for 6382.

Iteration 1 A^-1\*A deviation from orthogonality is 5.80D-08 for 5834 5723.

Iteration 2 A\*A^-1 deviation from unit magnitude is 4.88D-15 for 69.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.90D-15 for 3565 1965.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 5.

Iteration 2 A^-1\*A deviation from orthogonality is 1.56D-15 for 6397 759.

E= -2649.79549803113

DIIS: error= 9.99D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79549803113 IErMin= 1 ErrMin= 9.99D-05

ErrMax= 9.99D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.78D-05 BMatP= 4.78D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.685 Goal= None Shift= 0.000

Gap= 0.744 Goal= None Shift= 0.000

RMSDP=5.06D-06 MaxDP=2.12D-04 OVMax= 6.05D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.06D-06 CP: 1.00D+00

E= -2649.79552031087 Delta-E= -0.000022279743 Rises=F Damp=F

DIIS: error= 1.27D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79552031087 IErMin= 2 ErrMin= 1.27D-05

ErrMax= 1.27D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.61D-07 BMatP= 4.78D-05

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= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=6.67D-07 MaxDP=4.14D-05 DE=-2.23D-05 OVMax= 9.75D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 5.98D-07 CP: 1.00D+00 1.06D+00

E= -2649.79552057418 Delta-E= -0.000000263306 Rises=F Damp=F

DIIS: error= 6.79D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79552057418 IErMin= 3 ErrMin= 6.79D-06

ErrMax= 6.79D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.92D-07 BMatP= 5.61D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.299D-01 0.417D+00 0.613D+00

Coeff: -0.299D-01 0.417D+00 0.613D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=3.36D-07 MaxDP=2.63D-05 DE=-2.63D-07 OVMax= 1.05D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.90D-07 CP: 1.00D+00 1.07D+00 7.26D-01

E= -2649.79552059438 Delta-E= -0.000000020200 Rises=F Damp=F

DIIS: error= 5.84D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79552059438 IErMin= 4 ErrMin= 5.84D-06

ErrMax= 5.84D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.08D-07 BMatP= 1.92D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.793D-02 0.896D-01 0.421D+00 0.497D+00

Coeff: -0.793D-02 0.896D-01 0.421D+00 0.497D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.55D-07 MaxDP=1.38D-05 DE=-2.02D-08 OVMax= 3.99D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 7.82D-08 CP: 1.00D+00 1.07D+00 8.43D-01 6.06D-01

E= -2649.79552061883 Delta-E= -0.000000024451 Rises=F Damp=F

DIIS: error= 1.13D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79552061883 IErMin= 5 ErrMin= 1.13D-06

ErrMax= 1.13D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.11D-09 BMatP= 1.08D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.930D-03 0.573D-03 0.129D+00 0.214D+00 0.658D+00

Coeff: -0.930D-03 0.573D-03 0.129D+00 0.214D+00 0.658D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=3.84D-08 MaxDP=3.08D-06 DE=-2.45D-08 OVMax= 9.72D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.06D-08 CP: 1.00D+00 1.07D+00 8.61D-01 6.25D-01 7.51D-01

E= -2649.79552061921 Delta-E= -0.000000000386 Rises=F Damp=F

DIIS: error= 5.99D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79552061921 IErMin= 6 ErrMin= 5.99D-07

ErrMax= 5.99D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.28D-09 BMatP= 3.11D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.580D-03-0.138D-01 0.202D-01 0.643D-01 0.433D+00 0.495D+00

Coeff: 0.580D-03-0.138D-01 0.202D-01 0.643D-01 0.433D+00 0.495D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.80D-08 MaxDP=1.18D-06 DE=-3.86D-10 OVMax= 7.73D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 7.36D-09 CP: 1.00D+00 1.07D+00 8.62D-01 6.41D-01 8.16D-01

CP: 5.13D-01

E= -2649.79552061959 Delta-E= -0.000000000377 Rises=F Damp=F

DIIS: error= 9.09D-08 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2649.79552061959 IErMin= 7 ErrMin= 9.09D-08

ErrMax= 9.09D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.88D-11 BMatP= 1.28D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.303D-03-0.622D-02 0.282D-02 0.187D-01 0.164D+00 0.223D+00

Coeff-Com: 0.597D+00

Coeff: 0.303D-03-0.622D-02 0.282D-02 0.187D-01 0.164D+00 0.223D+00

Coeff: 0.597D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=3.62D-09 MaxDP=2.11D-07 DE=-3.77D-10 OVMax= 2.34D-06

Error on total polarization charges = 0.07299

SCF Done: E(UB3LYP) = -2649.79552062 A.U. after 7 cycles

NFock= 7 Conv=0.36D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0171 S= 1.0057

<L.S>= 0.000000000000E+00

KE= 2.690148008078D+03 PE=-2.236262040619D+04 EE= 8.980726421578D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0171, after 2.0002

Leave Link 502 at Sat Jul 6 03:39:16 2019, MaxMem= 1342177280 cpu: 4419.0

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44311 LenP2D= 111304.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 274

Leave Link 701 at Sat Jul 6 03:39:37 2019, MaxMem= 1342177280 cpu: 229.8

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 03:39:37 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 03:41:14 2019, MaxMem= 1342177280 cpu: 1170.2

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 1.29871951D-04 2.34412192D-04 1.94447339D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000002942 0.000009553 -0.000010092

2 7 -0.000037428 -0.000074776 0.000030652

3 6 0.000001866 0.000028441 -0.000027627

4 6 0.000025192 -0.000004168 -0.000000029

5 6 -0.000015556 0.000000846 -0.000009815

6 7 -0.000012098 0.000015668 0.000015336

7 6 -0.000014998 -0.000025338 0.000003908

8 7 0.000011093 0.000016459 0.000027341

9 6 -0.000005484 0.000008840 -0.000018212

10 6 0.000004640 0.000013691 -0.000005077

11 6 0.000010516 -0.000006702 -0.000018431

12 7 0.000025297 0.000017894 -0.000010709

13 6 -0.000006145 -0.000010482 -0.000013810

14 6 -0.000013500 0.000010386 -0.000001154

15 6 0.000023220 0.000004088 -0.000039038

16 7 -0.000008849 -0.000009119 0.000034131

17 6 0.000002924 -0.000012088 0.000003377

18 7 0.000022648 -0.000004707 0.000011028

19 7 0.000043881 0.000071634 -0.000002006

20 6 -0.000014112 -0.000019433 0.000013797

21 6 -0.000025055 0.000002945 -0.000013950

22 6 0.000014693 -0.000004116 -0.000020242

23 6 -0.000001878 -0.000008740 0.000025391

24 7 -0.000030426 -0.000017199 -0.000017109

25 30 -0.000006047 -0.000004390 -0.000004678

26 6 0.000013618 0.000008893 0.000013466

27 6 -0.000008569 -0.000009886 0.000001533

28 6 -0.000008187 0.000007152 -0.000000211

29 6 0.000011218 -0.000001760 0.000016683

30 6 -0.000001158 0.000000752 -0.000003149

31 6 0.000005856 -0.000001944 0.000000480

32 6 0.000000700 -0.000003934 0.000001036

33 6 0.000005358 0.000000453 -0.000002685

34 6 -0.000009767 0.000001374 0.000023162

35 6 0.000007632 -0.000008355 -0.000002879

36 6 0.000008217 0.000007127 0.000003574

37 6 -0.000012742 -0.000012105 0.000015104

38 6 0.000000185 0.000001537 -0.000013304

39 6 -0.000005201 0.000002088 0.000001604

40 6 -0.000002492 0.000005424 0.000001963

41 6 -0.000004632 -0.000001077 -0.000010193

42 1 0.000002573 0.000004232 -0.000003076

43 1 -0.000001745 -0.000002548 -0.000003757

44 1 -0.000003715 -0.000001826 0.000003054

45 1 0.000006475 0.000002628 0.000004935

46 1 0.000002716 0.000002691 -0.000003696

47 1 -0.000002391 -0.000002718 -0.000002206

48 1 0.000003041 0.000001157 0.000002618

49 1 -0.000006391 -0.000002986 0.000004248

50 8 -0.000000338 0.000009896 0.000011490

51 8 0.000001898 0.000013286 0.000022679

52 8 0.000005722 -0.000000355 -0.000023681

53 8 0.000025691 0.000006870 -0.000005354

54 8 -0.000007094 -0.000020154 0.000016102

55 8 0.000008394 -0.000017228 0.000005758

56 8 -0.000016623 0.000009976 -0.000012859

57 8 -0.000016349 0.000004131 -0.000011264

58 6 0.000012970 -0.000016989 -0.000015926

59 1 -0.000003009 0.000003568 0.000005688

60 1 -0.000003165 0.000001685 0.000011124

61 1 0.000000996 0.000004358 0.000000210

62 6 -0.000007748 0.000008188 0.000010136

63 1 -0.000001433 -0.000001481 -0.000002609

64 1 -0.000000100 -0.000002489 -0.000001652

65 1 0.000005147 0.000000201 -0.000003002

66 6 -0.000009660 -0.000000245 0.000004029

67 1 -0.000002075 0.000001221 -0.000000314

68 1 0.000000221 -0.000000061 -0.000002462

69 1 0.000004047 -0.000002151 0.000000658

70 6 -0.000002145 -0.000026345 -0.000007441

71 1 -0.000001807 0.000004191 0.000003814

72 1 0.000002778 0.000004907 0.000004013

73 1 -0.000000168 0.000004332 -0.000004394

74 6 0.000009921 0.000000862 0.000004737

75 1 0.000000180 0.000001545 -0.000000330

76 1 0.000000929 -0.000000145 -0.000002692

77 1 -0.000003234 0.000001653 -0.000001948

78 6 0.000006528 -0.000009852 0.000009988

79 1 0.000000374 0.000000608 -0.000002721

80 1 0.000002832 0.000004929 -0.000001369

81 1 -0.000006125 -0.000000711 0.000000314

82 6 -0.000012427 0.000015816 -0.000018825

83 1 0.000004581 -0.000003206 0.000005621

84 1 0.000001876 -0.000002902 0.000011615

85 1 -0.000001019 -0.000004163 -0.000002011

86 6 0.000002992 0.000025587 -0.000011494

87 1 0.000002789 -0.000005518 0.000004899

88 1 -0.000004346 -0.000004923 0.000004382

89 1 0.000000063 -0.000004446 -0.000006192

-------------------------------------------------------------------

Cartesian Forces: Max 0.000074776 RMS 0.000012897

Leave Link 716 at Sat Jul 6 03:41:14 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000039592 RMS 0.000007671

Search for a local minimum.

Step number 25 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .76712D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 6 5 7 9 11

14 13 16 17 18

19 20 21 22 23

24 25

DE= -3.05D-07 DEPred=-4.57D-07 R= 6.68D-01

Trust test= 6.68D-01 RLast= 6.66D-03 DXMaxT set to 2.35D-01

ITU= 0 1 1 1 1 1 1 1 0 0 -1 -1 0 -1 0 0 0 0 0 0

ITU= 1 1 1 1 0

Eigenvalues --- 0.00415 0.00641 0.01210 0.01281 0.01316

Eigenvalues --- 0.01316 0.01316 0.01316 0.01317 0.01318

Eigenvalues --- 0.01394 0.01575 0.01586 0.01591 0.01599

Eigenvalues --- 0.01627 0.01684 0.01707 0.01708 0.01712

Eigenvalues --- 0.01716 0.01730 0.01807 0.01835 0.01869

Eigenvalues --- 0.01877 0.01919 0.01943 0.01968 0.01978

Eigenvalues --- 0.01995 0.02018 0.02024 0.02029 0.02035

Eigenvalues --- 0.02042 0.02053 0.02053 0.02054 0.02057

Eigenvalues --- 0.02057 0.02057 0.02057 0.02058 0.02061

Eigenvalues --- 0.02067 0.02067 0.02070 0.02070 0.02071

Eigenvalues --- 0.02080 0.02082 0.02083 0.02146 0.02162

Eigenvalues --- 0.02229 0.02249 0.02260 0.02260 0.02260

Eigenvalues --- 0.02262 0.02309 0.02323 0.02348 0.02364

Eigenvalues --- 0.02463 0.02836 0.03180 0.03976 0.06054

Eigenvalues --- 0.09925 0.09976 0.09979 0.09982 0.09985

Eigenvalues --- 0.09985 0.09991 0.10215 0.10642 0.10647

Eigenvalues --- 0.10647 0.10648 0.10658 0.10658 0.10669

Eigenvalues --- 0.10672 0.12654 0.13321 0.13464 0.15632

Eigenvalues --- 0.15928 0.15964 0.15999 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16010 0.16013 0.16022 0.16092 0.16146

Eigenvalues --- 0.16803 0.17096 0.20710 0.21692 0.21946

Eigenvalues --- 0.22474 0.22475 0.22480 0.22496 0.23996

Eigenvalues --- 0.24246 0.24507 0.24516 0.24546 0.24588

Eigenvalues --- 0.24738 0.24771 0.24814 0.24902 0.24912

Eigenvalues --- 0.24915 0.24943 0.24985 0.24986 0.24992

Eigenvalues --- 0.24993 0.24998 0.24998 0.24999 0.24999

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25001 0.25016 0.25112

Eigenvalues --- 0.25221 0.25481 0.26358 0.28455 0.31069

Eigenvalues --- 0.33305 0.33662 0.33699 0.33701 0.33901

Eigenvalues --- 0.34060 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34063 0.34065 0.34076 0.34080 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34082 0.34092

Eigenvalues --- 0.34599 0.34681 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34686 0.34690 0.34737 0.34948

Eigenvalues --- 0.35088 0.35236 0.35614 0.35631 0.35632

Eigenvalues --- 0.35632 0.35632 0.35634 0.35640 0.36250

Eigenvalues --- 0.36556 0.37013 0.37133 0.37469 0.40698

Eigenvalues --- 0.41215 0.41215 0.41215 0.41215 0.41218

Eigenvalues --- 0.41220 0.41318 0.41410 0.41417 0.41419

Eigenvalues --- 0.41445 0.41616 0.41987 0.42207 0.42504

Eigenvalues --- 0.43182 0.44502 0.44561 0.44714 0.44789

Eigenvalues --- 0.44881 0.44998 0.45001 0.45003 0.45008

Eigenvalues --- 0.45365 0.45366 0.45654 0.46026 0.46498

Eigenvalues --- 0.47216 0.47386 0.49334 0.49415 0.49853

Eigenvalues --- 0.50059 0.51419 0.53549 0.53554 0.53554

Eigenvalues --- 0.53555 0.53576 0.53712 0.54825 0.55111

Eigenvalues --- 0.56052 0.56666 0.57415 0.57552 0.58032

Eigenvalues --- 0.62746

En-DIIS/RFO-DIIS IScMMF= 0 using points: 25 24 23 22 21

RFO step: Lambda=-8.15870843D-08.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 7.93D-06 SmlDif= 1.00D-05

RMS Error= 0.2512250167D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.83484 0.19640 -0.04653 -0.02110 0.03639

Iteration 1 RMS(Cart)= 0.00086320 RMS(Int)= 0.00000012

Iteration 2 RMS(Cart)= 0.00000023 RMS(Int)= 0.00000006

ITry= 1 IFail=0 DXMaxC= 4.84D-03 DCOld= 1.00D+10 DXMaxT= 2.35D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58250 -0.00001 0.00000 -0.00003 -0.00002 2.58248

R2 2.73962 0.00001 0.00000 0.00000 0.00000 2.73962

R3 2.56143 -0.00003 0.00000 -0.00003 -0.00003 2.56140

R4 2.58240 0.00002 0.00000 0.00003 0.00003 2.58243

R5 3.86938 -0.00002 0.00005 -0.00017 -0.00012 3.86926

R6 2.73966 0.00000 -0.00001 0.00000 0.00000 2.73966

R7 2.56144 -0.00001 -0.00001 0.00001 0.00000 2.56143

R8 2.69557 0.00001 0.00001 0.00001 0.00002 2.69559

R9 2.66243 0.00001 0.00000 0.00003 0.00003 2.66246

R10 2.66243 0.00001 0.00000 0.00003 0.00003 2.66246

R11 2.48235 0.00001 -0.00001 0.00001 0.00001 2.48236

R12 2.59620 -0.00002 -0.00001 0.00000 -0.00001 2.59619

R13 2.79452 0.00001 -0.00002 0.00007 0.00005 2.79457

R14 2.59616 0.00001 -0.00001 0.00005 0.00004 2.59620

R15 3.84171 0.00000 0.00006 -0.00003 0.00003 3.84174

R16 2.79449 0.00003 0.00001 0.00007 0.00007 2.79456

R17 2.48235 0.00002 0.00000 0.00002 0.00002 2.48237

R18 2.66401 0.00000 0.00001 -0.00002 -0.00001 2.66400

R19 2.64564 0.00002 0.00000 0.00003 0.00003 2.64566

R20 2.64565 0.00000 0.00000 0.00000 0.00000 2.64565

R21 2.48236 0.00001 0.00000 0.00000 0.00000 2.48236

R22 2.66401 0.00000 0.00001 -0.00001 0.00000 2.66401

R23 2.79452 0.00000 -0.00001 0.00002 0.00001 2.79454

R24 2.64565 0.00001 0.00000 0.00001 0.00001 2.64566

R25 2.79447 0.00004 0.00000 0.00012 0.00012 2.79459

R26 2.64565 0.00001 0.00000 0.00002 0.00002 2.64567

R27 2.59618 -0.00001 0.00000 0.00000 0.00000 2.59618

R28 2.48237 0.00002 0.00001 0.00000 0.00001 2.48238

R29 2.59617 0.00000 -0.00001 0.00003 0.00002 2.59619

R30 3.84177 0.00000 0.00008 -0.00009 -0.00001 3.84176

R31 2.56144 0.00000 0.00000 0.00002 0.00002 2.56147

R32 2.58238 0.00003 0.00000 0.00004 0.00005 2.58242

R33 2.58250 0.00000 0.00001 -0.00003 -0.00002 2.58248

R34 3.86944 -0.00002 0.00007 -0.00025 -0.00018 3.86926

R35 2.73965 0.00001 0.00000 0.00001 0.00001 2.73967

R36 2.69557 0.00001 0.00001 0.00003 0.00003 2.69560

R37 2.66242 0.00001 0.00000 0.00004 0.00004 2.66246

R38 2.73962 0.00001 0.00000 0.00002 0.00002 2.73964

R39 2.66243 0.00001 0.00000 0.00004 0.00004 2.66246

R40 2.56142 -0.00001 0.00000 -0.00001 -0.00001 2.56141

R41 2.65606 0.00000 0.00000 0.00001 0.00001 2.65607

R42 2.54969 0.00001 0.00000 0.00000 0.00001 2.54970

R43 2.62946 -0.00001 0.00000 -0.00003 -0.00002 2.62944

R44 2.04425 0.00000 0.00000 0.00000 0.00000 2.04425

R45 2.65605 0.00001 0.00000 0.00002 0.00002 2.65608

R46 2.04425 0.00000 0.00000 0.00001 0.00001 2.04426

R47 2.54968 -0.00001 0.00000 -0.00001 -0.00001 2.54967

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R49 2.55240 -0.00001 0.00000 0.00000 0.00000 2.55239

R50 2.64705 -0.00001 0.00000 -0.00002 -0.00002 2.64703

R51 2.04404 0.00000 0.00000 -0.00001 -0.00001 2.04404

R52 2.64330 0.00000 -0.00001 0.00001 0.00000 2.64331

R53 2.04405 0.00000 0.00000 -0.00002 -0.00001 2.04403

R54 2.55238 0.00000 -0.00001 0.00001 0.00001 2.55239

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R56 2.54968 0.00000 0.00001 -0.00001 0.00000 2.54968

R57 2.62946 0.00000 0.00001 -0.00003 -0.00002 2.62944

R58 2.04425 0.00000 0.00000 0.00002 0.00001 2.04426

R59 2.65605 0.00001 0.00000 0.00002 0.00002 2.65607

R60 2.04425 0.00000 0.00000 0.00000 0.00000 2.04425

R61 2.54970 -0.00001 0.00000 -0.00001 -0.00001 2.54969

R62 2.64330 0.00000 0.00000 0.00001 0.00000 2.64330

R63 2.55239 0.00000 0.00000 0.00001 0.00000 2.55240

R64 2.64704 0.00000 0.00000 -0.00001 -0.00001 2.64704

R65 2.04404 0.00000 0.00000 -0.00001 -0.00001 2.04404

R66 2.64330 0.00001 0.00000 0.00001 0.00001 2.64331

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R68 2.55238 0.00001 0.00000 0.00001 0.00001 2.55239

R69 2.69387 0.00000 0.00000 0.00000 0.00000 2.69387

R70 2.69390 -0.00001 0.00000 -0.00002 -0.00002 2.69388

R71 2.69566 0.00000 0.00000 0.00000 0.00000 2.69566

R72 2.69568 -0.00001 0.00000 -0.00001 -0.00001 2.69567

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R74 2.69387 0.00000 -0.00001 0.00000 0.00000 2.69387

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R76 2.69568 0.00000 0.00000 -0.00001 -0.00001 2.69567

R77 2.06726 0.00001 0.00001 0.00000 0.00001 2.06727

R78 2.06738 -0.00001 0.00000 -0.00003 -0.00003 2.06736

R79 2.05686 0.00000 0.00000 0.00000 0.00000 2.05686

R80 2.06715 0.00000 0.00000 0.00000 0.00000 2.06715

R81 2.06743 0.00000 0.00000 -0.00001 -0.00001 2.06742

R82 2.05669 0.00000 0.00000 -0.00001 -0.00001 2.05669

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R89 2.06743 0.00000 0.00000 -0.00001 -0.00001 2.06742

R90 2.06715 0.00000 0.00000 0.00000 0.00000 2.06715

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R92 2.06715 0.00000 0.00000 0.00000 0.00000 2.06715

R93 2.06743 0.00000 0.00000 -0.00001 -0.00001 2.06742

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R96 2.06738 -0.00001 0.00000 -0.00003 -0.00003 2.06736

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R99 2.06727 0.00001 0.00001 0.00000 0.00001 2.06728

R100 2.05686 0.00000 0.00000 0.00000 0.00000 2.05686

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A2 2.21491 -0.00001 0.00000 -0.00007 -0.00007 2.21483

A3 2.17912 0.00000 0.00001 0.00000 0.00000 2.17913

A4 1.93087 -0.00002 0.00000 -0.00009 -0.00009 1.93079

A5 2.17274 0.00002 -0.00002 0.00009 0.00007 2.17281

A6 2.17283 0.00000 -0.00003 0.00008 0.00005 2.17288

A7 1.88907 0.00002 0.00000 0.00007 0.00007 1.88914

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A12 2.10801 0.00000 0.00000 -0.00002 -0.00002 2.10799

A13 1.85788 0.00000 0.00000 -0.00001 -0.00002 1.85787

A14 2.31716 0.00000 0.00001 0.00001 0.00001 2.31717

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A16 2.18702 0.00000 0.00000 0.00002 0.00001 2.18704

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A18 2.16630 -0.00001 0.00000 0.00001 0.00001 2.16632

A19 1.88343 0.00001 0.00000 0.00001 0.00001 1.88344

A20 1.93249 0.00000 0.00001 -0.00001 0.00000 1.93249

A21 2.16277 0.00000 -0.00001 -0.00003 -0.00004 2.16272

A22 2.16273 0.00000 0.00001 -0.00007 -0.00006 2.16267

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A24 2.23307 -0.00001 -0.00002 0.00000 -0.00003 2.23305

A25 2.16628 0.00001 0.00003 0.00000 0.00003 2.16631

A26 1.86263 -0.00001 0.00000 0.00000 -0.00001 1.86263

A27 2.30397 0.00002 0.00001 0.00002 0.00003 2.30400

A28 2.11652 -0.00001 -0.00001 -0.00001 -0.00002 2.11649

A29 1.86264 0.00000 0.00000 0.00001 0.00001 1.86265

A30 2.30401 -0.00001 -0.00001 0.00000 -0.00001 2.30400

A31 2.11647 0.00001 0.00001 -0.00001 0.00000 2.11647

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A33 1.86263 0.00000 0.00000 0.00000 0.00000 1.86262

A34 2.11648 0.00001 0.00000 0.00004 0.00004 2.11651

A35 2.30402 -0.00001 0.00000 -0.00003 -0.00004 2.30398

A36 1.86264 0.00000 0.00000 0.00000 0.00000 1.86264

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A38 2.30397 0.00002 0.00001 0.00005 0.00005 2.30402

A39 1.88346 -0.00001 -0.00001 -0.00002 -0.00003 1.88343

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A41 2.23310 -0.00001 -0.00002 -0.00003 -0.00005 2.23305

A42 1.93248 0.00001 0.00001 0.00000 0.00002 1.93249

A43 2.16279 0.00000 0.00000 -0.00006 -0.00005 2.16274

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A48 2.18699 0.00001 0.00001 0.00004 0.00005 2.18704

A49 1.93086 -0.00002 0.00000 -0.00006 -0.00006 1.93080

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A51 2.17271 0.00002 -0.00003 0.00012 0.00009 2.17280

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A55 1.85787 0.00000 0.00000 -0.00003 -0.00003 1.85785

A56 2.31714 0.00001 0.00000 0.00005 0.00006 2.31720

A57 2.10802 -0.00001 -0.00001 -0.00002 -0.00003 2.10799

A58 1.85788 0.00000 0.00000 -0.00002 -0.00002 1.85787

A59 2.10800 0.00000 -0.00001 0.00000 -0.00001 2.10799

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A61 1.88907 0.00001 0.00000 0.00006 0.00005 1.88912

A62 2.21493 -0.00002 0.00000 -0.00009 -0.00009 2.21484

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A68 1.55936 0.00001 -0.00001 0.00006 0.00005 1.55941

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A70 2.07263 0.00001 -0.00001 0.00005 0.00005 2.07267

A71 2.16558 0.00000 0.00000 -0.00005 -0.00004 2.16553

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A73 2.09917 0.00000 0.00000 -0.00001 -0.00001 2.09915

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A79 2.07264 0.00002 0.00000 0.00006 0.00006 2.07270

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A81 2.05210 0.00001 0.00001 0.00001 0.00002 2.05212

A82 2.06560 0.00000 0.00001 -0.00002 0.00000 2.06560

A83 2.16548 -0.00001 -0.00002 0.00001 -0.00002 2.16546

A84 2.12308 0.00000 0.00000 -0.00001 -0.00001 2.12307

A85 2.10064 0.00001 0.00000 0.00006 0.00006 2.10070

A86 2.05946 -0.00001 0.00001 -0.00005 -0.00005 2.05941

A87 2.12306 0.00000 0.00000 0.00002 0.00001 2.12307

A88 2.05944 0.00000 0.00001 -0.00003 -0.00003 2.05941

A89 2.10068 0.00000 0.00000 0.00002 0.00002 2.10070

A90 2.05210 0.00001 0.00001 0.00001 0.00002 2.05212

A91 2.06560 0.00001 0.00002 -0.00001 0.00001 2.06561

A92 2.16548 -0.00001 -0.00003 0.00000 -0.00003 2.16545

A93 2.04496 0.00000 0.00000 0.00003 0.00002 2.04499

A94 2.07265 0.00000 -0.00001 0.00004 0.00003 2.07268

A95 2.16556 0.00000 0.00001 -0.00007 -0.00005 2.16551

A96 2.12174 0.00000 0.00000 -0.00002 -0.00002 2.12172

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A104 2.16560 -0.00002 0.00000 -0.00009 -0.00009 2.16551

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A106 2.06561 0.00000 0.00001 -0.00004 -0.00002 2.06559

A107 2.16547 0.00000 -0.00002 0.00004 0.00002 2.16548

A108 2.12308 0.00000 0.00000 -0.00001 -0.00001 2.12307

A109 2.10064 0.00001 -0.00001 0.00006 0.00006 2.10070

A110 2.05946 -0.00001 0.00001 -0.00006 -0.00005 2.05941

A111 2.12306 0.00000 0.00000 0.00002 0.00001 2.12307

A112 2.05944 0.00000 0.00000 -0.00003 -0.00003 2.05942

A113 2.10068 0.00000 0.00000 0.00001 0.00001 2.10069

A114 2.05211 0.00000 0.00000 0.00000 0.00000 2.05211

A115 2.06561 0.00000 0.00001 0.00000 0.00000 2.06561

A116 2.16546 0.00000 -0.00001 0.00000 -0.00001 2.16546

A117 2.06564 0.00002 0.00000 0.00011 0.00011 2.06575

A118 2.06562 0.00002 -0.00001 0.00014 0.00013 2.06575

A119 2.06935 0.00000 0.00004 -0.00004 0.00000 2.06935

A120 2.06934 0.00000 0.00002 0.00001 0.00003 2.06937

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A122 2.06564 0.00001 -0.00002 0.00013 0.00012 2.06575

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A124 2.06933 0.00001 0.00002 0.00003 0.00005 2.06938

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A126 1.94718 0.00000 0.00001 0.00003 0.00004 1.94722

A127 1.84232 0.00001 0.00000 0.00006 0.00006 1.84238

A128 1.91166 -0.00001 -0.00002 -0.00001 -0.00004 1.91162

A129 1.90850 0.00000 0.00001 -0.00001 0.00000 1.90850

A130 1.90812 0.00000 0.00002 -0.00001 0.00001 1.90813

A131 1.94763 -0.00001 0.00000 -0.00005 -0.00005 1.94758

A132 1.94494 0.00000 0.00001 -0.00003 -0.00002 1.94492

A133 1.84039 0.00001 -0.00001 0.00007 0.00005 1.84044

A134 1.91253 0.00000 0.00000 0.00000 0.00000 1.91253

A135 1.90783 0.00000 0.00000 -0.00001 -0.00001 1.90782

A136 1.90887 0.00000 -0.00001 0.00003 0.00003 1.90889

A137 1.94495 0.00000 0.00000 -0.00001 -0.00001 1.94494

A138 1.94761 0.00000 0.00000 -0.00002 -0.00001 1.94760

A139 1.84039 0.00001 0.00000 0.00003 0.00002 1.84041

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A146 1.91162 -0.00001 -0.00002 0.00000 -0.00002 1.91160

A147 1.90818 -0.00001 0.00002 -0.00007 -0.00005 1.90814

A148 1.90850 0.00000 0.00001 0.00001 0.00002 1.90852

A149 1.94493 0.00000 0.00001 0.00001 0.00002 1.94495

A150 1.94762 0.00000 0.00000 -0.00002 -0.00002 1.94759

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A153 1.90889 0.00000 0.00000 0.00000 0.00000 1.90889

A154 1.90783 0.00000 0.00000 -0.00002 -0.00002 1.90781

A155 1.94761 0.00000 0.00001 -0.00004 -0.00003 1.94758

A156 1.94496 -0.00001 0.00000 -0.00004 -0.00004 1.94492

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A159 1.90782 0.00000 0.00000 -0.00001 -0.00001 1.90782

A160 1.90887 0.00000 0.00000 0.00002 0.00002 1.90889

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A167 1.94720 0.00001 0.00001 0.00006 0.00006 1.94726

A168 1.94445 0.00000 -0.00001 -0.00002 -0.00003 1.94442

A169 1.84233 0.00000 0.00000 0.00002 0.00002 1.84235

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A171 1.90818 -0.00001 0.00002 -0.00007 -0.00005 1.90813

A172 1.90849 0.00000 0.00001 0.00002 0.00002 1.90852

A173 3.11883 0.00000 -0.00002 0.00005 0.00003 3.11886

A174 3.11883 0.00000 -0.00001 0.00006 0.00004 3.11887

A175 3.33435 0.00000 0.00002 -0.00001 0.00001 3.33436

A176 2.90752 0.00000 -0.00010 0.00014 0.00004 2.90756

D1 0.00364 -0.00002 -0.00002 -0.00042 -0.00044 0.00320

D2 3.02529 -0.00001 -0.00047 0.00035 -0.00012 3.02518

D3 3.13100 -0.00001 0.00005 -0.00042 -0.00037 3.13062

D4 -0.13054 -0.00001 -0.00040 0.00035 -0.00005 -0.13059

D5 -0.00219 0.00001 -0.00002 0.00034 0.00031 -0.00188

D6 -3.12489 0.00002 0.00012 0.00041 0.00053 -3.12436

D7 -3.12991 0.00000 -0.00009 0.00034 0.00025 -3.12966

D8 0.03058 0.00001 0.00006 0.00041 0.00047 0.03104

D9 0.17260 0.00000 0.00032 -0.00014 0.00018 0.17278

D10 -2.98547 0.00001 0.00040 -0.00015 0.00025 -2.98522

D11 -0.00362 0.00002 0.00005 0.00033 0.00038 -0.00323

D12 -3.13073 0.00001 -0.00005 0.00028 0.00024 -3.13049

D13 -3.02526 0.00001 0.00050 -0.00044 0.00006 -3.02520

D14 0.13081 0.00000 0.00040 -0.00049 -0.00009 0.13073

D15 -2.95650 -0.00001 0.00031 -0.00052 -0.00021 -2.95672

D16 -0.04899 0.00000 0.00021 -0.00037 -0.00016 -0.04915

D17 0.04880 0.00000 -0.00020 0.00034 0.00015 0.04894

D18 2.95631 0.00000 -0.00029 0.00049 0.00020 2.95651

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D20 3.12469 -0.00002 -0.00018 -0.00020 -0.00038 3.12432

D21 3.12960 0.00000 0.00003 -0.00006 -0.00003 3.12957

D22 -0.03101 -0.00001 -0.00008 -0.00015 -0.00023 -0.03124

D23 -0.17282 0.00000 -0.00035 0.00044 0.00009 -0.17273

D24 2.98553 -0.00001 -0.00046 0.00038 -0.00008 2.98544

D25 0.00004 0.00000 0.00005 -0.00014 -0.00008 -0.00004

D26 3.12549 -0.00001 -0.00007 -0.00019 -0.00027 3.12523

D27 -3.12530 0.00000 0.00015 -0.00006 0.00009 -3.12521

D28 0.00015 0.00000 0.00002 -0.00012 -0.00009 0.00005

D29 -3.12516 0.00001 0.00010 0.00018 0.00028 -3.12489

D30 0.01330 0.00000 0.00007 -0.00003 0.00004 0.01334

D31 -0.00480 0.00000 -0.00003 0.00008 0.00005 -0.00475

D32 3.13367 -0.00001 -0.00006 -0.00013 -0.00019 3.13348

D33 3.12509 -0.00001 -0.00017 0.00001 -0.00016 3.12493

D34 -0.01350 0.00000 -0.00013 0.00028 0.00014 -0.01336

D35 0.00459 0.00000 0.00000 0.00008 0.00008 0.00467

D36 -3.13401 0.00001 0.00003 0.00035 0.00038 -3.13362

D37 -0.05203 -0.00001 0.00008 -0.00033 -0.00024 -0.05228

D38 3.12256 -0.00001 0.00014 -0.00043 -0.00029 3.12228

D39 -3.09787 0.00000 0.00010 -0.00019 -0.00009 -3.09796

D40 0.27537 0.00001 0.00007 0.00030 0.00037 0.27574

D41 0.01501 0.00000 0.00005 -0.00010 -0.00005 0.01495

D42 -2.89494 0.00001 0.00002 0.00039 0.00041 -2.89453

D43 3.10551 -0.00001 -0.00014 0.00000 -0.00015 3.10537

D44 -0.02325 -0.00001 -0.00001 -0.00003 -0.00004 -0.02329

D45 -0.00873 -0.00001 -0.00010 -0.00009 -0.00018 -0.00891

D46 -3.13749 -0.00001 0.00003 -0.00011 -0.00008 -3.13757

D47 -0.01518 0.00000 0.00002 0.00024 0.00026 -0.01492

D48 3.09767 0.00000 -0.00008 0.00029 0.00022 3.09789

D49 2.89477 -0.00001 0.00004 -0.00024 -0.00020 2.89457

D50 -0.27556 -0.00001 -0.00005 -0.00019 -0.00024 -0.27580

D51 -0.22716 0.00000 -0.00001 -0.00026 -0.00027 -0.22742

D52 3.10720 0.00000 0.00001 -0.00028 -0.00026 3.10694

D53 -3.10702 0.00000 -0.00004 0.00029 0.00024 -3.10678

D54 0.22734 0.00000 -0.00002 0.00027 0.00025 0.22759

D55 0.00919 -0.00001 -0.00008 -0.00029 -0.00037 0.00882

D56 3.13790 -0.00001 -0.00018 -0.00018 -0.00036 3.13754

D57 -3.10503 -0.00001 0.00001 -0.00034 -0.00033 -3.10536

D58 0.02369 0.00000 -0.00009 -0.00023 -0.00032 0.02337

D59 0.05221 0.00000 -0.00006 0.00005 -0.00002 0.05220

D60 -3.12241 0.00000 -0.00017 0.00011 -0.00007 -3.12248

D61 -0.00027 0.00001 0.00010 0.00022 0.00033 0.00005

D62 3.13017 0.00001 -0.00001 0.00025 0.00024 3.13041

D63 -3.13067 0.00001 0.00019 0.00013 0.00032 -3.13035

D64 -0.00023 0.00001 0.00008 0.00015 0.00023 0.00000

D65 -3.12603 -0.00001 0.00004 -0.00025 -0.00021 -3.12623

D66 0.02068 0.00000 0.00000 -0.00013 -0.00013 0.02055

D67 0.00114 0.00000 -0.00007 -0.00013 -0.00020 0.00094

D68 -3.13534 0.00000 -0.00011 0.00000 -0.00012 -3.13546

D69 3.12636 0.00000 -0.00016 -0.00003 -0.00019 3.12617

D70 -0.02016 -0.00001 -0.00017 -0.00024 -0.00041 -0.02056

D71 -0.00086 0.00000 -0.00002 -0.00005 -0.00007 -0.00094

D72 3.13581 -0.00001 -0.00002 -0.00027 -0.00029 3.13552

D73 -3.12246 0.00000 -0.00016 0.00017 0.00001 -3.12245

D74 0.05218 0.00000 -0.00006 0.00010 0.00003 0.05222

D75 0.00012 -0.00001 -0.00009 -0.00018 -0.00028 -0.00015

D76 3.13053 -0.00001 -0.00019 -0.00011 -0.00030 3.13023

D77 -3.13037 -0.00001 0.00004 -0.00021 -0.00017 -3.13054

D78 0.00004 -0.00001 -0.00006 -0.00014 -0.00020 -0.00016

D79 -3.10529 0.00001 0.00015 -0.00004 0.00011 -3.10519

D80 0.00891 0.00001 0.00007 0.00002 0.00009 0.00899

D81 0.02353 0.00000 -0.00001 0.00000 -0.00001 0.02352

D82 3.13773 0.00000 -0.00009 0.00006 -0.00003 3.13770

D83 0.00098 0.00000 0.00000 0.00006 0.00006 0.00104

D84 -3.13553 0.00001 -0.00003 0.00024 0.00021 -3.13532

D85 -3.12630 0.00000 0.00017 0.00002 0.00019 -3.12611

D86 0.02037 0.00001 0.00014 0.00020 0.00034 0.02072

D87 -0.00912 0.00001 0.00009 0.00029 0.00038 -0.00874

D88 3.10530 0.00000 -0.00003 0.00024 0.00021 3.10551

D89 -3.13784 0.00001 0.00021 0.00020 0.00041 -3.13743

D90 -0.02343 0.00000 0.00008 0.00016 0.00024 -0.02319

D91 -0.00103 0.00000 0.00008 0.00010 0.00018 -0.00085

D92 3.13551 0.00000 0.00013 0.00000 0.00013 3.13564

D93 3.12615 0.00000 -0.00005 0.00020 0.00015 3.12630

D94 -0.02050 0.00000 0.00000 0.00010 0.00010 -0.02040

D95 0.01522 -0.00001 -0.00005 -0.00028 -0.00033 0.01489

D96 -2.89476 0.00000 -0.00008 0.00022 0.00014 -2.89462

D97 -3.09784 0.00000 0.00008 -0.00023 -0.00016 -3.09800

D98 0.27536 0.00001 0.00005 0.00027 0.00032 0.27568

D99 3.12236 0.00000 0.00024 -0.00028 -0.00004 3.12232

D100 -0.05202 -0.00001 0.00009 -0.00034 -0.00025 -0.05227

D101 3.09769 0.00000 -0.00009 0.00023 0.00014 3.09783

D102 -0.01515 0.00000 -0.00001 0.00017 0.00016 -0.01499

D103 -0.27549 -0.00001 -0.00006 -0.00027 -0.00034 -0.27583

D104 2.89485 -0.00001 0.00002 -0.00033 -0.00031 2.89454

D105 3.10720 0.00000 0.00003 -0.00023 -0.00020 3.10700

D106 -0.22716 -0.00001 0.00000 -0.00021 -0.00021 -0.22737

D107 0.22728 0.00000 -0.00001 0.00033 0.00033 0.22761

D108 -3.10707 0.00000 -0.00003 0.00035 0.00032 -3.10675

D109 -0.17280 0.00000 -0.00034 0.00043 0.00009 -0.17271

D110 2.98521 0.00001 -0.00033 0.00067 0.00034 2.98555

D111 -3.13071 0.00001 -0.00006 0.00023 0.00017 -3.13054

D112 -0.00331 0.00000 -0.00007 0.00003 -0.00004 -0.00335

D113 0.13078 0.00000 0.00040 -0.00045 -0.00005 0.13073

D114 -3.02500 0.00000 0.00039 -0.00065 -0.00026 -3.02526

D115 0.00335 0.00000 0.00005 -0.00004 0.00001 0.00336

D116 3.13095 -0.00001 0.00007 -0.00036 -0.00030 3.13066

D117 3.02506 0.00000 -0.00041 0.00064 0.00022 3.02528

D118 -0.13052 -0.00001 -0.00040 0.00031 -0.00009 -0.13060

D119 2.95634 0.00000 -0.00030 0.00044 0.00013 2.95647

D120 0.04882 0.00000 -0.00021 0.00030 0.00009 0.04891

D121 -0.04903 0.00000 0.00022 -0.00033 -0.00010 -0.04913

D122 -2.95655 0.00000 0.00032 -0.00047 -0.00015 -2.95669

D123 3.12969 0.00000 0.00006 -0.00021 -0.00015 3.12954

D124 -0.03100 -0.00001 -0.00004 -0.00016 -0.00020 -0.03120

D125 0.00192 0.00000 0.00007 -0.00001 0.00005 0.00197

D126 3.12441 0.00000 -0.00003 0.00004 0.00001 3.12442

D127 0.00006 0.00000 -0.00003 -0.00001 -0.00005 0.00002

D128 3.12542 0.00000 -0.00010 -0.00002 -0.00012 3.12530

D129 -3.12521 0.00000 0.00005 -0.00006 -0.00001 -3.12521

D130 0.00015 0.00000 -0.00001 -0.00007 -0.00008 0.00007

D131 -3.12510 0.00001 0.00013 0.00002 0.00015 -3.12495

D132 0.01325 0.00001 0.00013 -0.00004 0.00009 0.01334

D133 -0.00483 0.00000 0.00002 0.00007 0.00009 -0.00473

D134 3.13352 0.00000 0.00002 0.00001 0.00004 3.13356

D135 -0.00203 0.00000 -0.00001 0.00003 0.00002 -0.00201

D136 -3.12999 0.00001 -0.00002 0.00035 0.00032 -3.12967

D137 -3.12462 0.00001 0.00007 0.00004 0.00011 -3.12451

D138 0.03060 0.00001 0.00005 0.00036 0.00041 0.03101

D139 0.00462 0.00000 0.00000 0.00002 0.00002 0.00464

D140 -3.13383 0.00000 -0.00002 0.00015 0.00013 -3.13369

D141 3.12500 -0.00001 -0.00009 0.00001 -0.00008 3.12492

D142 -0.01345 0.00000 -0.00010 0.00014 0.00004 -0.01341

D143 0.17260 0.00000 0.00031 -0.00012 0.00019 0.17279

D144 -2.98518 0.00000 0.00033 -0.00049 -0.00016 -2.98534

D145 -0.00102 0.00000 0.00005 0.00004 0.00009 -0.00093

D146 -3.13778 0.00000 0.00001 0.00013 0.00015 -3.13764

D147 3.13519 0.00000 0.00008 -0.00015 -0.00007 3.13512

D148 -0.00157 0.00000 0.00004 -0.00005 -0.00001 -0.00158

D149 -3.09844 -0.00001 -0.00006 0.00004 -0.00002 -3.09845

D150 0.04862 0.00000 -0.00009 0.00023 0.00014 0.04876

D151 0.00003 0.00000 -0.00003 -0.00007 -0.00011 -0.00007

D152 -3.13685 0.00000 -0.00004 0.00004 0.00000 -3.13684

D153 3.13689 -0.00001 0.00000 -0.00017 -0.00016 3.13673

D154 0.00001 0.00000 0.00000 -0.00005 -0.00005 -0.00004

D155 0.00099 0.00000 -0.00003 0.00000 -0.00003 0.00096

D156 -3.13525 0.00000 -0.00009 0.00011 0.00002 -3.13523

D157 3.13777 0.00000 -0.00002 -0.00012 -0.00014 3.13763

D158 0.00154 0.00000 -0.00008 -0.00001 -0.00009 0.00144

D159 3.09894 -0.00001 0.00000 -0.00035 -0.00035 3.09858

D160 -0.04809 -0.00001 0.00006 -0.00046 -0.00040 -0.04849

D161 -0.00474 0.00000 0.00001 0.00002 0.00003 -0.00472

D162 3.14115 0.00000 0.00001 0.00006 0.00007 3.14123

D163 3.13350 0.00000 0.00003 -0.00012 -0.00009 3.13341

D164 -0.00378 0.00000 0.00003 -0.00008 -0.00005 -0.00383

D165 3.11405 0.00000 0.00015 -0.00006 0.00009 3.11414

D166 -0.02418 0.00000 0.00014 0.00008 0.00021 -0.02396

D167 0.00002 0.00000 -0.00001 -0.00001 -0.00001 0.00001

D168 -3.13734 0.00000 0.00001 -0.00001 0.00000 -3.13735

D169 3.13740 0.00000 0.00000 -0.00005 -0.00006 3.13735

D170 0.00004 0.00000 0.00001 -0.00006 -0.00005 -0.00001

D171 0.00479 0.00000 -0.00001 -0.00004 -0.00005 0.00474

D172 -3.13335 0.00000 -0.00001 0.00002 0.00001 -3.13334

D173 -3.14113 0.00000 -0.00002 -0.00004 -0.00006 -3.14119

D174 0.00391 0.00000 -0.00003 0.00003 0.00000 0.00391

D175 -3.11464 0.00001 -0.00020 0.00042 0.00023 -3.11441

D176 0.02348 0.00001 -0.00019 0.00036 0.00017 0.02365

D177 0.00104 0.00000 -0.00004 -0.00006 -0.00010 0.00094

D178 3.13779 0.00000 -0.00002 -0.00012 -0.00014 3.13764

D179 -3.13535 0.00001 -0.00004 0.00017 0.00013 -3.13522

D180 0.00140 0.00001 -0.00002 0.00011 0.00009 0.00149

D181 3.09876 0.00000 0.00009 -0.00018 -0.00009 3.09866

D182 -0.04812 -0.00001 0.00009 -0.00041 -0.00033 -0.04845

D183 -0.00012 0.00000 0.00004 0.00008 0.00013 0.00001

D184 3.13682 0.00000 0.00003 -0.00007 -0.00004 3.13679

D185 -3.13697 0.00001 0.00002 0.00014 0.00017 -3.13680

D186 -0.00002 0.00000 0.00001 -0.00001 0.00001 -0.00002

D187 -0.00097 0.00000 0.00002 0.00001 0.00003 -0.00095

D188 3.13521 0.00000 0.00006 -0.00012 -0.00006 3.13515

D189 -3.13782 0.00000 0.00003 0.00016 0.00019 -3.13763

D190 -0.00164 0.00000 0.00007 0.00004 0.00011 -0.00153

D191 -3.09852 0.00000 -0.00001 0.00016 0.00015 -3.09837

D192 0.04856 0.00000 -0.00005 0.00029 0.00024 0.04880

D193 -0.00472 0.00000 -0.00001 -0.00001 -0.00002 -0.00474

D194 3.14110 0.00001 0.00003 0.00009 0.00012 3.14123

D195 3.13369 -0.00001 -0.00005 -0.00029 -0.00035 3.13335

D196 -0.00367 0.00000 0.00000 -0.00019 -0.00020 -0.00387

D197 3.11420 -0.00001 0.00014 -0.00022 -0.00008 3.11412

D198 -0.02419 0.00000 0.00018 0.00007 0.00024 -0.02395

D199 0.00002 0.00000 0.00001 -0.00003 -0.00002 0.00000

D200 -3.13742 0.00000 0.00004 0.00006 0.00010 -3.13731

D201 3.13748 -0.00001 -0.00003 -0.00013 -0.00016 3.13732

D202 0.00004 0.00000 0.00000 -0.00004 -0.00004 0.00000

D203 0.00476 0.00000 0.00001 0.00000 0.00001 0.00477

D204 -3.13351 0.00001 0.00004 0.00022 0.00026 -3.13325

D205 -3.14108 -0.00001 -0.00002 -0.00009 -0.00012 -3.14120

D206 0.00383 0.00000 0.00001 0.00013 0.00013 0.00396

D207 -3.11476 0.00002 -0.00013 0.00050 0.00037 -3.11439

D208 0.02349 0.00001 -0.00016 0.00028 0.00012 0.02360

D209 1.05281 0.00000 0.00027 0.00029 0.00056 1.05338

D210 -1.08971 0.00001 0.00030 0.00032 0.00062 -1.08909

D211 3.12266 0.00000 0.00028 0.00028 0.00056 3.12322

D212 1.08975 0.00000 -0.00033 -0.00005 -0.00037 1.08938

D213 -1.05271 0.00000 -0.00029 -0.00008 -0.00037 -1.05308

D214 -3.12253 0.00000 -0.00030 -0.00010 -0.00039 -3.12292

D215 1.09380 0.00000 -0.00004 0.00022 0.00017 1.09398

D216 -1.05049 0.00000 -0.00006 0.00028 0.00022 -1.05027

D217 -3.11985 0.00000 -0.00005 0.00022 0.00017 -3.11968

D218 1.05021 0.00000 0.00002 -0.00021 -0.00019 1.05002

D219 -1.09407 0.00000 0.00001 -0.00020 -0.00019 -1.09425

D220 3.11960 0.00000 0.00001 -0.00019 -0.00018 3.11942

D221 1.08979 0.00000 -0.00034 -0.00007 -0.00041 1.08938

D222 -1.05267 0.00000 -0.00031 -0.00009 -0.00040 -1.05307

D223 -3.12249 -0.00001 -0.00032 -0.00011 -0.00043 -3.12292

D224 1.05281 0.00000 0.00027 0.00032 0.00059 1.05340

D225 -1.08971 0.00001 0.00030 0.00035 0.00065 -1.08906

D226 3.12266 0.00000 0.00028 0.00031 0.00059 3.12325

D227 1.09374 0.00000 0.00000 0.00027 0.00027 1.09401

D228 -1.05056 0.00001 -0.00001 0.00033 0.00032 -1.05024

D229 -3.11993 0.00000 0.00000 0.00028 0.00028 -3.11964

D230 1.05015 0.00000 0.00004 -0.00013 -0.00009 1.05006

D231 -1.09412 0.00000 0.00003 -0.00014 -0.00010 -1.09422

D232 3.11954 0.00000 0.00004 -0.00011 -0.00008 3.11946

Item Value Threshold Converged?

Maximum Force 0.000040 0.000450 YES

RMS Force 0.000008 0.000300 YES

Maximum Displacement 0.004844 0.001800 NO

RMS Displacement 0.000863 0.001200 YES

Predicted change in Energy=-1.599504D-07

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 03:41:16 2019, MaxMem= 1342177280 cpu: 14.2

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=3 Diff= 6.05D-04

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 -1.126012 2.799827 -0.018175

2 7 0 -0.001649 2.037876 -0.169173

3 6 0 1.121383 2.801693 -0.017926

4 6 0 0.709743 4.166147 0.247851

5 6 0 -0.716704 4.164939 0.247725

6 7 0 2.407757 2.385168 -0.112771

7 6 0 2.796718 1.132672 -0.187131

8 7 0 2.018933 0.001685 -0.129098

9 6 0 2.798582 -1.128014 -0.187311

10 6 0 4.208876 -0.701375 -0.313617

11 6 0 4.207707 0.708354 -0.313552

12 7 0 -2.411663 2.381156 -0.113161

13 6 0 -4.208848 0.701414 -0.313761

14 6 0 -4.207733 -0.708318 -0.313443

15 6 0 -2.796735 -1.132665 -0.187100

16 7 0 -2.018933 -0.001690 -0.129132

17 6 0 -2.798560 1.128015 -0.187395

18 7 0 -2.407775 -2.385172 -0.112710

19 7 0 0.001654 -2.037903 -0.169157

20 6 0 -1.121382 -2.801706 -0.017884

21 6 0 -0.709740 -4.166180 0.247807

22 6 0 0.716711 -4.164982 0.247644

23 6 0 1.126023 -2.799837 -0.018112

24 7 0 2.411676 -2.381158 -0.113072

25 30 0 0.000007 -0.000013 -0.367567

26 6 0 -5.402440 1.427102 -0.407419

27 6 0 -6.595880 0.690400 -0.499516

28 6 0 -6.594812 -0.701039 -0.499069

29 6 0 -5.400240 -1.435866 -0.406587

30 6 0 1.438710 -5.348606 0.498229

31 6 0 0.705889 -6.515410 0.739286

32 6 0 -0.694860 -6.516576 0.739490

33 6 0 -1.429696 -5.350994 0.498637

34 6 0 5.400158 1.435951 -0.406919

35 6 0 6.594772 0.701177 -0.499253

36 6 0 6.595921 -0.690261 -0.499313

37 6 0 5.402522 -1.427012 -0.407051

38 6 0 -1.438715 5.348516 0.498481

39 6 0 -0.705895 6.515305 0.739630

40 6 0 0.694856 6.516486 0.739788

41 6 0 1.429697 5.350933 0.498801

42 1 0 7.544867 1.212515 -0.577288

43 1 0 7.546857 -1.200016 -0.577411

44 1 0 1.201784 7.451386 0.937188

45 1 0 -1.214436 7.449353 0.936915

46 1 0 -7.546783 1.200191 -0.577763

47 1 0 -7.544942 -1.212336 -0.576953

48 1 0 -1.201789 -7.451498 0.936784

49 1 0 1.214430 -7.449487 0.936440

50 8 0 2.779166 5.294112 0.496501

51 8 0 -2.788089 5.289406 0.495765

52 8 0 5.339606 2.783820 -0.409413

53 8 0 5.344181 -2.774985 -0.409734

54 8 0 2.788084 -5.289552 0.495412

55 8 0 -2.779165 -5.294190 0.496288

56 8 0 -5.339797 -2.783738 -0.408699

57 8 0 -5.343985 2.775073 -0.410505

58 6 0 3.507533 6.485390 0.783705

59 1 0 3.271424 6.867046 1.781366

60 1 0 3.315070 7.263736 0.039416

61 1 0 4.557723 6.201959 0.745241

62 6 0 6.559929 3.521339 -0.451007

63 1 0 7.116529 3.326861 -1.372402

64 1 0 7.192072 3.297444 0.413386

65 1 0 6.266635 4.569026 -0.422045

66 6 0 6.565718 -3.510516 -0.451026

67 1 0 7.197342 -3.285526 0.413461

68 1 0 7.122179 -3.315243 -1.372338

69 1 0 6.274098 -4.558668 -0.422017

70 6 0 -3.518567 6.479363 0.783102

71 1 0 -3.327450 7.258175 0.038955

72 1 0 -3.283172 6.861290 1.780833

73 1 0 -4.568243 6.194061 0.744541

74 6 0 -6.565447 3.510712 -0.452129

75 1 0 -7.197159 3.286078 0.412385

76 1 0 -7.121857 3.315188 -1.373418

77 1 0 -6.273722 4.558845 -0.423453

78 6 0 -6.560189 -3.521164 -0.449967

79 1 0 -7.116845 -3.326931 -1.371380

80 1 0 -7.192244 -3.296937 0.414403

81 1 0 -6.266987 -4.568868 -0.420693

82 6 0 -3.507532 -6.485503 0.783348

83 1 0 -3.271480 -6.867239 1.780992

84 1 0 -3.315011 -7.263786 0.039007

85 1 0 -4.557725 -6.202087 0.744843

86 6 0 3.518523 -6.479580 0.782553

87 1 0 3.327317 -7.258297 0.038330

88 1 0 3.283176 -6.861610 1.780256

89 1 0 4.568212 -6.194328 0.743952

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0447620 0.0439718 0.0225229

Leave Link 202 at Sat Jul 6 03:41:17 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8042.1273089920 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= 89 NActive= 89 NUniq= 89 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= -0.2279730045 Hartrees.

Nuclear repulsion after empirical dispersion term = 8041.8993359875 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6400

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.23D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 402

GePol: Fraction of low-weight points (<1% of avg) = 6.28%

GePol: Cavity surface area = 703.214 Ang\*\*2

GePol: Cavity volume = 801.603 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0089860411 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8041.8903499464 Hartrees.

Leave Link 301 at Sat Jul 6 03:41:17 2019, MaxMem= 1342177280 cpu: 1.3

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44310 LenP2D= 111303.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.55D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 03:41:21 2019, MaxMem= 1342177280 cpu: 42.7

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 03:41:22 2019, MaxMem= 1342177280 cpu: 2.6

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000003 0.000000 -0.000214 Ang= -0.02 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>= 2.0171 S= 1.0057

Leave Link 401 at Sat Jul 6 03:41:28 2019, MaxMem= 1342177280 cpu: 72.4

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 122880000.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.02D-14 for 6396.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.49D-15 for 6380 6006.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.88D-15 for 6396.

Iteration 1 A^-1\*A deviation from orthogonality is 6.06D-09 for 5835 5724.

Iteration 2 A\*A^-1 deviation from unit magnitude is 4.00D-15 for 512.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.25D-15 for 3907 1318.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 1344.

Iteration 2 A^-1\*A deviation from orthogonality is 4.81D-16 for 6366 2617.

E= -2649.79551835308

DIIS: error= 3.32D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79551835308 IErMin= 1 ErrMin= 3.32D-05

ErrMax= 3.32D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.31D-06 BMatP= 5.31D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.685 Goal= None Shift= 0.000

Gap= 0.744 Goal= None Shift= 0.000

RMSDP=2.11D-06 MaxDP=9.61D-05 OVMax= 1.70D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.11D-06 CP: 1.00D+00

E= -2649.79552074590 Delta-E= -0.000002392826 Rises=F Damp=F

DIIS: error= 3.71D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79552074590 IErMin= 2 ErrMin= 3.71D-06

ErrMax= 3.71D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.15D-08 BMatP= 5.31D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.662D-01 0.107D+01

Coeff: -0.662D-01 0.107D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=2.45D-07 MaxDP=1.08D-05 DE=-2.39D-06 OVMax= 3.82D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.27D-07 CP: 1.00D+00 1.04D+00

E= -2649.79552076979 Delta-E= -0.000000023882 Rises=F Damp=F

DIIS: error= 3.11D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79552076979 IErMin= 3 ErrMin= 3.11D-06

ErrMax= 3.11D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.73D-08 BMatP= 6.15D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.366D-01 0.519D+00 0.517D+00

Coeff: -0.366D-01 0.519D+00 0.517D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.24D-07 MaxDP=1.23D-05 DE=-2.39D-08 OVMax= 3.56D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.00D-07 CP: 1.00D+00 1.05D+00 6.83D-01

E= -2649.79552077599 Delta-E= -0.000000006203 Rises=F Damp=F

DIIS: error= 1.86D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79552077599 IErMin= 4 ErrMin= 1.86D-06

ErrMax= 1.86D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-08 BMatP= 3.73D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.899D-02 0.106D+00 0.341D+00 0.562D+00

Coeff: -0.899D-02 0.106D+00 0.341D+00 0.562D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=4.91D-08 MaxDP=4.95D-06 DE=-6.20D-09 OVMax= 1.48D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.99D-08 CP: 1.00D+00 1.05D+00 7.80D-01 6.80D-01

E= -2649.79552077783 Delta-E= -0.000000001837 Rises=F Damp=F

DIIS: error= 3.24D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79552077783 IErMin= 5 ErrMin= 3.24D-07

ErrMax= 3.24D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.85D-10 BMatP= 1.02D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.125D-02 0.565D-02 0.112D+00 0.249D+00 0.635D+00

Coeff: -0.125D-02 0.565D-02 0.112D+00 0.249D+00 0.635D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.27D-08 MaxDP=7.85D-07 DE=-1.84D-09 OVMax= 7.51D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.07D-08 CP: 1.00D+00 1.05D+00 7.91D-01 7.25D-01 8.54D-01

E= -2649.79552077808 Delta-E= -0.000000000253 Rises=F Damp=F

DIIS: error= 1.89D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79552077808 IErMin= 6 ErrMin= 1.89D-07

ErrMax= 1.89D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.26D-10 BMatP= 3.85D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.543D-03-0.129D-01 0.198D-01 0.727D-01 0.401D+00 0.519D+00

Coeff: 0.543D-03-0.129D-01 0.198D-01 0.727D-01 0.401D+00 0.519D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=6.44D-09 MaxDP=3.95D-07 DE=-2.53D-10 OVMax= 5.33D-06

Error on total polarization charges = 0.07298

SCF Done: E(UB3LYP) = -2649.79552078 A.U. after 6 cycles

NFock= 6 Conv=0.64D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0171 S= 1.0057

<L.S>= 0.000000000000E+00

KE= 2.690147201859D+03 PE=-2.236249951653D+04 EE= 8.980666443943D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0171, after 2.0002

Leave Link 502 at Sat Jul 6 03:47:00 2019, MaxMem= 1342177280 cpu: 3887.3

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44310 LenP2D= 111303.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 275

Leave Link 701 at Sat Jul 6 03:47:19 2019, MaxMem= 1342177280 cpu: 225.5

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 03:47:19 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 03:48:57 2019, MaxMem= 1342177280 cpu: 1165.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 2.67829751D-05 1.31757623D-04 1.94602057D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000012508 -0.000006123 0.000017989

2 7 -0.000035141 -0.000010851 -0.000002362

3 6 0.000028880 0.000007600 0.000002397

4 6 0.000012509 -0.000002738 -0.000007449

5 6 -0.000007831 0.000008668 -0.000020577

6 7 -0.000007207 0.000013237 0.000007872

7 6 -0.000007354 -0.000022440 -0.000012565

8 7 0.000026339 0.000004541 0.000015456

9 6 -0.000002714 0.000012947 0.000010746

10 6 -0.000004912 -0.000006270 -0.000009600

11 6 0.000000252 0.000004914 -0.000000511

12 7 0.000012695 0.000014007 -0.000010605

13 6 0.000006074 0.000000272 -0.000004950

14 6 -0.000003906 -0.000007407 -0.000006450

15 6 0.000010687 0.000012958 0.000002054

16 7 -0.000022076 -0.000007283 0.000016308

17 6 -0.000001214 -0.000011310 -0.000001834

18 7 0.000011265 -0.000007221 0.000009590

19 7 0.000034707 0.000019634 0.000012162

20 6 -0.000037614 -0.000007627 -0.000008523

21 6 -0.000012826 0.000002751 -0.000007454

22 6 0.000007463 -0.000006881 -0.000012805

23 6 0.000010684 -0.000001134 -0.000000554

24 7 -0.000005674 -0.000009777 -0.000007735

25 30 -0.000001592 -0.000000656 -0.000007546

26 6 0.000002510 0.000008410 0.000000985

27 6 -0.000002356 -0.000005333 0.000002300

28 6 -0.000002159 0.000006055 -0.000001511

29 6 0.000001372 0.000000731 0.000007063

30 6 0.000005173 0.000003634 0.000005223

31 6 0.000004442 0.000003188 -0.000001160

32 6 -0.000001160 0.000003399 -0.000002032

33 6 -0.000002731 0.000000492 0.000006754

34 6 -0.000000063 0.000002095 0.000006221

35 6 0.000003153 -0.000004113 -0.000000334

36 6 0.000002082 0.000007417 0.000001537

37 6 -0.000003118 -0.000006293 0.000001481

38 6 -0.000005684 -0.000001629 0.000006072

39 6 -0.000007099 -0.000004799 -0.000001684

40 6 0.000001689 -0.000003645 -0.000002362

41 6 0.000001977 -0.000001058 0.000010762

42 1 -0.000000170 0.000000400 0.000000285

43 1 -0.000002497 -0.000000842 -0.000000457

44 1 0.000003896 0.000000784 0.000003829

45 1 -0.000003186 0.000003387 0.000004374

46 1 0.000001492 0.000001220 -0.000000329

47 1 0.000000864 -0.000000718 0.000000320

48 1 -0.000004342 -0.000000529 0.000004245

49 1 0.000002087 -0.000002528 0.000003976

50 8 -0.000001975 0.000001589 -0.000010042

51 8 0.000004890 0.000006433 0.000002154

52 8 -0.000000089 -0.000000638 -0.000007261

53 8 0.000001833 -0.000003621 -0.000000477

54 8 0.000000835 -0.000000701 0.000004216

55 8 -0.000001245 0.000002709 -0.000006213

56 8 0.000005256 -0.000004629 -0.000010698

57 8 -0.000007998 -0.000002965 0.000003815

58 6 -0.000001078 -0.000010301 -0.000008507

59 1 -0.000004813 0.000006526 0.000003701

60 1 -0.000003957 0.000004952 0.000004899

61 1 -0.000001568 -0.000001561 -0.000000239

62 6 -0.000003714 -0.000000084 0.000004287

63 1 0.000001473 0.000001452 -0.000001512

64 1 0.000000718 -0.000001718 0.000000453

65 1 0.000000774 0.000000888 0.000000649

66 6 -0.000007596 0.000004054 -0.000002125

67 1 0.000001212 -0.000001329 0.000001580

68 1 0.000001123 -0.000001071 -0.000001010

69 1 0.000000133 -0.000002027 -0.000000604

70 6 0.000009730 -0.000016989 -0.000003613

71 1 0.000001336 0.000006085 -0.000000686

72 1 0.000003517 0.000005830 0.000002119

73 1 0.000000880 -0.000000065 -0.000003152

74 6 0.000006896 -0.000005261 -0.000001603

75 1 -0.000000312 -0.000000038 0.000001740

76 1 -0.000001612 0.000000867 -0.000001190

77 1 -0.000000463 0.000002076 0.000001024

78 6 0.000004227 -0.000000087 0.000003623

79 1 -0.000000889 -0.000001211 -0.000001483

80 1 -0.000001323 0.000000729 0.000000411

81 1 -0.000000121 -0.000000764 -0.000000701

82 6 0.000001542 0.000010327 -0.000007903

83 1 0.000004976 -0.000006461 0.000003704

84 1 0.000003892 -0.000004591 0.000004656

85 1 0.000001750 0.000001911 0.000000319

86 6 -0.000008136 0.000017140 -0.000001935

87 1 -0.000001881 -0.000005246 -0.000000888

88 1 -0.000002462 -0.000006104 0.000002084

89 1 -0.000000922 0.000000354 -0.000002206

-------------------------------------------------------------------

Cartesian Forces: Max 0.000037614 RMS 0.000007665

Leave Link 716 at Sat Jul 6 03:48:57 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000026449 RMS 0.000005286

Search for a local minimum.

Step number 26 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .52858D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 6 5 7 9 11

14 13 16 17 18

19 20 21 22 23

24 25 26

DE= -1.58D-07 DEPred=-1.60D-07 R= 9.91D-01

Trust test= 9.91D-01 RLast= 3.53D-03 DXMaxT set to 2.35D-01

ITU= 0 0 1 1 1 1 1 1 1 0 0 -1 -1 0 -1 0 0 0 0 0

ITU= 0 1 1 1 1 0

Eigenvalues --- 0.00415 0.00668 0.01116 0.01220 0.01316

Eigenvalues --- 0.01316 0.01316 0.01317 0.01318 0.01319

Eigenvalues --- 0.01387 0.01579 0.01581 0.01592 0.01599

Eigenvalues --- 0.01635 0.01650 0.01707 0.01712 0.01713

Eigenvalues --- 0.01716 0.01770 0.01811 0.01837 0.01868

Eigenvalues --- 0.01885 0.01899 0.01919 0.01950 0.01979

Eigenvalues --- 0.02003 0.02020 0.02024 0.02029 0.02035

Eigenvalues --- 0.02043 0.02053 0.02053 0.02055 0.02057

Eigenvalues --- 0.02057 0.02057 0.02059 0.02059 0.02061

Eigenvalues --- 0.02067 0.02067 0.02070 0.02070 0.02071

Eigenvalues --- 0.02078 0.02080 0.02088 0.02162 0.02206

Eigenvalues --- 0.02234 0.02252 0.02260 0.02260 0.02260

Eigenvalues --- 0.02288 0.02329 0.02346 0.02350 0.02366

Eigenvalues --- 0.02526 0.02915 0.03574 0.04058 0.05829

Eigenvalues --- 0.09937 0.09960 0.09980 0.09982 0.09983

Eigenvalues --- 0.09985 0.09986 0.10212 0.10622 0.10645

Eigenvalues --- 0.10647 0.10647 0.10657 0.10658 0.10673

Eigenvalues --- 0.10682 0.12827 0.13463 0.13478 0.15535

Eigenvalues --- 0.15858 0.15975 0.15997 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16004

Eigenvalues --- 0.16008 0.16023 0.16038 0.16086 0.16276

Eigenvalues --- 0.16910 0.17111 0.20777 0.21694 0.21994

Eigenvalues --- 0.22473 0.22475 0.22480 0.22500 0.23928

Eigenvalues --- 0.24252 0.24507 0.24513 0.24538 0.24606

Eigenvalues --- 0.24742 0.24812 0.24820 0.24883 0.24907

Eigenvalues --- 0.24921 0.24956 0.24985 0.24987 0.24992

Eigenvalues --- 0.24993 0.24998 0.24998 0.24999 0.24999

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25000 0.25014 0.25029 0.25198

Eigenvalues --- 0.25500 0.25543 0.27532 0.29811 0.31180

Eigenvalues --- 0.33333 0.33651 0.33711 0.33741 0.34028

Eigenvalues --- 0.34059 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34064 0.34066 0.34077 0.34081 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34083 0.34601

Eigenvalues --- 0.34630 0.34683 0.34686 0.34686 0.34686

Eigenvalues --- 0.34686 0.34688 0.34702 0.34756 0.34975

Eigenvalues --- 0.35131 0.35552 0.35618 0.35627 0.35632

Eigenvalues --- 0.35632 0.35633 0.35634 0.35754 0.36195

Eigenvalues --- 0.36853 0.37065 0.37150 0.37605 0.40724

Eigenvalues --- 0.41191 0.41215 0.41215 0.41216 0.41216

Eigenvalues --- 0.41220 0.41318 0.41405 0.41417 0.41420

Eigenvalues --- 0.41522 0.41716 0.42248 0.42373 0.42663

Eigenvalues --- 0.43233 0.44508 0.44562 0.44714 0.44839

Eigenvalues --- 0.44888 0.44992 0.45001 0.45005 0.45014

Eigenvalues --- 0.45366 0.45367 0.45574 0.45945 0.46565

Eigenvalues --- 0.47269 0.47732 0.49354 0.49449 0.49862

Eigenvalues --- 0.50172 0.51490 0.53546 0.53554 0.53554

Eigenvalues --- 0.53564 0.53620 0.53733 0.55122 0.55281

Eigenvalues --- 0.56090 0.57202 0.57425 0.57572 0.58532

Eigenvalues --- 0.66543

En-DIIS/RFO-DIIS IScMMF= 0 using points: 26 25 24 23 22

RFO step: Lambda=-2.93846595D-08.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 3.85D-06 SmlDif= 1.00D-05

RMS Error= 0.1479697892D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 0.96055 0.10147 -0.08711 -0.02248 0.04756

Iteration 1 RMS(Cart)= 0.00049738 RMS(Int)= 0.00000007

Iteration 2 RMS(Cart)= 0.00000010 RMS(Int)= 0.00000002

ITry= 1 IFail=0 DXMaxC= 2.55D-03 DCOld= 1.00D+10 DXMaxT= 2.35D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58248 0.00000 0.00000 -0.00001 -0.00001 2.58247

R2 2.73962 0.00000 0.00000 0.00002 0.00001 2.73964

R3 2.56140 -0.00001 -0.00001 -0.00002 -0.00002 2.56138

R4 2.58243 0.00003 0.00000 0.00005 0.00005 2.58248

R5 3.86926 -0.00001 -0.00003 -0.00004 -0.00007 3.86919

R6 2.73966 0.00000 -0.00001 0.00000 -0.00001 2.73965

R7 2.56143 0.00000 -0.00001 -0.00001 -0.00002 2.56141

R8 2.69559 0.00001 0.00002 0.00002 0.00004 2.69563

R9 2.66246 0.00000 0.00000 0.00000 0.00000 2.66246

R10 2.66246 0.00000 0.00001 0.00000 0.00000 2.66246

R11 2.48236 0.00001 -0.00001 0.00000 -0.00001 2.48235

R12 2.59619 -0.00001 -0.00001 -0.00003 -0.00004 2.59615

R13 2.79457 0.00001 0.00000 0.00003 0.00003 2.79460

R14 2.59620 -0.00001 -0.00001 0.00000 -0.00001 2.59619

R15 3.84174 0.00001 -0.00001 0.00016 0.00015 3.84189

R16 2.79456 -0.00002 0.00000 -0.00002 -0.00002 2.79454

R17 2.48237 0.00000 -0.00001 0.00000 -0.00001 2.48236

R18 2.66400 0.00000 0.00000 0.00001 0.00001 2.66401

R19 2.64566 -0.00001 0.00000 0.00000 0.00000 2.64566

R20 2.64565 0.00000 0.00000 0.00000 0.00000 2.64566

R21 2.48236 0.00001 -0.00001 0.00001 0.00000 2.48236

R22 2.66401 0.00000 0.00000 0.00001 0.00001 2.66402

R23 2.79454 0.00000 0.00001 0.00000 0.00001 2.79455

R24 2.64566 0.00000 0.00000 0.00001 0.00001 2.64567

R25 2.79459 -0.00001 0.00001 0.00001 0.00001 2.79460

R26 2.64567 -0.00001 0.00000 -0.00001 -0.00001 2.64566

R27 2.59618 -0.00001 -0.00001 -0.00003 -0.00004 2.59615

R28 2.48238 0.00000 0.00000 -0.00001 -0.00001 2.48237

R29 2.59619 0.00000 -0.00001 0.00000 -0.00001 2.59618

R30 3.84176 0.00001 0.00000 0.00013 0.00013 3.84189

R31 2.56147 -0.00002 0.00000 -0.00002 -0.00002 2.56145

R32 2.58242 0.00002 0.00000 0.00005 0.00005 2.58247

R33 2.58248 0.00000 0.00000 -0.00002 -0.00002 2.58245

R34 3.86926 -0.00001 -0.00002 -0.00006 -0.00008 3.86919

R35 2.73967 -0.00001 0.00000 -0.00001 -0.00001 2.73965

R36 2.69560 0.00001 0.00002 0.00002 0.00004 2.69564

R37 2.66246 -0.00001 0.00000 -0.00001 0.00000 2.66246

R38 2.73964 0.00000 -0.00001 0.00001 0.00000 2.73963

R39 2.66246 -0.00001 0.00000 -0.00001 0.00000 2.66246

R40 2.56141 -0.00002 -0.00001 -0.00003 -0.00004 2.56137

R41 2.65607 0.00000 0.00000 0.00001 0.00001 2.65608

R42 2.54970 -0.00001 0.00000 0.00001 0.00000 2.54970

R43 2.62944 0.00000 0.00000 0.00000 0.00000 2.62944

R44 2.04425 0.00000 0.00000 0.00000 0.00000 2.04425

R45 2.65608 0.00000 0.00001 0.00001 0.00001 2.65609

R46 2.04426 0.00000 0.00000 0.00000 0.00000 2.04426

R47 2.54967 0.00001 0.00000 0.00002 0.00002 2.54969

R48 2.64330 0.00000 0.00000 0.00000 0.00000 2.64330

R49 2.55239 -0.00001 0.00001 -0.00001 0.00000 2.55239

R50 2.64703 0.00000 0.00000 0.00000 0.00000 2.64703

R51 2.04404 0.00000 0.00000 0.00000 0.00000 2.04404

R52 2.64331 0.00000 0.00000 0.00000 0.00000 2.64331

R53 2.04403 0.00000 0.00000 0.00000 0.00000 2.04403

R54 2.55239 -0.00001 0.00001 0.00000 0.00000 2.55239

R55 2.65607 0.00001 0.00001 0.00001 0.00002 2.65609

R56 2.54968 0.00000 0.00000 0.00001 0.00001 2.54969

R57 2.62944 0.00000 0.00000 0.00000 0.00000 2.62944

R58 2.04426 0.00000 0.00000 0.00000 0.00000 2.04426

R59 2.65607 0.00000 0.00001 0.00001 0.00001 2.65608

R60 2.04425 0.00000 0.00000 -0.00001 -0.00001 2.04424

R61 2.54969 0.00000 0.00000 0.00002 0.00001 2.54970

R62 2.64330 -0.00001 0.00000 -0.00001 -0.00001 2.64330

R63 2.55240 -0.00002 0.00000 -0.00002 -0.00001 2.55239

R64 2.64704 0.00000 0.00000 -0.00001 -0.00001 2.64703

R65 2.04404 0.00001 0.00000 0.00001 0.00001 2.04404

R66 2.64331 -0.00001 0.00000 0.00000 0.00000 2.64331

R67 2.04403 0.00000 0.00000 0.00000 0.00000 2.04403

R68 2.55239 -0.00001 0.00001 0.00000 0.00000 2.55239

R69 2.69387 -0.00001 0.00000 0.00000 -0.00001 2.69386

R70 2.69388 -0.00001 0.00000 -0.00002 -0.00003 2.69385

R71 2.69566 0.00000 0.00000 0.00001 0.00000 2.69567

R72 2.69567 0.00000 0.00000 0.00000 -0.00001 2.69566

R73 2.69388 -0.00001 0.00000 -0.00002 -0.00003 2.69385

R74 2.69387 -0.00001 0.00000 0.00000 -0.00001 2.69386

R75 2.69566 0.00000 0.00000 0.00001 0.00000 2.69567

R76 2.69567 -0.00001 0.00000 0.00000 -0.00001 2.69566

R77 2.06727 0.00001 0.00001 0.00002 0.00003 2.06730

R78 2.06736 0.00000 0.00000 -0.00001 0.00000 2.06735

R79 2.05686 0.00000 0.00000 0.00000 0.00000 2.05686

R80 2.06715 0.00000 0.00000 0.00001 0.00001 2.06716

R81 2.06742 0.00000 0.00000 0.00000 0.00001 2.06743

R82 2.05669 0.00000 0.00000 0.00000 0.00000 2.05669

R83 2.06742 0.00000 0.00000 0.00000 0.00001 2.06743

R84 2.06715 0.00000 0.00000 0.00001 0.00001 2.06716

R85 2.05669 0.00000 0.00000 0.00001 0.00001 2.05669

R86 2.06735 0.00001 0.00000 0.00001 0.00001 2.06737

R87 2.06728 0.00000 0.00001 0.00001 0.00002 2.06730

R88 2.05686 0.00000 0.00000 0.00000 0.00000 2.05686

R89 2.06742 0.00000 0.00000 0.00000 0.00001 2.06743

R90 2.06715 0.00000 0.00000 0.00001 0.00001 2.06716

R91 2.05669 0.00000 0.00000 0.00001 0.00001 2.05669

R92 2.06715 0.00000 0.00000 0.00001 0.00001 2.06716

R93 2.06742 0.00000 0.00000 0.00000 0.00001 2.06743

R94 2.05669 0.00000 0.00000 0.00000 0.00000 2.05669

R95 2.06727 0.00001 0.00001 0.00002 0.00003 2.06730

R96 2.06736 0.00000 0.00000 -0.00001 0.00000 2.06735

R97 2.05686 0.00000 0.00000 0.00000 0.00000 2.05686

R98 2.06735 0.00000 0.00000 0.00001 0.00001 2.06737

R99 2.06728 0.00000 0.00001 0.00001 0.00002 2.06730

R100 2.05686 0.00000 0.00000 0.00000 0.00000 2.05686

A1 1.88913 0.00000 0.00001 0.00000 0.00000 1.88913

A2 2.21483 0.00000 -0.00001 -0.00002 -0.00003 2.21480

A3 2.17913 0.00001 0.00000 0.00002 0.00003 2.17915

A4 1.93079 0.00001 -0.00001 0.00001 0.00000 1.93079

A5 2.17281 0.00001 0.00000 0.00003 0.00003 2.17284

A6 2.17288 -0.00001 0.00000 -0.00003 -0.00003 2.17285

A7 1.88914 -0.00001 0.00001 -0.00001 0.00000 1.88914

A8 2.21481 0.00001 -0.00001 0.00002 0.00001 2.21482

A9 2.17914 0.00000 0.00000 -0.00001 -0.00001 2.17913

A10 1.85784 0.00000 0.00000 0.00000 0.00000 1.85784

A11 2.31720 0.00000 0.00000 0.00002 0.00002 2.31722

A12 2.10799 -0.00001 0.00000 -0.00002 -0.00002 2.10797

A13 1.85787 0.00000 0.00000 0.00000 0.00000 1.85787

A14 2.31717 0.00000 0.00000 0.00000 0.00001 2.31718

A15 2.10800 0.00000 0.00000 -0.00001 -0.00001 2.10799

A16 2.18704 0.00000 0.00000 0.00004 0.00004 2.18708

A17 2.23306 0.00000 0.00000 -0.00004 -0.00004 2.23303

A18 2.16632 0.00001 0.00000 0.00004 0.00005 2.16636

A19 1.88344 0.00000 -0.00001 -0.00001 -0.00001 1.88342

A20 1.93249 0.00000 0.00001 0.00001 0.00003 1.93252

A21 2.16272 0.00000 0.00000 -0.00004 -0.00004 2.16268

A22 2.16267 -0.00001 0.00000 -0.00007 -0.00007 2.16261

A23 1.88345 0.00000 -0.00001 0.00000 -0.00001 1.88345

A24 2.23305 0.00001 0.00001 0.00000 0.00000 2.23305

A25 2.16631 -0.00001 0.00001 0.00000 0.00000 2.16631

A26 1.86263 0.00000 0.00000 0.00000 0.00000 1.86263

A27 2.30400 -0.00001 0.00000 -0.00002 -0.00002 2.30398

A28 2.11649 0.00001 0.00000 0.00002 0.00002 2.11651

A29 1.86265 0.00000 0.00000 -0.00001 -0.00001 1.86264

A30 2.30400 0.00001 0.00000 0.00002 0.00002 2.30402

A31 2.11647 0.00000 0.00000 -0.00001 -0.00001 2.11646

A32 2.18706 0.00000 0.00001 0.00002 0.00003 2.18709

A33 1.86262 0.00000 0.00000 0.00000 0.00000 1.86262

A34 2.11651 -0.00001 0.00000 -0.00001 -0.00001 2.11651

A35 2.30398 0.00001 0.00000 0.00001 0.00001 2.30398

A36 1.86264 0.00000 0.00000 0.00000 0.00000 1.86264

A37 2.11645 0.00001 0.00000 0.00001 0.00001 2.11646

A38 2.30402 -0.00001 0.00000 -0.00001 -0.00001 2.30401

A39 1.88343 0.00000 -0.00001 0.00000 -0.00001 1.88342

A40 2.16633 -0.00001 0.00001 0.00002 0.00003 2.16636

A41 2.23305 0.00001 0.00000 -0.00002 -0.00002 2.23303

A42 1.93249 0.00000 0.00002 0.00002 0.00004 1.93253

A43 2.16274 -0.00001 0.00000 -0.00008 -0.00008 2.16266

A44 2.16266 0.00000 0.00000 -0.00004 -0.00004 2.16262

A45 2.16628 0.00001 0.00001 0.00003 0.00004 2.16633

A46 2.23307 0.00000 0.00000 -0.00003 -0.00002 2.23304

A47 1.88346 -0.00001 -0.00001 -0.00001 -0.00002 1.88344

A48 2.18704 0.00000 0.00001 0.00004 0.00005 2.18708

A49 1.93080 0.00000 0.00000 0.00000 -0.00001 1.93080

A50 2.17288 -0.00001 0.00000 -0.00004 -0.00004 2.17283

A51 2.17280 0.00001 0.00000 0.00006 0.00006 2.17285

A52 2.21482 0.00000 -0.00001 0.00001 0.00000 2.21482

A53 2.17914 0.00000 0.00000 -0.00001 0.00000 2.17913

A54 1.88913 0.00000 0.00000 0.00000 0.00000 1.88914

A55 1.85785 0.00000 0.00000 0.00000 -0.00001 1.85784

A56 2.31720 0.00000 0.00000 0.00002 0.00002 2.31722

A57 2.10799 0.00000 0.00000 -0.00002 -0.00002 2.10797

A58 1.85787 0.00000 0.00000 0.00000 0.00000 1.85787

A59 2.10799 0.00000 0.00000 0.00000 0.00000 2.10799

A60 2.31718 0.00000 0.00000 -0.00001 -0.00001 2.31717

A61 1.88912 0.00000 0.00001 0.00001 0.00001 1.88913

A62 2.21484 0.00000 -0.00001 -0.00003 -0.00004 2.21480

A63 2.17913 0.00000 0.00000 0.00003 0.00003 2.17916

A64 2.18707 -0.00001 0.00000 0.00000 0.00001 2.18708

A65 1.55940 0.00001 0.00001 0.00000 0.00001 1.55941

A66 1.55945 0.00000 0.00001 -0.00003 -0.00002 1.55943

A67 1.55946 -0.00001 0.00001 -0.00004 -0.00003 1.55943

A68 1.55941 0.00000 0.00001 0.00002 0.00004 1.55945

A69 2.04497 0.00000 0.00000 -0.00001 0.00000 2.04497

A70 2.07267 0.00000 0.00001 0.00001 0.00002 2.07269

A71 2.16553 0.00000 -0.00001 -0.00001 -0.00002 2.16551

A72 2.12172 0.00000 0.00000 0.00001 0.00001 2.12173

A73 2.09915 0.00000 -0.00001 -0.00002 -0.00003 2.09913

A74 2.06230 0.00000 0.00001 0.00001 0.00002 2.06232

A75 2.12173 0.00000 0.00000 -0.00001 -0.00001 2.12172

A76 2.06230 0.00000 0.00001 0.00000 0.00002 2.06231

A77 2.09915 0.00000 -0.00001 0.00000 -0.00001 2.09914

A78 2.04499 0.00000 0.00000 0.00000 0.00000 2.04499

A79 2.07270 -0.00001 0.00001 -0.00002 -0.00002 2.07268

A80 2.16549 0.00001 -0.00001 0.00002 0.00001 2.16550

A81 2.05212 0.00000 0.00000 0.00001 0.00001 2.05213

A82 2.06560 0.00000 0.00001 0.00000 0.00001 2.06561

A83 2.16546 0.00000 -0.00001 -0.00001 -0.00002 2.16544

A84 2.12307 0.00000 0.00000 -0.00001 -0.00001 2.12306

A85 2.10070 0.00000 0.00000 0.00002 0.00002 2.10072

A86 2.05941 0.00000 0.00000 -0.00001 -0.00001 2.05940

A87 2.12307 0.00000 0.00000 0.00000 0.00001 2.12308

A88 2.05941 0.00000 0.00000 0.00001 0.00001 2.05943

A89 2.10070 0.00000 0.00000 -0.00002 -0.00002 2.10068

A90 2.05212 0.00000 0.00000 0.00001 0.00001 2.05213

A91 2.06561 0.00001 0.00001 0.00001 0.00002 2.06564

A92 2.16545 -0.00001 -0.00001 -0.00002 -0.00003 2.16541

A93 2.04499 0.00000 0.00000 0.00000 0.00001 2.04499

A94 2.07268 0.00000 0.00000 0.00000 0.00000 2.07268

A95 2.16551 0.00000 0.00000 0.00000 -0.00001 2.16550

A96 2.12172 0.00000 0.00000 0.00000 0.00000 2.12172

A97 2.09915 0.00000 -0.00001 0.00000 -0.00001 2.09914

A98 2.06230 0.00000 0.00001 0.00000 0.00001 2.06232

A99 2.12172 0.00000 0.00000 0.00001 0.00000 2.12172

A100 2.06230 0.00000 0.00001 0.00001 0.00002 2.06232

A101 2.09915 0.00000 -0.00001 -0.00001 -0.00002 2.09913

A102 2.04498 -0.00001 0.00000 -0.00001 -0.00001 2.04496

A103 2.07269 -0.00001 0.00000 -0.00001 0.00000 2.07269

A104 2.16551 0.00001 -0.00001 0.00002 0.00001 2.16552

A105 2.05211 0.00001 0.00000 0.00002 0.00002 2.05213

A106 2.06559 0.00001 0.00001 0.00002 0.00003 2.06561

A107 2.16548 -0.00002 -0.00001 -0.00004 -0.00005 2.16543

A108 2.12307 0.00000 0.00000 -0.00002 -0.00001 2.12306

A109 2.10070 0.00000 0.00000 0.00002 0.00002 2.10072

A110 2.05941 0.00000 0.00000 0.00000 0.00000 2.05941

A111 2.12307 0.00000 0.00000 0.00000 0.00001 2.12307

A112 2.05942 0.00000 0.00000 0.00001 0.00001 2.05943

A113 2.10069 0.00000 0.00000 -0.00001 -0.00002 2.10068

A114 2.05211 0.00001 0.00000 0.00002 0.00002 2.05213

A115 2.06561 0.00001 0.00001 0.00002 0.00003 2.06564

A116 2.16546 -0.00001 -0.00001 -0.00004 -0.00005 2.16541

A117 2.06575 -0.00003 0.00000 -0.00003 -0.00003 2.06572

A118 2.06575 -0.00003 0.00000 -0.00003 -0.00002 2.06573

A119 2.06935 0.00000 0.00000 0.00002 0.00002 2.06937

A120 2.06937 0.00001 0.00000 0.00006 0.00006 2.06943

A121 2.06574 -0.00002 0.00000 -0.00001 0.00000 2.06574

A122 2.06575 -0.00003 0.00000 -0.00003 -0.00003 2.06572

A123 2.06935 0.00001 0.00000 0.00004 0.00003 2.06938

A124 2.06938 0.00000 0.00000 0.00004 0.00004 2.06942

A125 1.94444 0.00000 -0.00002 -0.00002 -0.00004 1.94440

A126 1.94722 0.00000 0.00002 0.00001 0.00003 1.94725

A127 1.84238 0.00000 0.00001 0.00000 0.00002 1.84239

A128 1.91162 -0.00001 -0.00003 -0.00004 -0.00006 1.91156

A129 1.90850 0.00000 0.00002 0.00001 0.00002 1.90852

A130 1.90813 0.00000 0.00000 0.00003 0.00004 1.90816

A131 1.94758 0.00000 0.00000 0.00000 0.00000 1.94758

A132 1.94492 0.00000 0.00000 -0.00001 -0.00001 1.94491

A133 1.84044 0.00000 0.00000 0.00001 0.00000 1.84044

A134 1.91253 0.00000 0.00000 0.00000 0.00000 1.91253

A135 1.90782 0.00000 0.00000 -0.00001 -0.00001 1.90781

A136 1.90889 0.00000 0.00000 0.00001 0.00001 1.90890

A137 1.94494 0.00000 0.00001 0.00001 0.00002 1.94495

A138 1.94760 0.00000 0.00000 0.00001 0.00001 1.94761

A139 1.84041 0.00000 -0.00001 -0.00001 -0.00002 1.84039

A140 1.91253 0.00000 0.00000 0.00001 0.00001 1.91254

A141 1.90889 0.00000 0.00000 -0.00001 -0.00001 1.90888

A142 1.90781 0.00000 0.00000 -0.00002 -0.00002 1.90780

A143 1.94725 0.00000 0.00002 0.00000 0.00002 1.94727

A144 1.94443 0.00000 -0.00002 0.00002 0.00000 1.94443

A145 1.84235 0.00000 0.00001 -0.00001 0.00000 1.84235

A146 1.91160 -0.00001 -0.00002 -0.00001 -0.00004 1.91157

A147 1.90814 0.00000 0.00000 -0.00002 -0.00002 1.90812

A148 1.90852 0.00000 0.00002 0.00002 0.00004 1.90856

A149 1.94495 0.00000 0.00000 0.00000 0.00001 1.94495

A150 1.94759 0.00000 0.00000 0.00001 0.00002 1.94761

A151 1.84041 0.00000 -0.00001 -0.00001 -0.00001 1.84039

A152 1.91253 0.00000 0.00000 0.00001 0.00001 1.91254

A153 1.90889 0.00000 0.00000 -0.00001 -0.00001 1.90888

A154 1.90781 0.00000 0.00000 -0.00001 -0.00001 1.90780

A155 1.94758 0.00000 0.00000 0.00000 0.00000 1.94758

A156 1.94492 0.00000 0.00001 -0.00001 0.00000 1.94491

A157 1.84044 0.00000 -0.00001 0.00001 0.00000 1.84044

A158 1.91253 0.00000 0.00000 0.00001 0.00000 1.91253

A159 1.90782 0.00000 0.00000 -0.00001 -0.00001 1.90781

A160 1.90889 0.00000 0.00000 0.00001 0.00001 1.90890

A161 1.94444 0.00000 -0.00002 -0.00002 -0.00004 1.94440

A162 1.94722 0.00000 0.00001 0.00002 0.00003 1.94725

A163 1.84238 0.00000 0.00001 0.00000 0.00001 1.84239

A164 1.91162 -0.00001 -0.00003 -0.00003 -0.00006 1.91156

A165 1.90850 0.00000 0.00001 0.00001 0.00003 1.90852

A166 1.90813 0.00000 0.00001 0.00003 0.00004 1.90816

A167 1.94726 0.00000 0.00002 0.00000 0.00002 1.94728

A168 1.94442 0.00000 -0.00002 0.00002 0.00000 1.94443

A169 1.84235 0.00000 0.00001 -0.00002 0.00000 1.84235

A170 1.91160 -0.00001 -0.00003 -0.00001 -0.00004 1.91156

A171 1.90813 0.00000 0.00000 -0.00002 -0.00001 1.90812

A172 1.90852 0.00000 0.00002 0.00002 0.00004 1.90855

A173 3.11886 0.00000 0.00003 0.00000 0.00002 3.11888

A174 3.11887 0.00000 0.00002 -0.00002 0.00001 3.11888

A175 3.33436 0.00000 -0.00010 0.00004 -0.00006 3.33431

A176 2.90756 0.00000 0.00010 -0.00016 -0.00006 2.90750

D1 0.00320 0.00000 0.00006 -0.00007 -0.00002 0.00319

D2 3.02518 0.00000 -0.00005 0.00003 -0.00002 3.02516

D3 3.13062 0.00000 -0.00003 -0.00013 -0.00016 3.13047

D4 -0.13059 0.00000 -0.00013 -0.00003 -0.00016 -0.13074

D5 -0.00188 0.00000 -0.00003 0.00003 0.00000 -0.00188

D6 -3.12436 0.00000 0.00005 0.00021 0.00026 -3.12411

D7 -3.12966 0.00000 0.00005 0.00008 0.00013 -3.12953

D8 0.03104 0.00000 0.00013 0.00026 0.00039 0.03143

D9 0.17278 0.00000 0.00010 0.00011 0.00021 0.17299

D10 -2.98522 0.00000 0.00000 0.00005 0.00005 -2.98517

D11 -0.00323 0.00000 -0.00006 0.00009 0.00003 -0.00320

D12 -3.13049 0.00000 0.00003 -0.00003 0.00000 -3.13050

D13 -3.02520 0.00000 0.00004 -0.00002 0.00003 -3.02517

D14 0.13073 0.00000 0.00013 -0.00014 -0.00001 0.13072

D15 -2.95672 0.00000 0.00001 0.00004 0.00005 -2.95666

D16 -0.04915 0.00000 0.00011 -0.00011 -0.00001 -0.04916

D17 0.04894 0.00000 -0.00011 0.00016 0.00005 0.04900

D18 2.95651 0.00000 -0.00001 0.00000 -0.00001 2.95650

D19 0.00194 0.00000 0.00004 -0.00007 -0.00003 0.00191

D20 3.12432 0.00000 -0.00004 -0.00013 -0.00017 3.12414

D21 3.12957 0.00000 -0.00005 0.00005 0.00000 3.12957

D22 -0.03124 0.00000 -0.00013 -0.00001 -0.00014 -0.03138

D23 -0.17273 0.00000 -0.00009 0.00013 0.00004 -0.17269

D24 2.98544 0.00000 0.00001 -0.00001 0.00000 2.98544

D25 -0.00004 0.00000 0.00000 0.00003 0.00002 -0.00002

D26 3.12523 0.00000 -0.00007 -0.00013 -0.00020 3.12503

D27 -3.12521 0.00000 0.00006 0.00007 0.00014 -3.12507

D28 0.00005 0.00000 0.00000 -0.00008 -0.00008 -0.00003

D29 -3.12489 0.00000 0.00012 0.00018 0.00031 -3.12458

D30 0.01334 0.00001 0.00019 0.00014 0.00033 0.01367

D31 -0.00475 0.00000 0.00003 0.00012 0.00015 -0.00460

D32 3.13348 0.00000 0.00010 0.00007 0.00018 3.13365

D33 3.12493 -0.00001 -0.00012 -0.00020 -0.00032 3.12461

D34 -0.01336 -0.00001 -0.00019 -0.00007 -0.00026 -0.01362

D35 0.00467 0.00000 -0.00003 0.00000 -0.00003 0.00464

D36 -3.13362 0.00000 -0.00010 0.00013 0.00003 -3.13359

D37 -0.05228 0.00000 0.00007 -0.00025 -0.00018 -0.05246

D38 3.12228 0.00000 -0.00002 -0.00011 -0.00012 3.12215

D39 -3.09796 0.00000 -0.00002 -0.00010 -0.00012 -3.09808

D40 0.27574 0.00000 -0.00009 0.00034 0.00025 0.27599

D41 0.01495 0.00000 0.00005 -0.00023 -0.00017 0.01478

D42 -2.89453 0.00000 -0.00001 0.00021 0.00020 -2.89433

D43 3.10537 0.00000 0.00006 0.00005 0.00012 3.10548

D44 -0.02329 0.00000 0.00011 0.00009 0.00020 -0.02309

D45 -0.00891 0.00000 -0.00001 0.00017 0.00017 -0.00874

D46 -3.13757 0.00000 0.00004 0.00022 0.00025 -3.13732

D47 -0.01492 0.00000 -0.00008 0.00019 0.00011 -0.01481

D48 3.09789 0.00000 0.00002 0.00014 0.00016 3.09805

D49 2.89457 0.00000 -0.00001 -0.00025 -0.00026 2.89432

D50 -0.27580 0.00000 0.00009 -0.00029 -0.00021 -0.27601

D51 -0.22742 0.00000 0.00009 -0.00025 -0.00016 -0.22759

D52 3.10694 0.00000 -0.00001 -0.00021 -0.00022 3.10672

D53 -3.10678 0.00000 0.00001 0.00023 0.00024 -3.10653

D54 0.22759 0.00000 -0.00009 0.00027 0.00018 0.22777

D55 0.00882 0.00000 0.00008 -0.00008 0.00000 0.00882

D56 3.13754 0.00000 0.00002 -0.00016 -0.00014 3.13740

D57 -3.10536 0.00000 -0.00002 -0.00003 -0.00005 -3.10540

D58 0.02337 0.00000 -0.00007 -0.00011 -0.00019 0.02318

D59 0.05220 0.00000 -0.00006 0.00006 -0.00001 0.05219

D60 -3.12248 0.00000 0.00005 0.00000 0.00005 -3.12243

D61 0.00005 0.00000 -0.00004 -0.00006 -0.00010 -0.00004

D62 3.13041 0.00000 -0.00008 -0.00009 -0.00017 3.13023

D63 -3.13035 0.00000 0.00001 0.00002 0.00002 -3.13033

D64 0.00000 0.00000 -0.00003 -0.00002 -0.00005 -0.00005

D65 -3.12623 0.00000 0.00008 0.00009 0.00017 -3.12607

D66 0.02055 0.00000 0.00007 0.00015 0.00022 0.02077

D67 0.00094 0.00000 0.00002 -0.00001 0.00001 0.00095

D68 -3.13546 0.00000 0.00001 0.00005 0.00006 -3.13540

D69 3.12617 0.00000 -0.00003 -0.00002 -0.00005 3.12612

D70 -0.02056 0.00000 0.00000 -0.00009 -0.00009 -0.02066

D71 -0.00094 0.00000 0.00002 0.00003 0.00005 -0.00089

D72 3.13552 0.00000 0.00005 -0.00004 0.00000 3.13552

D73 -3.12245 0.00000 0.00003 -0.00005 -0.00003 -3.12248

D74 0.05222 0.00000 -0.00008 0.00005 -0.00003 0.05219

D75 -0.00015 0.00001 0.00004 0.00012 0.00017 0.00001

D76 3.13023 0.00000 0.00000 0.00004 0.00005 3.13028

D77 -3.13054 0.00001 0.00007 0.00020 0.00027 -3.13027

D78 -0.00016 0.00000 0.00003 0.00012 0.00015 -0.00001

D79 -3.10519 -0.00001 -0.00008 -0.00017 -0.00025 -3.10544

D80 0.00899 0.00000 0.00001 -0.00026 -0.00025 0.00875

D81 0.02352 -0.00001 -0.00011 -0.00026 -0.00037 0.02315

D82 3.13770 -0.00001 -0.00002 -0.00035 -0.00037 3.13733

D83 0.00104 0.00000 -0.00002 -0.00011 -0.00012 0.00092

D84 -3.13532 0.00000 -0.00004 -0.00012 -0.00015 -3.13547

D85 -3.12611 0.00000 0.00002 -0.00001 0.00001 -3.12610

D86 0.02072 0.00000 0.00000 -0.00002 -0.00002 0.02070

D87 -0.00874 0.00000 -0.00008 0.00005 -0.00003 -0.00877

D88 3.10551 0.00000 0.00003 -0.00011 -0.00008 3.10543

D89 -3.13743 0.00000 -0.00004 0.00014 0.00010 -3.13733

D90 -0.02319 0.00000 0.00008 -0.00002 0.00006 -0.02313

D91 -0.00085 0.00000 -0.00002 -0.00004 -0.00006 -0.00091

D92 3.13564 -0.00001 -0.00002 -0.00012 -0.00014 3.13551

D93 3.12630 0.00000 -0.00007 -0.00015 -0.00022 3.12608

D94 -0.02040 -0.00001 -0.00007 -0.00022 -0.00029 -0.02069

D95 0.01489 0.00000 0.00009 -0.00022 -0.00013 0.01476

D96 -2.89462 0.00000 0.00003 0.00023 0.00026 -2.89436

D97 -3.09800 0.00000 -0.00003 -0.00005 -0.00008 -3.09807

D98 0.27568 0.00000 -0.00009 0.00040 0.00031 0.27599

D99 3.12232 0.00000 -0.00007 -0.00006 -0.00013 3.12219

D100 -0.05227 0.00000 0.00007 -0.00026 -0.00019 -0.05246

D101 3.09783 0.00000 0.00003 0.00021 0.00024 3.09806

D102 -0.01499 0.00000 -0.00007 0.00030 0.00023 -0.01476

D103 -0.27583 0.00000 0.00009 -0.00025 -0.00016 -0.27599

D104 2.89454 0.00000 0.00000 -0.00016 -0.00016 2.89437

D105 3.10700 0.00000 -0.00001 -0.00027 -0.00028 3.10672

D106 -0.22737 0.00000 0.00009 -0.00031 -0.00022 -0.22759

D107 0.22761 0.00000 -0.00009 0.00024 0.00015 0.22776

D108 -3.10675 0.00000 0.00001 0.00020 0.00021 -3.10655

D109 -0.17271 0.00000 -0.00008 0.00008 0.00001 -0.17270

D110 2.98555 0.00000 -0.00007 -0.00002 -0.00009 2.98545

D111 -3.13054 0.00000 0.00002 0.00003 0.00005 -3.13049

D112 -0.00335 0.00001 0.00001 0.00012 0.00013 -0.00321

D113 0.13073 0.00000 0.00011 -0.00011 -0.00001 0.13072

D114 -3.02526 0.00000 0.00010 -0.00002 0.00008 -3.02518

D115 0.00336 -0.00001 -0.00001 -0.00018 -0.00019 0.00316

D116 3.13066 0.00000 -0.00003 -0.00017 -0.00020 3.13045

D117 3.02528 -0.00001 -0.00011 -0.00004 -0.00015 3.02513

D118 -0.13060 0.00000 -0.00012 -0.00003 -0.00016 -0.13076

D119 2.95647 0.00000 0.00000 0.00003 0.00003 2.95650

D120 0.04891 0.00000 -0.00010 0.00019 0.00009 0.04900

D121 -0.04913 0.00000 0.00011 -0.00013 -0.00003 -0.04916

D122 -2.95669 0.00000 0.00001 0.00003 0.00004 -2.95666

D123 3.12954 0.00000 -0.00001 0.00007 0.00006 3.12960

D124 -0.03120 0.00000 -0.00012 -0.00005 -0.00017 -0.03137

D125 0.00197 0.00000 0.00000 -0.00002 -0.00002 0.00196

D126 3.12442 -0.00001 -0.00011 -0.00014 -0.00025 3.12417

D127 0.00002 0.00000 -0.00001 -0.00009 -0.00010 -0.00008

D128 3.12530 0.00000 -0.00011 -0.00022 -0.00032 3.12498

D129 -3.12521 0.00000 0.00009 0.00002 0.00011 -3.12511

D130 0.00007 0.00000 -0.00001 -0.00011 -0.00012 -0.00005

D131 -3.12495 0.00001 0.00015 0.00025 0.00040 -3.12455

D132 0.01334 0.00001 0.00019 0.00017 0.00036 0.01370

D133 -0.00473 0.00000 0.00002 0.00011 0.00014 -0.00459

D134 3.13356 0.00000 0.00007 0.00003 0.00010 3.13366

D135 -0.00201 0.00000 0.00001 0.00016 0.00018 -0.00183

D136 -3.12967 0.00000 0.00003 0.00016 0.00019 -3.12948

D137 -3.12451 0.00001 0.00013 0.00031 0.00044 -3.12407

D138 0.03101 0.00001 0.00014 0.00031 0.00045 0.03147

D139 0.00464 0.00000 -0.00001 0.00004 0.00003 0.00467

D140 -3.13369 0.00000 -0.00005 0.00016 0.00011 -3.13358

D141 3.12492 0.00000 -0.00014 -0.00012 -0.00027 3.12465

D142 -0.01341 0.00000 -0.00018 -0.00001 -0.00018 -0.01359

D143 0.17279 0.00000 0.00009 0.00013 0.00021 0.17301

D144 -2.98534 0.00001 0.00007 0.00014 0.00020 -2.98514

D145 -0.00093 0.00000 -0.00001 0.00002 0.00001 -0.00092

D146 -3.13764 0.00000 0.00002 0.00007 0.00009 -3.13755

D147 3.13512 0.00000 0.00001 0.00003 0.00004 3.13516

D148 -0.00158 0.00000 0.00004 0.00008 0.00012 -0.00147

D149 -3.09845 0.00000 -0.00004 0.00016 0.00012 -3.09834

D150 0.04876 0.00000 -0.00006 0.00015 0.00009 0.04884

D151 -0.00007 0.00000 0.00002 0.00006 0.00007 0.00000

D152 -3.13684 0.00000 0.00003 0.00005 0.00008 -3.13677

D153 3.13673 0.00000 -0.00001 0.00001 0.00000 3.13673

D154 -0.00004 0.00000 0.00000 0.00000 0.00000 -0.00003

D155 0.00096 0.00000 0.00000 -0.00004 -0.00005 0.00092

D156 -3.13523 0.00000 -0.00001 0.00004 0.00003 -3.13520

D157 3.13763 0.00000 -0.00002 -0.00003 -0.00005 3.13758

D158 0.00144 0.00000 -0.00002 0.00004 0.00003 0.00147

D159 3.09858 0.00000 0.00006 -0.00024 -0.00018 3.09840

D160 -0.04849 0.00000 0.00006 -0.00032 -0.00026 -0.04875

D161 -0.00472 0.00000 0.00002 0.00002 0.00004 -0.00468

D162 3.14123 0.00000 0.00003 0.00008 0.00011 3.14134

D163 3.13341 0.00000 0.00006 -0.00010 -0.00005 3.13336

D164 -0.00383 0.00000 0.00006 -0.00004 0.00002 -0.00381

D165 3.11414 0.00000 -0.00010 0.00022 0.00012 3.11426

D166 -0.02396 0.00000 -0.00013 0.00034 0.00021 -0.02376

D167 0.00001 0.00000 0.00000 -0.00001 -0.00002 -0.00001

D168 -3.13735 0.00000 0.00000 0.00004 0.00004 -3.13730

D169 3.13735 0.00000 -0.00001 -0.00007 -0.00009 3.13726

D170 -0.00001 0.00000 0.00000 -0.00002 -0.00002 -0.00003

D171 0.00474 0.00000 -0.00002 -0.00005 -0.00007 0.00467

D172 -3.13334 0.00000 -0.00006 0.00003 -0.00003 -3.13337

D173 -3.14119 0.00000 -0.00003 -0.00011 -0.00014 -3.14133

D174 0.00391 0.00000 -0.00007 -0.00002 -0.00009 0.00382

D175 -3.11441 0.00000 0.00011 0.00011 0.00022 -3.11419

D176 0.02365 0.00000 0.00015 0.00003 0.00018 0.02382

D177 0.00094 0.00000 0.00001 -0.00001 -0.00001 0.00093

D178 3.13764 0.00000 -0.00001 -0.00006 -0.00007 3.13757

D179 -3.13522 0.00000 -0.00003 0.00006 0.00004 -3.13518

D180 0.00149 0.00000 -0.00004 0.00002 -0.00002 0.00147

D181 3.09866 -0.00001 0.00002 -0.00029 -0.00027 3.09839

D182 -0.04845 0.00000 0.00005 -0.00037 -0.00032 -0.04877

D183 0.00001 0.00000 -0.00002 -0.00001 -0.00003 -0.00003

D184 3.13679 0.00000 -0.00002 -0.00006 -0.00008 3.13670

D185 -3.13680 0.00000 0.00000 0.00003 0.00003 -3.13677

D186 -0.00002 0.00000 -0.00001 -0.00002 -0.00002 -0.00004

D187 -0.00095 0.00000 0.00000 0.00003 0.00003 -0.00092

D188 3.13515 0.00000 0.00001 -0.00004 -0.00002 3.13513

D189 -3.13763 0.00000 0.00001 0.00007 0.00008 -3.13754

D190 -0.00153 0.00000 0.00002 0.00001 0.00003 -0.00150

D191 -3.09837 0.00000 -0.00006 0.00005 -0.00001 -3.09838

D192 0.04880 0.00000 -0.00007 0.00011 0.00004 0.04885

D193 -0.00474 0.00000 0.00003 0.00004 0.00007 -0.00467

D194 3.14123 0.00000 0.00002 0.00011 0.00012 3.14135

D195 3.13335 0.00000 0.00011 -0.00010 0.00001 3.13336

D196 -0.00387 0.00000 0.00009 -0.00004 0.00006 -0.00381

D197 3.11412 0.00000 -0.00006 0.00021 0.00015 3.11427

D198 -0.02395 0.00000 -0.00013 0.00035 0.00022 -0.02373

D199 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D200 -3.13731 0.00000 -0.00001 0.00002 0.00001 -3.13731

D201 3.13732 0.00000 0.00001 -0.00006 -0.00005 3.13727

D202 0.00000 0.00000 0.00000 -0.00004 -0.00004 -0.00004

D203 0.00477 0.00000 -0.00003 -0.00008 -0.00011 0.00465

D204 -3.13325 0.00000 -0.00011 -0.00003 -0.00014 -3.13339

D205 -3.14120 0.00000 -0.00002 -0.00010 -0.00012 -3.14132

D206 0.00396 0.00000 -0.00009 -0.00005 -0.00015 0.00382

D207 -3.11439 0.00000 0.00008 0.00013 0.00021 -3.11418

D208 0.02360 0.00000 0.00015 0.00008 0.00023 0.02383

D209 1.05338 0.00000 -0.00002 0.00031 0.00029 1.05367

D210 -1.08909 0.00001 0.00002 0.00036 0.00038 -1.08871

D211 3.12322 0.00000 0.00000 0.00031 0.00031 3.12353

D212 1.08938 0.00000 -0.00001 -0.00023 -0.00024 1.08914

D213 -1.05308 0.00000 0.00003 -0.00023 -0.00020 -1.05328

D214 -3.12292 0.00000 0.00001 -0.00025 -0.00025 -3.12317

D215 1.09398 0.00000 -0.00001 0.00023 0.00022 1.09420

D216 -1.05027 0.00000 -0.00001 0.00024 0.00022 -1.05005

D217 -3.11968 0.00000 -0.00001 0.00023 0.00022 -3.11946

D218 1.05002 0.00000 0.00004 -0.00006 -0.00002 1.05000

D219 -1.09425 0.00000 0.00003 -0.00009 -0.00005 -1.09431

D220 3.11942 0.00000 0.00004 -0.00007 -0.00003 3.11939

D221 1.08938 0.00000 -0.00001 -0.00023 -0.00023 1.08915

D222 -1.05307 0.00000 0.00003 -0.00023 -0.00020 -1.05327

D223 -3.12292 0.00000 0.00001 -0.00026 -0.00024 -3.12316

D224 1.05340 0.00000 -0.00002 0.00028 0.00026 1.05366

D225 -1.08906 0.00000 0.00002 0.00033 0.00034 -1.08872

D226 3.12325 0.00000 -0.00001 0.00028 0.00028 3.12352

D227 1.09401 0.00000 -0.00003 0.00022 0.00019 1.09420

D228 -1.05024 0.00000 -0.00003 0.00022 0.00019 -1.05005

D229 -3.11964 0.00000 -0.00003 0.00021 0.00018 -3.11947

D230 1.05006 0.00000 0.00002 -0.00009 -0.00007 1.04999

D231 -1.09422 0.00000 0.00002 -0.00011 -0.00010 -1.09432

D232 3.11946 0.00000 0.00001 -0.00010 -0.00009 3.11937

Item Value Threshold Converged?

Maximum Force 0.000026 0.000450 YES

RMS Force 0.000005 0.000300 YES

Maximum Displacement 0.002553 0.001800 NO

RMS Displacement 0.000497 0.001200 YES

Predicted change in Energy=-5.535442D-08

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Jul 6 03:48:58 2019, MaxMem= 1342177280 cpu: 15.3

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=0 Diff= 6.82D-05

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 -1.126174 2.799765 -0.018207

2 7 0 -0.001792 2.037851 -0.169207

3 6 0 1.121239 2.801729 -0.018007

4 6 0 0.709557 4.166162 0.247780

5 6 0 -0.716909 4.164903 0.247667

6 7 0 2.407623 2.385263 -0.112861

7 6 0 2.796686 1.132806 -0.187231

8 7 0 2.018991 0.001793 -0.128998

9 6 0 2.798653 -1.127880 -0.187446

10 6 0 4.208901 -0.701195 -0.313988

11 6 0 4.207693 0.708540 -0.313816

12 7 0 -2.411788 2.381046 -0.113322

13 6 0 -4.208922 0.701204 -0.313965

14 6 0 -4.207703 -0.708535 -0.313847

15 6 0 -2.796692 -1.132795 -0.187274

16 7 0 -2.019010 -0.001777 -0.129031

17 6 0 -2.798665 1.127894 -0.187483

18 7 0 -2.407621 -2.385263 -0.112890

19 7 0 0.001808 -2.037864 -0.169191

20 6 0 -1.121224 -2.801736 -0.018004

21 6 0 -0.709539 -4.166171 0.247782

22 6 0 0.716930 -4.164895 0.247744

23 6 0 1.126188 -2.799764 -0.018165

24 7 0 2.411792 -2.381037 -0.113280

25 30 0 -0.000007 -0.000009 -0.367537

26 6 0 -5.402583 1.426812 -0.407440

27 6 0 -6.595962 0.690018 -0.499716

28 6 0 -6.594777 -0.701422 -0.499596

29 6 0 -5.400138 -1.436165 -0.407195

30 6 0 1.438976 -5.348382 0.498824

31 6 0 0.706213 -6.515155 0.740209

32 6 0 -0.694537 -6.516418 0.740210

33 6 0 -1.429428 -5.350975 0.498840

34 6 0 5.400133 1.436161 -0.407149

35 6 0 6.594763 0.701413 -0.499621

36 6 0 6.595932 -0.690028 -0.499835

37 6 0 5.402547 -1.426814 -0.407559

38 6 0 -1.438949 5.348412 0.498674

39 6 0 -0.706184 6.515175 0.740096

40 6 0 0.694565 6.516413 0.740191

41 6 0 1.429450 5.350957 0.498870

42 1 0 7.544838 1.212786 -0.577704

43 1 0 7.546852 -1.199778 -0.578113

44 1 0 1.201474 7.451276 0.937816

45 1 0 -1.214753 7.449147 0.937691

46 1 0 -7.546891 1.199764 -0.577915

47 1 0 -7.544850 -1.212797 -0.577676

48 1 0 -1.201441 -7.451286 0.937817

49 1 0 1.214783 -7.449117 0.937848

50 8 0 2.778926 5.294292 0.496359

51 8 0 -2.788316 5.289297 0.496004

52 8 0 5.339562 2.784035 -0.409536

53 8 0 5.344210 -2.774794 -0.410412

54 8 0 2.788345 -5.289234 0.496237

55 8 0 -2.778905 -5.294327 0.496255

56 8 0 -5.339551 -2.784039 -0.409652

57 8 0 -5.344282 2.774793 -0.410164

58 6 0 3.507162 6.485550 0.783963

59 1 0 3.271323 6.866566 1.781947

60 1 0 3.314214 7.264327 0.040253

61 1 0 4.557400 6.202370 0.744928

62 6 0 6.559875 3.521596 -0.450752

63 1 0 7.116614 3.327394 -1.372126

64 1 0 7.191899 3.297466 0.413670

65 1 0 6.266554 4.569272 -0.421543

66 6 0 6.565700 -3.510389 -0.451854

67 1 0 7.197399 -3.285539 0.412617

68 1 0 7.122113 -3.315082 -1.373193

69 1 0 6.274002 -4.558527 -0.422929

70 6 0 -3.518752 6.479245 0.783413

71 1 0 -3.327481 7.258181 0.039424

72 1 0 -3.283457 6.861019 1.781237

73 1 0 -4.568443 6.194019 0.744632

74 6 0 -6.565798 3.510349 -0.451459

75 1 0 -7.197441 3.285381 0.413024

76 1 0 -7.122257 3.315122 -1.372788

77 1 0 -6.274136 4.558495 -0.422433

78 6 0 -6.559847 -3.521629 -0.450898

79 1 0 -7.116597 -3.327394 -1.372259

80 1 0 -7.191871 -3.297561 0.413540

81 1 0 -6.266499 -4.569298 -0.421747

82 6 0 -3.507142 -6.485594 0.783817

83 1 0 -3.271347 -6.866611 1.781811

84 1 0 -3.314153 -7.264367 0.040114

85 1 0 -4.557381 -6.202423 0.744733

86 6 0 3.518804 -6.479147 0.783733

87 1 0 3.327613 -7.258115 0.039757

88 1 0 3.283453 -6.860897 1.781553

89 1 0 4.568488 -6.193886 0.745017

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0447620 0.0439710 0.0225232

Leave Link 202 at Sat Jul 6 03:48:59 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 1187 symmetry adapted cartesian basis functions of A symmetry.

There are 1128 symmetry adapted basis functions of A symmetry.

1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

203 alpha electrons 201 beta electrons

nuclear repulsion energy 8042.1115213372 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= 89 NActive= 89 NUniq= 89 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= -0.2279722483 Hartrees.

Nuclear repulsion after empirical dispersion term = 8041.8835490889 Hartrees.

No density basis found on file 724.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

GePol: Number of exposed spheres = 89 (100.00%)

GePol: Number of points = 6400

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.13D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 402

GePol: Fraction of low-weight points (<1% of avg) = 6.28%

GePol: Cavity surface area = 703.219 Ang\*\*2

GePol: Cavity volume = 801.603 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = -0.0089874220 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 8041.8745616668 Hartrees.

Leave Link 301 at Sat Jul 6 03:49:00 2019, MaxMem= 1342177280 cpu: 1.6

(Enter /apps/gaussian/g09d01/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44310 LenP2D= 111303.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1128 RedAO= T EigKep= 5.55D-05 NBF= 1128

NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 1128

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= 1148 1148 1148 1148 1148 MxSgAt= 89 MxSgA2= 89.

Leave Link 302 at Sat Jul 6 03:49:03 2019, MaxMem= 1342177280 cpu: 42.7

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Jul 6 03:49:04 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "ZnOMPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000001 0.000000 -0.000024 Ang= 0.00 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>= 2.0171 S= 1.0057

Leave Link 401 at Sat Jul 6 03:49:10 2019, MaxMem= 1342177280 cpu: 72.6

(Enter /apps/gaussian/g09d01/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4268513 IEndB= 4268513 NGot= 1342177280 MDV= 1339335564

LenX= 1339335564 LenY= 1337925408

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= 540000000 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= 122880000.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.77D-15 for 6400.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.56D-15 for 3587 206.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.99D-15 for 6400.

Iteration 1 A^-1\*A deviation from orthogonality is 3.38D-09 for 5076 5009.

Iteration 2 A\*A^-1 deviation from unit magnitude is 4.44D-15 for 136.

Iteration 2 A\*A^-1 deviation from orthogonality is 5.18D-15 for 1925 1037.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 367.

Iteration 2 A^-1\*A deviation from orthogonality is 5.78D-16 for 6366 2621.

E= -2649.79551968650

DIIS: error= 2.36D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2649.79551968650 IErMin= 1 ErrMin= 2.36D-05

ErrMax= 2.36D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.47D-06 BMatP= 2.47D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.685 Goal= None Shift= 0.000

Gap= 0.744 Goal= None Shift= 0.000

RMSDP=1.39D-06 MaxDP=8.66D-05 OVMax= 1.38D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.39D-06 CP: 1.00D+00

E= -2649.79552082454 Delta-E= -0.000001138042 Rises=F Damp=F

DIIS: error= 2.20D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2649.79552082454 IErMin= 2 ErrMin= 2.20D-06

ErrMax= 2.20D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.23D-08 BMatP= 2.47D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.682D-01 0.107D+01

Coeff: -0.682D-01 0.107D+01

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.67D-07 MaxDP=8.20D-06 DE=-1.14D-06 OVMax= 3.35D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.55D-07 CP: 1.00D+00 1.04D+00

E= -2649.79552083604 Delta-E= -0.000000011505 Rises=F Damp=F

DIIS: error= 2.72D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2649.79552083604 IErMin= 2 ErrMin= 2.20D-06

ErrMax= 2.72D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.04D-08 BMatP= 3.23D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.379D-01 0.522D+00 0.516D+00

Coeff: -0.379D-01 0.522D+00 0.516D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=9.20D-08 MaxDP=8.92D-06 DE=-1.15D-08 OVMax= 2.46D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 7.61D-08 CP: 1.00D+00 1.05D+00 6.87D-01

E= -2649.79552083906 Delta-E= -0.000000003021 Rises=F Damp=F

DIIS: error= 1.64D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2649.79552083906 IErMin= 4 ErrMin= 1.64D-06

ErrMax= 1.64D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.11D-09 BMatP= 2.04D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.966D-02 0.114D+00 0.349D+00 0.546D+00

Coeff: -0.966D-02 0.114D+00 0.349D+00 0.546D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=3.79D-08 MaxDP=3.38D-06 DE=-3.02D-09 OVMax= 1.36D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.28D-08 CP: 1.00D+00 1.05D+00 7.94D-01 6.77D-01

E= -2649.79552084063 Delta-E= -0.000000001564 Rises=F Damp=F

DIIS: error= 2.43D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2649.79552084063 IErMin= 5 ErrMin= 2.43D-07

ErrMax= 2.43D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.67D-10 BMatP= 6.11D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.150D-02 0.100D-01 0.109D+00 0.225D+00 0.657D+00

Coeff: -0.150D-02 0.100D-01 0.109D+00 0.225D+00 0.657D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=1.04D-08 MaxDP=6.69D-07 DE=-1.56D-09 OVMax= 8.96D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.23D-09 CP: 1.00D+00 1.05D+00 8.10D-01 7.27D-01 9.40D-01

E= -2649.79552084063 Delta-E= -0.000000000004 Rises=F Damp=F

DIIS: error= 1.68D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2649.79552084063 IErMin= 6 ErrMin= 1.68D-07

ErrMax= 1.68D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.31D-11 BMatP= 1.67D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.646D-03-0.137D-01 0.107D-01 0.522D-01 0.429D+00 0.521D+00

Coeff: 0.646D-03-0.137D-01 0.107D-01 0.522D-01 0.429D+00 0.521D+00

Gap= 0.044 Goal= None Shift= 0.000

Gap= 0.066 Goal= None Shift= 0.000

RMSDP=6.13D-09 MaxDP=4.13D-07 DE=-3.64D-12 OVMax= 6.76D-06

Error on total polarization charges = 0.07299

SCF Done: E(UB3LYP) = -2649.79552084 A.U. after 6 cycles

NFock= 6 Conv=0.61D-08 -V/T= 1.9850

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0171 S= 1.0057

<L.S>= 0.000000000000E+00

KE= 2.690146913247D+03 PE=-2.236246715931D+04 EE= 8.980650163554D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0171, after 2.0002

Leave Link 502 at Sat Jul 6 03:54:39 2019, MaxMem= 1342177280 cpu: 3848.7

(Enter /apps/gaussian/g09d01/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44310 LenP2D= 111303.

LDataN: DoStor=T MaxTD1= 6 Len= 172

D1PCM: PCM CHGder 1st derivatives, ID1Alg=3 FixD1E=F DoIter=F DoCFld=F I1PDM=0.

GePol: Maximum number of non-zero 1st derivatives = 275

Leave Link 701 at Sat Jul 6 03:55:00 2019, MaxMem= 1342177280 cpu: 226.0

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Jul 6 03:55:00 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=T IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 2127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FMM levels: 10 Number of levels for PrismC: 9

Leave Link 703 at Sat Jul 6 03:56:37 2019, MaxMem= 1342177280 cpu: 1169.2

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 3.02753565D-05-1.09302027D-05 1.95916588D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000000498 -0.000004026 0.000002794

2 7 -0.000018920 0.000002049 0.000000076

3 6 0.000018424 0.000001193 0.000005118

4 6 -0.000002505 -0.000001651 -0.000006054

5 6 -0.000000071 0.000006975 -0.000007558

6 7 0.000000504 0.000021283 0.000000181

7 6 0.000001116 -0.000026467 0.000001099

8 7 0.000002341 -0.000006030 0.000003378

9 6 -0.000003242 0.000016993 0.000001923

10 6 -0.000001630 -0.000006510 -0.000001857

11 6 0.000002187 0.000007850 0.000001344

12 7 -0.000006680 0.000015642 -0.000001311

13 6 0.000002606 0.000005296 -0.000005286

14 6 -0.000002140 -0.000006528 0.000000733

15 6 0.000002596 0.000014592 0.000003066

16 7 0.000003818 0.000000241 0.000001115

17 6 0.000000976 -0.000016657 0.000009609

18 7 0.000006839 -0.000014520 0.000000287

19 7 0.000014141 0.000004261 -0.000001704

20 6 -0.000030606 0.000001574 0.000000351

21 6 0.000002327 0.000002906 -0.000002656

22 6 -0.000002499 -0.000007061 -0.000010179

23 6 0.000000305 0.000001283 0.000007848

24 7 0.000008532 -0.000012114 -0.000001433

25 30 0.000000181 0.000001043 -0.000003400

26 6 -0.000002233 0.000004873 -0.000002211

27 6 0.000002357 -0.000005641 -0.000000494

28 6 0.000002433 0.000003216 -0.000000685

29 6 -0.000003564 -0.000003266 0.000000418

30 6 0.000004764 0.000000080 0.000003840

31 6 0.000000183 0.000003693 -0.000000319

32 6 0.000000381 0.000005385 -0.000002235

33 6 -0.000003365 -0.000002823 0.000009456

34 6 0.000003003 0.000003072 -0.000000788

35 6 -0.000002081 -0.000003918 -0.000001161

36 6 -0.000003087 0.000003806 0.000000088

37 6 0.000003207 -0.000005812 -0.000004718

38 6 -0.000004344 -0.000001147 0.000006594

39 6 0.000000577 -0.000003165 -0.000000806

40 6 0.000000088 -0.000005039 -0.000002825

41 6 0.000003542 0.000002865 0.000008715

42 1 -0.000000573 -0.000000876 0.000001650

43 1 0.000001387 -0.000000862 0.000001588

44 1 0.000001495 0.000000681 0.000003044

45 1 -0.000001528 0.000000009 0.000001522

46 1 -0.000000965 0.000000278 0.000001362

47 1 0.000000095 -0.000000071 0.000001354

48 1 -0.000001580 -0.000000933 0.000002655

49 1 0.000002255 -0.000000654 0.000001856

50 8 -0.000001847 -0.000004653 -0.000009977

51 8 0.000002015 -0.000002943 -0.000002205

52 8 -0.000002947 -0.000002823 -0.000003716

53 8 0.000000224 0.000009103 0.000004672

54 8 -0.000004927 0.000001308 -0.000002364

55 8 0.000002188 0.000004169 -0.000010687

56 8 0.000003764 0.000003453 -0.000004207

57 8 0.000002748 -0.000006315 0.000002038

58 6 -0.000001776 -0.000005438 -0.000000555

59 1 -0.000001251 0.000004390 -0.000001594

60 1 -0.000000805 0.000002627 0.000001723

61 1 -0.000003224 -0.000000676 0.000001271

62 6 -0.000001885 -0.000002402 0.000001431

63 1 -0.000000167 0.000000795 0.000001239

64 1 0.000000354 0.000000106 -0.000001361

65 1 0.000000561 -0.000000897 0.000000462

66 6 -0.000003849 0.000002957 -0.000002289

67 1 -0.000000350 0.000000635 -0.000000463

68 1 -0.000000095 0.000000716 0.000001621

69 1 0.000001782 0.000000593 0.000000474

70 6 0.000003273 -0.000006544 -0.000000987

71 1 0.000001871 0.000001624 0.000000515

72 1 -0.000001428 0.000002560 -0.000002229

73 1 0.000001519 0.000000990 0.000001515

74 6 0.000004207 -0.000002134 -0.000002707

75 1 0.000000001 -0.000000084 -0.000000593

76 1 0.000000259 -0.000000505 0.000001888

77 1 -0.000001708 -0.000000576 -0.000000197

78 6 0.000001817 0.000003678 0.000001480

79 1 0.000000121 -0.000000378 0.000001229

80 1 -0.000000267 0.000000227 -0.000001293

81 1 -0.000000502 0.000000851 0.000000670

82 6 0.000001477 0.000005541 0.000000116

83 1 0.000001067 -0.000004529 -0.000001588

84 1 0.000001302 -0.000002406 0.000001650

85 1 0.000003151 0.000000621 0.000001305

86 6 -0.000004865 0.000006128 -0.000000404

87 1 -0.000001880 -0.000001641 0.000000088

88 1 0.000001236 -0.000002666 -0.000002291

89 1 -0.000001712 -0.000000828 0.000000936

-------------------------------------------------------------------

Cartesian Forces: Max 0.000030606 RMS 0.000005163

Leave Link 716 at Sat Jul 6 03:56:38 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000016637 RMS 0.000003308

Search for a local minimum.

Step number 27 out of a maximum of 518

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .33079D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 6 5 7 9 11

14 13 16 17 18

19 20 21 22 23

24 25 26 27

DE= -6.26D-08 DEPred=-5.54D-08 R= 1.13D+00

Trust test= 1.13D+00 RLast= 2.58D-03 DXMaxT set to 2.35D-01

ITU= 0 0 0 1 1 1 1 1 1 1 0 0 -1 -1 0 -1 0 0 0 0

ITU= 0 0 1 1 1 1 0

Eigenvalues --- 0.00422 0.00642 0.00914 0.01218 0.01316

Eigenvalues --- 0.01316 0.01316 0.01318 0.01318 0.01329

Eigenvalues --- 0.01390 0.01565 0.01587 0.01592 0.01600

Eigenvalues --- 0.01644 0.01667 0.01708 0.01712 0.01715

Eigenvalues --- 0.01716 0.01781 0.01788 0.01838 0.01873

Eigenvalues --- 0.01891 0.01919 0.01921 0.01966 0.01980

Eigenvalues --- 0.02003 0.02018 0.02024 0.02030 0.02035

Eigenvalues --- 0.02050 0.02053 0.02054 0.02055 0.02057

Eigenvalues --- 0.02057 0.02058 0.02059 0.02060 0.02066

Eigenvalues --- 0.02067 0.02067 0.02068 0.02070 0.02074

Eigenvalues --- 0.02077 0.02081 0.02109 0.02166 0.02205

Eigenvalues --- 0.02239 0.02253 0.02256 0.02260 0.02261

Eigenvalues --- 0.02273 0.02329 0.02334 0.02351 0.02399

Eigenvalues --- 0.02704 0.03008 0.03663 0.04089 0.05994

Eigenvalues --- 0.09890 0.09972 0.09980 0.09983 0.09985

Eigenvalues --- 0.09986 0.09987 0.10211 0.10629 0.10646

Eigenvalues --- 0.10647 0.10650 0.10657 0.10658 0.10674

Eigenvalues --- 0.10683 0.13023 0.13466 0.13585 0.15456

Eigenvalues --- 0.15860 0.15990 0.15996 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16004 0.16007

Eigenvalues --- 0.16024 0.16029 0.16051 0.16088 0.16417

Eigenvalues --- 0.16955 0.17131 0.20829 0.21695 0.22131

Eigenvalues --- 0.22468 0.22475 0.22480 0.22501 0.24077

Eigenvalues --- 0.24313 0.24497 0.24517 0.24546 0.24607

Eigenvalues --- 0.24758 0.24816 0.24823 0.24902 0.24907

Eigenvalues --- 0.24923 0.24979 0.24985 0.24989 0.24993

Eigenvalues --- 0.24995 0.24998 0.24998 0.24999 0.24999

Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

Eigenvalues --- 0.25000 0.25010 0.25020 0.25189 0.25278

Eigenvalues --- 0.25517 0.26428 0.28025 0.29705 0.31253

Eigenvalues --- 0.33506 0.33679 0.33724 0.33948 0.34021

Eigenvalues --- 0.34059 0.34063 0.34063 0.34063 0.34063

Eigenvalues --- 0.34064 0.34068 0.34078 0.34081 0.34081

Eigenvalues --- 0.34081 0.34081 0.34081 0.34117 0.34531

Eigenvalues --- 0.34655 0.34685 0.34686 0.34686 0.34686

Eigenvalues --- 0.34687 0.34687 0.34720 0.34840 0.35032

Eigenvalues --- 0.35152 0.35588 0.35619 0.35632 0.35632

Eigenvalues --- 0.35633 0.35634 0.35645 0.35960 0.36180

Eigenvalues --- 0.36759 0.37091 0.37142 0.37807 0.40487

Eigenvalues --- 0.41174 0.41215 0.41216 0.41216 0.41217

Eigenvalues --- 0.41222 0.41318 0.41404 0.41417 0.41419

Eigenvalues --- 0.41539 0.41776 0.42114 0.42355 0.42747

Eigenvalues --- 0.43331 0.44521 0.44563 0.44753 0.44854

Eigenvalues --- 0.44888 0.44998 0.45004 0.45007 0.45032

Eigenvalues --- 0.45366 0.45369 0.45758 0.45904 0.46686

Eigenvalues --- 0.47318 0.47838 0.49365 0.49483 0.49833

Eigenvalues --- 0.50155 0.51822 0.53545 0.53554 0.53558

Eigenvalues --- 0.53581 0.53639 0.53843 0.55173 0.55680

Eigenvalues --- 0.56227 0.57178 0.57422 0.57743 0.58541

Eigenvalues --- 0.65010

En-DIIS/RFO-DIIS IScMMF= 0 using points: 27 26 25 24 23

RFO step: Lambda=-1.04689573D-08.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 1.54D-06 SmlDif= 1.00D-05

RMS Error= 0.8344800784D-05 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.06363 -0.03806 -0.06265 0.00098 0.03610

Iteration 1 RMS(Cart)= 0.00021120 RMS(Int)= 0.00000001

Iteration 2 RMS(Cart)= 0.00000003 RMS(Int)= 0.00000001

ITry= 1 IFail=0 DXMaxC= 1.46D-03 DCOld= 1.00D+10 DXMaxT= 2.35D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58247 0.00000 0.00000 -0.00001 -0.00001 2.58246

R2 2.73964 0.00000 0.00000 -0.00001 -0.00001 2.73963

R3 2.56138 0.00000 0.00000 -0.00001 -0.00001 2.56137

R4 2.58248 0.00001 0.00001 0.00002 0.00003 2.58252

R5 3.86919 0.00000 -0.00002 -0.00001 -0.00004 3.86916

R6 2.73965 0.00000 0.00000 -0.00001 -0.00001 2.73964

R7 2.56141 0.00000 0.00000 -0.00001 -0.00001 2.56141

R8 2.69563 0.00000 0.00000 0.00000 0.00001 2.69564

R9 2.66246 -0.00001 0.00000 -0.00001 -0.00001 2.66245

R10 2.66246 -0.00001 0.00000 -0.00001 -0.00001 2.66245

R11 2.48235 0.00002 0.00001 0.00001 0.00002 2.48237

R12 2.59615 0.00000 0.00000 -0.00002 -0.00002 2.59613

R13 2.79460 -0.00001 0.00000 -0.00001 -0.00001 2.79459

R14 2.59619 0.00000 0.00000 -0.00001 -0.00001 2.59618

R15 3.84189 0.00000 -0.00002 0.00004 0.00003 3.84192

R16 2.79454 0.00000 0.00000 0.00000 0.00000 2.79454

R17 2.48236 0.00001 0.00001 0.00001 0.00002 2.48237

R18 2.66401 0.00000 0.00000 0.00000 0.00000 2.66402

R19 2.64566 0.00000 0.00000 0.00000 0.00000 2.64566

R20 2.64566 0.00000 0.00000 -0.00001 0.00000 2.64565

R21 2.48236 0.00001 0.00001 0.00000 0.00001 2.48237

R22 2.66402 0.00000 0.00000 0.00000 0.00000 2.66402

R23 2.79455 -0.00001 0.00000 -0.00001 -0.00001 2.79454

R24 2.64567 -0.00001 0.00000 -0.00001 -0.00001 2.64566

R25 2.79460 -0.00001 0.00000 -0.00001 0.00000 2.79460

R26 2.64566 -0.00001 0.00000 -0.00001 -0.00001 2.64565

R27 2.59615 0.00000 0.00000 -0.00001 -0.00002 2.59613

R28 2.48237 0.00000 0.00000 0.00000 0.00000 2.48238

R29 2.59618 0.00000 0.00000 -0.00001 -0.00001 2.59617

R30 3.84189 0.00000 -0.00001 0.00003 0.00002 3.84191

R31 2.56145 -0.00002 -0.00001 -0.00002 -0.00003 2.56142

R32 2.58247 0.00001 0.00001 0.00003 0.00004 2.58251

R33 2.58245 0.00000 0.00001 -0.00001 0.00000 2.58246

R34 3.86919 0.00000 -0.00002 -0.00003 -0.00004 3.86914

R35 2.73965 -0.00001 0.00000 -0.00002 -0.00002 2.73963

R36 2.69564 0.00000 0.00000 0.00000 0.00001 2.69564

R37 2.66246 -0.00001 0.00000 -0.00001 -0.00001 2.66245

R38 2.73963 0.00000 0.00000 0.00000 0.00000 2.73964

R39 2.66246 -0.00001 0.00000 -0.00001 -0.00001 2.66245

R40 2.56137 0.00001 0.00000 0.00000 0.00000 2.56137

R41 2.65608 0.00000 0.00000 0.00000 0.00000 2.65608

R42 2.54970 -0.00001 -0.00001 -0.00001 -0.00001 2.54969

R43 2.62944 0.00000 -0.00001 0.00000 -0.00001 2.62943

R44 2.04425 0.00000 0.00000 0.00000 0.00000 2.04425

R45 2.65609 0.00000 0.00000 0.00000 0.00000 2.65609

R46 2.04426 0.00000 0.00000 0.00000 0.00000 2.04426

R47 2.54969 -0.00001 0.00000 -0.00001 -0.00001 2.54968

R48 2.64330 0.00000 0.00000 0.00000 0.00000 2.64330

R49 2.55239 -0.00001 0.00000 -0.00001 -0.00001 2.55238

R50 2.64703 0.00000 0.00000 0.00000 0.00000 2.64703

R51 2.04404 0.00000 0.00000 0.00000 0.00000 2.04405

R52 2.64331 -0.00001 0.00000 0.00000 0.00000 2.64330

R53 2.04403 0.00000 0.00000 0.00000 0.00000 2.04404

R54 2.55239 -0.00001 0.00000 0.00000 -0.00001 2.55239

R55 2.65609 0.00000 0.00000 0.00000 0.00000 2.65609

R56 2.54969 -0.00001 -0.00001 0.00000 -0.00001 2.54968

R57 2.62944 -0.00001 -0.00001 0.00000 -0.00001 2.62943

R58 2.04426 0.00000 0.00000 0.00000 0.00000 2.04426

R59 2.65608 0.00000 0.00000 0.00000 0.00000 2.65608

R60 2.04424 0.00000 0.00000 0.00000 0.00000 2.04425

R61 2.54970 -0.00001 -0.00001 -0.00001 -0.00002 2.54968

R62 2.64330 0.00000 0.00000 0.00000 0.00000 2.64330

R63 2.55239 -0.00001 0.00000 0.00000 -0.00001 2.55238

R64 2.64703 0.00000 0.00000 0.00000 0.00000 2.64703

R65 2.04404 0.00000 0.00000 0.00000 0.00000 2.04404

R66 2.64331 0.00000 0.00000 0.00000 0.00000 2.64330

R67 2.04403 0.00000 0.00000 0.00000 0.00000 2.04404

R68 2.55239 -0.00001 0.00000 0.00000 0.00000 2.55239

R69 2.69386 0.00000 0.00000 0.00000 -0.00001 2.69386

R70 2.69385 0.00000 -0.00001 -0.00001 -0.00002 2.69383

R71 2.69567 0.00000 0.00000 0.00000 0.00000 2.69566

R72 2.69566 0.00000 0.00000 -0.00001 -0.00001 2.69565

R73 2.69385 0.00000 -0.00001 -0.00001 -0.00002 2.69383

R74 2.69386 0.00000 0.00000 0.00000 -0.00001 2.69386

R75 2.69567 0.00000 0.00000 0.00000 -0.00001 2.69566

R76 2.69566 0.00000 0.00000 -0.00001 -0.00001 2.69565

R77 2.06730 0.00000 0.00000 0.00000 0.00001 2.06731

R78 2.06735 0.00000 0.00000 0.00000 0.00000 2.06735

R79 2.05686 0.00000 0.00000 0.00000 -0.00001 2.05686

R80 2.06716 0.00000 0.00000 0.00000 0.00000 2.06716

R81 2.06743 0.00000 0.00000 0.00000 0.00000 2.06743

R82 2.05669 0.00000 0.00000 0.00000 0.00000 2.05669

R83 2.06743 0.00000 0.00000 0.00000 0.00000 2.06743

R84 2.06716 0.00000 0.00000 0.00000 0.00000 2.06716

R85 2.05669 0.00000 0.00000 0.00000 0.00000 2.05670

R86 2.06737 0.00000 0.00000 0.00001 0.00001 2.06737

R87 2.06730 0.00000 0.00000 0.00000 0.00000 2.06730

R88 2.05686 0.00000 0.00000 0.00000 0.00000 2.05686

R89 2.06743 0.00000 0.00000 0.00000 0.00000 2.06743

R90 2.06716 0.00000 0.00000 0.00000 0.00000 2.06716

R91 2.05669 0.00000 0.00000 0.00000 0.00000 2.05670

R92 2.06716 0.00000 0.00000 0.00000 0.00000 2.06716

R93 2.06743 0.00000 0.00000 0.00000 0.00000 2.06743

R94 2.05669 0.00000 0.00000 0.00000 0.00000 2.05669

R95 2.06730 0.00000 0.00000 0.00000 0.00001 2.06731

R96 2.06735 0.00000 0.00000 0.00000 0.00000 2.06735

R97 2.05686 0.00000 0.00000 0.00000 -0.00001 2.05686

R98 2.06737 0.00000 0.00000 0.00001 0.00001 2.06737

R99 2.06730 0.00000 0.00000 0.00000 0.00000 2.06730

R100 2.05686 0.00000 0.00000 0.00000 0.00000 2.05686

A1 1.88913 0.00000 0.00000 0.00000 0.00000 1.88913

A2 2.21480 0.00000 0.00000 0.00000 0.00000 2.21480

A3 2.17915 0.00000 0.00000 0.00000 0.00000 2.17915

A4 1.93079 0.00000 -0.00001 0.00001 0.00001 1.93079

A5 2.17284 0.00000 0.00001 0.00002 0.00003 2.17287

A6 2.17285 -0.00001 0.00000 -0.00002 -0.00002 2.17283

A7 1.88914 -0.00001 0.00000 -0.00002 -0.00002 1.88913

A8 2.21482 0.00000 0.00000 0.00002 0.00002 2.21484

A9 2.17913 0.00000 0.00000 0.00000 0.00000 2.17913

A10 1.85784 0.00000 0.00000 0.00001 0.00001 1.85785

A11 2.31722 0.00000 0.00000 -0.00001 -0.00001 2.31721

A12 2.10797 0.00000 0.00000 0.00000 -0.00001 2.10797

A13 1.85787 0.00000 0.00000 0.00000 0.00000 1.85787

A14 2.31718 0.00000 0.00000 -0.00001 -0.00001 2.31717

A15 2.10799 0.00000 0.00000 0.00001 0.00001 2.10799

A16 2.18708 -0.00001 0.00000 0.00000 0.00000 2.18707

A17 2.23303 0.00000 0.00000 0.00001 0.00001 2.23303

A18 2.16636 -0.00001 -0.00001 -0.00001 -0.00002 2.16635

A19 1.88342 0.00000 0.00000 0.00000 0.00001 1.88343

A20 1.93252 0.00000 0.00000 0.00001 0.00000 1.93252

A21 2.16268 0.00000 0.00000 -0.00003 -0.00003 2.16265

A22 2.16261 0.00000 0.00001 -0.00001 0.00000 2.16261

A23 1.88345 0.00000 0.00000 -0.00001 0.00000 1.88344

A24 2.23305 0.00000 0.00000 0.00001 0.00001 2.23306

A25 2.16631 0.00000 -0.00001 0.00000 0.00000 2.16631

A26 1.86263 0.00000 0.00000 0.00000 0.00000 1.86263

A27 2.30398 0.00000 0.00000 0.00001 0.00001 2.30399

A28 2.11651 0.00000 0.00000 -0.00001 -0.00001 2.11650

A29 1.86264 0.00000 0.00000 -0.00001 -0.00001 1.86263

A30 2.30402 0.00000 0.00000 0.00000 0.00000 2.30402

A31 2.11646 0.00000 0.00000 0.00001 0.00001 2.11647

A32 2.18709 -0.00001 -0.00001 -0.00002 -0.00003 2.18706

A33 1.86262 0.00000 0.00000 0.00001 0.00000 1.86263

A34 2.11651 0.00000 0.00000 0.00000 0.00000 2.11650

A35 2.30398 0.00000 0.00000 -0.00001 0.00000 2.30398

A36 1.86264 0.00000 0.00000 -0.00001 -0.00001 1.86263

A37 2.11646 0.00000 0.00000 0.00000 0.00000 2.11646

A38 2.30401 0.00000 0.00000 0.00000 0.00001 2.30402

A39 1.88342 0.00000 0.00001 0.00000 0.00001 1.88343

A40 2.16636 -0.00001 -0.00001 0.00000 -0.00001 2.16635

A41 2.23303 0.00000 0.00000 0.00000 0.00000 2.23304

A42 1.93253 0.00000 -0.00001 0.00000 0.00000 1.93253

A43 2.16266 0.00000 0.00001 -0.00003 -0.00002 2.16264

A44 2.16262 0.00000 0.00001 -0.00001 0.00000 2.16262

A45 2.16633 -0.00001 -0.00001 0.00000 -0.00001 2.16631

A46 2.23304 0.00000 0.00000 0.00001 0.00002 2.23306

A47 1.88344 0.00000 0.00001 0.00000 0.00000 1.88344

A48 2.18708 -0.00001 -0.00001 0.00000 -0.00001 2.18708

A49 1.93080 0.00000 -0.00001 0.00001 0.00000 1.93080

A50 2.17283 -0.00001 0.00000 -0.00003 -0.00002 2.17281

A51 2.17285 0.00000 0.00001 0.00003 0.00003 2.17288

A52 2.21482 0.00001 0.00000 0.00002 0.00002 2.21484

A53 2.17913 0.00000 -0.00001 0.00000 -0.00001 2.17912

A54 1.88914 -0.00001 0.00001 -0.00002 -0.00001 1.88912

A55 1.85784 0.00000 0.00000 0.00001 0.00001 1.85785

A56 2.31722 0.00000 0.00000 -0.00001 -0.00001 2.31721

A57 2.10797 0.00000 0.00000 0.00000 0.00000 2.10797

A58 1.85787 0.00000 0.00000 0.00000 0.00000 1.85787

A59 2.10799 0.00000 0.00000 0.00000 0.00000 2.10799

A60 2.31717 0.00000 0.00000 -0.00001 0.00000 2.31717

A61 1.88913 0.00000 0.00001 -0.00001 -0.00001 1.88913

A62 2.21480 0.00000 0.00000 0.00000 -0.00001 2.21479

A63 2.17916 0.00000 0.00000 0.00001 0.00001 2.17917

A64 2.18708 -0.00001 -0.00001 -0.00001 -0.00002 2.18706

A65 1.55941 0.00001 0.00001 0.00001 0.00002 1.55944

A66 1.55943 0.00000 0.00000 -0.00002 -0.00002 1.55941

A67 1.55943 0.00000 0.00000 -0.00002 -0.00002 1.55942

A68 1.55945 0.00000 0.00000 0.00002 0.00001 1.55946

A69 2.04497 0.00000 0.00000 0.00000 0.00000 2.04496

A70 2.07269 0.00000 0.00000 -0.00001 -0.00001 2.07269

A71 2.16551 0.00000 0.00000 0.00001 0.00001 2.16552

A72 2.12173 0.00000 0.00000 0.00000 0.00000 2.12173

A73 2.09913 0.00000 0.00000 0.00000 -0.00001 2.09912

A74 2.06232 0.00000 0.00000 0.00000 0.00000 2.06232

A75 2.12172 0.00000 0.00000 0.00000 0.00000 2.12172

A76 2.06231 0.00000 0.00000 0.00000 0.00000 2.06232

A77 2.09914 0.00000 0.00000 0.00000 0.00000 2.09914

A78 2.04499 0.00000 0.00000 0.00000 0.00000 2.04499

A79 2.07268 0.00000 0.00000 0.00000 0.00000 2.07268

A80 2.16550 0.00000 0.00000 0.00000 0.00000 2.16551

A81 2.05213 0.00000 0.00000 0.00000 0.00000 2.05213

A82 2.06561 0.00000 0.00000 0.00000 0.00001 2.06562

A83 2.16544 0.00000 -0.00001 -0.00001 -0.00001 2.16543

A84 2.12306 0.00000 0.00000 0.00000 0.00000 2.12305

A85 2.10072 0.00000 0.00000 0.00000 0.00000 2.10072

A86 2.05940 0.00000 0.00000 0.00001 0.00000 2.05941

A87 2.12308 0.00000 0.00000 0.00000 0.00000 2.12308

A88 2.05943 0.00000 0.00000 0.00000 0.00000 2.05943

A89 2.10068 0.00000 0.00000 -0.00001 0.00000 2.10067

A90 2.05213 0.00000 0.00000 0.00000 0.00000 2.05213

A91 2.06564 0.00000 0.00000 0.00000 0.00000 2.06564

A92 2.16541 0.00000 0.00000 0.00000 0.00000 2.16541

A93 2.04499 0.00000 0.00000 0.00000 0.00000 2.04499

A94 2.07268 0.00000 0.00000 -0.00001 -0.00001 2.07268

A95 2.16550 0.00000 -0.00001 0.00001 0.00001 2.16551

A96 2.12172 0.00000 0.00000 0.00000 0.00000 2.12172

A97 2.09914 0.00000 0.00000 0.00000 0.00000 2.09914

A98 2.06232 0.00000 0.00000 0.00000 0.00000 2.06232

A99 2.12172 0.00000 0.00000 0.00000 0.00000 2.12173

A100 2.06232 0.00000 0.00000 0.00000 0.00001 2.06232

A101 2.09913 0.00000 0.00000 -0.00001 -0.00001 2.09912

A102 2.04496 0.00000 0.00000 0.00000 0.00000 2.04497

A103 2.07269 0.00000 0.00000 0.00000 0.00001 2.07269

A104 2.16552 0.00000 -0.00001 -0.00001 -0.00001 2.16551

A105 2.05213 0.00000 0.00000 -0.00001 0.00000 2.05213

A106 2.06561 0.00000 0.00000 0.00000 0.00000 2.06561

A107 2.16543 0.00000 -0.00001 0.00001 0.00000 2.16544

A108 2.12306 0.00000 0.00000 0.00000 0.00000 2.12305

A109 2.10072 0.00000 0.00000 0.00000 0.00000 2.10072

A110 2.05941 0.00000 0.00000 0.00000 0.00000 2.05941

A111 2.12307 0.00000 0.00000 0.00000 0.00000 2.12308

A112 2.05943 0.00000 0.00000 0.00000 0.00000 2.05943

A113 2.10068 0.00000 0.00000 -0.00001 0.00000 2.10067

A114 2.05213 0.00000 0.00000 0.00000 0.00000 2.05213

A115 2.06564 0.00000 0.00000 -0.00001 0.00000 2.06564

A116 2.16541 0.00000 -0.00001 0.00001 0.00000 2.16541

A117 2.06572 -0.00001 -0.00001 -0.00002 -0.00003 2.06570

A118 2.06573 -0.00001 -0.00001 -0.00001 -0.00001 2.06572

A119 2.06937 0.00000 0.00000 0.00000 0.00000 2.06937

A120 2.06943 -0.00001 0.00000 -0.00002 -0.00002 2.06941

A121 2.06574 -0.00002 0.00000 -0.00002 -0.00003 2.06571

A122 2.06572 -0.00001 -0.00001 -0.00002 -0.00003 2.06570

A123 2.06938 -0.00001 0.00000 -0.00002 -0.00002 2.06936

A124 2.06942 -0.00001 0.00000 -0.00001 -0.00001 2.06941

A125 1.94440 0.00000 0.00000 0.00000 0.00000 1.94440

A126 1.94725 0.00000 0.00001 0.00002 0.00002 1.94727

A127 1.84239 0.00000 0.00001 -0.00001 0.00000 1.84239

A128 1.91156 -0.00001 -0.00002 -0.00003 -0.00005 1.91151

A129 1.90852 0.00000 0.00000 0.00000 0.00001 1.90853

A130 1.90816 0.00000 0.00000 0.00002 0.00002 1.90818

A131 1.94758 0.00000 0.00000 0.00001 0.00000 1.94759

A132 1.94491 0.00000 0.00000 0.00001 0.00001 1.94492

A133 1.84044 0.00000 0.00001 -0.00001 0.00000 1.84044

A134 1.91253 0.00000 0.00000 0.00000 -0.00001 1.91252

A135 1.90781 0.00000 0.00000 0.00000 0.00000 1.90780

A136 1.90890 0.00000 0.00000 0.00000 0.00000 1.90890

A137 1.94495 0.00000 0.00000 0.00000 0.00000 1.94495

A138 1.94761 0.00000 0.00000 0.00000 0.00000 1.94761

A139 1.84039 0.00000 0.00001 0.00000 0.00001 1.84041

A140 1.91254 0.00000 0.00000 0.00000 -0.00001 1.91253

A141 1.90888 0.00000 0.00000 0.00000 0.00000 1.90888

A142 1.90780 0.00000 0.00000 0.00000 0.00000 1.90780

A143 1.94727 0.00000 0.00001 0.00000 0.00000 1.94727

A144 1.94443 0.00000 0.00000 0.00002 0.00002 1.94445

A145 1.84235 0.00000 0.00001 0.00001 0.00001 1.84236

A146 1.91157 0.00000 -0.00002 -0.00001 -0.00003 1.91153

A147 1.90812 0.00000 0.00000 0.00000 0.00000 1.90812

A148 1.90856 0.00000 0.00001 -0.00001 0.00000 1.90856

A149 1.94495 0.00000 0.00000 0.00000 0.00000 1.94495

A150 1.94761 0.00000 0.00000 0.00000 0.00000 1.94761

A151 1.84039 0.00000 0.00001 0.00000 0.00001 1.84040

A152 1.91254 0.00000 0.00000 0.00000 -0.00001 1.91253

A153 1.90888 0.00000 0.00000 0.00000 0.00000 1.90888

A154 1.90780 0.00000 0.00000 0.00000 0.00000 1.90780

A155 1.94758 0.00000 0.00000 0.00000 0.00000 1.94759

A156 1.94491 0.00000 0.00000 0.00001 0.00000 1.94492

A157 1.84044 0.00000 0.00001 -0.00001 0.00000 1.84044

A158 1.91253 0.00000 0.00000 -0.00001 -0.00001 1.91252

A159 1.90781 0.00000 0.00000 0.00000 0.00000 1.90781

A160 1.90890 0.00000 0.00000 0.00000 0.00000 1.90890

A161 1.94440 0.00000 0.00000 0.00001 0.00001 1.94440

A162 1.94725 0.00000 0.00001 0.00001 0.00002 1.94727

A163 1.84239 0.00000 0.00001 -0.00001 0.00000 1.84239

A164 1.91156 0.00000 -0.00002 -0.00003 -0.00005 1.91151

A165 1.90852 0.00000 0.00001 0.00000 0.00001 1.90853

A166 1.90816 0.00000 0.00000 0.00002 0.00002 1.90818

A167 1.94728 0.00000 0.00001 -0.00001 0.00000 1.94727

A168 1.94443 0.00000 0.00000 0.00002 0.00002 1.94445

A169 1.84235 0.00000 0.00001 0.00000 0.00001 1.84236

A170 1.91156 0.00000 -0.00002 -0.00001 -0.00003 1.91153

A171 1.90812 0.00000 0.00000 0.00000 0.00000 1.90812

A172 1.90855 0.00000 0.00001 0.00000 0.00000 1.90856

A173 3.11888 0.00000 0.00000 0.00000 -0.00001 3.11887

A174 3.11888 0.00000 0.00000 0.00000 0.00000 3.11888

A175 3.33431 0.00000 -0.00002 -0.00001 -0.00003 3.33427

A176 2.90750 0.00000 0.00002 -0.00005 -0.00003 2.90747

D1 0.00319 0.00000 -0.00004 0.00001 -0.00003 0.00316

D2 3.02516 0.00000 -0.00004 0.00010 0.00006 3.02522

D3 3.13047 0.00000 -0.00001 -0.00009 -0.00009 3.13038

D4 -0.13074 0.00000 0.00000 0.00000 0.00000 -0.13074

D5 -0.00188 0.00000 0.00003 0.00004 0.00007 -0.00181

D6 -3.12411 0.00000 0.00011 0.00010 0.00021 -3.12389

D7 -3.12953 0.00000 0.00000 0.00013 0.00013 -3.12940

D8 0.03143 0.00000 0.00008 0.00020 0.00028 0.03171

D9 0.17299 0.00000 0.00000 0.00002 0.00002 0.17301

D10 -2.98517 0.00000 0.00004 -0.00009 -0.00005 -2.98522

D11 -0.00320 0.00000 0.00004 -0.00005 -0.00002 -0.00322

D12 -3.13050 0.00000 -0.00001 0.00000 -0.00001 -3.13051

D13 -3.02517 0.00000 0.00003 -0.00015 -0.00012 -3.02529

D14 0.13072 0.00000 -0.00002 -0.00009 -0.00011 0.13061

D15 -2.95666 0.00000 -0.00001 0.00002 0.00001 -2.95665

D16 -0.04916 0.00000 0.00001 -0.00003 -0.00002 -0.04918

D17 0.04900 0.00000 0.00000 0.00012 0.00012 0.04912

D18 2.95650 0.00000 0.00002 0.00007 0.00009 2.95659

D19 0.00191 0.00000 -0.00002 0.00008 0.00006 0.00197

D20 3.12414 0.00000 -0.00009 0.00003 -0.00007 3.12408

D21 3.12957 0.00000 0.00003 0.00002 0.00005 3.12962

D22 -0.03138 0.00000 -0.00005 -0.00003 -0.00008 -0.03145

D23 -0.17269 0.00000 0.00001 0.00001 0.00003 -0.17267

D24 2.98544 0.00000 -0.00004 0.00008 0.00004 2.98548

D25 -0.00002 0.00000 -0.00001 -0.00007 -0.00007 -0.00009

D26 3.12503 0.00000 -0.00008 -0.00012 -0.00020 3.12482

D27 -3.12507 0.00000 0.00006 -0.00002 0.00003 -3.12504

D28 -0.00003 0.00000 -0.00001 -0.00008 -0.00009 -0.00012

D29 -3.12458 0.00000 0.00014 0.00013 0.00028 -3.12430

D30 0.01367 0.00000 0.00014 0.00020 0.00033 0.01400

D31 -0.00460 0.00000 0.00006 0.00008 0.00014 -0.00446

D32 3.13365 0.00000 0.00005 0.00014 0.00019 3.13384

D33 3.12461 0.00000 -0.00013 -0.00004 -0.00018 3.12444

D34 -0.01362 0.00000 -0.00011 -0.00009 -0.00021 -0.01383

D35 0.00464 0.00000 -0.00004 0.00003 -0.00001 0.00463

D36 -3.13359 0.00000 -0.00002 -0.00002 -0.00004 -3.13363

D37 -0.05246 0.00000 0.00002 -0.00003 -0.00001 -0.05247

D38 3.12215 0.00000 0.00004 -0.00008 -0.00004 3.12211

D39 -3.09808 0.00000 -0.00001 -0.00005 -0.00005 -3.09814

D40 0.27599 0.00000 -0.00004 0.00011 0.00006 0.27605

D41 0.01478 0.00000 -0.00002 -0.00001 -0.00003 0.01475

D42 -2.89433 0.00000 -0.00006 0.00015 0.00009 -2.89424

D43 3.10548 0.00000 -0.00001 0.00001 0.00000 3.10549

D44 -0.02309 0.00000 0.00001 0.00004 0.00005 -0.02304

D45 -0.00874 0.00000 0.00001 -0.00003 -0.00002 -0.00876

D46 -3.13732 0.00000 0.00003 0.00000 0.00003 -3.13729

D47 -0.01481 0.00000 0.00003 0.00004 0.00006 -0.01475

D48 3.09805 0.00000 0.00001 0.00013 0.00014 3.09819

D49 2.89432 0.00000 0.00006 -0.00012 -0.00006 2.89425

D50 -0.27601 0.00000 0.00005 -0.00003 0.00002 -0.27599

D51 -0.22759 0.00000 0.00002 -0.00013 -0.00010 -0.22769

D52 3.10672 0.00000 0.00001 -0.00014 -0.00013 3.10659

D53 -3.10653 0.00000 -0.00001 0.00005 0.00003 -3.10650

D54 0.22777 0.00000 -0.00003 0.00003 0.00000 0.22777

D55 0.00882 0.00000 -0.00002 -0.00005 -0.00007 0.00874

D56 3.13740 0.00000 -0.00004 -0.00010 -0.00014 3.13726

D57 -3.10540 0.00000 -0.00001 -0.00014 -0.00015 -3.10555

D58 0.02318 0.00000 -0.00003 -0.00018 -0.00021 0.02297

D59 0.05219 0.00000 -0.00003 0.00001 -0.00002 0.05217

D60 -3.12243 0.00000 -0.00005 0.00012 0.00007 -3.12236

D61 -0.00004 0.00000 0.00001 0.00005 0.00006 0.00001

D62 3.13023 0.00000 -0.00001 0.00002 0.00001 3.13025

D63 -3.13033 0.00000 0.00002 0.00009 0.00011 -3.13022

D64 -0.00005 0.00000 0.00001 0.00006 0.00007 0.00002

D65 -3.12607 0.00000 0.00001 0.00004 0.00005 -3.12602

D66 0.02077 0.00000 0.00001 -0.00004 -0.00003 0.02074

D67 0.00095 0.00000 -0.00001 -0.00001 -0.00002 0.00093

D68 -3.13540 0.00000 -0.00001 -0.00009 -0.00010 -3.13550

D69 3.12612 0.00000 -0.00002 -0.00010 -0.00012 3.12600

D70 -0.02066 0.00000 -0.00003 -0.00007 -0.00010 -0.02075

D71 -0.00089 0.00000 0.00000 -0.00006 -0.00006 -0.00095

D72 3.13552 0.00000 -0.00001 -0.00003 -0.00004 3.13548

D73 -3.12248 0.00000 -0.00004 0.00021 0.00017 -3.12231

D74 0.05219 0.00000 -0.00003 0.00000 -0.00002 0.05217

D75 0.00001 0.00000 0.00000 -0.00003 -0.00003 -0.00002

D76 3.13028 0.00000 -0.00001 -0.00002 -0.00004 3.13024

D77 -3.13027 0.00000 0.00002 -0.00001 0.00001 -3.13026

D78 -0.00001 0.00000 0.00001 0.00000 0.00001 0.00000

D79 -3.10544 0.00000 0.00000 -0.00011 -0.00011 -3.10555

D80 0.00875 0.00000 -0.00002 0.00006 0.00005 0.00879

D81 0.02315 0.00000 -0.00003 -0.00014 -0.00016 0.02298

D82 3.13733 0.00000 -0.00004 0.00004 0.00000 3.13733

D83 0.00092 0.00000 -0.00001 0.00003 0.00002 0.00094

D84 -3.13547 0.00000 -0.00001 0.00003 0.00001 -3.13545

D85 -3.12610 0.00000 0.00002 0.00006 0.00008 -3.12601

D86 0.02070 0.00000 0.00001 0.00006 0.00007 0.02077

D87 -0.00877 0.00000 0.00001 -0.00001 0.00000 -0.00877

D88 3.10543 0.00000 -0.00001 0.00010 0.00008 3.10551

D89 -3.13733 0.00000 0.00003 -0.00002 0.00001 -3.13732

D90 -0.02313 0.00000 0.00001 0.00009 0.00009 -0.02304

D91 -0.00091 0.00000 0.00000 -0.00004 -0.00004 -0.00095

D92 3.13551 0.00000 0.00000 -0.00004 -0.00004 3.13547

D93 3.12608 0.00000 -0.00002 -0.00003 -0.00005 3.12603

D94 -0.02069 0.00000 -0.00002 -0.00003 -0.00005 -0.02074

D95 0.01476 0.00000 -0.00003 0.00005 0.00003 0.01479

D96 -2.89436 0.00000 -0.00006 0.00021 0.00015 -2.89421

D97 -3.09807 0.00000 0.00000 -0.00006 -0.00006 -3.09813

D98 0.27599 0.00000 -0.00003 0.00009 0.00006 0.27605

D99 3.12219 0.00000 0.00005 -0.00016 -0.00011 3.12207

D100 -0.05246 0.00000 0.00002 -0.00004 -0.00002 -0.05247

D101 3.09806 0.00000 0.00001 0.00011 0.00012 3.09819

D102 -0.01476 0.00000 0.00003 -0.00007 -0.00004 -0.01480

D103 -0.27599 0.00000 0.00005 -0.00005 0.00000 -0.27599

D104 2.89437 0.00000 0.00006 -0.00023 -0.00017 2.89421

D105 3.10672 0.00000 0.00000 -0.00013 -0.00012 3.10659

D106 -0.22759 0.00000 0.00002 -0.00011 -0.00009 -0.22768

D107 0.22776 0.00000 -0.00003 0.00005 0.00002 0.22777

D108 -3.10655 0.00000 -0.00002 0.00006 0.00005 -3.10650

D109 -0.17270 0.00000 0.00001 0.00003 0.00004 -0.17266

D110 2.98545 0.00000 -0.00002 0.00003 0.00000 2.98546

D111 -3.13049 0.00000 0.00000 -0.00001 -0.00001 -3.13051

D112 -0.00321 0.00000 0.00002 0.00000 0.00002 -0.00320

D113 0.13072 0.00000 -0.00001 -0.00010 -0.00011 0.13061

D114 -3.02518 0.00000 0.00002 -0.00010 -0.00008 -3.02526

D115 0.00316 0.00000 -0.00002 0.00003 0.00001 0.00317

D116 3.13045 0.00000 -0.00001 -0.00006 -0.00007 3.13039

D117 3.02513 0.00000 -0.00001 0.00012 0.00010 3.02524

D118 -0.13076 0.00000 -0.00001 0.00003 0.00003 -0.13074

D119 2.95650 0.00000 0.00002 0.00007 0.00009 2.95659

D120 0.04900 0.00000 0.00000 0.00012 0.00012 0.04912

D121 -0.04916 0.00000 0.00001 -0.00004 -0.00002 -0.04918

D122 -2.95666 0.00000 -0.00001 0.00001 0.00001 -2.95665

D123 3.12960 0.00000 0.00001 -0.00002 -0.00001 3.12959

D124 -0.03137 0.00000 -0.00006 -0.00003 -0.00009 -0.03147

D125 0.00196 0.00000 -0.00002 -0.00002 -0.00004 0.00192

D126 3.12417 0.00000 -0.00009 -0.00004 -0.00012 3.12404

D127 -0.00008 0.00000 0.00000 0.00004 0.00004 -0.00004

D128 3.12498 0.00000 -0.00007 -0.00004 -0.00011 3.12487

D129 -3.12511 0.00000 0.00006 0.00005 0.00012 -3.12499

D130 -0.00005 0.00000 -0.00001 -0.00003 -0.00003 -0.00009

D131 -3.12455 0.00000 0.00013 0.00008 0.00021 -3.12434

D132 0.01370 0.00000 0.00013 0.00014 0.00027 0.01397

D133 -0.00459 0.00000 0.00005 0.00006 0.00011 -0.00448

D134 3.13366 0.00000 0.00005 0.00012 0.00017 3.13383

D135 -0.00183 0.00000 0.00001 -0.00004 -0.00003 -0.00186

D136 -3.12948 0.00000 0.00000 0.00004 0.00004 -3.12944

D137 -3.12407 0.00000 0.00009 0.00005 0.00014 -3.12392

D138 0.03147 0.00000 0.00008 0.00013 0.00022 0.03168

D139 0.00467 0.00000 -0.00004 -0.00002 -0.00006 0.00461

D140 -3.13358 0.00000 -0.00004 -0.00004 -0.00008 -3.13366

D141 3.12465 0.00000 -0.00013 -0.00012 -0.00026 3.12440

D142 -0.01359 0.00000 -0.00013 -0.00014 -0.00027 -0.01386

D143 0.17301 0.00000 0.00001 -0.00001 0.00000 0.17300

D144 -2.98514 0.00000 0.00002 -0.00011 -0.00009 -2.98523

D145 -0.00092 0.00000 0.00000 -0.00003 -0.00002 -0.00094

D146 -3.13755 0.00000 0.00000 -0.00003 -0.00003 -3.13758

D147 3.13516 0.00000 0.00001 -0.00002 -0.00001 3.13515

D148 -0.00147 0.00000 0.00001 -0.00003 -0.00002 -0.00149

D149 -3.09834 0.00000 -0.00005 -0.00001 -0.00006 -3.09840

D150 0.04884 0.00000 -0.00006 -0.00001 -0.00007 0.04878

D151 0.00000 0.00000 0.00000 -0.00001 -0.00001 -0.00001

D152 -3.13677 0.00000 0.00000 0.00000 0.00000 -3.13677

D153 3.13673 0.00000 0.00000 0.00000 0.00000 3.13673

D154 -0.00003 0.00000 0.00000 0.00000 0.00000 -0.00003

D155 0.00092 0.00000 0.00000 0.00004 0.00004 0.00096

D156 -3.13520 0.00000 0.00000 0.00004 0.00004 -3.13516

D157 3.13758 0.00000 0.00000 0.00004 0.00003 3.13762

D158 0.00147 0.00000 0.00000 0.00004 0.00004 0.00150

D159 3.09840 0.00000 0.00004 -0.00017 -0.00013 3.09827

D160 -0.04875 0.00000 0.00004 -0.00017 -0.00013 -0.04888

D161 -0.00468 0.00000 0.00004 0.00003 0.00007 -0.00460

D162 3.14134 0.00000 0.00005 0.00004 0.00009 3.14142

D163 3.13336 0.00000 0.00004 0.00005 0.00009 3.13345

D164 -0.00381 0.00000 0.00005 0.00005 0.00010 -0.00371

D165 3.11426 0.00000 -0.00008 0.00018 0.00010 3.11436

D166 -0.02376 0.00000 -0.00008 0.00016 0.00009 -0.02367

D167 -0.00001 0.00000 0.00000 0.00001 0.00001 0.00000

D168 -3.13730 0.00000 0.00000 0.00000 0.00000 -3.13730

D169 3.13726 0.00000 0.00000 0.00000 0.00000 3.13726

D170 -0.00003 0.00000 0.00000 0.00000 -0.00001 -0.00004

D171 0.00467 0.00000 -0.00005 -0.00005 -0.00010 0.00457

D172 -3.13337 0.00000 -0.00005 -0.00011 -0.00016 -3.13353

D173 -3.14133 0.00000 -0.00005 -0.00005 -0.00010 -3.14142

D174 0.00382 0.00000 -0.00005 -0.00011 -0.00016 0.00366

D175 -3.11419 0.00000 0.00011 0.00002 0.00013 -3.11407

D176 0.02382 0.00000 0.00011 0.00008 0.00019 0.02401

D177 0.00093 0.00000 -0.00001 0.00002 0.00001 0.00094

D178 3.13757 0.00000 0.00000 0.00006 0.00006 3.13763

D179 -3.13518 0.00000 0.00000 -0.00001 -0.00001 -3.13519

D180 0.00147 0.00000 0.00000 0.00003 0.00003 0.00150

D181 3.09839 0.00000 0.00005 -0.00017 -0.00013 3.09826

D182 -0.04877 0.00000 0.00004 -0.00014 -0.00010 -0.04887

D183 -0.00003 0.00000 0.00000 0.00003 0.00003 0.00000

D184 3.13670 0.00000 0.00000 0.00005 0.00005 3.13675

D185 -3.13677 0.00000 0.00000 -0.00001 -0.00001 -3.13678

D186 -0.00004 0.00000 0.00000 0.00001 0.00001 -0.00003

D187 -0.00092 0.00000 0.00000 -0.00003 -0.00002 -0.00094

D188 3.13513 0.00000 0.00001 0.00005 0.00006 3.13519

D189 -3.13754 0.00000 0.00001 -0.00005 -0.00005 -3.13759

D190 -0.00150 0.00000 0.00001 0.00003 0.00004 -0.00146

D191 -3.09838 0.00000 -0.00006 0.00007 0.00002 -3.09836

D192 0.04885 0.00000 -0.00006 -0.00001 -0.00007 0.04878

D193 -0.00467 0.00000 0.00005 0.00002 0.00006 -0.00460

D194 3.14135 0.00000 0.00005 0.00001 0.00007 3.14142

D195 3.13336 0.00000 0.00003 0.00007 0.00010 3.13345

D196 -0.00381 0.00000 0.00004 0.00006 0.00010 -0.00372

D197 3.11427 0.00000 -0.00010 0.00017 0.00008 3.11435

D198 -0.02373 0.00000 -0.00008 0.00012 0.00004 -0.02368

D199 0.00000 0.00000 0.00000 -0.00002 -0.00002 -0.00002

D200 -3.13731 0.00000 0.00001 0.00000 0.00001 -3.13730

D201 3.13727 0.00000 -0.00001 -0.00001 -0.00002 3.13725

D202 -0.00004 0.00000 0.00000 0.00001 0.00000 -0.00003

D203 0.00465 0.00000 -0.00005 -0.00003 -0.00008 0.00457

D204 -3.13339 0.00000 -0.00004 -0.00010 -0.00014 -3.13353

D205 -3.14132 0.00000 -0.00006 -0.00005 -0.00011 -3.14143

D206 0.00382 0.00000 -0.00005 -0.00012 -0.00017 0.00365

D207 -3.11418 0.00000 0.00012 -0.00002 0.00010 -3.11408

D208 0.02383 0.00000 0.00011 0.00005 0.00016 0.02399

D209 1.05367 0.00000 -0.00005 -0.00005 -0.00011 1.05357

D210 -1.08871 0.00000 -0.00003 -0.00003 -0.00006 -1.08877

D211 3.12353 0.00000 -0.00004 -0.00005 -0.00009 3.12344

D212 1.08914 0.00000 0.00003 -0.00006 -0.00003 1.08911

D213 -1.05328 0.00000 0.00005 -0.00005 0.00000 -1.05329

D214 -3.12317 0.00000 0.00004 -0.00006 -0.00002 -3.12319

D215 1.09420 0.00000 -0.00003 0.00015 0.00012 1.09432

D216 -1.05005 0.00000 -0.00003 0.00015 0.00012 -1.04993

D217 -3.11946 0.00000 -0.00003 0.00015 0.00012 -3.11935

D218 1.05000 0.00000 0.00004 -0.00004 0.00000 1.05000

D219 -1.09431 0.00000 0.00004 -0.00004 0.00001 -1.09430

D220 3.11939 0.00000 0.00004 -0.00004 0.00000 3.11938

D221 1.08915 0.00000 0.00003 -0.00007 -0.00003 1.08912

D222 -1.05327 0.00000 0.00005 -0.00006 -0.00001 -1.05328

D223 -3.12316 0.00000 0.00004 -0.00007 -0.00003 -3.12319

D224 1.05366 0.00000 -0.00005 -0.00005 -0.00010 1.05356

D225 -1.08872 0.00000 -0.00003 -0.00002 -0.00005 -1.08877

D226 3.12352 0.00000 -0.00004 -0.00004 -0.00009 3.12344

D227 1.09420 0.00000 -0.00003 0.00014 0.00011 1.09431

D228 -1.05005 0.00000 -0.00003 0.00014 0.00012 -1.04993

D229 -3.11947 0.00000 -0.00003 0.00014 0.00011 -3.11935

D230 1.04999 0.00000 0.00004 -0.00002 0.00002 1.05001

D231 -1.09432 0.00000 0.00005 -0.00002 0.00003 -1.09429

D232 3.11937 0.00000 0.00004 -0.00001 0.00003 3.11940

Item Value Threshold Converged?

Maximum Force 0.000017 0.000450 YES

RMS Force 0.000003 0.000300 YES

Maximum Displacement 0.001463 0.001800 YES

RMS Displacement 0.000211 0.001200 YES

Predicted change in Energy=-1.761788D-08

Optimization completed.

-- Stationary point found.

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! Optimized Parameters !

! (Angstroms and Degrees) !

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! Name Definition Value Derivative Info. !

--------------------------------------------------------------------------------

! R1 R(1,2) 1.3666 -DE/DX = 0.0 !

! R2 R(1,5) 1.4498 -DE/DX = 0.0 !

! R3 R(1,12) 1.3554 -DE/DX = 0.0 !

! R4 R(2,3) 1.3666 -DE/DX = 0.0 !

! R5 R(2,25) 2.0475 -DE/DX = 0.0 !

! R6 R(3,4) 1.4498 -DE/DX = 0.0 !

! R7 R(3,6) 1.3554 -DE/DX = 0.0 !

! R8 R(4,5) 1.4265 -DE/DX = 0.0 !

! R9 R(4,41) 1.4089 -DE/DX = 0.0 !

! R10 R(5,38) 1.4089 -DE/DX = 0.0 !

! R11 R(6,7) 1.3136 -DE/DX = 0.0 !

! R12 R(7,8) 1.3738 -DE/DX = 0.0 !

! R13 R(7,11) 1.4788 -DE/DX = 0.0 !

! R14 R(8,9) 1.3738 -DE/DX = 0.0 !

! R15 R(8,25) 2.033 -DE/DX = 0.0 !

! R16 R(9,10) 1.4788 -DE/DX = 0.0 !

! R17 R(9,24) 1.3136 -DE/DX = 0.0 !

! R18 R(10,11) 1.4097 -DE/DX = 0.0 !

! R19 R(10,37) 1.4 -DE/DX = 0.0 !

! R20 R(11,34) 1.4 -DE/DX = 0.0 !

! R21 R(12,17) 1.3136 -DE/DX = 0.0 !

! R22 R(13,14) 1.4097 -DE/DX = 0.0 !

! R23 R(13,17) 1.4788 -DE/DX = 0.0 !

! R24 R(13,26) 1.4 -DE/DX = 0.0 !

! R25 R(14,15) 1.4788 -DE/DX = 0.0 !

! R26 R(14,29) 1.4 -DE/DX = 0.0 !

! R27 R(15,16) 1.3738 -DE/DX = 0.0 !

! R28 R(15,18) 1.3136 -DE/DX = 0.0 !

! R29 R(16,17) 1.3738 -DE/DX = 0.0 !

! R30 R(16,25) 2.033 -DE/DX = 0.0 !

! R31 R(18,20) 1.3555 -DE/DX = 0.0 !

! R32 R(19,20) 1.3666 -DE/DX = 0.0 !

! R33 R(19,23) 1.3666 -DE/DX = 0.0 !

! R34 R(19,25) 2.0475 -DE/DX = 0.0 !

! R35 R(20,21) 1.4498 -DE/DX = 0.0 !

! R36 R(21,22) 1.4265 -DE/DX = 0.0 !

! R37 R(21,33) 1.4089 -DE/DX = 0.0 !

! R38 R(22,23) 1.4498 -DE/DX = 0.0 !

! R39 R(22,30) 1.4089 -DE/DX = 0.0 !

! R40 R(23,24) 1.3554 -DE/DX = 0.0 !

! R41 R(26,27) 1.4055 -DE/DX = 0.0 !

! R42 R(26,57) 1.3492 -DE/DX = 0.0 !

! R43 R(27,28) 1.3914 -DE/DX = 0.0 !

! R44 R(27,46) 1.0818 -DE/DX = 0.0 !

! R45 R(28,29) 1.4055 -DE/DX = 0.0 !

! R46 R(28,47) 1.0818 -DE/DX = 0.0 !

! R47 R(29,56) 1.3492 -DE/DX = 0.0 !

! R48 R(30,31) 1.3988 -DE/DX = 0.0 !

! R49 R(30,54) 1.3507 -DE/DX = 0.0 !

! R50 R(31,32) 1.4008 -DE/DX = 0.0 !

! R51 R(31,49) 1.0817 -DE/DX = 0.0 !

! R52 R(32,33) 1.3988 -DE/DX = 0.0 !

! R53 R(32,48) 1.0817 -DE/DX = 0.0 !

! R54 R(33,55) 1.3507 -DE/DX = 0.0 !

! R55 R(34,35) 1.4055 -DE/DX = 0.0 !

! R56 R(34,52) 1.3492 -DE/DX = 0.0 !

! R57 R(35,36) 1.3914 -DE/DX = 0.0 !

! R58 R(35,42) 1.0818 -DE/DX = 0.0 !

! R59 R(36,37) 1.4055 -DE/DX = 0.0 !

! R60 R(36,43) 1.0818 -DE/DX = 0.0 !

! R61 R(37,53) 1.3492 -DE/DX = 0.0 !

! R62 R(38,39) 1.3988 -DE/DX = 0.0 !

! R63 R(38,51) 1.3507 -DE/DX = 0.0 !

! R64 R(39,40) 1.4007 -DE/DX = 0.0 !

! R65 R(39,45) 1.0817 -DE/DX = 0.0 !

! R66 R(40,41) 1.3988 -DE/DX = 0.0 !

! R67 R(40,44) 1.0817 -DE/DX = 0.0 !

! R68 R(41,50) 1.3507 -DE/DX = 0.0 !

! R69 R(50,58) 1.4255 -DE/DX = 0.0 !

! R70 R(51,70) 1.4255 -DE/DX = 0.0 !

! R71 R(52,62) 1.4265 -DE/DX = 0.0 !

! R72 R(53,66) 1.4265 -DE/DX = 0.0 !

! R73 R(54,86) 1.4255 -DE/DX = 0.0 !

! R74 R(55,82) 1.4255 -DE/DX = 0.0 !

! R75 R(56,78) 1.4265 -DE/DX = 0.0 !

! R76 R(57,74) 1.4265 -DE/DX = 0.0 !

! R77 R(58,59) 1.094 -DE/DX = 0.0 !

! R78 R(58,60) 1.094 -DE/DX = 0.0 !

! R79 R(58,61) 1.0884 -DE/DX = 0.0 !

! R80 R(62,63) 1.0939 -DE/DX = 0.0 !

! R81 R(62,64) 1.094 -DE/DX = 0.0 !

! R82 R(62,65) 1.0884 -DE/DX = 0.0 !

! R83 R(66,67) 1.094 -DE/DX = 0.0 !

! R84 R(66,68) 1.0939 -DE/DX = 0.0 !

! R85 R(66,69) 1.0884 -DE/DX = 0.0 !

! R86 R(70,71) 1.094 -DE/DX = 0.0 !

! R87 R(70,72) 1.094 -DE/DX = 0.0 !

! R88 R(70,73) 1.0884 -DE/DX = 0.0 !

! R89 R(74,75) 1.094 -DE/DX = 0.0 !

! R90 R(74,76) 1.0939 -DE/DX = 0.0 !

! R91 R(74,77) 1.0884 -DE/DX = 0.0 !

! R92 R(78,79) 1.0939 -DE/DX = 0.0 !

! R93 R(78,80) 1.094 -DE/DX = 0.0 !

! R94 R(78,81) 1.0884 -DE/DX = 0.0 !

! R95 R(82,83) 1.094 -DE/DX = 0.0 !

! R96 R(82,84) 1.094 -DE/DX = 0.0 !

! R97 R(82,85) 1.0884 -DE/DX = 0.0 !

! R98 R(86,87) 1.094 -DE/DX = 0.0 !

! R99 R(86,88) 1.094 -DE/DX = 0.0 !

! R100 R(86,89) 1.0884 -DE/DX = 0.0 !

! A1 A(2,1,5) 108.2394 -DE/DX = 0.0 !

! A2 A(2,1,12) 126.8989 -DE/DX = 0.0 !

! A3 A(5,1,12) 124.8563 -DE/DX = 0.0 !

! A4 A(1,2,3) 110.6259 -DE/DX = 0.0 !

! A5 A(1,2,25) 124.4947 -DE/DX = 0.0 !

! A6 A(3,2,25) 124.4953 -DE/DX = 0.0 !

! A7 A(2,3,4) 108.2398 -DE/DX = 0.0 !

! A8 A(2,3,6) 126.9 -DE/DX = 0.0 !

! A9 A(4,3,6) 124.8548 -DE/DX = 0.0 !

! A10 A(3,4,5) 106.4466 -DE/DX = 0.0 !

! A11 A(3,4,41) 132.7667 -DE/DX = 0.0 !

! A12 A(5,4,41) 120.778 -DE/DX = 0.0 !

! A13 A(1,5,4) 106.448 -DE/DX = 0.0 !

! A14 A(1,5,38) 132.7645 -DE/DX = 0.0 !

! A15 A(4,5,38) 120.7787 -DE/DX = 0.0 !

! A16 A(3,6,7) 125.3103 -DE/DX = 0.0 !

! A17 A(6,7,8) 127.9429 -DE/DX = 0.0 !

! A18 A(6,7,11) 124.1235 -DE/DX = 0.0 !

! A19 A(8,7,11) 107.9121 -DE/DX = 0.0 !

! A20 A(7,8,9) 110.7252 -DE/DX = 0.0 !

! A21 A(7,8,25) 123.9126 -DE/DX = 0.0 !

! A22 A(9,8,25) 123.9081 -DE/DX = 0.0 !

! A23 A(8,9,10) 107.9135 -DE/DX = 0.0 !

! A24 A(8,9,24) 127.9445 -DE/DX = 0.0 !

! A25 A(10,9,24) 124.1205 -DE/DX = 0.0 !

! A26 A(9,10,11) 106.7207 -DE/DX = 0.0 !

! A27 A(9,10,37) 132.0082 -DE/DX = 0.0 !

! A28 A(11,10,37) 121.2671 -DE/DX = 0.0 !

! A29 A(7,11,10) 106.7214 -DE/DX = 0.0 !

! A30 A(7,11,34) 132.0104 -DE/DX = 0.0 !

! A31 A(10,11,34) 121.2641 -DE/DX = 0.0 !

! A32 A(1,12,17) 125.3108 -DE/DX = 0.0 !

! A33 A(14,13,17) 106.7205 -DE/DX = 0.0 !

! A34 A(14,13,26) 121.2668 -DE/DX = 0.0 !

! A35 A(17,13,26) 132.0086 -DE/DX = 0.0 !

! A36 A(13,14,15) 106.7214 -DE/DX = 0.0 !

! A37 A(13,14,29) 121.2642 -DE/DX = 0.0 !

! A38 A(15,14,29) 132.0103 -DE/DX = 0.0 !

! A39 A(14,15,16) 107.9119 -DE/DX = 0.0 !

! A40 A(14,15,18) 124.1234 -DE/DX = 0.0 !

! A41 A(16,15,18) 127.9432 -DE/DX = 0.0 !

! A42 A(15,16,17) 110.7259 -DE/DX = 0.0 !

! A43 A(15,16,25) 123.9111 -DE/DX = 0.0 !

! A44 A(17,16,25) 123.909 -DE/DX = 0.0 !

! A45 A(12,17,13) 124.1213 -DE/DX = 0.0 !

! A46 A(12,17,16) 127.9439 -DE/DX = 0.0 !

! A47 A(13,17,16) 107.9132 -DE/DX = 0.0 !

! A48 A(15,18,20) 125.3107 -DE/DX = 0.0 !

! A49 A(20,19,23) 110.6264 -DE/DX = 0.0 !

! A50 A(20,19,25) 124.4942 -DE/DX = 0.0 !

! A51 A(23,19,25) 124.4953 -DE/DX = 0.0 !

! A52 A(18,20,19) 126.8999 -DE/DX = 0.0 !

! A53 A(18,20,21) 124.8552 -DE/DX = 0.0 !

! A54 A(19,20,21) 108.2395 -DE/DX = 0.0 !

! A55 A(20,21,22) 106.4465 -DE/DX = 0.0 !

! A56 A(20,21,33) 132.7668 -DE/DX = 0.0 !

! A57 A(22,21,33) 120.7778 -DE/DX = 0.0 !

! A58 A(21,22,23) 106.4478 -DE/DX = 0.0 !

! A59 A(21,22,30) 120.779 -DE/DX = 0.0 !

! A60 A(23,22,30) 132.7643 -DE/DX = 0.0 !

! A61 A(19,23,22) 108.2394 -DE/DX = 0.0 !

! A62 A(19,23,24) 126.8987 -DE/DX = 0.0 !

! A63 A(22,23,24) 124.8564 -DE/DX = 0.0 !

! A64 A(9,24,23) 125.3105 -DE/DX = 0.0 !

! A65 A(2,25,8) 89.3478 -DE/DX = 0.0 !

! A66 A(2,25,16) 89.3489 -DE/DX = 0.0 !

! A67 A(8,25,19) 89.3489 -DE/DX = 0.0 !

! A68 A(16,25,19) 89.3497 -DE/DX = 0.0 !

! A69 A(13,26,27) 117.168 -DE/DX = 0.0 !

! A70 A(13,26,57) 118.7566 -DE/DX = 0.0 !

! A71 A(27,26,57) 124.0747 -DE/DX = 0.0 !

! A72 A(26,27,28) 121.5659 -DE/DX = 0.0 !

! A73 A(26,27,46) 120.2712 -DE/DX = 0.0 !

! A74 A(28,27,46) 118.1623 -DE/DX = 0.0 !

! A75 A(27,28,29) 121.5658 -DE/DX = 0.0 !

! A76 A(27,28,47) 118.1618 -DE/DX = 0.0 !

! A77 A(29,28,47) 120.2718 -DE/DX = 0.0 !

! A78 A(14,29,28) 117.1693 -DE/DX = 0.0 !

! A79 A(14,29,56) 118.7558 -DE/DX = 0.0 !

! A80 A(28,29,56) 124.0742 -DE/DX = 0.0 !

! A81 A(22,30,31) 117.5783 -DE/DX = 0.0 !

! A82 A(22,30,54) 118.3506 -DE/DX = 0.0 !

! A83 A(31,30,54) 124.0708 -DE/DX = 0.0 !

! A84 A(30,31,32) 121.6422 -DE/DX = 0.0 !

! A85 A(30,31,49) 120.3621 -DE/DX = 0.0 !

! A86 A(32,31,49) 117.9952 -DE/DX = 0.0 !

! A87 A(31,32,33) 121.6433 -DE/DX = 0.0 !

! A88 A(31,32,48) 117.9964 -DE/DX = 0.0 !

! A89 A(33,32,48) 120.3598 -DE/DX = 0.0 !

! A90 A(21,33,32) 117.5783 -DE/DX = 0.0 !

! A91 A(21,33,55) 118.3524 -DE/DX = 0.0 !

! A92 A(32,33,55) 124.0691 -DE/DX = 0.0 !

! A93 A(11,34,35) 117.1694 -DE/DX = 0.0 !

! A94 A(11,34,52) 118.7559 -DE/DX = 0.0 !

! A95 A(35,34,52) 124.074 -DE/DX = 0.0 !

! A96 A(34,35,36) 121.5657 -DE/DX = 0.0 !

! A97 A(34,35,42) 120.2717 -DE/DX = 0.0 !

! A98 A(36,35,42) 118.162 -DE/DX = 0.0 !

! A99 A(35,36,37) 121.5659 -DE/DX = 0.0 !

! A100 A(35,36,43) 118.1622 -DE/DX = 0.0 !

! A101 A(37,36,43) 120.2714 -DE/DX = 0.0 !

! A102 A(10,37,36) 117.1678 -DE/DX = 0.0 !

! A103 A(10,37,53) 118.7561 -DE/DX = 0.0 !

! A104 A(36,37,53) 124.0753 -DE/DX = 0.0 !

! A105 A(5,38,39) 117.5786 -DE/DX = 0.0 !

! A106 A(5,38,51) 118.3509 -DE/DX = 0.0 !

! A107 A(39,38,51) 124.0702 -DE/DX = 0.0 !

! A108 A(38,39,40) 121.6421 -DE/DX = 0.0 !

! A109 A(38,39,45) 120.3621 -DE/DX = 0.0 !

! A110 A(40,39,45) 117.9953 -DE/DX = 0.0 !

! A111 A(39,40,41) 121.6432 -DE/DX = 0.0 !

! A112 A(39,40,44) 117.9965 -DE/DX = 0.0 !

! A113 A(41,40,44) 120.3598 -DE/DX = 0.0 !

! A114 A(4,41,40) 117.5783 -DE/DX = 0.0 !

! A115 A(4,41,50) 118.3525 -DE/DX = 0.0 !

! A116 A(40,41,50) 124.0689 -DE/DX = 0.0 !

! A117 A(41,50,58) 118.3573 -DE/DX = 0.0 !

! A118 A(38,51,70) 118.3576 -DE/DX = 0.0 !

! A119 A(34,52,62) 118.5661 -DE/DX = 0.0 !

! A120 A(37,53,66) 118.5695 -DE/DX = 0.0 !

! A121 A(30,54,86) 118.3581 -DE/DX = 0.0 !

! A122 A(33,55,82) 118.3573 -DE/DX = 0.0 !

! A123 A(29,56,78) 118.5668 -DE/DX = 0.0 !

! A124 A(26,57,74) 118.569 -DE/DX = 0.0 !

! A125 A(50,58,59) 111.4058 -DE/DX = 0.0 !

! A126 A(50,58,60) 111.5692 -DE/DX = 0.0 !

! A127 A(50,58,61) 105.5615 -DE/DX = 0.0 !

! A128 A(59,58,60) 109.5244 -DE/DX = 0.0 !

! A129 A(59,58,61) 109.3504 -DE/DX = 0.0 !

! A130 A(60,58,61) 109.3297 -DE/DX = 0.0 !

! A131 A(52,62,63) 111.5883 -DE/DX = 0.0 !

! A132 A(52,62,64) 111.4353 -DE/DX = 0.0 !

! A133 A(52,62,65) 105.4496 -DE/DX = 0.0 !

! A134 A(63,62,64) 109.5798 -DE/DX = 0.0 !

! A135 A(63,62,65) 109.3094 -DE/DX = 0.0 !

! A136 A(64,62,65) 109.3719 -DE/DX = 0.0 !

! A137 A(53,66,67) 111.4377 -DE/DX = 0.0 !

! A138 A(53,66,68) 111.5897 -DE/DX = 0.0 !

! A139 A(53,66,69) 105.4467 -DE/DX = 0.0 !

! A140 A(67,66,68) 109.5804 -DE/DX = 0.0 !

! A141 A(67,66,69) 109.3709 -DE/DX = 0.0 !

! A142 A(68,66,69) 109.3087 -DE/DX = 0.0 !

! A143 A(51,70,71) 111.5705 -DE/DX = 0.0 !

! A144 A(51,70,72) 111.4075 -DE/DX = 0.0 !

! A145 A(51,70,73) 105.5588 -DE/DX = 0.0 !

! A146 A(71,70,72) 109.5247 -DE/DX = 0.0 !

! A147 A(71,70,73) 109.3271 -DE/DX = 0.0 !

! A148 A(72,70,73) 109.3522 -DE/DX = 0.0 !

! A149 A(57,74,75) 111.4375 -DE/DX = 0.0 !

! A150 A(57,74,76) 111.5897 -DE/DX = 0.0 !

! A151 A(57,74,77) 105.4467 -DE/DX = 0.0 !

! A152 A(75,74,76) 109.5804 -DE/DX = 0.0 !

! A153 A(75,74,77) 109.3709 -DE/DX = 0.0 !

! A154 A(76,74,77) 109.3088 -DE/DX = 0.0 !

! A155 A(56,78,79) 111.5884 -DE/DX = 0.0 !

! A156 A(56,78,80) 111.4354 -DE/DX = 0.0 !

! A157 A(56,78,81) 105.4496 -DE/DX = 0.0 !

! A158 A(79,78,80) 109.5798 -DE/DX = 0.0 !

! A159 A(79,78,81) 109.3093 -DE/DX = 0.0 !

! A160 A(80,78,81) 109.3719 -DE/DX = 0.0 !

! A161 A(55,82,83) 111.4057 -DE/DX = 0.0 !

! A162 A(55,82,84) 111.5694 -DE/DX = 0.0 !

! A163 A(55,82,85) 105.5614 -DE/DX = 0.0 !

! A164 A(83,82,84) 109.5244 -DE/DX = 0.0 !

! A165 A(83,82,85) 109.3504 -DE/DX = 0.0 !

! A166 A(84,82,85) 109.3297 -DE/DX = 0.0 !

! A167 A(54,86,87) 111.5706 -DE/DX = 0.0 !

! A168 A(54,86,88) 111.4073 -DE/DX = 0.0 !

! A169 A(54,86,89) 105.5589 -DE/DX = 0.0 !

! A170 A(87,86,88) 109.5246 -DE/DX = 0.0 !

! A171 A(87,86,89) 109.3271 -DE/DX = 0.0 !

! A172 A(88,86,89) 109.3521 -DE/DX = 0.0 !

! A173 L(2,25,19,16,-1) 178.6986 -DE/DX = 0.0 !

! A174 L(8,25,16,19,-1) 178.6986 -DE/DX = 0.0 !

! A175 L(2,25,19,16,-2) 191.0416 -DE/DX = 0.0 !

! A176 L(8,25,16,19,-2) 166.5875 -DE/DX = 0.0 !

! D1 D(5,1,2,3) 0.1825 -DE/DX = 0.0 !

! D2 D(5,1,2,25) 173.3288 -DE/DX = 0.0 !

! D3 D(12,1,2,3) 179.3626 -DE/DX = 0.0 !

! D4 D(12,1,2,25) -7.4911 -DE/DX = 0.0 !

! D5 D(2,1,5,4) -0.1076 -DE/DX = 0.0 !

! D6 D(2,1,5,38) -178.9981 -DE/DX = 0.0 !

! D7 D(12,1,5,4) -179.3086 -DE/DX = 0.0 !

! D8 D(12,1,5,38) 1.801 -DE/DX = 0.0 !

! D9 D(2,1,12,17) 9.9115 -DE/DX = 0.0 !

! D10 D(5,1,12,17) -171.0375 -DE/DX = 0.0 !

! D11 D(1,2,3,4) -0.1832 -DE/DX = 0.0 !

! D12 D(1,2,3,6) -179.3642 -DE/DX = 0.0 !

! D13 D(25,2,3,4) -173.3294 -DE/DX = 0.0 !

! D14 D(25,2,3,6) 7.4896 -DE/DX = 0.0 !

! D15 D(1,2,25,8) -169.4044 -DE/DX = 0.0 !

! D16 D(1,2,25,16) -2.8167 -DE/DX = 0.0 !

! D17 D(3,2,25,8) 2.8074 -DE/DX = 0.0 !

! D18 D(3,2,25,16) 169.395 -DE/DX = 0.0 !

! D19 D(2,3,4,5) 0.1094 -DE/DX = 0.0 !

! D20 D(2,3,4,41) 179.0003 -DE/DX = 0.0 !

! D21 D(6,3,4,5) 179.3113 -DE/DX = 0.0 !

! D22 D(6,3,4,41) -1.7978 -DE/DX = 0.0 !

! D23 D(2,3,6,7) -9.8946 -DE/DX = 0.0 !

! D24 D(4,3,6,7) 171.0533 -DE/DX = 0.0 !

! D25 D(3,4,5,1) -0.0011 -DE/DX = 0.0 !

! D26 D(3,4,5,38) 179.0508 -DE/DX = 0.0 !

! D27 D(41,4,5,1) -179.0534 -DE/DX = 0.0 !

! D28 D(41,4,5,38) -0.0015 -DE/DX = 0.0 !

! D29 D(3,4,41,40) -179.0253 -DE/DX = 0.0 !

! D30 D(3,4,41,50) 0.7832 -DE/DX = 0.0 !

! D31 D(5,4,41,40) -0.2634 -DE/DX = 0.0 !

! D32 D(5,4,41,50) 179.5451 -DE/DX = 0.0 !

! D33 D(1,5,38,39) 179.027 -DE/DX = 0.0 !

! D34 D(1,5,38,51) -0.7804 -DE/DX = 0.0 !

! D35 D(4,5,38,39) 0.2657 -DE/DX = 0.0 !

! D36 D(4,5,38,51) -179.5418 -DE/DX = 0.0 !

! D37 D(3,6,7,8) -3.0058 -DE/DX = 0.0 !

! D38 D(3,6,7,11) 178.8861 -DE/DX = 0.0 !

! D39 D(6,7,8,9) -177.5072 -DE/DX = 0.0 !

! D40 D(6,7,8,25) 15.8129 -DE/DX = 0.0 !

! D41 D(11,7,8,9) 0.8469 -DE/DX = 0.0 !

! D42 D(11,7,8,25) -165.833 -DE/DX = 0.0 !

! D43 D(6,7,11,10) 177.9311 -DE/DX = 0.0 !

! D44 D(6,7,11,34) -1.323 -DE/DX = 0.0 !

! D45 D(8,7,11,10) -0.5009 -DE/DX = 0.0 !

! D46 D(8,7,11,34) -179.7551 -DE/DX = 0.0 !

! D47 D(7,8,9,10) -0.8485 -DE/DX = 0.0 !

! D48 D(7,8,9,24) 177.5052 -DE/DX = 0.0 !

! D49 D(25,8,9,10) 165.8321 -DE/DX = 0.0 !

! D50 D(25,8,9,24) -15.8142 -DE/DX = 0.0 !

! D51 D(7,8,25,2) -13.0397 -DE/DX = 0.0 !

! D52 D(7,8,25,19) 178.0017 -DE/DX = 0.0 !

! D53 D(9,8,25,2) -177.9911 -DE/DX = 0.0 !

! D54 D(9,8,25,19) 13.0503 -DE/DX = 0.0 !

! D55 D(8,9,10,11) 0.5052 -DE/DX = 0.0 !

! D56 D(8,9,10,37) 179.76 -DE/DX = 0.0 !

! D57 D(24,9,10,11) -177.9266 -DE/DX = 0.0 !

! D58 D(24,9,10,37) 1.3282 -DE/DX = 0.0 !

! D59 D(8,9,24,23) 2.9904 -DE/DX = 0.0 !

! D60 D(10,9,24,23) -178.9019 -DE/DX = 0.0 !

! D61 D(9,10,11,7) -0.0026 -DE/DX = 0.0 !

! D62 D(9,10,11,34) 179.3491 -DE/DX = 0.0 !

! D63 D(37,10,11,7) -179.3547 -DE/DX = 0.0 !

! D64 D(37,10,11,34) -0.0031 -DE/DX = 0.0 !

! D65 D(9,10,37,36) -179.1105 -DE/DX = 0.0 !

! D66 D(9,10,37,53) 1.19 -DE/DX = 0.0 !

! D67 D(11,10,37,36) 0.0545 -DE/DX = 0.0 !

! D68 D(11,10,37,53) -179.645 -DE/DX = 0.0 !

! D69 D(7,11,34,35) 179.1135 -DE/DX = 0.0 !

! D70 D(7,11,34,52) -1.1836 -DE/DX = 0.0 !

! D71 D(10,11,34,35) -0.0508 -DE/DX = 0.0 !

! D72 D(10,11,34,52) 179.6521 -DE/DX = 0.0 !

! D73 D(1,12,17,13) -178.9048 -DE/DX = 0.0 !

! D74 D(1,12,17,16) 2.9902 -DE/DX = 0.0 !

! D75 D(17,13,14,15) 0.0008 -DE/DX = 0.0 !

! D76 D(17,13,14,29) 179.3516 -DE/DX = 0.0 !

! D77 D(26,13,14,15) -179.3513 -DE/DX = 0.0 !

! D78 D(26,13,14,29) -0.0004 -DE/DX = 0.0 !

! D79 D(14,13,17,12) -177.9284 -DE/DX = 0.0 !

! D80 D(14,13,17,16) 0.5012 -DE/DX = 0.0 !

! D81 D(26,13,17,12) 1.3263 -DE/DX = 0.0 !

! D82 D(26,13,17,16) 179.7559 -DE/DX = 0.0 !

! D83 D(14,13,26,27) 0.0528 -DE/DX = 0.0 !

! D84 D(14,13,26,57) -179.649 -DE/DX = 0.0 !

! D85 D(17,13,26,27) -179.1121 -DE/DX = 0.0 !

! D86 D(17,13,26,57) 1.1861 -DE/DX = 0.0 !

! D87 D(13,14,15,16) -0.5025 -DE/DX = 0.0 !

! D88 D(13,14,15,18) 177.928 -DE/DX = 0.0 !

! D89 D(29,14,15,16) -179.7557 -DE/DX = 0.0 !

! D90 D(29,14,15,18) -1.3252 -DE/DX = 0.0 !

! D91 D(13,14,29,28) -0.0522 -DE/DX = 0.0 !

! D92 D(13,14,29,56) 179.6513 -DE/DX = 0.0 !

! D93 D(15,14,29,28) 179.1111 -DE/DX = 0.0 !

! D94 D(15,14,29,56) -1.1854 -DE/DX = 0.0 !

! D95 D(14,15,16,17) 0.8459 -DE/DX = 0.0 !

! D96 D(14,15,16,25) -165.8347 -DE/DX = 0.0 !

! D97 D(18,15,16,17) -177.5065 -DE/DX = 0.0 !

! D98 D(18,15,16,25) 15.8129 -DE/DX = 0.0 !

! D99 D(14,15,18,20) 178.8882 -DE/DX = 0.0 !

! D100 D(16,15,18,20) -3.0056 -DE/DX = 0.0 !

! D101 D(15,16,17,12) 177.506 -DE/DX = 0.0 !

! D102 D(15,16,17,13) -0.8454 -DE/DX = 0.0 !

! D103 D(25,16,17,12) -15.8131 -DE/DX = 0.0 !

! D104 D(25,16,17,13) 165.8355 -DE/DX = 0.0 !

! D105 D(15,16,25,2) 178.0017 -DE/DX = 0.0 !

! D106 D(15,16,25,19) -13.0399 -DE/DX = 0.0 !

! D107 D(17,16,25,2) 13.0496 -DE/DX = 0.0 !

! D108 D(17,16,25,19) -177.992 -DE/DX = 0.0 !

! D109 D(15,18,20,19) -9.8952 -DE/DX = 0.0 !

! D110 D(15,18,20,21) 171.054 -DE/DX = 0.0 !

! D111 D(23,19,20,18) -179.3641 -DE/DX = 0.0 !

! D112 D(23,19,20,21) -0.1841 -DE/DX = 0.0 !

! D113 D(25,19,20,18) 7.4898 -DE/DX = 0.0 !

! D114 D(25,19,20,21) -173.3303 -DE/DX = 0.0 !

! D115 D(20,19,23,22) 0.1813 -DE/DX = 0.0 !

! D116 D(20,19,23,24) 179.3618 -DE/DX = 0.0 !

! D117 D(25,19,23,22) 173.3274 -DE/DX = 0.0 !

! D118 D(25,19,23,24) -7.4922 -DE/DX = 0.0 !

! D119 D(20,19,25,8) 169.395 -DE/DX = 0.0 !

! D120 D(20,19,25,16) 2.8075 -DE/DX = 0.0 !

! D121 D(23,19,25,8) -2.8166 -DE/DX = 0.0 !

! D122 D(23,19,25,16) -169.4041 -DE/DX = 0.0 !

! D123 D(18,20,21,22) 179.313 -DE/DX = 0.0 !

! D124 D(18,20,21,33) -1.7976 -DE/DX = 0.0 !

! D125 D(19,20,21,22) 0.1121 -DE/DX = 0.0 !

! D126 D(19,20,21,33) 179.0016 -DE/DX = 0.0 !

! D127 D(20,21,22,23) -0.0044 -DE/DX = 0.0 !

! D128 D(20,21,22,30) 179.048 -DE/DX = 0.0 !

! D129 D(33,21,22,23) -179.0555 -DE/DX = 0.0 !

! D130 D(33,21,22,30) -0.0031 -DE/DX = 0.0 !

! D131 D(20,21,33,32) -179.0235 -DE/DX = 0.0 !

! D132 D(20,21,33,55) 0.7849 -DE/DX = 0.0 !

! D133 D(22,21,33,32) -0.2632 -DE/DX = 0.0 !

! D134 D(22,21,33,55) 179.5452 -DE/DX = 0.0 !

! D135 D(21,22,23,19) -0.1048 -DE/DX = 0.0 !

! D136 D(21,22,23,24) -179.3061 -DE/DX = 0.0 !

! D137 D(30,22,23,19) -178.9958 -DE/DX = 0.0 !

! D138 D(30,22,23,24) 1.8028 -DE/DX = 0.0 !

! D139 D(21,22,30,31) 0.2674 -DE/DX = 0.0 !

! D140 D(21,22,30,54) -179.5409 -DE/DX = 0.0 !

! D141 D(23,22,30,31) 179.0295 -DE/DX = 0.0 !

! D142 D(23,22,30,54) -0.7788 -DE/DX = 0.0 !

! D143 D(19,23,24,9) 9.9125 -DE/DX = 0.0 !

! D144 D(22,23,24,9) -171.036 -DE/DX = 0.0 !

! D145 D(13,26,27,28) -0.0527 -DE/DX = 0.0 !

! D146 D(13,26,27,46) -179.7684 -DE/DX = 0.0 !

! D147 D(57,26,27,28) 179.6317 -DE/DX = 0.0 !

! D148 D(57,26,27,46) -0.0841 -DE/DX = 0.0 !

! D149 D(13,26,57,74) -177.5217 -DE/DX = 0.0 !

! D150 D(27,26,57,74) 2.7986 -DE/DX = 0.0 !

! D151 D(26,27,28,29) -0.0001 -DE/DX = 0.0 !

! D152 D(26,27,28,47) -179.7235 -DE/DX = 0.0 !

! D153 D(46,27,28,29) 179.7215 -DE/DX = 0.0 !

! D154 D(46,27,28,47) -0.002 -DE/DX = 0.0 !

! D155 D(27,28,29,14) 0.0526 -DE/DX = 0.0 !

! D156 D(27,28,29,56) -179.6336 -DE/DX = 0.0 !

! D157 D(47,28,29,14) 179.7703 -DE/DX = 0.0 !

! D158 D(47,28,29,56) 0.0842 -DE/DX = 0.0 !

! D159 D(14,29,56,78) 177.5254 -DE/DX = 0.0 !

! D160 D(28,29,56,78) -2.7931 -DE/DX = 0.0 !

! D161 D(22,30,31,32) -0.268 -DE/DX = 0.0 !

! D162 D(22,30,31,49) 179.9854 -DE/DX = 0.0 !

! D163 D(54,30,31,32) 179.5283 -DE/DX = 0.0 !

! D164 D(54,30,31,49) -0.2183 -DE/DX = 0.0 !

! D165 D(22,30,54,86) 178.4338 -DE/DX = 0.0 !

! D166 D(31,30,54,86) -1.3611 -DE/DX = 0.0 !

! D167 D(30,31,32,33) -0.0006 -DE/DX = 0.0 !

! D168 D(30,31,32,48) -179.7542 -DE/DX = 0.0 !

! D169 D(49,31,32,33) 179.7518 -DE/DX = 0.0 !

! D170 D(49,31,32,48) -0.0018 -DE/DX = 0.0 !

! D171 D(31,32,33,21) 0.2674 -DE/DX = 0.0 !

! D172 D(31,32,33,55) -179.529 -DE/DX = 0.0 !

! D173 D(48,32,33,21) -179.9848 -DE/DX = 0.0 !

! D174 D(48,32,33,55) 0.2188 -DE/DX = 0.0 !

! D175 D(21,33,55,82) -178.43 -DE/DX = 0.0 !

! D176 D(32,33,55,82) 1.3649 -DE/DX = 0.0 !

! D177 D(11,34,35,36) 0.0532 -DE/DX = 0.0 !

! D178 D(11,34,35,42) 179.7696 -DE/DX = 0.0 !

! D179 D(52,34,35,36) -179.6324 -DE/DX = 0.0 !

! D180 D(52,34,35,42) 0.084 -DE/DX = 0.0 !

! D181 D(11,34,52,62) 177.5247 -DE/DX = 0.0 !

! D182 D(35,34,52,62) -2.7944 -DE/DX = 0.0 !

! D183 D(34,35,36,37) -0.0015 -DE/DX = 0.0 !

! D184 D(34,35,36,43) 179.7198 -DE/DX = 0.0 !

! D185 D(42,35,36,37) -179.7236 -DE/DX = 0.0 !

! D186 D(42,35,36,43) -0.0023 -DE/DX = 0.0 !

! D187 D(35,36,37,10) -0.0525 -DE/DX = 0.0 !

! D188 D(35,36,37,53) 179.6295 -DE/DX = 0.0 !

! D189 D(43,36,37,10) -179.768 -DE/DX = 0.0 !

! D190 D(43,36,37,53) -0.086 -DE/DX = 0.0 !

! D191 D(10,37,53,66) -177.5241 -DE/DX = 0.0 !

! D192 D(36,37,53,66) 2.7986 -DE/DX = 0.0 !

! D193 D(5,38,39,40) -0.2674 -DE/DX = 0.0 !

! D194 D(5,38,39,45) 179.9861 -DE/DX = 0.0 !

! D195 D(51,38,39,40) 179.528 -DE/DX = 0.0 !

! D196 D(51,38,39,45) -0.2185 -DE/DX = 0.0 !

! D197 D(5,38,51,70) 178.4345 -DE/DX = 0.0 !

! D198 D(39,38,51,70) -1.3595 -DE/DX = 0.0 !

! D199 D(38,39,40,41) 0.0 -DE/DX = 0.0 !

! D200 D(38,39,40,44) -179.7545 -DE/DX = 0.0 !

! D201 D(45,39,40,41) 179.7524 -DE/DX = 0.0 !

! D202 D(45,39,40,44) -0.0022 -DE/DX = 0.0 !

! D203 D(39,40,41,4) 0.2666 -DE/DX = 0.0 !

! D204 D(39,40,41,50) -179.53 -DE/DX = 0.0 !

! D205 D(44,40,41,4) -179.9846 -DE/DX = 0.0 !

! D206 D(44,40,41,50) 0.2189 -DE/DX = 0.0 !

! D207 D(4,41,50,58) -178.4296 -DE/DX = 0.0 !

! D208 D(40,41,50,58) 1.3655 -DE/DX = 0.0 !

! D209 D(41,50,58,59) 60.3709 -DE/DX = 0.0 !

! D210 D(41,50,58,60) -62.3785 -DE/DX = 0.0 !

! D211 D(41,50,58,61) 178.9651 -DE/DX = 0.0 !

! D212 D(38,51,70,71) 62.4032 -DE/DX = 0.0 !

! D213 D(38,51,70,72) -60.3487 -DE/DX = 0.0 !

! D214 D(38,51,70,73) -178.9444 -DE/DX = 0.0 !

! D215 D(34,52,62,63) 62.693 -DE/DX = 0.0 !

! D216 D(34,52,62,64) -60.1633 -DE/DX = 0.0 !

! D217 D(34,52,62,65) -178.7321 -DE/DX = 0.0 !

! D218 D(37,53,66,67) 60.1606 -DE/DX = 0.0 !

! D219 D(37,53,66,68) -62.6992 -DE/DX = 0.0 !

! D220 D(37,53,66,69) 178.7277 -DE/DX = 0.0 !

! D221 D(30,54,86,87) 62.4036 -DE/DX = 0.0 !

! D222 D(30,54,86,88) -60.3482 -DE/DX = 0.0 !

! D223 D(30,54,86,89) -178.9438 -DE/DX = 0.0 !

! D224 D(33,55,82,83) 60.3705 -DE/DX = 0.0 !

! D225 D(33,55,82,84) -62.3789 -DE/DX = 0.0 !

! D226 D(33,55,82,85) 178.9647 -DE/DX = 0.0 !

! D227 D(29,56,78,79) 62.693 -DE/DX = 0.0 !

! D228 D(29,56,78,80) -60.1634 -DE/DX = 0.0 !

! D229 D(29,56,78,81) -178.7323 -DE/DX = 0.0 !

! D230 D(26,57,74,75) 60.1599 -DE/DX = 0.0 !

! D231 D(26,57,74,76) -62.6999 -DE/DX = 0.0 !

! D232 D(26,57,74,77) 178.7269 -DE/DX = 0.0 !

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Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Largest change from initial coordinates is atom 25 0.247 Angstoms.

Leave Link 103 at Sat Jul 6 03:56:39 2019, MaxMem= 1342177280 cpu: 14.7

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Stoichiometry C40H32N8O8Zn(3)

Framework group C1[X(C40H32N8O8Zn)]

Deg. of freedom 261

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.74D-14

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 -1.126174 2.799765 -0.018207

2 7 0 -0.001792 2.037851 -0.169207

3 6 0 1.121239 2.801729 -0.018007

4 6 0 0.709557 4.166162 0.247780

5 6 0 -0.716909 4.164903 0.247667

6 7 0 2.407623 2.385263 -0.112861

7 6 0 2.796686 1.132806 -0.187231

8 7 0 2.018991 0.001793 -0.128998

9 6 0 2.798653 -1.127880 -0.187446

10 6 0 4.208901 -0.701195 -0.313988

11 6 0 4.207693 0.708540 -0.313816

12 7 0 -2.411788 2.381046 -0.113322

13 6 0 -4.208922 0.701204 -0.313965

14 6 0 -4.207703 -0.708535 -0.313847

15 6 0 -2.796692 -1.132795 -0.187274

16 7 0 -2.019010 -0.001777 -0.129031

17 6 0 -2.798665 1.127894 -0.187483

18 7 0 -2.407621 -2.385263 -0.112890

19 7 0 0.001808 -2.037864 -0.169191

20 6 0 -1.121224 -2.801736 -0.018004

21 6 0 -0.709539 -4.166171 0.247782

22 6 0 0.716930 -4.164895 0.247744

23 6 0 1.126188 -2.799764 -0.018165

24 7 0 2.411792 -2.381037 -0.113280

25 30 0 -0.000007 -0.000009 -0.367537

26 6 0 -5.402583 1.426812 -0.407440

27 6 0 -6.595962 0.690018 -0.499716

28 6 0 -6.594777 -0.701422 -0.499596

29 6 0 -5.400138 -1.436165 -0.407195

30 6 0 1.438976 -5.348382 0.498824

31 6 0 0.706213 -6.515155 0.740209

32 6 0 -0.694537 -6.516418 0.740210

33 6 0 -1.429428 -5.350975 0.498840

34 6 0 5.400133 1.436161 -0.407149

35 6 0 6.594763 0.701413 -0.499621

36 6 0 6.595932 -0.690028 -0.499835

37 6 0 5.402547 -1.426814 -0.407559

38 6 0 -1.438949 5.348412 0.498674

39 6 0 -0.706184 6.515175 0.740096

40 6 0 0.694565 6.516413 0.740191

41 6 0 1.429450 5.350957 0.498870

42 1 0 7.544838 1.212786 -0.577704

43 1 0 7.546852 -1.199778 -0.578113

44 1 0 1.201474 7.451276 0.937816

45 1 0 -1.214753 7.449147 0.937691

46 1 0 -7.546891 1.199764 -0.577915

47 1 0 -7.544850 -1.212797 -0.577676

48 1 0 -1.201441 -7.451286 0.937817

49 1 0 1.214783 -7.449117 0.937848

50 8 0 2.778926 5.294292 0.496359

51 8 0 -2.788316 5.289297 0.496004

52 8 0 5.339562 2.784035 -0.409536

53 8 0 5.344210 -2.774794 -0.410412

54 8 0 2.788345 -5.289234 0.496237

55 8 0 -2.778905 -5.294327 0.496255

56 8 0 -5.339551 -2.784039 -0.409652

57 8 0 -5.344282 2.774793 -0.410164

58 6 0 3.507162 6.485550 0.783963

59 1 0 3.271323 6.866566 1.781947

60 1 0 3.314214 7.264327 0.040253

61 1 0 4.557400 6.202370 0.744928

62 6 0 6.559875 3.521596 -0.450752

63 1 0 7.116614 3.327394 -1.372126

64 1 0 7.191899 3.297466 0.413670

65 1 0 6.266554 4.569272 -0.421543

66 6 0 6.565700 -3.510389 -0.451854

67 1 0 7.197399 -3.285539 0.412617

68 1 0 7.122113 -3.315082 -1.373193

69 1 0 6.274002 -4.558527 -0.422929

70 6 0 -3.518752 6.479245 0.783413

71 1 0 -3.327481 7.258181 0.039424

72 1 0 -3.283457 6.861019 1.781237

73 1 0 -4.568443 6.194019 0.744632

74 6 0 -6.565798 3.510349 -0.451459

75 1 0 -7.197441 3.285381 0.413024

76 1 0 -7.122257 3.315122 -1.372788

77 1 0 -6.274136 4.558495 -0.422433

78 6 0 -6.559847 -3.521629 -0.450898

79 1 0 -7.116597 -3.327394 -1.372259

80 1 0 -7.191871 -3.297561 0.413540

81 1 0 -6.266499 -4.569298 -0.421747

82 6 0 -3.507142 -6.485594 0.783817

83 1 0 -3.271347 -6.866611 1.781811

84 1 0 -3.314153 -7.264367 0.040114

85 1 0 -4.557381 -6.202423 0.744733

86 6 0 3.518804 -6.479147 0.783733

87 1 0 3.327613 -7.258115 0.039757

88 1 0 3.283453 -6.860897 1.781553

89 1 0 4.568488 -6.193886 0.745017

---------------------------------------------------------------------

Rotational constants (GHZ): 0.0447620 0.0439710 0.0225232

Leave Link 202 at Sat Jul 6 03:56:40 2019, MaxMem= 1342177280 cpu: 0.5

(Enter /apps/gaussian/g09d01/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 1 IROHF=0.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Population analysis using the SCF density.

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Orbital symmetries:

Alpha Orbitals:

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The electronic state is 3-A.

Alpha occ. eigenvalues -- -19.14785 -19.14785 -19.14785 -19.14785 -19.14676

Alpha occ. eigenvalues -- -19.14676 -19.14676 -19.14676 -14.30395 -14.30395

Alpha occ. eigenvalues -- -14.29658 -14.29658 -14.29380 -14.29380 -14.29380

Alpha occ. eigenvalues -- -14.29380 -10.24733 -10.24732 -10.24731 -10.24731

Alpha occ. eigenvalues -- -10.24011 -10.24011 -10.24009 -10.24009 -10.23879

Alpha occ. eigenvalues -- -10.23879 -10.23877 -10.23877 -10.23710 -10.23710

Alpha occ. eigenvalues -- -10.23708 -10.23708 -10.20951 -10.20951 -10.20951

Alpha occ. eigenvalues -- -10.20951 -10.20858 -10.20858 -10.20858 -10.20858

Alpha occ. eigenvalues -- -10.18075 -10.18075 -10.18027 -10.18027 -10.17894

Alpha occ. eigenvalues -- -10.17894 -10.17841 -10.17841 -10.17365 -10.17365

Alpha occ. eigenvalues -- -10.17322 -10.17322 -10.17287 -10.17287 -10.17238

Alpha occ. eigenvalues -- -10.17238 -1.06948 -1.06947 -1.06849 -1.06847

Alpha occ. eigenvalues -- -1.06788 -1.06786 -1.06694 -1.06694 -0.99372

Alpha occ. eigenvalues -- -0.98004 -0.97998 -0.95386 -0.93009 -0.89334

Alpha occ. eigenvalues -- -0.88732 -0.86226 -0.85224 -0.85023 -0.84723

Alpha occ. eigenvalues -- -0.84515 -0.77504 -0.76643 -0.76533 -0.76424

Alpha occ. eigenvalues -- -0.76318 -0.76258 -0.75819 -0.75793 -0.72508

Alpha occ. eigenvalues -- -0.71473 -0.71387 -0.71175 -0.71165 -0.69726

Alpha occ. eigenvalues -- -0.68824 -0.68073 -0.67930 -0.67912 -0.67882

Alpha occ. eigenvalues -- -0.63372 -0.63192 -0.61693 -0.61519 -0.61339

Alpha occ. eigenvalues -- -0.59746 -0.59554 -0.59534 -0.59526 -0.58820

Alpha occ. eigenvalues -- -0.56965 -0.56062 -0.55506 -0.55344 -0.55137

Alpha occ. eigenvalues -- -0.55026 -0.54810 -0.54489 -0.53829 -0.52962

Alpha occ. eigenvalues -- -0.52543 -0.51915 -0.51751 -0.51642 -0.51501

Alpha occ. eigenvalues -- -0.50900 -0.50682 -0.50396 -0.50286 -0.49150

Alpha occ. eigenvalues -- -0.48818 -0.47824 -0.47640 -0.47284 -0.47081

Alpha occ. eigenvalues -- -0.46986 -0.46910 -0.46356 -0.46344 -0.46335

Alpha occ. eigenvalues -- -0.46281 -0.46271 -0.45006 -0.44832 -0.44722

Alpha occ. eigenvalues -- -0.44477 -0.43788 -0.43674 -0.43581 -0.43579

Alpha occ. eigenvalues -- -0.43488 -0.43365 -0.43135 -0.41526 -0.41231

Alpha occ. eigenvalues -- -0.41109 -0.40691 -0.40568 -0.40372 -0.39626

Alpha occ. eigenvalues -- -0.39255 -0.39185 -0.38377 -0.38265 -0.38118

Alpha occ. eigenvalues -- -0.38097 -0.37985 -0.37950 -0.37751 -0.37709

Alpha occ. eigenvalues -- -0.37687 -0.36265 -0.35435 -0.35319 -0.35268

Alpha occ. eigenvalues -- -0.34578 -0.34220 -0.33925 -0.33828 -0.33336

Alpha occ. eigenvalues -- -0.33032 -0.32903 -0.32835 -0.31994 -0.31890

Alpha occ. eigenvalues -- -0.31817 -0.31639 -0.31124 -0.29635 -0.29434

Alpha occ. eigenvalues -- -0.29399 -0.29302 -0.28241 -0.25906 -0.25644

Alpha occ. eigenvalues -- -0.25625 -0.25609 -0.25184 -0.24629 -0.24568

Alpha occ. eigenvalues -- -0.24565 -0.23903 -0.23208 -0.21236 -0.21034

Alpha occ. eigenvalues -- -0.20988 -0.17826 -0.13658

Alpha virt. eigenvalues -- -0.09211 -0.04874 -0.01705 -0.00559 -0.00498

Alpha virt. eigenvalues -- -0.00324 0.01794 0.02450 0.02782 0.03715

Alpha virt. eigenvalues -- 0.04957 0.04989 0.05081 0.05327 0.05855

Alpha virt. eigenvalues -- 0.05916 0.06091 0.06099 0.06397 0.06539

Alpha virt. eigenvalues -- 0.06851 0.06871 0.07910 0.07976 0.09193

Alpha virt. eigenvalues -- 0.09252 0.09830 0.11056 0.11099 0.11164

Alpha virt. eigenvalues -- 0.11367 0.11454 0.11520 0.11593 0.11648

Alpha virt. eigenvalues -- 0.11838 0.11908 0.12079 0.12660 0.12662

Alpha virt. eigenvalues -- 0.12742 0.12882 0.12956 0.13040 0.13075

Alpha virt. eigenvalues -- 0.13203 0.13262 0.13271 0.13305 0.13372

Alpha virt. eigenvalues -- 0.16894 0.16896 0.17011 0.17016 0.17949

Alpha virt. eigenvalues -- 0.18260 0.18394 0.18484 0.18544 0.18793

Alpha virt. eigenvalues -- 0.18986 0.19086 0.19332 0.20789 0.20908

Alpha virt. eigenvalues -- 0.21085 0.21276 0.21596 0.21606 0.21732

Alpha virt. eigenvalues -- 0.22416 0.23263 0.23527 0.24408 0.24536

Alpha virt. eigenvalues -- 0.24690 0.25113 0.25322 0.25811 0.25976

Alpha virt. eigenvalues -- 0.26417 0.26619 0.26807 0.28674 0.28675

Alpha virt. eigenvalues -- 0.29616 0.29911 0.29937 0.29972 0.30463

Alpha virt. eigenvalues -- 0.31018 0.31124 0.31235 0.32091 0.32254

Alpha virt. eigenvalues -- 0.32736 0.32783 0.32873 0.33088 0.33295

Alpha virt. eigenvalues -- 0.33343 0.33376 0.33458 0.33767 0.34646

Alpha virt. eigenvalues -- 0.34889 0.34965 0.35123 0.35305 0.35727

Alpha virt. eigenvalues -- 0.35751 0.36239 0.36654 0.36797 0.37292

Alpha virt. eigenvalues -- 0.37467 0.38008 0.38202 0.38215 0.38283

Alpha virt. eigenvalues -- 0.38298 0.38500 0.39003 0.39094 0.39245

Alpha virt. eigenvalues -- 0.39425 0.39486 0.39692 0.39777 0.39977

Alpha virt. eigenvalues -- 0.39985 0.40420 0.40974 0.41023 0.41364

Alpha virt. eigenvalues -- 0.41925 0.41962 0.42123 0.42292 0.43087

Alpha virt. eigenvalues -- 0.43282 0.43391 0.43520 0.43701 0.43883

Alpha virt. eigenvalues -- 0.44298 0.44304 0.44478 0.44484 0.44905

Alpha virt. eigenvalues -- 0.45204 0.45372 0.45858 0.46195 0.46236

Alpha virt. eigenvalues -- 0.46439 0.46978 0.47531 0.48005 0.48525

Alpha virt. eigenvalues -- 0.48627 0.48913 0.48995 0.49292 0.49397

Alpha virt. eigenvalues -- 0.49584 0.49688 0.50056 0.50213 0.50239

Alpha virt. eigenvalues -- 0.50288 0.50712 0.50797 0.50972 0.51503

Alpha virt. eigenvalues -- 0.51771 0.52002 0.52003 0.52187 0.52528

Alpha virt. eigenvalues -- 0.52787 0.52940 0.53165 0.53919 0.54146

Alpha virt. eigenvalues -- 0.54613 0.54626 0.54751 0.55170 0.55675

Alpha virt. eigenvalues -- 0.56034 0.56880 0.57004 0.57115 0.57430

Alpha virt. eigenvalues -- 0.57907 0.57916 0.58186 0.58454 0.58462

Alpha virt. eigenvalues -- 0.58523 0.58809 0.59085 0.59421 0.59892

Alpha virt. eigenvalues -- 0.59999 0.60437 0.61231 0.61379 0.61461

Alpha virt. eigenvalues -- 0.61656 0.61981 0.62352 0.62598 0.62992

Alpha virt. eigenvalues -- 0.63006 0.63258 0.63346 0.63500 0.63560

Alpha virt. eigenvalues -- 0.63815 0.63823 0.64079 0.64111 0.64520

Alpha virt. eigenvalues -- 0.64691 0.64782 0.64914 0.65050 0.65260

Alpha virt. eigenvalues -- 0.65389 0.65418 0.65578 0.65620 0.67138

Alpha virt. eigenvalues -- 0.67198 0.67641 0.67952 0.68771 0.69058

Alpha virt. eigenvalues -- 0.69601 0.69736 0.70067 0.70479 0.70503

Alpha virt. eigenvalues -- 0.71458 0.72455 0.72503 0.72602 0.72745

Alpha virt. eigenvalues -- 0.72873 0.73540 0.73591 0.74623 0.74655

Alpha virt. eigenvalues -- 0.74933 0.75694 0.75905 0.76161 0.76315

Alpha virt. eigenvalues -- 0.76552 0.77939 0.78891 0.79093 0.79186

Alpha virt. eigenvalues -- 0.79188 0.79425 0.79951 0.80201 0.80442

Alpha virt. eigenvalues -- 0.80684 0.81000 0.81103 0.81121 0.81642

Alpha virt. eigenvalues -- 0.81815 0.81949 0.82532 0.82766 0.83203

Alpha virt. eigenvalues -- 0.84227 0.84238 0.85395 0.85583 0.85796

Alpha virt. eigenvalues -- 0.85824 0.86349 0.86477 0.87409 0.87523

Alpha virt. eigenvalues -- 0.87674 0.88213 0.88608 0.88666 0.90420

Alpha virt. eigenvalues -- 0.90449 0.90620 0.91929 0.92492 0.92730

Alpha virt. eigenvalues -- 0.92911 0.92974 0.93249 0.93557 0.93827

Alpha virt. eigenvalues -- 0.94452 0.95277 0.95668 0.95682 0.96336

Alpha virt. eigenvalues -- 0.96752 0.97337 0.97408 0.97646 0.98077

Alpha virt. eigenvalues -- 0.98464 0.98514 0.98777 0.99167 0.99626

Alpha virt. eigenvalues -- 0.99862 1.00512 1.01314 1.01934 1.02529

Alpha virt. eigenvalues -- 1.02572 1.03859 1.04199 1.04796 1.06233

Alpha virt. eigenvalues -- 1.06843 1.07492 1.07876 1.08189 1.08576

Alpha virt. eigenvalues -- 1.08660 1.09056 1.09226 1.10411 1.10910

Alpha virt. eigenvalues -- 1.11150 1.11305 1.11482 1.11646 1.12012

Alpha virt. eigenvalues -- 1.12057 1.13518 1.13588 1.13936 1.14057

Alpha virt. eigenvalues -- 1.14506 1.14951 1.15615 1.15710 1.15803

Alpha virt. eigenvalues -- 1.18292 1.18436 1.18858 1.19140 1.19166

Alpha virt. eigenvalues -- 1.19189 1.19491 1.19644 1.19701 1.20596

Alpha virt. eigenvalues -- 1.21786 1.22594 1.23545 1.23632 1.23652

Alpha virt. eigenvalues -- 1.23969 1.24255 1.24526 1.24637 1.25800

Alpha virt. eigenvalues -- 1.26083 1.26303 1.26789 1.27202 1.27314

Alpha virt. eigenvalues -- 1.27755 1.27806 1.29301 1.30020 1.31090

Alpha virt. eigenvalues -- 1.31636 1.31806 1.32180 1.33499 1.33516

Alpha virt. eigenvalues -- 1.33586 1.33603 1.33890 1.34534 1.34614

Alpha virt. eigenvalues -- 1.35064 1.35648 1.36181 1.36607 1.37649

Alpha virt. eigenvalues -- 1.37910 1.38350 1.38354 1.40032 1.41020

Alpha virt. eigenvalues -- 1.41173 1.41478 1.43728 1.44583 1.44745

Alpha virt. eigenvalues -- 1.46184 1.46785 1.47097 1.47828 1.48164

Alpha virt. eigenvalues -- 1.48169 1.48466 1.50642 1.50904 1.50984

Alpha virt. eigenvalues -- 1.51169 1.51646 1.51752 1.52041 1.52066

Alpha virt. eigenvalues -- 1.52187 1.52330 1.52347 1.52380 1.52590

Alpha virt. eigenvalues -- 1.52603 1.52623 1.52666 1.52779 1.53043

Alpha virt. eigenvalues -- 1.53558 1.53882 1.53990 1.54328 1.54587

Alpha virt. eigenvalues -- 1.55406 1.55928 1.56020 1.56893 1.57363

Alpha virt. eigenvalues -- 1.57407 1.58225 1.58905 1.59202 1.59295

Alpha virt. eigenvalues -- 1.59345 1.59455 1.59811 1.60073 1.61318

Alpha virt. eigenvalues -- 1.61343 1.61626 1.61724 1.61950 1.62936

Alpha virt. eigenvalues -- 1.63083 1.64846 1.66162 1.66581 1.66972

Alpha virt. eigenvalues -- 1.67274 1.68195 1.68215 1.68621 1.68764

Alpha virt. eigenvalues -- 1.68976 1.69168 1.69520 1.70592 1.71192

Alpha virt. eigenvalues -- 1.71843 1.71981 1.72316 1.73207 1.73263

Alpha virt. eigenvalues -- 1.73408 1.74478 1.74955 1.75050 1.75195

Alpha virt. eigenvalues -- 1.77072 1.77148 1.78179 1.78474 1.78759

Alpha virt. eigenvalues -- 1.79385 1.79412 1.79817 1.80121 1.80267

Alpha virt. eigenvalues -- 1.80344 1.80583 1.80915 1.81603 1.81782

Alpha virt. eigenvalues -- 1.82432 1.84095 1.84126 1.84326 1.84558

Alpha virt. eigenvalues -- 1.85650 1.87545 1.87671 1.87939 1.88694

Alpha virt. eigenvalues -- 1.88709 1.89512 1.89745 1.90264 1.90339

Alpha virt. eigenvalues -- 1.90450 1.90690 1.90829 1.91545 1.91592

Alpha virt. eigenvalues -- 1.91850 1.94938 1.95995 1.96028 1.96141

Alpha virt. eigenvalues -- 1.96659 1.97165 1.97736 1.98014 1.98658

Alpha virt. eigenvalues -- 1.99641 1.99887 1.99994 2.01171 2.01220

Alpha virt. eigenvalues -- 2.01603 2.02485 2.03172 2.05016 2.07398

Alpha virt. eigenvalues -- 2.08235 2.08609 2.08625 2.10050 2.10818

Alpha virt. eigenvalues -- 2.11015 2.12454 2.13767 2.14247 2.15057

Alpha virt. eigenvalues -- 2.15644 2.15667 2.16285 2.16879 2.19273

Alpha virt. eigenvalues -- 2.20211 2.21462 2.23008 2.23632 2.24672

Alpha virt. eigenvalues -- 2.25244 2.25349 2.25624 2.25873 2.26120

Alpha virt. eigenvalues -- 2.26230 2.26670 2.27849 2.28118 2.28168

Alpha virt. eigenvalues -- 2.28775 2.29852 2.29951 2.30862 2.32135

Alpha virt. eigenvalues -- 2.32761 2.33602 2.33676 2.34060 2.34097

Alpha virt. eigenvalues -- 2.34169 2.34195 2.34208 2.34447 2.34548

Alpha virt. eigenvalues -- 2.34594 2.34713 2.35050 2.35337 2.35862

Alpha virt. eigenvalues -- 2.36025 2.36582 2.39379 2.40167 2.40210

Alpha virt. eigenvalues -- 2.40837 2.40963 2.41164 2.42550 2.42839

Alpha virt. eigenvalues -- 2.43044 2.43413 2.43718 2.43724 2.43836

Alpha virt. eigenvalues -- 2.44357 2.47299 2.48579 2.48627 2.49645

Alpha virt. eigenvalues -- 2.50203 2.50688 2.50789 2.50798 2.50831

Alpha virt. eigenvalues -- 2.51489 2.51839 2.52386 2.54084 2.54752

Alpha virt. eigenvalues -- 2.56630 2.57057 2.57528 2.59027 2.59040

Alpha virt. eigenvalues -- 2.60875 2.61671 2.62105 2.64347 2.64416

Alpha virt. eigenvalues -- 2.64786 2.65583 2.66077 2.67102 2.67282

Alpha virt. eigenvalues -- 2.67339 2.67603 2.68275 2.68541 2.71428

Alpha virt. eigenvalues -- 2.72742 2.72982 2.73010 2.74548 2.74669

Alpha virt. eigenvalues -- 2.74968 2.75454 2.78345 2.78461 2.78776

Alpha virt. eigenvalues -- 2.79067 2.79643 2.80043 2.80077 2.81264

Alpha virt. eigenvalues -- 2.81448 2.81557 2.81602 2.82872 2.82912

Alpha virt. eigenvalues -- 2.82957 2.83787 2.85356 2.85570 2.86282

Alpha virt. eigenvalues -- 2.86403 2.86461 2.86558 2.86683 2.87155

Alpha virt. eigenvalues -- 2.87234 2.88564 2.88618 2.88640 2.91002

Alpha virt. eigenvalues -- 2.91720 2.93840 2.93977 2.94589 2.95503

Alpha virt. eigenvalues -- 2.95663 2.95756 2.95796 2.97027 2.98399

Alpha virt. eigenvalues -- 2.98903 2.99540 3.00465 3.00478 3.00667

Alpha virt. eigenvalues -- 3.01096 3.01706 3.02728 3.02854 3.03608

Alpha virt. eigenvalues -- 3.05170 3.06149 3.06334 3.06358 3.07671

Alpha virt. eigenvalues -- 3.07732 3.08889 3.11744 3.13572 3.13595

Alpha virt. eigenvalues -- 3.13627 3.13638 3.14706 3.14761 3.14813

Alpha virt. eigenvalues -- 3.15233 3.15303 3.15810 3.16678 3.16771

Alpha virt. eigenvalues -- 3.17609 3.17758 3.17825 3.18017 3.18978

Alpha virt. eigenvalues -- 3.19472 3.20015 3.20253 3.20313 3.20379

Alpha virt. eigenvalues -- 3.20702 3.20721 3.21103 3.21164 3.21167

Alpha virt. eigenvalues -- 3.21421 3.21716 3.21972 3.22517 3.22908

Alpha virt. eigenvalues -- 3.24866 3.24944 3.26596 3.27981 3.28732

Alpha virt. eigenvalues -- 3.28735 3.28741 3.29073 3.29313 3.29868

Alpha virt. eigenvalues -- 3.30141 3.31218 3.31254 3.32657 3.32940

Alpha virt. eigenvalues -- 3.35602 3.36496 3.36755 3.37259 3.37543

Alpha virt. eigenvalues -- 3.40383 3.40390 3.40960 3.41214 3.41326

Alpha virt. eigenvalues -- 3.41539 3.41599 3.42974 3.45741 3.47119

Alpha virt. eigenvalues -- 3.47204 3.48746 3.55734 3.59977 3.60609

Alpha virt. eigenvalues -- 3.61079 3.61742 3.61857 3.63230 3.67161

Alpha virt. eigenvalues -- 3.67342 3.68406 3.68663 3.75000 3.76560

Alpha virt. eigenvalues -- 3.76947 3.76953 3.77201 3.78203 3.78951

Alpha virt. eigenvalues -- 3.79598 3.81886 3.84362 3.84365 3.84559

Alpha virt. eigenvalues -- 3.87794 3.90595 3.90671 3.91425 3.92819

Alpha virt. eigenvalues -- 3.96036 3.96848 3.96907 3.97498 3.98455

Alpha virt. eigenvalues -- 3.98536 3.99023 3.99251 4.01255 4.01387

Alpha virt. eigenvalues -- 4.01769 4.01822 4.11431 4.14153 4.14687

Alpha virt. eigenvalues -- 4.17075 4.17666 4.17721 4.19075 4.21173

Alpha virt. eigenvalues -- 4.22039 4.22459 4.24142 4.26010 4.36105

Alpha virt. eigenvalues -- 4.42119 4.42771 4.43844 4.48369 4.52806

Alpha virt. eigenvalues -- 4.56013 4.60702 4.81957 4.82036 4.82252

Alpha virt. eigenvalues -- 4.82316 4.87819 4.88161 4.88203 4.88706

Alpha virt. eigenvalues -- 4.89190 4.89487 4.89565 4.89723 5.12031

Alpha virt. eigenvalues -- 5.12708 5.12750 5.17104 5.20841 5.25999

Alpha virt. eigenvalues -- 5.26246 5.26246 5.26638 5.29740 5.29747

Alpha virt. eigenvalues -- 5.29873 5.30328 5.36897 5.37496 5.53739

Alpha virt. eigenvalues -- 5.67532 5.68993 5.68999 5.69367 5.75869

Alpha virt. eigenvalues -- 5.76121 5.76334 5.76887 7.80586 7.83647

Alpha virt. eigenvalues -- 7.88330 7.94741 8.19165 11.15097 23.34438

Alpha virt. eigenvalues -- 23.37236 23.38029 23.39517 23.44448 23.44703

Alpha virt. eigenvalues -- 23.44845 23.45337 23.45466 23.45789 23.45881

Alpha virt. eigenvalues -- 23.45976 23.76593 23.77647 23.79825 23.80639

Alpha virt. eigenvalues -- 23.82117 23.82173 23.84181 23.84194 23.86306

Alpha virt. eigenvalues -- 23.86779 23.88265 23.89359 23.90188 23.90879

Alpha virt. eigenvalues -- 23.91364 23.91858 24.01798 24.01836 24.02341

Alpha virt. eigenvalues -- 24.02394 24.03889 24.03902 24.04983 24.05204

Alpha virt. eigenvalues -- 24.10924 24.10959 24.11513 24.11589 35.58469

Alpha virt. eigenvalues -- 35.61374 35.61858 35.62418 35.71065 35.71969

Alpha virt. eigenvalues -- 35.72046 35.72065 49.91750 49.92145 49.92181

Alpha virt. eigenvalues -- 49.92414 49.92615 49.92928 49.92989 49.93182

Beta occ. eigenvalues -- -19.14756 -19.14756 -19.14756 -19.14756 -19.14625

Beta occ. eigenvalues -- -19.14625 -19.14624 -19.14624 -14.30532 -14.30532

Beta occ. eigenvalues -- -14.29533 -14.29533 -14.29340 -14.29340 -14.29340

Beta occ. eigenvalues -- -14.29339 -10.24577 -10.24577 -10.24576 -10.24576

Beta occ. eigenvalues -- -10.23969 -10.23969 -10.23967 -10.23967 -10.23635

Beta occ. eigenvalues -- -10.23635 -10.23634 -10.23634 -10.23514 -10.23514

Beta occ. eigenvalues -- -10.23513 -10.23513 -10.20952 -10.20952 -10.20952

Beta occ. eigenvalues -- -10.20952 -10.20860 -10.20860 -10.20859 -10.20859

Beta occ. eigenvalues -- -10.18099 -10.18099 -10.18051 -10.18051 -10.17862

Beta occ. eigenvalues -- -10.17862 -10.17808 -10.17808 -10.17364 -10.17363

Beta occ. eigenvalues -- -10.17320 -10.17320 -10.17184 -10.17184 -10.17134

Beta occ. eigenvalues -- -10.17134 -1.06886 -1.06886 -1.06788 -1.06787

Beta occ. eigenvalues -- -1.06677 -1.06676 -1.06585 -1.06585 -0.99029

Beta occ. eigenvalues -- -0.97669 -0.97654 -0.95097 -0.92637 -0.89089

Beta occ. eigenvalues -- -0.88442 -0.86103 -0.85093 -0.84852 -0.84535

Beta occ. eigenvalues -- -0.84354 -0.77262 -0.76567 -0.76344 -0.76330

Beta occ. eigenvalues -- -0.76181 -0.76152 -0.75653 -0.75636 -0.71970

Beta occ. eigenvalues -- -0.71447 -0.71361 -0.71145 -0.71137 -0.69115

Beta occ. eigenvalues -- -0.68606 -0.67989 -0.67789 -0.67709 -0.67625

Beta occ. eigenvalues -- -0.63082 -0.62984 -0.61571 -0.61386 -0.61204

Beta occ. eigenvalues -- -0.59625 -0.59432 -0.59393 -0.59379 -0.58625

Beta occ. eigenvalues -- -0.56929 -0.56022 -0.55454 -0.55350 -0.55066

Beta occ. eigenvalues -- -0.54932 -0.54772 -0.54395 -0.53764 -0.52763

Beta occ. eigenvalues -- -0.52372 -0.51856 -0.51720 -0.51565 -0.51445

Beta occ. eigenvalues -- -0.50850 -0.50615 -0.50292 -0.50200 -0.48973

Beta occ. eigenvalues -- -0.48657 -0.47601 -0.47517 -0.47020 -0.46930

Beta occ. eigenvalues -- -0.46698 -0.46681 -0.46262 -0.46261 -0.46254

Beta occ. eigenvalues -- -0.46110 -0.46106 -0.44662 -0.44637 -0.44387

Beta occ. eigenvalues -- -0.44304 -0.43753 -0.43499 -0.43478 -0.43302

Beta occ. eigenvalues -- -0.43086 -0.43003 -0.42625 -0.41197 -0.41080

Beta occ. eigenvalues -- -0.40920 -0.40622 -0.40504 -0.40339 -0.39592

Beta occ. eigenvalues -- -0.39215 -0.39110 -0.38236 -0.38035 -0.37951

Beta occ. eigenvalues -- -0.37935 -0.37880 -0.37584 -0.37504 -0.37211

Beta occ. eigenvalues -- -0.36896 -0.35631 -0.35214 -0.34998 -0.34923

Beta occ. eigenvalues -- -0.34167 -0.34134 -0.33887 -0.33776 -0.33290

Beta occ. eigenvalues -- -0.32976 -0.32889 -0.32718 -0.31919 -0.31854

Beta occ. eigenvalues -- -0.31687 -0.30821 -0.30088 -0.29412 -0.28932

Beta occ. eigenvalues -- -0.28909 -0.28717 -0.28041 -0.25765 -0.25472

Beta occ. eigenvalues -- -0.25466 -0.25450 -0.24808 -0.24455 -0.24388

Beta occ. eigenvalues -- -0.24056 -0.23432 -0.22248 -0.20625 -0.20312

Beta occ. eigenvalues -- -0.20194

Beta virt. eigenvalues -- -0.13627 -0.08822 -0.08384 -0.03813 -0.00771

Beta virt. eigenvalues -- 0.00042 0.00241 0.00286 0.02688 0.03366

Beta virt. eigenvalues -- 0.03685 0.03795 0.04973 0.05016 0.05092

Beta virt. eigenvalues -- 0.05333 0.06132 0.06177 0.06414 0.06555

Beta virt. eigenvalues -- 0.06865 0.06895 0.07002 0.07146 0.07924

Beta virt. eigenvalues -- 0.08005 0.09211 0.09273 0.09855 0.11083

Beta virt. eigenvalues -- 0.11203 0.11247 0.11553 0.11671 0.11686

Beta virt. eigenvalues -- 0.11852 0.11952 0.12148 0.12243 0.12370

Beta virt. eigenvalues -- 0.12677 0.12684 0.12790 0.12925 0.13006

Beta virt. eigenvalues -- 0.13243 0.13284 0.13289 0.13363 0.13404

Beta virt. eigenvalues -- 0.13541 0.13887 0.16921 0.16923 0.17077

Beta virt. eigenvalues -- 0.17085 0.18258 0.18560 0.18653 0.18829

Beta virt. eigenvalues -- 0.18837 0.18971 0.19263 0.19598 0.19614

Beta virt. eigenvalues -- 0.20904 0.21019 0.21218 0.21467 0.21827

Beta virt. eigenvalues -- 0.21877 0.21880 0.22606 0.23366 0.23851

Beta virt. eigenvalues -- 0.24701 0.24823 0.24910 0.25343 0.25635

Beta virt. eigenvalues -- 0.25926 0.26172 0.26583 0.26779 0.27003

Beta virt. eigenvalues -- 0.28894 0.28912 0.29904 0.30001 0.30154

Beta virt. eigenvalues -- 0.30182 0.30613 0.31116 0.31268 0.31366

Beta virt. eigenvalues -- 0.32241 0.32446 0.32784 0.32888 0.32984

Beta virt. eigenvalues -- 0.33113 0.33322 0.33373 0.33405 0.33579

Beta virt. eigenvalues -- 0.33848 0.34839 0.35039 0.35094 0.35336

Beta virt. eigenvalues -- 0.35468 0.35807 0.35900 0.36367 0.36845

Beta virt. eigenvalues -- 0.37018 0.37632 0.37735 0.38096 0.38319

Beta virt. eigenvalues -- 0.38330 0.38374 0.38648 0.38689 0.39109

Beta virt. eigenvalues -- 0.39202 0.39431 0.39495 0.39629 0.39876

Beta virt. eigenvalues -- 0.39893 0.40071 0.40106 0.40727 0.41290

Beta virt. eigenvalues -- 0.41413 0.41513 0.42025 0.42342 0.42345

Beta virt. eigenvalues -- 0.42643 0.43224 0.43408 0.43661 0.43682

Beta virt. eigenvalues -- 0.43956 0.44278 0.44452 0.44491 0.44611

Beta virt. eigenvalues -- 0.44659 0.45035 0.45577 0.45627 0.45938

Beta virt. eigenvalues -- 0.46278 0.46497 0.46546 0.47081 0.47699

Beta virt. eigenvalues -- 0.48167 0.48608 0.48801 0.48971 0.49260

Beta virt. eigenvalues -- 0.49476 0.49502 0.49695 0.49762 0.50163

Beta virt. eigenvalues -- 0.50332 0.50404 0.50557 0.50760 0.51044

Beta virt. eigenvalues -- 0.51110 0.51587 0.52029 0.52133 0.52137

Beta virt. eigenvalues -- 0.52272 0.52964 0.52971 0.53098 0.53443

Beta virt. eigenvalues -- 0.54061 0.54346 0.54696 0.54781 0.54803

Beta virt. eigenvalues -- 0.55332 0.55822 0.56117 0.56950 0.57135

Beta virt. eigenvalues -- 0.57184 0.57546 0.58006 0.58049 0.58295

Beta virt. eigenvalues -- 0.58518 0.58562 0.58603 0.58870 0.59156

Beta virt. eigenvalues -- 0.59570 0.59948 0.60077 0.60485 0.61305

Beta virt. eigenvalues -- 0.61465 0.61586 0.61765 0.62156 0.62478

Beta virt. eigenvalues -- 0.62728 0.63049 0.63089 0.63385 0.63404

Beta virt. eigenvalues -- 0.63608 0.63679 0.64035 0.64076 0.64266

Beta virt. eigenvalues -- 0.64356 0.64624 0.64869 0.64878 0.65024

Beta virt. eigenvalues -- 0.65158 0.65350 0.65549 0.65554 0.65660

Beta virt. eigenvalues -- 0.65922 0.67301 0.67447 0.67711 0.68070

Beta virt. eigenvalues -- 0.68879 0.69095 0.69714 0.69785 0.70170

Beta virt. eigenvalues -- 0.70557 0.70561 0.71578 0.72543 0.72611

Beta virt. eigenvalues -- 0.72683 0.72867 0.72872 0.73734 0.73766

Beta virt. eigenvalues -- 0.74752 0.74753 0.75017 0.75867 0.75987

Beta virt. eigenvalues -- 0.76372 0.76427 0.76676 0.78085 0.79063

Beta virt. eigenvalues -- 0.79284 0.79335 0.79356 0.79652 0.80046

Beta virt. eigenvalues -- 0.80440 0.80598 0.80732 0.81039 0.81164

Beta virt. eigenvalues -- 0.81240 0.81728 0.81935 0.81991 0.82659

Beta virt. eigenvalues -- 0.82865 0.83290 0.84410 0.84413 0.85438

Beta virt. eigenvalues -- 0.85627 0.85897 0.85906 0.86550 0.86559

Beta virt. eigenvalues -- 0.87480 0.87626 0.87759 0.88314 0.88744

Beta virt. eigenvalues -- 0.88747 0.90514 0.90574 0.90762 0.92003

Beta virt. eigenvalues -- 0.92623 0.92922 0.93086 0.93133 0.93423

Beta virt. eigenvalues -- 0.93746 0.93955 0.94627 0.95428 0.95835

Beta virt. eigenvalues -- 0.95851 0.96424 0.97028 0.97504 0.97545

Beta virt. eigenvalues -- 0.97725 0.98212 0.98649 0.98740 0.98947

Beta virt. eigenvalues -- 0.99267 0.99748 1.00011 1.00675 1.01424

Beta virt. eigenvalues -- 1.02004 1.02588 1.02614 1.03964 1.04256

Beta virt. eigenvalues -- 1.04903 1.06469 1.07018 1.07699 1.08069

Beta virt. eigenvalues -- 1.08395 1.08705 1.08782 1.09208 1.09476

Beta virt. eigenvalues -- 1.10537 1.11108 1.11412 1.11490 1.11745

Beta virt. eigenvalues -- 1.12141 1.12232 1.12413 1.13717 1.13752

Beta virt. eigenvalues -- 1.14235 1.14243 1.14761 1.15319 1.15791

Beta virt. eigenvalues -- 1.16036 1.16076 1.18587 1.18955 1.18991

Beta virt. eigenvalues -- 1.19258 1.19333 1.19419 1.19807 1.19895

Beta virt. eigenvalues -- 1.20060 1.20756 1.21904 1.22796 1.23715

Beta virt. eigenvalues -- 1.23781 1.23818 1.24088 1.24409 1.24690

Beta virt. eigenvalues -- 1.24723 1.25892 1.26317 1.26361 1.26865

Beta virt. eigenvalues -- 1.27293 1.27423 1.27891 1.27952 1.29643

Beta virt. eigenvalues -- 1.30075 1.31247 1.31739 1.31981 1.32380

Beta virt. eigenvalues -- 1.33546 1.33565 1.33697 1.33717 1.34030

Beta virt. eigenvalues -- 1.34772 1.34803 1.35193 1.35754 1.36411

Beta virt. eigenvalues -- 1.36816 1.37951 1.38188 1.38583 1.38739

Beta virt. eigenvalues -- 1.40576 1.41170 1.41271 1.41941 1.44081

Beta virt. eigenvalues -- 1.44680 1.44898 1.46256 1.46870 1.47184

Beta virt. eigenvalues -- 1.47870 1.48224 1.48246 1.48561 1.50987

Beta virt. eigenvalues -- 1.51242 1.51307 1.51585 1.51754 1.51898

Beta virt. eigenvalues -- 1.52087 1.52091 1.52244 1.52394 1.52397

Beta virt. eigenvalues -- 1.52433 1.52667 1.52691 1.52771 1.52816

Beta virt. eigenvalues -- 1.52831 1.53150 1.53749 1.53961 1.54053

Beta virt. eigenvalues -- 1.54482 1.54636 1.55538 1.56087 1.56163

Beta virt. eigenvalues -- 1.57058 1.57441 1.57521 1.58279 1.59206

Beta virt. eigenvalues -- 1.59317 1.59417 1.59553 1.59830 1.60053

Beta virt. eigenvalues -- 1.60296 1.61369 1.61642 1.61778 1.61870

Beta virt. eigenvalues -- 1.61976 1.63388 1.63400 1.64907 1.66213

Beta virt. eigenvalues -- 1.66622 1.66987 1.67409 1.68226 1.68367

Beta virt. eigenvalues -- 1.68670 1.68824 1.69102 1.69332 1.69662

Beta virt. eigenvalues -- 1.70667 1.71312 1.71941 1.72060 1.72416

Beta virt. eigenvalues -- 1.73261 1.73365 1.73477 1.74602 1.75030

Beta virt. eigenvalues -- 1.75216 1.75329 1.77195 1.77256 1.78366

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Beta virt. eigenvalues -- 1.80391 1.80445 1.80537 1.80727 1.81280

Beta virt. eigenvalues -- 1.81859 1.81947 1.82843 1.84266 1.84425

Beta virt. eigenvalues -- 1.84532 1.84713 1.85733 1.87676 1.87860

Beta virt. eigenvalues -- 1.88222 1.88821 1.88909 1.89803 1.90111

Beta virt. eigenvalues -- 1.90524 1.90669 1.90742 1.90784 1.91001

Beta virt. eigenvalues -- 1.91736 1.91740 1.92012 1.95092 1.96111

Beta virt. eigenvalues -- 1.96180 1.96376 1.96870 1.97428 1.98045

Beta virt. eigenvalues -- 1.98412 1.98951 1.99986 2.00330 2.00401

Beta virt. eigenvalues -- 2.01460 2.01602 2.02258 2.02694 2.03594

Beta virt. eigenvalues -- 2.05198 2.07628 2.08810 2.08825 2.09159

Beta virt. eigenvalues -- 2.10377 2.11046 2.11183 2.12690 2.13895

Beta virt. eigenvalues -- 2.14679 2.15315 2.15734 2.15777 2.16432

Beta virt. eigenvalues -- 2.17010 2.19310 2.20277 2.21536 2.23299

Beta virt. eigenvalues -- 2.23791 2.24751 2.25446 2.25506 2.25670

Beta virt. eigenvalues -- 2.26154 2.26269 2.26347 2.26870 2.27972

Beta virt. eigenvalues -- 2.28216 2.28254 2.28852 2.29984 2.30018

Beta virt. eigenvalues -- 2.30978 2.32234 2.32773 2.33613 2.33686

Beta virt. eigenvalues -- 2.34082 2.34113 2.34195 2.34228 2.34379

Beta virt. eigenvalues -- 2.34573 2.34599 2.34605 2.34759 2.35090

Beta virt. eigenvalues -- 2.35495 2.35876 2.36052 2.36606 2.39858

Beta virt. eigenvalues -- 2.40417 2.40736 2.40985 2.41339 2.41403

Beta virt. eigenvalues -- 2.42560 2.42861 2.43074 2.43437 2.43897

Beta virt. eigenvalues -- 2.44032 2.44236 2.44505 2.47441 2.48623

Beta virt. eigenvalues -- 2.48731 2.49694 2.50437 2.50765 2.50928

Beta virt. eigenvalues -- 2.50930 2.51034 2.51697 2.52223 2.52534

Beta virt. eigenvalues -- 2.54456 2.54819 2.56541 2.57366 2.57641

Beta virt. eigenvalues -- 2.59119 2.59193 2.60938 2.61825 2.62493

Beta virt. eigenvalues -- 2.64719 2.64946 2.65268 2.65731 2.66279

Beta virt. eigenvalues -- 2.67366 2.67683 2.67737 2.67960 2.68649

Beta virt. eigenvalues -- 2.68799 2.71549 2.72949 2.73139 2.73321

Beta virt. eigenvalues -- 2.74926 2.74987 2.75278 2.75743 2.78846

Beta virt. eigenvalues -- 2.79161 2.79226 2.79735 2.80302 2.80451

Beta virt. eigenvalues -- 2.80575 2.81331 2.81519 2.81620 2.81678

Beta virt. eigenvalues -- 2.82987 2.83050 2.83367 2.84198 2.85516

Beta virt. eigenvalues -- 2.85638 2.86385 2.86521 2.86525 2.86641

Beta virt. eigenvalues -- 2.86816 2.87330 2.87647 2.88663 2.88743

Beta virt. eigenvalues -- 2.88891 2.91638 2.92130 2.94131 2.94370

Beta virt. eigenvalues -- 2.94828 2.95600 2.95797 2.95844 2.95948

Beta virt. eigenvalues -- 2.97171 2.98731 2.99585 2.99625 3.00572

Beta virt. eigenvalues -- 3.00731 3.01079 3.01186 3.01797 3.02806

Beta virt. eigenvalues -- 3.02936 3.03673 3.05374 3.06257 3.06426

Beta virt. eigenvalues -- 3.06720 3.07781 3.07817 3.09241 3.11841

Beta virt. eigenvalues -- 3.13615 3.13633 3.13699 3.13704 3.14762

Beta virt. eigenvalues -- 3.14842 3.14850 3.15317 3.15344 3.15860

Beta virt. eigenvalues -- 3.16726 3.16813 3.17680 3.17794 3.17913

Beta virt. eigenvalues -- 3.18050 3.19047 3.19579 3.20116 3.20374

Beta virt. eigenvalues -- 3.20498 3.20548 3.20786 3.20806 3.21232

Beta virt. eigenvalues -- 3.21318 3.21345 3.21509 3.21798 3.22034

Beta virt. eigenvalues -- 3.22623 3.22968 3.24962 3.25010 3.26677

Beta virt. eigenvalues -- 3.28095 3.28769 3.28797 3.28807 3.29118

Beta virt. eigenvalues -- 3.29398 3.30015 3.30219 3.31304 3.31323

Beta virt. eigenvalues -- 3.32706 3.33007 3.35656 3.36585 3.36834

Beta virt. eigenvalues -- 3.37370 3.37608 3.40421 3.40422 3.41008

Beta virt. eigenvalues -- 3.41286 3.41393 3.41600 3.41647 3.43018

Beta virt. eigenvalues -- 3.45812 3.47221 3.47247 3.48828 3.55925

Beta virt. eigenvalues -- 3.60087 3.60738 3.61181 3.61806 3.61928

Beta virt. eigenvalues -- 3.63416 3.67369 3.67522 3.68494 3.68755

Beta virt. eigenvalues -- 3.75150 3.76662 3.77012 3.77052 3.77357

Beta virt. eigenvalues -- 3.78357 3.79096 3.79799 3.82001 3.84398

Beta virt. eigenvalues -- 3.84540 3.84817 3.87938 3.90754 3.90873

Beta virt. eigenvalues -- 3.91808 3.92973 3.96129 3.96886 3.96981

Beta virt. eigenvalues -- 3.97537 3.98548 3.98588 3.99061 3.99320

Beta virt. eigenvalues -- 4.01294 4.01448 4.01837 4.01871 4.11503

Beta virt. eigenvalues -- 4.14259 4.14748 4.17153 4.17781 4.17781

Beta virt. eigenvalues -- 4.19161 4.21233 4.22152 4.22544 4.24301

Beta virt. eigenvalues -- 4.26153 4.36319 4.42352 4.43029 4.44098

Beta virt. eigenvalues -- 4.48538 4.52925 4.56204 4.60759 4.82165

Beta virt. eigenvalues -- 4.82245 4.82326 4.82391 4.87989 4.88333

Beta virt. eigenvalues -- 4.88369 4.88875 4.89361 4.89696 4.89696

Beta virt. eigenvalues -- 4.89891 5.12252 5.12941 5.12999 5.17356

Beta virt. eigenvalues -- 5.21101 5.26038 5.26279 5.26303 5.26689

Beta virt. eigenvalues -- 5.29793 5.29808 5.29918 5.30376 5.37151

Beta virt. eigenvalues -- 5.37759 5.54031 5.67577 5.69034 5.69068

Beta virt. eigenvalues -- 5.69421 5.75919 5.76182 5.76367 5.76932

Beta virt. eigenvalues -- 7.80575 7.83678 7.88330 7.94746 8.19169

Beta virt. eigenvalues -- 11.15103 23.34500 23.37265 23.38127 23.39583

Beta virt. eigenvalues -- 23.44448 23.44703 23.44845 23.45337 23.45469

Beta virt. eigenvalues -- 23.45790 23.45881 23.45976 23.76857 23.77935

Beta virt. eigenvalues -- 23.79942 23.80766 23.82213 23.82272 23.84218

Beta virt. eigenvalues -- 23.84235 23.86418 23.86867 23.88605 23.89699

Beta virt. eigenvalues -- 23.90357 23.91101 23.91536 23.92044 24.01823

Beta virt. eigenvalues -- 24.01861 24.02415 24.02468 24.03960 24.03966

Beta virt. eigenvalues -- 24.04989 24.05216 24.11010 24.11044 24.11534

Beta virt. eigenvalues -- 24.11610 35.58482 35.61494 35.61734 35.62403

Beta virt. eigenvalues -- 35.71110 35.72026 35.72085 35.72095 49.91788

Beta virt. eigenvalues -- 49.92176 49.92229 49.92455 49.92653 49.92960

Beta virt. eigenvalues -- 49.93037 49.93223

Condensed to atoms (all electrons):

Atomic-Atomic Spin Densities.

Mulliken charges and spin densities:

1 2

1 C 0.373141 0.226696

2 N -0.672333 -0.074651

3 C 0.373125 0.226681

4 C -0.099518 -0.003841

5 C -0.099520 -0.003853

6 N -0.359626 0.005163

7 C 0.392871 0.098981

8 N -0.709117 0.054755

9 C 0.392856 0.098998

10 C -0.087387 -0.018061

11 C -0.087383 -0.018045

12 N -0.359636 0.005136

13 C -0.087388 -0.018062

14 C -0.087385 -0.018045

15 C 0.392873 0.098980

16 N -0.709117 0.054754

17 C 0.392862 0.098999

18 N -0.359638 0.005165

19 N -0.672334 -0.074651

20 C 0.373127 0.226685

21 C -0.099517 -0.003841

22 C -0.099523 -0.003852

23 C 0.373142 0.226692

24 N -0.359630 0.005140

25 Zn 1.410968 -0.000506

26 C 0.205330 0.029810

27 C -0.295150 0.022834

28 C -0.295147 0.022851

29 C 0.205315 0.029797

30 C 0.205019 0.055059

31 C -0.311922 0.073385

32 C -0.311938 0.073396

33 C 0.205005 0.055052

34 C 0.205313 0.029797

35 C -0.295147 0.022851

36 C -0.295148 0.022835

37 C 0.205329 0.029810

38 C 0.205018 0.055060

39 C -0.311924 0.073384

40 C -0.311939 0.073397

41 C 0.205006 0.055052

42 H 0.260290 -0.001438

43 H 0.260289 -0.001437

44 H 0.255640 -0.004521

45 H 0.255630 -0.004520

46 H 0.260291 -0.001437

47 H 0.260288 -0.001438

48 H 0.255640 -0.004521

49 H 0.255629 -0.004520

50 O -0.311656 0.015496

51 O -0.311650 0.015496

52 O -0.311377 0.008773

53 O -0.311387 0.008775

54 O -0.311655 0.015495

55 O -0.311656 0.015495

56 O -0.311379 0.008773

57 O -0.311386 0.008775

58 C -0.500174 -0.001688

59 H 0.229100 0.001618

60 H 0.229003 0.001421

61 H 0.251483 -0.000095

62 C -0.500441 -0.000860

63 H 0.230847 0.000765

64 H 0.230640 0.000615

65 H 0.251919 -0.000033

66 C -0.500411 -0.000861

67 H 0.230635 0.000615

68 H 0.230844 0.000766

69 H 0.251905 -0.000033

70 C -0.500174 -0.001688

71 H 0.228994 0.001421

72 H 0.229103 0.001618

73 H 0.251484 -0.000095

74 C -0.500421 -0.000861

75 H 0.230636 0.000615

76 H 0.230845 0.000766

77 H 0.251912 -0.000033

78 C -0.500438 -0.000860

79 H 0.230846 0.000765

80 H 0.230639 0.000615

81 H 0.251919 -0.000033

82 C -0.500174 -0.001688

83 H 0.229099 0.001618

84 H 0.229003 0.001421

85 H 0.251483 -0.000095

86 C -0.500164 -0.001688

87 H 0.228994 0.001421

88 H 0.229103 0.001618

89 H 0.251478 -0.000095

Sum of Mulliken charges = 0.00000 2.00000

Mulliken charges and spin densities with hydrogens summed into heavy atoms:

1 2

1 C 0.373141 0.226696

2 N -0.672333 -0.074651

3 C 0.373125 0.226681

4 C -0.099518 -0.003841

5 C -0.099520 -0.003853

6 N -0.359626 0.005163

7 C 0.392871 0.098981

8 N -0.709117 0.054755

9 C 0.392856 0.098998

10 C -0.087387 -0.018061

11 C -0.087383 -0.018045

12 N -0.359636 0.005136

13 C -0.087388 -0.018062

14 C -0.087385 -0.018045

15 C 0.392873 0.098980

16 N -0.709117 0.054754

17 C 0.392862 0.098999

18 N -0.359638 0.005165

19 N -0.672334 -0.074651

20 C 0.373127 0.226685

21 C -0.099517 -0.003841

22 C -0.099523 -0.003852

23 C 0.373142 0.226692

24 N -0.359630 0.005140

25 Zn 1.410968 -0.000506

26 C 0.205330 0.029810

27 C -0.034860 0.021397

28 C -0.034858 0.021413

29 C 0.205315 0.029797

30 C 0.205019 0.055059

31 C -0.056293 0.068865

32 C -0.056298 0.068875

33 C 0.205005 0.055052

34 C 0.205313 0.029797

35 C -0.034857 0.021413

36 C -0.034859 0.021398

37 C 0.205329 0.029810

38 C 0.205018 0.055060

39 C -0.056294 0.068864

40 C -0.056298 0.068876

41 C 0.205006 0.055052

50 O -0.311656 0.015496

51 O -0.311650 0.015496

52 O -0.311377 0.008773

53 O -0.311387 0.008775

54 O -0.311655 0.015495

55 O -0.311656 0.015495

56 O -0.311379 0.008773

57 O -0.311386 0.008775

58 C 0.209411 0.001256

62 C 0.212964 0.000486

66 C 0.212974 0.000486

70 C 0.209407 0.001256

74 C 0.212972 0.000486

78 C 0.212967 0.000486

82 C 0.209411 0.001256

86 C 0.209410 0.001256

Electronic spatial extent (au): <R\*\*2>= 44350.3567

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0001 Y= 0.0000 Z= 0.4980 Tot= 0.4980

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -173.9323 YY= -204.2616 ZZ= -331.9083

XY= 0.0212 XZ= -0.0010 YZ= 0.0007

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 62.7684 YY= 32.4392 ZZ= -95.2076

XY= 0.0212 XZ= -0.0010 YZ= 0.0007

Octapole moment (field-independent basis, Debye-Ang\*\*2):

XXX= -0.0089 YYY= 0.0046 ZZZ= -16.3235 XYY= -0.0022

XXY= 0.0002 XXZ= -56.5601 XZZ= 0.0048 YZZ= -0.0036

YYZ= 148.8632 XYZ= -0.1473

Hexadecapole moment (field-independent basis, Debye-Ang\*\*3):

XXXX= -19416.8334 YYYY= -20555.9699 ZZZZ= -819.0200 XXXY= 0.0042

XXXZ= -0.0860 YYYX= 1.3190 YYYZ= -0.0177 ZZZX= 0.0029

ZZZY= 0.0039 XXYY= -6413.8960 XXZZ= -5134.6924 YYZZ= -4983.2480

XXYZ= 0.0692 YYXZ= 0.0396 ZZXY= -0.0639

N-N= 8.041874561667D+03 E-N=-2.236246719581D+04 KE= 2.690146913247D+03

Isotropic Fermi Contact Couplings

Atom a.u. MegaHertz Gauss 10(-4) cm-1

1 C(13) 0.01549 8.70623 3.10660 2.90408

2 N(14) -0.01460 -2.35930 -0.84186 -0.78698

3 C(13) 0.01549 8.70542 3.10631 2.90381

4 C(13) -0.00768 -4.31918 -1.54119 -1.44072

5 C(13) -0.00769 -4.32037 -1.54161 -1.44112

6 N(14) -0.00025 -0.04017 -0.01433 -0.01340

7 C(13) 0.00615 3.45464 1.23270 1.15235

8 N(14) 0.00533 0.86064 0.30710 0.28708

9 C(13) 0.00615 3.45841 1.23405 1.15360

10 C(13) -0.00442 -2.48232 -0.88575 -0.82801

11 C(13) -0.00441 -2.48109 -0.88531 -0.82760

12 N(14) -0.00025 -0.04065 -0.01450 -0.01356

13 C(13) -0.00442 -2.48232 -0.88575 -0.82801

14 C(13) -0.00441 -2.48108 -0.88531 -0.82760

15 C(13) 0.00615 3.45443 1.23263 1.15227

16 N(14) 0.00533 0.86058 0.30708 0.28706

17 C(13) 0.00615 3.45784 1.23384 1.15341

18 N(14) -0.00025 -0.04021 -0.01435 -0.01341

19 N(14) -0.01460 -2.35934 -0.84187 -0.78699

20 C(13) 0.01549 8.70565 3.10639 2.90389

21 C(13) -0.00768 -4.31923 -1.54121 -1.44074

22 C(13) -0.00769 -4.32031 -1.54159 -1.44110

23 C(13) 0.01549 8.70598 3.10651 2.90400

24 N(14) -0.00025 -0.04020 -0.01434 -0.01341

25 Zn(67) 0.00000 0.00000 0.00000 0.00000

26 C(13) 0.00083 0.46630 0.16639 0.15554

27 C(13) -0.00027 -0.15050 -0.05370 -0.05020

28 C(13) -0.00027 -0.14958 -0.05337 -0.04989

29 C(13) 0.00083 0.46541 0.16607 0.15524

30 C(13) -0.00040 -0.22481 -0.08022 -0.07499

31 C(13) 0.00026 0.14575 0.05201 0.04862

32 C(13) 0.00026 0.14651 0.05228 0.04887

33 C(13) -0.00040 -0.22549 -0.08046 -0.07522

34 C(13) 0.00083 0.46542 0.16607 0.15525

35 C(13) -0.00027 -0.14959 -0.05338 -0.04990

36 C(13) -0.00027 -0.15048 -0.05369 -0.05019

37 C(13) 0.00083 0.46629 0.16638 0.15554

38 C(13) -0.00040 -0.22477 -0.08020 -0.07498

39 C(13) 0.00026 0.14571 0.05199 0.04860

40 C(13) 0.00026 0.14653 0.05229 0.04888

41 C(13) -0.00040 -0.22552 -0.08047 -0.07523

42 H(1) -0.00041 -0.90590 -0.32325 -0.30218

43 H(1) -0.00041 -0.90536 -0.32306 -0.30200

44 H(1) -0.00125 -2.78955 -0.99538 -0.93049

45 H(1) -0.00125 -2.78902 -0.99519 -0.93032

46 H(1) -0.00041 -0.90534 -0.32305 -0.30199

47 H(1) -0.00041 -0.90590 -0.32325 -0.30218

48 H(1) -0.00125 -2.78954 -0.99538 -0.93049

49 H(1) -0.00125 -2.78904 -0.99520 -0.93032

50 O(17) 0.00265 -0.80450 -0.28707 -0.26835

51 O(17) 0.00265 -0.80450 -0.28706 -0.26835

52 O(17) 0.00165 -0.49886 -0.17801 -0.16640

53 O(17) 0.00165 -0.49914 -0.17811 -0.16649

54 O(17) 0.00265 -0.80450 -0.28707 -0.26835

55 O(17) 0.00265 -0.80449 -0.28706 -0.26835

56 O(17) 0.00165 -0.49888 -0.17801 -0.16641

57 O(17) 0.00165 -0.49908 -0.17809 -0.16648

58 C(13) -0.00044 -0.24873 -0.08875 -0.08297

59 H(1) 0.00013 0.28261 0.10084 0.09427

60 H(1) 0.00010 0.23201 0.08279 0.07739

61 H(1) -0.00004 -0.08191 -0.02923 -0.02732

62 C(13) -0.00025 -0.14184 -0.05061 -0.04731

63 H(1) 0.00013 0.30067 0.10729 0.10029

64 H(1) 0.00007 0.15633 0.05578 0.05215

65 H(1) -0.00001 -0.02847 -0.01016 -0.00950

66 C(13) -0.00025 -0.14189 -0.05063 -0.04733

67 H(1) 0.00007 0.15645 0.05583 0.05219

68 H(1) 0.00013 0.30094 0.10738 0.10038

69 H(1) -0.00001 -0.02845 -0.01015 -0.00949

70 C(13) -0.00044 -0.24874 -0.08876 -0.08297

71 H(1) 0.00010 0.23200 0.08278 0.07739

72 H(1) 0.00013 0.28271 0.10088 0.09430

73 H(1) -0.00004 -0.08190 -0.02922 -0.02732

74 C(13) -0.00025 -0.14189 -0.05063 -0.04733

75 H(1) 0.00007 0.15644 0.05582 0.05218

76 H(1) 0.00013 0.30091 0.10737 0.10037

77 H(1) -0.00001 -0.02846 -0.01015 -0.00949

78 C(13) -0.00025 -0.14185 -0.05061 -0.04731

79 H(1) 0.00013 0.30068 0.10729 0.10030

80 H(1) 0.00007 0.15636 0.05579 0.05216

81 H(1) -0.00001 -0.02847 -0.01016 -0.00950

82 C(13) -0.00044 -0.24872 -0.08875 -0.08296

83 H(1) 0.00013 0.28259 0.10084 0.09426

84 H(1) 0.00010 0.23201 0.08279 0.07739

85 H(1) -0.00004 -0.08191 -0.02923 -0.02732

86 C(13) -0.00044 -0.24873 -0.08875 -0.08297

87 H(1) 0.00010 0.23201 0.08279 0.07739

88 H(1) 0.00013 0.28273 0.10088 0.09431

89 H(1) -0.00004 -0.08190 -0.02922 -0.02732

--------------------------------------------------------

Center ---- Spin Dipole Couplings ----

3XX-RR 3YY-RR 3ZZ-RR

--------------------------------------------------------

1 Atom -0.148106 -0.130754 0.278860

2 Atom 0.065169 0.051679 -0.116848

3 Atom -0.148088 -0.130757 0.278845

4 Atom -0.013320 -0.000929 0.014249

5 Atom -0.013310 -0.000929 0.014239

6 Atom -0.031341 -0.022372 0.053713

7 Atom -0.064681 -0.058932 0.123612

8 Atom -0.077370 -0.070552 0.147922

9 Atom -0.064691 -0.058939 0.123630

10 Atom 0.010263 0.004552 -0.014815

11 Atom 0.010254 0.004547 -0.014801

12 Atom -0.031312 -0.022351 0.053663

13 Atom 0.010264 0.004552 -0.014815

14 Atom 0.010254 0.004547 -0.014801

15 Atom -0.064679 -0.058930 0.123610

16 Atom -0.077370 -0.070552 0.147922

17 Atom -0.064692 -0.058940 0.123631

18 Atom -0.031345 -0.022377 0.053722

19 Atom 0.065169 0.051678 -0.116847

20 Atom -0.148092 -0.130762 0.278854

21 Atom -0.013320 -0.000929 0.014249

22 Atom -0.013311 -0.000930 0.014240

23 Atom -0.148103 -0.130747 0.278850

24 Atom -0.031313 -0.022351 0.053664

25 Atom 0.014562 -0.011353 -0.003209

26 Atom -0.015786 -0.018897 0.034683

27 Atom -0.013449 -0.014832 0.028281

28 Atom -0.013456 -0.014841 0.028297

29 Atom -0.015776 -0.018894 0.034670

30 Atom -0.035674 -0.026117 0.061791

31 Atom -0.045732 -0.039570 0.085302

32 Atom -0.045736 -0.039577 0.085312

33 Atom -0.035664 -0.026123 0.061787

34 Atom -0.015776 -0.018894 0.034670

35 Atom -0.013456 -0.014841 0.028297

36 Atom -0.013449 -0.014832 0.028281

37 Atom -0.015786 -0.018897 0.034683

38 Atom -0.035674 -0.026119 0.061793

39 Atom -0.045732 -0.039569 0.085301

40 Atom -0.045736 -0.039578 0.085314

41 Atom -0.035664 -0.026122 0.061786

42 Atom 0.002911 -0.001703 -0.001208

43 Atom 0.002916 -0.001708 -0.001208

44 Atom -0.004710 0.006544 -0.001833

45 Atom -0.004693 0.006526 -0.001834

46 Atom 0.002916 -0.001708 -0.001208

47 Atom 0.002911 -0.001703 -0.001208

48 Atom -0.004710 0.006544 -0.001834

49 Atom -0.004693 0.006526 -0.001834

50 Atom -0.042888 -0.036752 0.079640

51 Atom -0.042880 -0.036765 0.079644

52 Atom -0.021853 -0.024747 0.046600

53 Atom -0.021856 -0.024759 0.046615

54 Atom -0.042878 -0.036763 0.079641

55 Atom -0.042888 -0.036751 0.079639

56 Atom -0.021853 -0.024747 0.046600

57 Atom -0.021856 -0.024759 0.046615

58 Atom 0.001333 0.000465 -0.001799

59 Atom 0.001048 0.000114 -0.001163

60 Atom 0.001053 0.000681 -0.001734

61 Atom 0.001321 -0.000032 -0.001289

62 Atom 0.001117 0.000300 -0.001417

63 Atom 0.000709 0.000156 -0.000865

64 Atom 0.000851 0.000157 -0.001008

65 Atom 0.000666 0.000358 -0.001025

66 Atom 0.001121 0.000296 -0.001417

67 Atom 0.000854 0.000154 -0.001008

68 Atom 0.000711 0.000153 -0.000865

69 Atom 0.000669 0.000356 -0.001025

70 Atom 0.001340 0.000459 -0.001799

71 Atom 0.001059 0.000674 -0.001733

72 Atom 0.001054 0.000110 -0.001164

73 Atom 0.001325 -0.000036 -0.001289

74 Atom 0.001121 0.000296 -0.001417

75 Atom 0.000854 0.000154 -0.001008

76 Atom 0.000711 0.000153 -0.000865

77 Atom 0.000669 0.000356 -0.001025

78 Atom 0.001117 0.000300 -0.001417

79 Atom 0.000709 0.000156 -0.000865

80 Atom 0.000851 0.000157 -0.001008

81 Atom 0.000666 0.000358 -0.001025

82 Atom 0.001333 0.000465 -0.001799

83 Atom 0.001049 0.000115 -0.001163

84 Atom 0.001053 0.000681 -0.001734

85 Atom 0.001321 -0.000032 -0.001289

86 Atom 0.001340 0.000459 -0.001799

87 Atom 0.001059 0.000674 -0.001733

88 Atom 0.001054 0.000110 -0.001163

89 Atom 0.001325 -0.000036 -0.001289

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XY XZ YZ

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1 Atom 0.000940 0.013320 -0.081747

2 Atom 0.000009 -0.000013 0.033463

3 Atom -0.000955 -0.013264 -0.081747

4 Atom 0.001167 -0.000089 -0.003239

5 Atom -0.001188 0.000093 -0.003235

6 Atom 0.001535 -0.020057 -0.023358

7 Atom -0.000049 0.013141 0.009372

8 Atom -0.000007 0.023658 0.000005

9 Atom 0.000035 0.013158 -0.009400

10 Atom -0.000622 -0.002815 0.000487

11 Atom 0.000632 -0.002810 -0.000488

12 Atom -0.001544 0.020085 -0.023309

13 Atom -0.000622 0.002813 -0.000487

14 Atom 0.000632 0.002810 0.000487

15 Atom -0.000049 -0.013143 -0.009370

16 Atom -0.000007 -0.023657 -0.000007

17 Atom 0.000035 -0.013152 0.009398

18 Atom 0.001534 0.020054 0.023358

19 Atom 0.000009 0.000018 -0.033464

20 Atom -0.000957 0.013256 0.081745

21 Atom 0.001166 0.000085 0.003239

22 Atom -0.001189 -0.000096 0.003236

23 Atom 0.000938 -0.013328 0.081758

24 Atom -0.001548 -0.020091 0.023314

25 Atom 0.000024 0.000000 0.000000

26 Atom 0.001018 -0.003035 0.000491

27 Atom 0.000335 -0.004016 -0.000058

28 Atom -0.000333 -0.004016 0.000059

29 Atom -0.001013 -0.003033 -0.000485

30 Atom 0.001730 -0.001332 0.018694

31 Atom 0.000441 -0.000252 0.027654

32 Atom -0.000452 0.000200 0.027655

33 Atom -0.001747 0.001298 0.018691

34 Atom -0.001013 0.003033 0.000482

35 Atom -0.000333 0.004018 -0.000061

36 Atom 0.000335 0.004018 0.000056

37 Atom 0.001018 0.003038 -0.000496

38 Atom 0.001732 0.001324 -0.018692

39 Atom 0.000443 0.000242 -0.027653

40 Atom -0.000450 -0.000209 -0.027654

41 Atom -0.001746 -0.001304 -0.018691

42 Atom 0.001594 -0.000368 -0.000137

43 Atom -0.001585 -0.000369 0.000136

44 Atom 0.004735 0.000964 0.001778

45 Atom -0.004755 -0.000968 0.001776

46 Atom -0.001585 0.000368 -0.000136

47 Atom 0.001594 0.000368 0.000137

48 Atom 0.004735 -0.000964 -0.001778

49 Atom -0.004755 0.000967 -0.001776

50 Atom 0.003133 -0.002773 -0.022390

51 Atom -0.003141 0.002795 -0.022385

52 Atom 0.001391 -0.000859 0.001537

53 Atom -0.001386 -0.000860 -0.001563

54 Atom -0.003143 -0.002804 0.022386

55 Atom 0.003132 0.002765 0.022390

56 Atom 0.001391 0.000860 -0.001541

57 Atom -0.001386 0.000861 0.001555

58 Atom 0.001725 0.000341 0.000402

59 Atom 0.001440 0.001142 0.001040

60 Atom 0.001775 -0.000382 -0.000218

61 Atom 0.001186 0.000275 0.000262

62 Atom 0.000961 -0.000181 -0.000065

63 Atom 0.000777 -0.000529 -0.000352

64 Atom 0.000807 0.000288 0.000303

65 Atom 0.000802 -0.000177 -0.000019

66 Atom -0.000960 -0.000181 0.000065

67 Atom -0.000806 0.000288 -0.000303

68 Atom -0.000776 -0.000529 0.000351

69 Atom -0.000801 -0.000178 0.000019

70 Atom -0.001723 -0.000341 0.000401

71 Atom -0.001773 0.000383 -0.000218

72 Atom -0.001439 -0.001144 0.001038

73 Atom -0.001184 -0.000276 0.000261

74 Atom -0.000960 0.000181 -0.000065

75 Atom -0.000806 -0.000288 0.000303

76 Atom -0.000776 0.000529 -0.000351

77 Atom -0.000801 0.000178 -0.000019

78 Atom 0.000961 0.000181 0.000065

79 Atom 0.000777 0.000529 0.000352

80 Atom 0.000807 -0.000287 -0.000303

81 Atom 0.000802 0.000177 0.000019

82 Atom 0.001725 -0.000341 -0.000402

83 Atom 0.001440 -0.001142 -0.001040

84 Atom 0.001775 0.000382 0.000218

85 Atom 0.001187 -0.000275 -0.000261

86 Atom -0.001723 0.000342 -0.000402

87 Atom -0.001773 -0.000383 0.000217

88 Atom -0.001439 0.001144 -0.001038

89 Atom -0.001184 0.000276 -0.000261

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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 -0.1511 -20.270 -7.233 -6.761 0.8001 -0.5842 -0.1359

1 C(13) Bbb -0.1439 -19.309 -6.890 -6.441 0.5991 0.7894 0.1338

Bcc 0.2949 39.579 14.123 13.202 0.0291 -0.1884 0.9817

Baa -0.1232 -4.753 -1.696 -1.586 0.0001 -0.1879 0.9822

2 N(14) Bbb 0.0581 2.240 0.799 0.747 -0.0008 0.9822 0.1879

Bcc 0.0652 2.513 0.897 0.838 1.0000 0.0008 0.0001

Baa -0.1510 -20.269 -7.232 -6.761 0.7990 0.5857 0.1360

3 C(13) Bbb -0.1439 -19.308 -6.890 -6.440 -0.6006 0.7883 0.1336

Bcc 0.2949 39.577 14.122 13.201 -0.0290 -0.1884 0.9817

Baa -0.0134 -1.802 -0.643 -0.601 0.9955 -0.0949 -0.0079

4 C(13) Bbb -0.0015 -0.199 -0.071 -0.066 0.0946 0.9750 0.2012

Bcc 0.0149 2.001 0.714 0.668 -0.0114 -0.2011 0.9795

Baa -0.0134 -1.801 -0.643 -0.601 0.9953 0.0967 0.0080

5 C(13) Bbb -0.0015 -0.198 -0.071 -0.066 -0.0963 0.9748 0.2012

Bcc 0.0149 2.000 0.714 0.667 0.0117 -0.2010 0.9795

Baa -0.0372 -1.436 -0.512 -0.479 0.8866 0.3616 0.2884

6 N(14) Bbb -0.0271 -1.047 -0.374 -0.349 -0.4160 0.8960 0.1556

Bcc 0.0644 2.483 0.886 0.828 -0.2021 -0.2580 0.9448

Baa -0.0657 -8.812 -3.144 -2.939 0.9911 0.1105 -0.0743

7 C(13) Bbb -0.0593 -7.961 -2.841 -2.656 -0.1138 0.9926 -0.0427

Bcc 0.1250 16.774 5.985 5.595 0.0690 0.0507 0.9963

Baa -0.0798 -3.079 -1.099 -1.027 0.9946 0.0008 -0.1033

8 N(14) Bbb -0.0706 -2.721 -0.971 -0.908 -0.0008 1.0000 0.0001

Bcc 0.1504 5.800 2.070 1.935 0.1033 0.0000 0.9946

Baa -0.0657 -8.814 -3.145 -2.940 0.9913 -0.1087 -0.0743

9 C(13) Bbb -0.0593 -7.963 -2.841 -2.656 0.1121 0.9928 0.0429

Bcc 0.1250 16.777 5.986 5.596 0.0691 -0.0509 0.9963

Baa -0.0151 -2.031 -0.725 -0.677 0.1096 -0.0211 0.9938

10 C(13) Bbb 0.0045 0.602 0.215 0.201 0.1112 0.9938 0.0088

Bcc 0.0106 1.429 0.510 0.477 0.9877 -0.1096 -0.1113

Baa -0.0151 -2.029 -0.724 -0.677 0.1095 0.0211 0.9938

11 C(13) Bbb 0.0045 0.601 0.214 0.201 -0.1129 0.9936 -0.0087

Bcc 0.0106 1.428 0.510 0.476 0.9876 0.1113 -0.1112

Baa -0.0372 -1.435 -0.512 -0.479 0.8872 -0.3601 -0.2884

12 N(14) Bbb -0.0271 -1.046 -0.373 -0.349 0.4146 0.8966 0.1556

Bcc 0.0643 2.481 0.885 0.828 0.2026 -0.2577 0.9448

Baa -0.0151 -2.031 -0.725 -0.678 -0.1095 0.0211 0.9938

13 C(13) Bbb 0.0045 0.602 0.215 0.201 0.1113 0.9938 -0.0088

Bcc 0.0106 1.429 0.510 0.477 0.9877 -0.1096 0.1112

Baa -0.0151 -2.029 -0.724 -0.677 -0.1095 -0.0211 0.9938

14 C(13) Bbb 0.0045 0.601 0.214 0.201 -0.1129 0.9936 0.0087

Bcc 0.0106 1.428 0.510 0.476 0.9876 0.1112 0.1112

Baa -0.0657 -8.812 -3.144 -2.939 0.9911 0.1104 0.0743

15 C(13) Bbb -0.0593 -7.961 -2.841 -2.656 -0.1138 0.9926 0.0427

Bcc 0.1250 16.773 5.985 5.595 -0.0690 -0.0507 0.9963

Baa -0.0798 -3.079 -1.099 -1.027 0.9946 0.0008 0.1033

16 N(14) Bbb -0.0706 -2.721 -0.971 -0.908 -0.0008 1.0000 -0.0001

Bcc 0.1504 5.800 2.070 1.935 -0.1033 0.0000 0.9946

Baa -0.0657 -8.814 -3.145 -2.940 0.9913 -0.1087 0.0743

17 C(13) Bbb -0.0593 -7.963 -2.841 -2.656 0.1121 0.9928 -0.0429

Bcc 0.1250 16.777 5.986 5.596 -0.0691 0.0509 0.9963

Baa -0.0372 -1.436 -0.513 -0.479 0.8866 0.3616 -0.2883

18 N(14) Bbb -0.0271 -1.047 -0.374 -0.349 -0.4160 0.8960 -0.1556

Bcc 0.0644 2.483 0.886 0.828 0.2021 0.2579 0.9448

Baa -0.1232 -4.753 -1.696 -1.586 -0.0001 0.1879 0.9822

19 N(14) Bbb 0.0581 2.240 0.799 0.747 -0.0008 0.9822 -0.1879

Bcc 0.0652 2.513 0.897 0.838 1.0000 0.0008 0.0000

Baa -0.1510 -20.269 -7.233 -6.761 0.7990 0.5857 -0.1360

20 C(13) Bbb -0.1439 -19.308 -6.890 -6.441 -0.6006 0.7883 -0.1336

Bcc 0.2949 39.578 14.122 13.202 0.0290 0.1884 0.9817

Baa -0.0134 -1.802 -0.643 -0.601 0.9955 -0.0949 0.0080

21 C(13) Bbb -0.0015 -0.199 -0.071 -0.066 0.0946 0.9750 -0.2012

Bcc 0.0149 2.001 0.714 0.668 0.0113 0.2010 0.9795

Baa -0.0134 -1.802 -0.643 -0.601 0.9953 0.0967 -0.0079

22 C(13) Bbb -0.0015 -0.199 -0.071 -0.066 -0.0963 0.9748 -0.2013

Bcc 0.0149 2.000 0.714 0.667 -0.0118 0.2011 0.9795

Baa -0.1511 -20.270 -7.233 -6.761 0.8001 -0.5842 0.1359

23 C(13) Bbb -0.1439 -19.309 -6.890 -6.441 0.5991 0.7894 -0.1338

Bcc 0.2949 39.578 14.123 13.202 -0.0291 0.1885 0.9816

Baa -0.0372 -1.435 -0.512 -0.479 0.8872 -0.3600 0.2885

24 N(14) Bbb -0.0271 -1.046 -0.373 -0.349 0.4145 0.8966 -0.1557

Bcc 0.0643 2.481 0.885 0.828 -0.2026 0.2577 0.9447

Baa -0.0114 -0.380 -0.136 -0.127 -0.0009 1.0000 0.0000

25 Zn(67) Bbb -0.0032 -0.107 -0.038 -0.036 0.0000 0.0000 1.0000

Bcc 0.0146 0.487 0.174 0.162 1.0000 0.0009 0.0000

Baa -0.0192 -2.581 -0.921 -0.861 -0.3038 0.9524 -0.0258

26 C(13) Bbb -0.0156 -2.098 -0.749 -0.700 0.9509 0.3048 0.0544

Bcc 0.0349 4.679 1.670 1.561 -0.0597 0.0080 0.9982

Baa -0.0149 -2.003 -0.715 -0.668 -0.2851 0.9582 -0.0252

27 C(13) Bbb -0.0137 -1.843 -0.658 -0.615 0.9538 0.2862 0.0916

Bcc 0.0287 3.846 1.373 1.283 -0.0949 -0.0021 0.9955

Baa -0.0149 -2.005 -0.715 -0.669 0.2831 0.9588 0.0250

28 C(13) Bbb -0.0137 -1.844 -0.658 -0.615 0.9544 -0.2842 0.0916

Bcc 0.0287 3.849 1.373 1.284 -0.0949 0.0021 0.9955

Baa -0.0192 -2.580 -0.921 -0.861 0.3022 0.9529 0.0256

29 C(13) Bbb -0.0156 -2.097 -0.748 -0.699 0.9514 -0.3031 0.0544

Bcc 0.0349 4.677 1.669 1.560 -0.0596 -0.0079 0.9982

Baa -0.0363 -4.869 -1.738 -1.624 0.9556 -0.2869 0.0677

30 C(13) Bbb -0.0293 -3.935 -1.404 -1.313 0.2947 0.9369 -0.1879

Bcc 0.0656 8.804 3.142 2.937 -0.0095 0.1995 0.9798

Baa -0.0461 -6.184 -2.207 -2.063 0.8086 -0.5754 0.1227

31 C(13) Bbb -0.0451 -6.048 -2.158 -2.017 0.5884 0.7912 -0.1667

Bcc 0.0912 12.232 4.365 4.080 -0.0011 0.2070 0.9783

Baa -0.0461 -6.185 -2.207 -2.063 0.8076 0.5768 -0.1226

32 C(13) Bbb -0.0451 -6.048 -2.158 -2.018 -0.5897 0.7902 -0.1667

Bcc 0.0912 12.233 4.365 4.081 0.0007 0.2069 0.9784

Baa -0.0363 -4.869 -1.737 -1.624 0.9550 0.2887 -0.0677

33 C(13) Bbb -0.0293 -3.934 -1.404 -1.312 -0.2964 0.9364 -0.1879

Bcc 0.0656 8.803 3.141 2.937 0.0091 0.1995 0.9799

Baa -0.0192 -2.580 -0.921 -0.861 0.3022 0.9529 -0.0255

34 C(13) Bbb -0.0156 -2.097 -0.748 -0.699 0.9514 -0.3031 -0.0545

Bcc 0.0349 4.677 1.669 1.560 0.0596 0.0078 0.9982

Baa -0.0149 -2.005 -0.715 -0.669 0.2831 0.9588 -0.0250

35 C(13) Bbb -0.0137 -1.844 -0.658 -0.615 0.9544 -0.2842 -0.0916

Bcc 0.0287 3.849 1.373 1.284 0.0949 -0.0021 0.9955

Baa -0.0149 -2.003 -0.715 -0.668 -0.2851 0.9582 0.0253

36 C(13) Bbb -0.0137 -1.843 -0.658 -0.615 0.9538 0.2862 -0.0916

Bcc 0.0287 3.846 1.373 1.283 0.0950 0.0020 0.9955

Baa -0.0192 -2.581 -0.921 -0.861 -0.3038 0.9524 0.0259

37 C(13) Bbb -0.0156 -2.098 -0.749 -0.700 0.9509 0.3048 -0.0544

Bcc 0.0349 4.679 1.670 1.561 0.0597 -0.0081 0.9982

Baa -0.0363 -4.870 -1.738 -1.624 0.9556 -0.2870 -0.0676

38 C(13) Bbb -0.0293 -3.935 -1.404 -1.313 0.2947 0.9369 0.1879

Bcc 0.0656 8.804 3.142 2.937 0.0094 -0.1995 0.9799

Baa -0.0461 -6.184 -2.207 -2.063 0.8086 -0.5755 -0.1226

39 C(13) Bbb -0.0451 -6.048 -2.158 -2.017 0.5884 0.7912 0.1667

Bcc 0.0912 12.232 4.365 4.080 0.0011 -0.2070 0.9783

Baa -0.0461 -6.185 -2.207 -2.063 0.8076 0.5768 0.1227

40 C(13) Bbb -0.0451 -6.048 -2.158 -2.018 -0.5897 0.7902 0.1667

Bcc 0.0912 12.233 4.365 4.081 -0.0008 -0.2069 0.9784

Baa -0.0363 -4.869 -1.737 -1.624 0.9550 0.2887 0.0677

41 C(13) Bbb -0.0293 -3.934 -1.404 -1.312 -0.2964 0.9364 0.1879

Bcc 0.0656 8.803 3.141 2.936 -0.0092 -0.1995 0.9799

Baa -0.0022 -1.174 -0.419 -0.392 -0.2961 0.9549 0.0223

42 H(1) Bbb -0.0012 -0.662 -0.236 -0.221 0.0869 0.0037 0.9962

Bcc 0.0034 1.836 0.655 0.612 0.9512 0.2969 -0.0841

Baa -0.0022 -1.174 -0.419 -0.391 0.2944 0.9554 -0.0219

43 H(1) Bbb -0.0012 -0.662 -0.236 -0.221 0.0869 -0.0039 0.9962

Bcc 0.0034 1.835 0.655 0.612 0.9517 -0.2952 -0.0842

Baa -0.0065 -3.446 -1.229 -1.149 0.9404 -0.3332 -0.0679

44 H(1) Bbb -0.0022 -1.171 -0.418 -0.391 0.0001 -0.1994 0.9799

Bcc 0.0087 4.617 1.647 1.540 0.3401 0.9215 0.1875

Baa -0.0065 -3.445 -1.229 -1.149 0.9398 0.3349 0.0681

45 H(1) Bbb -0.0022 -1.171 -0.418 -0.391 0.0001 -0.1995 0.9799

Bcc 0.0087 4.616 1.647 1.540 -0.3417 0.9209 0.1875

Baa -0.0022 -1.174 -0.419 -0.391 0.2944 0.9554 0.0220

46 H(1) Bbb -0.0012 -0.662 -0.236 -0.221 -0.0869 0.0038 0.9962

Bcc 0.0034 1.835 0.655 0.612 0.9517 -0.2952 0.0841

Baa -0.0022 -1.174 -0.419 -0.392 -0.2961 0.9549 -0.0222

47 H(1) Bbb -0.0012 -0.662 -0.236 -0.221 -0.0869 -0.0038 0.9962

Bcc 0.0034 1.836 0.655 0.612 0.9512 0.2969 0.0841

Baa -0.0065 -3.446 -1.229 -1.149 0.9404 -0.3332 0.0680

48 H(1) Bbb -0.0022 -1.171 -0.418 -0.391 -0.0002 0.1995 0.9799

Bcc 0.0087 4.617 1.647 1.540 0.3401 0.9215 -0.1875

Baa -0.0065 -3.445 -1.229 -1.149 0.9398 0.3349 -0.0680

49 H(1) Bbb -0.0022 -1.171 -0.418 -0.391 -0.0002 0.1995 0.9799

Bcc 0.0087 4.616 1.647 1.540 -0.3417 0.9209 -0.1875

Baa -0.0447 3.236 1.155 1.079 0.8280 -0.5548 -0.0814

50 O(17) Bbb -0.0392 2.834 1.011 0.945 0.5601 0.8116 0.1660

Bcc 0.0839 -6.070 -2.166 -2.025 -0.0260 -0.1831 0.9828

Baa -0.0447 3.236 1.155 1.079 0.8270 0.5562 0.0815

51 O(17) Bbb -0.0392 2.834 1.011 0.945 -0.5615 0.8106 0.1659

Bcc 0.0839 -6.070 -2.166 -2.025 0.0262 -0.1830 0.9828

Baa -0.0253 1.834 0.655 0.612 -0.3746 0.9269 -0.0243

52 O(17) Bbb -0.0213 1.541 0.550 0.514 0.9271 0.3748 0.0032

Bcc 0.0466 -3.375 -1.204 -1.126 -0.0121 0.0213 0.9997

Baa -0.0254 1.835 0.655 0.612 0.3730 0.9275 0.0246

53 O(17) Bbb -0.0213 1.541 0.550 0.514 0.9277 -0.3732 0.0032

Bcc 0.0467 -3.376 -1.205 -1.126 -0.0121 -0.0216 0.9997

Baa -0.0447 3.236 1.155 1.079 0.8270 0.5562 -0.0815

54 O(17) Bbb -0.0392 2.834 1.011 0.945 -0.5615 0.8106 -0.1660

Bcc 0.0839 -6.070 -2.166 -2.025 -0.0263 0.1830 0.9828

Baa -0.0447 3.235 1.155 1.079 0.8280 -0.5547 0.0815

55 O(17) Bbb -0.0392 2.834 1.011 0.945 0.5601 0.8116 -0.1660

Bcc 0.0839 -6.070 -2.166 -2.025 0.0260 0.1831 0.9828

Baa -0.0253 1.834 0.655 0.612 -0.3746 0.9269 0.0243

56 O(17) Bbb -0.0213 1.541 0.550 0.514 0.9271 0.3748 -0.0032

Bcc 0.0466 -3.375 -1.204 -1.126 0.0121 -0.0213 0.9997

Baa -0.0254 1.835 0.655 0.612 0.3730 0.9275 -0.0245

57 O(17) Bbb -0.0213 1.541 0.550 0.514 0.9277 -0.3732 -0.0032

Bcc 0.0467 -3.376 -1.205 -1.126 0.0121 0.0215 0.9997

Baa -0.0019 -0.251 -0.089 -0.084 -0.0227 -0.1534 0.9879

58 C(13) Bbb -0.0009 -0.116 -0.042 -0.039 -0.6234 0.7746 0.1060

Bcc 0.0027 0.367 0.131 0.122 0.7815 0.6135 0.1132

Baa -0.0018 -0.961 -0.343 -0.321 -0.1868 -0.3565 0.9154

59 H(1) Bbb -0.0009 -0.483 -0.172 -0.161 -0.6446 0.7477 0.1597

Bcc 0.0027 1.444 0.515 0.482 0.7414 0.5603 0.3694

Baa -0.0018 -0.953 -0.340 -0.318 0.1427 -0.0153 0.9896

60 H(1) Bbb -0.0009 -0.484 -0.173 -0.161 -0.6558 0.7474 0.1061

Bcc 0.0027 1.437 0.513 0.479 0.7413 0.6642 -0.0966

Baa -0.0013 -0.716 -0.256 -0.239 -0.0240 -0.1748 0.9843

61 H(1) Bbb -0.0007 -0.378 -0.135 -0.126 -0.5137 0.8468 0.1379

Bcc 0.0021 1.094 0.390 0.365 0.8576 0.5024 0.1101

Baa -0.0014 -0.192 -0.068 -0.064 0.0716 -0.0023 0.9974

62 C(13) Bbb -0.0003 -0.045 -0.016 -0.015 -0.5481 0.8354 0.0413

Bcc 0.0018 0.237 0.084 0.079 0.8333 0.5497 -0.0585

Baa -0.0010 -0.555 -0.198 -0.185 0.2323 0.1323 0.9636

63 H(1) Bbb -0.0004 -0.209 -0.075 -0.070 -0.5689 0.8221 0.0243

Bcc 0.0014 0.764 0.273 0.255 0.7889 0.5538 -0.2663

Baa -0.0011 -0.580 -0.207 -0.194 -0.0627 -0.1979 0.9782

64 H(1) Bbb -0.0004 -0.194 -0.069 -0.065 -0.5701 0.8116 0.1277

Bcc 0.0015 0.774 0.276 0.258 0.8192 0.5497 0.1637

Baa -0.0010 -0.559 -0.199 -0.186 0.1311 -0.0614 0.9895

65 H(1) Bbb -0.0003 -0.155 -0.055 -0.052 -0.6222 0.7719 0.1303

Bcc 0.0013 0.714 0.255 0.238 0.7718 0.6328 -0.0630

Baa -0.0014 -0.192 -0.068 -0.064 0.0717 0.0022 0.9974

66 C(13) Bbb -0.0003 -0.045 -0.016 -0.015 0.5466 0.8364 -0.0412

Bcc 0.0018 0.237 0.084 0.079 0.8343 -0.5482 -0.0588

Baa -0.0011 -0.580 -0.207 -0.194 -0.0629 0.1976 0.9783

67 H(1) Bbb -0.0004 -0.194 -0.069 -0.065 0.5687 0.8126 -0.1276

Bcc 0.0015 0.774 0.276 0.258 0.8201 -0.5483 0.1635

Baa -0.0010 -0.555 -0.198 -0.185 0.2327 -0.1321 0.9635

68 H(1) Bbb -0.0004 -0.209 -0.075 -0.070 0.5674 0.8231 -0.0241

Bcc 0.0014 0.764 0.273 0.255 0.7899 -0.5523 -0.2665

Baa -0.0010 -0.559 -0.199 -0.186 0.1312 0.0615 0.9894

69 H(1) Bbb -0.0003 -0.155 -0.055 -0.052 0.6209 0.7730 -0.1304

Bcc 0.0013 0.714 0.255 0.238 0.7728 -0.6314 -0.0632

Baa -0.0019 -0.251 -0.089 -0.084 0.0226 -0.1536 0.9879

70 C(13) Bbb -0.0009 -0.116 -0.042 -0.039 0.6220 0.7757 0.1063

Bcc 0.0027 0.367 0.131 0.122 0.7827 -0.6121 -0.1131

Baa -0.0018 -0.953 -0.340 -0.318 -0.1429 -0.0155 0.9896

71 H(1) Bbb -0.0009 -0.484 -0.173 -0.161 0.6545 0.7486 0.1063

Bcc 0.0027 1.437 0.513 0.479 0.7425 -0.6628 0.0968

Baa -0.0018 -0.961 -0.343 -0.321 0.1872 -0.3561 0.9155

72 H(1) Bbb -0.0009 -0.483 -0.172 -0.161 0.6433 0.7488 0.1597

Bcc 0.0027 1.444 0.515 0.482 0.7424 -0.5590 -0.3692

Baa -0.0013 -0.716 -0.256 -0.239 0.0242 -0.1748 0.9843

73 H(1) Bbb -0.0007 -0.378 -0.135 -0.126 0.5122 0.8477 0.1379

Bcc 0.0021 1.094 0.391 0.365 0.8585 -0.5008 -0.1100

Baa -0.0014 -0.192 -0.068 -0.064 -0.0717 -0.0023 0.9974

74 C(13) Bbb -0.0003 -0.045 -0.016 -0.015 0.5466 0.8364 0.0412

Bcc 0.0018 0.237 0.084 0.079 0.8343 -0.5482 0.0587

Baa -0.0011 -0.580 -0.207 -0.194 0.0630 -0.1977 0.9782

75 H(1) Bbb -0.0004 -0.194 -0.069 -0.065 0.5687 0.8126 0.1276

Bcc 0.0015 0.774 0.276 0.258 0.8201 -0.5483 -0.1636

Baa -0.0010 -0.555 -0.198 -0.185 -0.2326 0.1321 0.9636

76 H(1) Bbb -0.0004 -0.209 -0.075 -0.070 0.5674 0.8231 0.0242

Bcc 0.0014 0.764 0.273 0.255 0.7899 -0.5523 0.2664

Baa -0.0010 -0.559 -0.199 -0.186 -0.1311 -0.0616 0.9895

77 H(1) Bbb -0.0003 -0.155 -0.055 -0.052 0.6209 0.7730 0.1304

Bcc 0.0013 0.714 0.255 0.238 0.7728 -0.6314 0.0631

Baa -0.0014 -0.192 -0.068 -0.064 -0.0716 0.0023 0.9974

78 C(13) Bbb -0.0003 -0.045 -0.016 -0.015 -0.5481 0.8354 -0.0413

Bcc 0.0018 0.237 0.084 0.079 0.8333 0.5497 0.0586

Baa -0.0010 -0.555 -0.198 -0.185 -0.2323 -0.1323 0.9636

79 H(1) Bbb -0.0004 -0.209 -0.075 -0.070 -0.5689 0.8221 -0.0243

Bcc 0.0014 0.764 0.273 0.255 0.7889 0.5538 0.2663

Baa -0.0011 -0.580 -0.207 -0.194 0.0627 0.1979 0.9782

80 H(1) Bbb -0.0004 -0.194 -0.069 -0.065 -0.5701 0.8116 -0.1277

Bcc 0.0015 0.774 0.276 0.258 0.8192 0.5497 -0.1637

Baa -0.0010 -0.559 -0.199 -0.186 -0.1311 0.0614 0.9895

81 H(1) Bbb -0.0003 -0.155 -0.055 -0.052 -0.6222 0.7719 -0.1303

Bcc 0.0013 0.714 0.255 0.238 0.7718 0.6328 0.0630

Baa -0.0019 -0.251 -0.089 -0.084 0.0226 0.1534 0.9879

82 C(13) Bbb -0.0009 -0.116 -0.042 -0.039 -0.6235 0.7746 -0.1060

Bcc 0.0027 0.367 0.131 0.122 0.7815 0.6135 -0.1132

Baa -0.0018 -0.961 -0.343 -0.321 0.1867 0.3565 0.9154

83 H(1) Bbb -0.0009 -0.483 -0.172 -0.161 -0.6446 0.7477 -0.1597

Bcc 0.0027 1.444 0.515 0.482 0.7414 0.5603 -0.3694

Baa -0.0018 -0.953 -0.340 -0.318 -0.1428 0.0153 0.9896

84 H(1) Bbb -0.0009 -0.484 -0.173 -0.161 -0.6558 0.7474 -0.1062

Bcc 0.0027 1.437 0.513 0.479 0.7413 0.6642 0.0967

Baa -0.0013 -0.716 -0.256 -0.239 0.0239 0.1748 0.9843

85 H(1) Bbb -0.0007 -0.378 -0.135 -0.126 -0.5137 0.8468 -0.1379

Bcc 0.0021 1.094 0.390 0.365 0.8576 0.5024 -0.1100

Baa -0.0019 -0.251 -0.089 -0.084 -0.0227 0.1536 0.9879

86 C(13) Bbb -0.0009 -0.116 -0.042 -0.039 0.6220 0.7757 -0.1063

Bcc 0.0027 0.367 0.131 0.122 0.7827 -0.6121 0.1132

Baa -0.0018 -0.952 -0.340 -0.318 0.1429 0.0156 0.9896

87 H(1) Bbb -0.0009 -0.484 -0.173 -0.161 0.6544 0.7486 -0.1063

Bcc 0.0027 1.436 0.513 0.479 0.7425 -0.6628 -0.0968

Baa -0.0018 -0.961 -0.343 -0.321 -0.1873 0.3561 0.9155

88 H(1) Bbb -0.0009 -0.483 -0.172 -0.161 0.6433 0.7488 -0.1597

Bcc 0.0027 1.444 0.515 0.482 0.7424 -0.5590 0.3693

Baa -0.0013 -0.716 -0.256 -0.239 -0.0243 0.1748 0.9843

89 H(1) Bbb -0.0007 -0.378 -0.135 -0.126 0.5122 0.8477 -0.1380

Bcc 0.0021 1.094 0.390 0.365 0.8585 -0.5008 0.1101

---------------------------------------------------------------------------------

No NMR shielding tensors so no spin-rotation constants.

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SEEN ON A WALL AT THE UNIVERSITY OF ILLINOIS AT CHICAGO CIRCLE:

TO DO IS TO BE -- SOCRATES

TO BE IS TO DO -- SARTRE

OO BE DO BE DO -- SINATRA

Job cpu time: 2 days 8 hours 20 minutes 30.4 seconds.

File lengths (MBytes): RWF= 2606 Int= 0 D2E= 0 Chk= 125 Scr= 2

Normal termination of Gaussian 09 at Sat Jul 6 03:56:45 2019.