Entering Gaussian System, Link 0=g09

Initial command:

/apps/gaussian/g09d01/g09/l1.exe "/srv/scratch/z5105842/Gau-11839.inp" -scrdir="/srv/scratch/z5105842/"

Entering Link 1 = /apps/gaussian/g09d01/g09/l1.exe PID= 11858.

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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

30-Jun-2019

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

%nprocshared=12

Will use up to 12 processors via shared memory.

%mem=10GB

%chk=ZnNPC3.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 Sun Jun 30 19:49:26 2019, MaxMem= 1342177280 cpu: 1.0

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

------

ZnNPC3

------

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C 1.1221 2.79961 0.14333

N 0. 2.02367 0.24353

C -1.1221 2.79961 0.14333

C -0.71905 4.18799 -0.01344

C 0.71905 4.18799 -0.01344

N -2.41564 2.38956 0.15046

C -2.79904 1.12837 0.17949

N -2.01082 0. 0.23312

C -2.79904 -1.12837 0.17949

C -4.21437 -0.71383 0.11787

C -4.21437 0.71383 0.11787

N 2.41564 2.38956 0.15046

C 4.21437 0.71383 0.11787

C 4.21437 -0.71383 0.11787

C 2.79904 -1.12837 0.17949

N 2.01082 0. 0.23312

C 2.79904 1.12837 0.17949

N 2.41564 -2.38956 0.15046

N 0. -2.02367 0.24353

C 1.1221 -2.79961 0.14333

C 0.71905 -4.18799 -0.01344

C -0.71905 -4.18799 -0.01344

C -1.1221 -2.79961 0.14333

N -2.41564 -2.38956 0.15046

Zn 0. 0. 0.75754

C 5.38287 1.43019 0.05768

C 6.62018 0.72025 0.00147

C 6.62018 -0.72025 0.00147

C 5.38287 -1.43019 0.05768

C -1.43217 -5.36076 -0.156

C -0.72262 -6.58326 -0.29796

C 0.72262 -6.58326 -0.29796

C 1.43217 -5.36076 -0.156

C -5.38287 1.43019 0.05768

C -6.62018 0.72025 0.00147

C -6.62018 -0.72025 0.00147

C -5.38287 -1.43019 0.05768

C 1.43217 5.36076 -0.156

C 0.72262 6.58326 -0.29796

C -0.72262 6.58326 -0.29796

C -1.43217 5.36076 -0.156

C 1.40597 -7.82298 -0.44352

C 0.70976 -9.00533 -0.58237

C -0.70976 -9.00533 -0.58237

C -1.40597 -7.82298 -0.44352

C 7.86198 -1.40505 -0.0555

C 9.05377 -0.70773 -0.10946

C 9.05377 0.70773 -0.10946

C 7.86198 1.40505 -0.0555

C -1.40597 7.82298 -0.44352

C -0.70976 9.00533 -0.58237

C 0.70976 9.00533 -0.58237

C 1.40597 7.82298 -0.44352

C -7.86198 -1.40505 -0.0555

C -9.05377 -0.70773 -0.10946

C -9.05377 0.70773 -0.10946

C -7.86198 1.40505 -0.0555

H 5.38506 2.51643 0.053

H 5.38506 -2.51643 0.053

H -2.51856 -5.36582 -0.16062

H 2.51856 -5.36582 -0.16062

H -5.38506 2.51643 0.053

H -5.38506 -2.51643 0.053

H 2.51856 5.36582 -0.16062

H -2.51856 5.36582 -0.16062

H 2.4928 -7.81942 -0.44334

H 1.24648 -9.943 -0.69315

H -1.24648 -9.943 -0.69315

H -2.4928 -7.81942 -0.44334

H 7.85814 -2.4917 -0.05573

H 9.99623 -1.24559 -0.15272

H 9.99623 1.24559 -0.15272

H 7.85814 2.4917 -0.05573

H -2.4928 7.81942 -0.44334

H -1.24648 9.943 -0.69315

H 1.24648 9.943 -0.69315

H 2.4928 7.81942 -0.44334

H -7.85814 -2.4917 -0.05573

H -9.99623 -1.24559 -0.15272

H -9.99623 1.24559 -0.15272

H -7.85814 2.4917 -0.05573

NAtoms= 81 NQM= 81 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 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 51 52 53 54 55 56 57 58 59 60

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

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

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

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

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

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

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

Atom 61 62 63 64 65 66 67 68 69 70

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

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

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

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

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

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

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

Atom 71 72 73 74 75 76 77 78 79 80

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

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

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

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

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

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

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

Atom 81

IAtWgt= 1

AtmWgt= 1.0078250

NucSpn= 1

AtZEff= 0.0000000

NQMom= 0.0000000

NMagM= 2.7928460

AtZNuc= 1.0000000

Leave Link 101 at Sun Jun 30 19:49:27 2019, MaxMem= 1342177280 cpu: 4.2

(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) 1.3679 estimate D2E/DX2 !

! R2 R(1,5) 1.4542 estimate D2E/DX2 !

! R3 R(1,12) 1.357 estimate D2E/DX2 !

! R4 R(2,3) 1.3679 estimate D2E/DX2 !

! R5 R(2,25) 2.0879 estimate D2E/DX2 !

! R6 R(3,4) 1.4542 estimate D2E/DX2 !

! R7 R(3,6) 1.357 estimate D2E/DX2 !

! R8 R(4,5) 1.4381 estimate D2E/DX2 !

! R9 R(4,41) 1.3799 estimate D2E/DX2 !

! R10 R(5,38) 1.3799 estimate D2E/DX2 !

! R11 R(6,7) 1.3185 estimate D2E/DX2 !

! R12 R(7,8) 1.3775 estimate D2E/DX2 !

! R13 R(7,11) 1.4761 estimate D2E/DX2 !

! R14 R(8,9) 1.3775 estimate D2E/DX2 !

! R15 R(8,25) 2.0781 estimate D2E/DX2 !

! R16 R(9,10) 1.4761 estimate D2E/DX2 !

! R17 R(9,24) 1.3185 estimate D2E/DX2 !

! R18 R(10,11) 1.4277 estimate D2E/DX2 !

! R19 R(10,37) 1.3719 estimate D2E/DX2 !

! R20 R(11,34) 1.3719 estimate D2E/DX2 !

! R21 R(12,17) 1.3185 estimate D2E/DX2 !

! R22 R(13,14) 1.4277 estimate D2E/DX2 !

! R23 R(13,17) 1.4761 estimate D2E/DX2 !

! R24 R(13,26) 1.3719 estimate D2E/DX2 !

! R25 R(14,15) 1.4761 estimate D2E/DX2 !

! R26 R(14,29) 1.3719 estimate D2E/DX2 !

! R27 R(15,16) 1.3775 estimate D2E/DX2 !

! R28 R(15,18) 1.3185 estimate D2E/DX2 !

! R29 R(16,17) 1.3775 estimate D2E/DX2 !

! R30 R(16,25) 2.0781 estimate D2E/DX2 !

! R31 R(18,20) 1.357 estimate D2E/DX2 !

! R32 R(19,20) 1.3679 estimate D2E/DX2 !

! R33 R(19,23) 1.3679 estimate D2E/DX2 !

! R34 R(19,25) 2.0879 estimate D2E/DX2 !

! R35 R(20,21) 1.4542 estimate D2E/DX2 !

! R36 R(21,22) 1.4381 estimate D2E/DX2 !

! R37 R(21,33) 1.3799 estimate D2E/DX2 !

! R38 R(22,23) 1.4542 estimate D2E/DX2 !

! R39 R(22,30) 1.3799 estimate D2E/DX2 !

! R40 R(23,24) 1.357 estimate D2E/DX2 !

! R41 R(26,27) 1.4276 estimate D2E/DX2 !

! R42 R(26,58) 1.0863 estimate D2E/DX2 !

! R43 R(27,28) 1.4405 estimate D2E/DX2 !

! R44 R(27,49) 1.4192 estimate D2E/DX2 !

! R45 R(28,29) 1.4276 estimate D2E/DX2 !

! R46 R(28,46) 1.4192 estimate D2E/DX2 !

! R47 R(29,59) 1.0863 estimate D2E/DX2 !

! R48 R(30,31) 1.4206 estimate D2E/DX2 !

! R49 R(30,60) 1.0864 estimate D2E/DX2 !

! R50 R(31,32) 1.4452 estimate D2E/DX2 !

! R51 R(31,45) 1.423 estimate D2E/DX2 !

! R52 R(32,33) 1.4206 estimate D2E/DX2 !

! R53 R(32,42) 1.423 estimate D2E/DX2 !

! R54 R(33,61) 1.0864 estimate D2E/DX2 !

! R55 R(34,35) 1.4276 estimate D2E/DX2 !

! R56 R(34,62) 1.0863 estimate D2E/DX2 !

! R57 R(35,36) 1.4405 estimate D2E/DX2 !

! R58 R(35,57) 1.4192 estimate D2E/DX2 !

! R59 R(36,37) 1.4276 estimate D2E/DX2 !

! R60 R(36,54) 1.4192 estimate D2E/DX2 !

! R61 R(37,63) 1.0863 estimate D2E/DX2 !

! R62 R(38,39) 1.4206 estimate D2E/DX2 !

! R63 R(38,64) 1.0864 estimate D2E/DX2 !

! R64 R(39,40) 1.4452 estimate D2E/DX2 !

! R65 R(39,53) 1.423 estimate D2E/DX2 !

! R66 R(40,41) 1.4206 estimate D2E/DX2 !

! R67 R(40,50) 1.423 estimate D2E/DX2 !

! R68 R(41,65) 1.0864 estimate D2E/DX2 !

! R69 R(42,43) 1.3791 estimate D2E/DX2 !

! R70 R(42,66) 1.0868 estimate D2E/DX2 !

! R71 R(43,44) 1.4195 estimate D2E/DX2 !

! R72 R(43,67) 1.0861 estimate D2E/DX2 !

! R73 R(44,45) 1.3791 estimate D2E/DX2 !

! R74 R(44,68) 1.0861 estimate D2E/DX2 !

! R75 R(45,69) 1.0868 estimate D2E/DX2 !

! R76 R(46,47) 1.3819 estimate D2E/DX2 !

! R77 R(46,70) 1.0867 estimate D2E/DX2 !

! R78 R(47,48) 1.4155 estimate D2E/DX2 !

! R79 R(47,71) 1.086 estimate D2E/DX2 !

! R80 R(48,49) 1.3819 estimate D2E/DX2 !

! R81 R(48,72) 1.086 estimate D2E/DX2 !

! R82 R(49,73) 1.0867 estimate D2E/DX2 !

! R83 R(50,51) 1.3791 estimate D2E/DX2 !

! R84 R(50,74) 1.0868 estimate D2E/DX2 !

! R85 R(51,52) 1.4195 estimate D2E/DX2 !

! R86 R(51,75) 1.0861 estimate D2E/DX2 !

! R87 R(52,53) 1.3791 estimate D2E/DX2 !

! R88 R(52,76) 1.0861 estimate D2E/DX2 !

! R89 R(53,77) 1.0868 estimate D2E/DX2 !

! R90 R(54,55) 1.3819 estimate D2E/DX2 !

! R91 R(54,78) 1.0867 estimate D2E/DX2 !

! R92 R(55,56) 1.4155 estimate D2E/DX2 !

! R93 R(55,79) 1.086 estimate D2E/DX2 !

! R94 R(56,57) 1.3819 estimate D2E/DX2 !

! R95 R(56,80) 1.086 estimate D2E/DX2 !

! R96 R(57,81) 1.0867 estimate D2E/DX2 !

! A1 A(2,1,5) 108.7908 estimate D2E/DX2 !

! A2 A(2,1,12) 127.6 estimate D2E/DX2 !

! A3 A(5,1,12) 123.5918 estimate D2E/DX2 !

! A4 A(1,2,3) 110.2278 estimate D2E/DX2 !

! A5 A(1,2,25) 124.5978 estimate D2E/DX2 !

! A6 A(3,2,25) 124.5978 estimate D2E/DX2 !

! A7 A(2,3,4) 108.7908 estimate D2E/DX2 !

! A8 A(2,3,6) 127.6 estimate D2E/DX2 !

! A9 A(4,3,6) 123.5918 estimate D2E/DX2 !

! A10 A(3,4,5) 106.0911 estimate D2E/DX2 !

! A11 A(3,4,41) 132.7907 estimate D2E/DX2 !

! A12 A(5,4,41) 121.1159 estimate D2E/DX2 !

! A13 A(1,5,4) 106.0911 estimate D2E/DX2 !

! A14 A(1,5,38) 132.7907 estimate D2E/DX2 !

! A15 A(4,5,38) 121.1159 estimate D2E/DX2 !

! A16 A(3,6,7) 124.4955 estimate D2E/DX2 !

! A17 A(6,7,8) 128.1722 estimate D2E/DX2 !

! A18 A(6,7,11) 123.1292 estimate D2E/DX2 !

! A19 A(8,7,11) 108.6782 estimate D2E/DX2 !

! A20 A(7,8,9) 110.0035 estimate D2E/DX2 !

! A21 A(7,8,25) 124.3006 estimate D2E/DX2 !

! A22 A(9,8,25) 124.3006 estimate D2E/DX2 !

! A23 A(8,9,10) 108.6782 estimate D2E/DX2 !

! A24 A(8,9,24) 128.1722 estimate D2E/DX2 !

! A25 A(10,9,24) 123.1292 estimate D2E/DX2 !

! A26 A(9,10,11) 106.3102 estimate D2E/DX2 !

! A27 A(9,10,37) 132.2108 estimate D2E/DX2 !

! A28 A(11,10,37) 121.477 estimate D2E/DX2 !

! A29 A(7,11,10) 106.3102 estimate D2E/DX2 !

! A30 A(7,11,34) 132.2108 estimate D2E/DX2 !

! A31 A(10,11,34) 121.477 estimate D2E/DX2 !

! A32 A(1,12,17) 124.4955 estimate D2E/DX2 !

! A33 A(14,13,17) 106.3102 estimate D2E/DX2 !

! A34 A(14,13,26) 121.477 estimate D2E/DX2 !

! A35 A(17,13,26) 132.2108 estimate D2E/DX2 !

! A36 A(13,14,15) 106.3102 estimate D2E/DX2 !

! A37 A(13,14,29) 121.477 estimate D2E/DX2 !

! A38 A(15,14,29) 132.2108 estimate D2E/DX2 !

! A39 A(14,15,16) 108.6782 estimate D2E/DX2 !

! A40 A(14,15,18) 123.1292 estimate D2E/DX2 !

! A41 A(16,15,18) 128.1722 estimate D2E/DX2 !

! A42 A(15,16,17) 110.0035 estimate D2E/DX2 !

! A43 A(15,16,25) 124.3006 estimate D2E/DX2 !

! A44 A(17,16,25) 124.3006 estimate D2E/DX2 !

! A45 A(12,17,13) 123.1292 estimate D2E/DX2 !

! A46 A(12,17,16) 128.1722 estimate D2E/DX2 !

! A47 A(13,17,16) 108.6782 estimate D2E/DX2 !

! A48 A(15,18,20) 124.4955 estimate D2E/DX2 !

! A49 A(20,19,23) 110.2278 estimate D2E/DX2 !

! A50 A(20,19,25) 124.5978 estimate D2E/DX2 !

! A51 A(23,19,25) 124.5978 estimate D2E/DX2 !

! A52 A(18,20,19) 127.6 estimate D2E/DX2 !

! A53 A(18,20,21) 123.5918 estimate D2E/DX2 !

! A54 A(19,20,21) 108.7908 estimate D2E/DX2 !

! A55 A(20,21,22) 106.0911 estimate D2E/DX2 !

! A56 A(20,21,33) 132.7907 estimate D2E/DX2 !

! A57 A(22,21,33) 121.1159 estimate D2E/DX2 !

! A58 A(21,22,23) 106.0911 estimate D2E/DX2 !

! A59 A(21,22,30) 121.1159 estimate D2E/DX2 !

! A60 A(23,22,30) 132.7907 estimate D2E/DX2 !

! A61 A(19,23,22) 108.7908 estimate D2E/DX2 !

! A62 A(19,23,24) 127.6 estimate D2E/DX2 !

! A63 A(22,23,24) 123.5918 estimate D2E/DX2 !

! A64 A(9,24,23) 124.4955 estimate D2E/DX2 !

! A65 A(2,25,8) 86.4382 estimate D2E/DX2 !

! A66 A(2,25,16) 86.4382 estimate D2E/DX2 !

! A67 A(2,25,19) 151.497 estimate D2E/DX2 !

! A68 A(8,25,16) 150.7661 estimate D2E/DX2 !

! A69 A(8,25,19) 86.4382 estimate D2E/DX2 !

! A70 A(16,25,19) 86.4382 estimate D2E/DX2 !

! A71 A(13,26,27) 118.7015 estimate D2E/DX2 !

! A72 A(13,26,58) 121.6049 estimate D2E/DX2 !

! A73 A(27,26,58) 119.6935 estimate D2E/DX2 !

! A74 A(26,27,28) 119.8206 estimate D2E/DX2 !

! A75 A(26,27,49) 121.3298 estimate D2E/DX2 !

! A76 A(28,27,49) 118.8496 estimate D2E/DX2 !

! A77 A(27,28,29) 119.8206 estimate D2E/DX2 !

! A78 A(27,28,46) 118.8496 estimate D2E/DX2 !

! A79 A(29,28,46) 121.3298 estimate D2E/DX2 !

! A80 A(14,29,28) 118.7015 estimate D2E/DX2 !

! A81 A(14,29,59) 121.6049 estimate D2E/DX2 !

! A82 A(28,29,59) 119.6935 estimate D2E/DX2 !

! A83 A(22,30,31) 118.9183 estimate D2E/DX2 !

! A84 A(22,30,60) 121.4097 estimate D2E/DX2 !

! A85 A(31,30,60) 119.672 estimate D2E/DX2 !

! A86 A(30,31,32) 119.9651 estimate D2E/DX2 !

! A87 A(30,31,45) 121.3363 estimate D2E/DX2 !

! A88 A(32,31,45) 118.6986 estimate D2E/DX2 !

! A89 A(31,32,33) 119.9651 estimate D2E/DX2 !

! A90 A(31,32,42) 118.6986 estimate D2E/DX2 !

! A91 A(33,32,42) 121.3363 estimate D2E/DX2 !

! A92 A(21,33,32) 118.9183 estimate D2E/DX2 !

! A93 A(21,33,61) 121.4097 estimate D2E/DX2 !

! A94 A(32,33,61) 119.672 estimate D2E/DX2 !

! A95 A(11,34,35) 118.7015 estimate D2E/DX2 !

! A96 A(11,34,62) 121.6049 estimate D2E/DX2 !

! A97 A(35,34,62) 119.6935 estimate D2E/DX2 !

! A98 A(34,35,36) 119.8206 estimate D2E/DX2 !

! A99 A(34,35,57) 121.3298 estimate D2E/DX2 !

! A100 A(36,35,57) 118.8496 estimate D2E/DX2 !

! A101 A(35,36,37) 119.8206 estimate D2E/DX2 !

! A102 A(35,36,54) 118.8496 estimate D2E/DX2 !

! A103 A(37,36,54) 121.3298 estimate D2E/DX2 !

! A104 A(10,37,36) 118.7015 estimate D2E/DX2 !

! A105 A(10,37,63) 121.6049 estimate D2E/DX2 !

! A106 A(36,37,63) 119.6935 estimate D2E/DX2 !

! A107 A(5,38,39) 118.9183 estimate D2E/DX2 !

! A108 A(5,38,64) 121.4097 estimate D2E/DX2 !

! A109 A(39,38,64) 119.672 estimate D2E/DX2 !

! A110 A(38,39,40) 119.9651 estimate D2E/DX2 !

! A111 A(38,39,53) 121.3363 estimate D2E/DX2 !

! A112 A(40,39,53) 118.6986 estimate D2E/DX2 !

! A113 A(39,40,41) 119.9651 estimate D2E/DX2 !

! A114 A(39,40,50) 118.6986 estimate D2E/DX2 !

! A115 A(41,40,50) 121.3363 estimate D2E/DX2 !

! A116 A(4,41,40) 118.9183 estimate D2E/DX2 !

! A117 A(4,41,65) 121.4097 estimate D2E/DX2 !

! A118 A(40,41,65) 119.672 estimate D2E/DX2 !

! A119 A(32,42,43) 120.9818 estimate D2E/DX2 !

! A120 A(32,42,66) 118.5111 estimate D2E/DX2 !

! A121 A(43,42,66) 120.5072 estimate D2E/DX2 !

! A122 A(42,43,44) 120.3197 estimate D2E/DX2 !

! A123 A(42,43,67) 120.0644 estimate D2E/DX2 !

! A124 A(44,43,67) 119.6159 estimate D2E/DX2 !

! A125 A(43,44,45) 120.3197 estimate D2E/DX2 !

! A126 A(43,44,68) 119.6159 estimate D2E/DX2 !

! A127 A(45,44,68) 120.0644 estimate D2E/DX2 !

! A128 A(31,45,44) 120.9818 estimate D2E/DX2 !

! A129 A(31,45,69) 118.5111 estimate D2E/DX2 !

! A130 A(44,45,69) 120.5072 estimate D2E/DX2 !

! A131 A(28,46,47) 120.8438 estimate D2E/DX2 !

! A132 A(28,46,70) 118.648 estimate D2E/DX2 !

! A133 A(47,46,70) 120.5082 estimate D2E/DX2 !

! A134 A(46,47,48) 120.3065 estimate D2E/DX2 !

! A135 A(46,47,71) 120.0061 estimate D2E/DX2 !

! A136 A(48,47,71) 119.6873 estimate D2E/DX2 !

! A137 A(47,48,49) 120.3065 estimate D2E/DX2 !

! A138 A(47,48,72) 119.6873 estimate D2E/DX2 !

! A139 A(49,48,72) 120.0061 estimate D2E/DX2 !

! A140 A(27,49,48) 120.8438 estimate D2E/DX2 !

! A141 A(27,49,73) 118.648 estimate D2E/DX2 !

! A142 A(48,49,73) 120.5082 estimate D2E/DX2 !

! A143 A(40,50,51) 120.9818 estimate D2E/DX2 !

! A144 A(40,50,74) 118.5111 estimate D2E/DX2 !

! A145 A(51,50,74) 120.5072 estimate D2E/DX2 !

! A146 A(50,51,52) 120.3197 estimate D2E/DX2 !

! A147 A(50,51,75) 120.0644 estimate D2E/DX2 !

! A148 A(52,51,75) 119.6159 estimate D2E/DX2 !

! A149 A(51,52,53) 120.3197 estimate D2E/DX2 !

! A150 A(51,52,76) 119.6159 estimate D2E/DX2 !

! A151 A(53,52,76) 120.0644 estimate D2E/DX2 !

! A152 A(39,53,52) 120.9818 estimate D2E/DX2 !

! A153 A(39,53,77) 118.5111 estimate D2E/DX2 !

! A154 A(52,53,77) 120.5072 estimate D2E/DX2 !

! A155 A(36,54,55) 120.8438 estimate D2E/DX2 !

! A156 A(36,54,78) 118.648 estimate D2E/DX2 !

! A157 A(55,54,78) 120.5082 estimate D2E/DX2 !

! A158 A(54,55,56) 120.3065 estimate D2E/DX2 !

! A159 A(54,55,79) 120.0061 estimate D2E/DX2 !

! A160 A(56,55,79) 119.6873 estimate D2E/DX2 !

! A161 A(55,56,57) 120.3065 estimate D2E/DX2 !

! A162 A(55,56,80) 119.6873 estimate D2E/DX2 !

! A163 A(57,56,80) 120.0061 estimate D2E/DX2 !

! A164 A(35,57,56) 120.8438 estimate D2E/DX2 !

! A165 A(35,57,81) 118.648 estimate D2E/DX2 !

! A166 A(56,57,81) 120.5082 estimate D2E/DX2 !

! D1 D(5,1,2,3) 0.9301 estimate D2E/DX2 !

! D2 D(5,1,2,25) -170.6864 estimate D2E/DX2 !

! D3 D(12,1,2,3) -177.5772 estimate D2E/DX2 !

! D4 D(12,1,2,25) 10.8063 estimate D2E/DX2 !

! D5 D(2,1,5,4) -0.5536 estimate D2E/DX2 !

! D6 D(2,1,5,38) -179.9832 estimate D2E/DX2 !

! D7 D(12,1,5,4) 178.0266 estimate D2E/DX2 !

! D8 D(12,1,5,38) -1.4029 estimate D2E/DX2 !

! D9 D(2,1,12,17) 4.2138 estimate D2E/DX2 !

! D10 D(5,1,12,17) -174.0897 estimate D2E/DX2 !

! D11 D(1,2,3,4) -0.9301 estimate D2E/DX2 !

! D12 D(1,2,3,6) 177.5772 estimate D2E/DX2 !

! D13 D(25,2,3,4) 170.6864 estimate D2E/DX2 !

! D14 D(25,2,3,6) -10.8063 estimate D2E/DX2 !

! D15 D(1,2,25,8) -170.5979 estimate D2E/DX2 !

! D16 D(1,2,25,16) -18.9689 estimate D2E/DX2 !

! D17 D(1,2,25,19) -94.7834 estimate D2E/DX2 !

! D18 D(3,2,25,8) 18.9689 estimate D2E/DX2 !

! D19 D(3,2,25,16) 170.5979 estimate D2E/DX2 !

! D20 D(3,2,25,19) 94.7834 estimate D2E/DX2 !

! D21 D(2,3,4,5) 0.5536 estimate D2E/DX2 !

! D22 D(2,3,4,41) 179.9832 estimate D2E/DX2 !

! D23 D(6,3,4,5) -178.0266 estimate D2E/DX2 !

! D24 D(6,3,4,41) 1.4029 estimate D2E/DX2 !

! D25 D(2,3,6,7) -4.2138 estimate D2E/DX2 !

! D26 D(4,3,6,7) 174.0897 estimate D2E/DX2 !

! D27 D(3,4,5,1) 0.0 estimate D2E/DX2 !

! D28 D(3,4,5,38) 179.511 estimate D2E/DX2 !

! D29 D(41,4,5,1) -179.511 estimate D2E/DX2 !

! D30 D(41,4,5,38) 0.0 estimate D2E/DX2 !

! D31 D(3,4,41,40) -179.664 estimate D2E/DX2 !

! D32 D(3,4,41,65) 0.3949 estimate D2E/DX2 !

! D33 D(5,4,41,40) -0.3042 estimate D2E/DX2 !

! D34 D(5,4,41,65) 179.7547 estimate D2E/DX2 !

! D35 D(1,5,38,39) 179.664 estimate D2E/DX2 !

! D36 D(1,5,38,64) -0.3949 estimate D2E/DX2 !

! D37 D(4,5,38,39) 0.3042 estimate D2E/DX2 !

! D38 D(4,5,38,64) -179.7547 estimate D2E/DX2 !

! D39 D(3,6,7,8) 1.3449 estimate D2E/DX2 !

! D40 D(3,6,7,11) -176.8191 estimate D2E/DX2 !

! D41 D(6,7,8,9) -176.9588 estimate D2E/DX2 !

! D42 D(6,7,8,25) 16.0591 estimate D2E/DX2 !

! D43 D(11,7,8,9) 1.4182 estimate D2E/DX2 !

! D44 D(11,7,8,25) -165.5639 estimate D2E/DX2 !

! D45 D(6,7,11,10) 177.6289 estimate D2E/DX2 !

! D46 D(6,7,11,34) -1.8461 estimate D2E/DX2 !

! D47 D(8,7,11,10) -0.8475 estimate D2E/DX2 !

! D48 D(8,7,11,34) 179.6775 estimate D2E/DX2 !

! D49 D(7,8,9,10) -1.4182 estimate D2E/DX2 !

! D50 D(7,8,9,24) 176.9588 estimate D2E/DX2 !

! D51 D(25,8,9,10) 165.5639 estimate D2E/DX2 !

! D52 D(25,8,9,24) -16.0591 estimate D2E/DX2 !

! D53 D(7,8,25,2) -21.2313 estimate D2E/DX2 !

! D54 D(7,8,25,16) -97.4231 estimate D2E/DX2 !

! D55 D(7,8,25,19) -173.6149 estimate D2E/DX2 !

! D56 D(9,8,25,2) 173.6149 estimate D2E/DX2 !

! D57 D(9,8,25,16) 97.4231 estimate D2E/DX2 !

! D58 D(9,8,25,19) 21.2313 estimate D2E/DX2 !

! D59 D(8,9,10,11) 0.8475 estimate D2E/DX2 !

! D60 D(8,9,10,37) -179.6775 estimate D2E/DX2 !

! D61 D(24,9,10,11) -177.6289 estimate D2E/DX2 !

! D62 D(24,9,10,37) 1.8461 estimate D2E/DX2 !

! D63 D(8,9,24,23) -1.3449 estimate D2E/DX2 !

! D64 D(10,9,24,23) 176.8191 estimate D2E/DX2 !

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

! D66 D(9,10,11,34) 179.544 estimate D2E/DX2 !

! D67 D(37,10,11,7) -179.544 estimate D2E/DX2 !

! D68 D(37,10,11,34) 0.0 estimate D2E/DX2 !

! D69 D(9,10,37,36) -179.7532 estimate D2E/DX2 !

! D70 D(9,10,37,63) 0.3084 estimate D2E/DX2 !

! D71 D(11,10,37,36) -0.344 estimate D2E/DX2 !

! D72 D(11,10,37,63) 179.7176 estimate D2E/DX2 !

! D73 D(7,11,34,35) 179.7532 estimate D2E/DX2 !

! D74 D(7,11,34,62) -0.3084 estimate D2E/DX2 !

! D75 D(10,11,34,35) 0.344 estimate D2E/DX2 !

! D76 D(10,11,34,62) -179.7176 estimate D2E/DX2 !

! D77 D(1,12,17,13) 176.8191 estimate D2E/DX2 !

! D78 D(1,12,17,16) -1.3449 estimate D2E/DX2 !

! D79 D(17,13,14,15) 0.0 estimate D2E/DX2 !

! D80 D(17,13,14,29) 179.544 estimate D2E/DX2 !

! D81 D(26,13,14,15) -179.544 estimate D2E/DX2 !

! D82 D(26,13,14,29) 0.0 estimate D2E/DX2 !

! D83 D(14,13,17,12) -177.6289 estimate D2E/DX2 !

! D84 D(14,13,17,16) 0.8475 estimate D2E/DX2 !

! D85 D(26,13,17,12) 1.8461 estimate D2E/DX2 !

! D86 D(26,13,17,16) -179.6775 estimate D2E/DX2 !

! D87 D(14,13,26,27) -0.344 estimate D2E/DX2 !

! D88 D(14,13,26,58) 179.7176 estimate D2E/DX2 !

! D89 D(17,13,26,27) -179.7532 estimate D2E/DX2 !

! D90 D(17,13,26,58) 0.3084 estimate D2E/DX2 !

! D91 D(13,14,15,16) -0.8475 estimate D2E/DX2 !

! D92 D(13,14,15,18) 177.6289 estimate D2E/DX2 !

! D93 D(29,14,15,16) 179.6775 estimate D2E/DX2 !

! D94 D(29,14,15,18) -1.8461 estimate D2E/DX2 !

! D95 D(13,14,29,28) 0.344 estimate D2E/DX2 !

! D96 D(13,14,29,59) -179.7176 estimate D2E/DX2 !

! D97 D(15,14,29,28) 179.7532 estimate D2E/DX2 !

! D98 D(15,14,29,59) -0.3084 estimate D2E/DX2 !

! D99 D(14,15,16,17) 1.4182 estimate D2E/DX2 !

! D100 D(14,15,16,25) -165.5639 estimate D2E/DX2 !

! D101 D(18,15,16,17) -176.9588 estimate D2E/DX2 !

! D102 D(18,15,16,25) 16.0591 estimate D2E/DX2 !

! D103 D(14,15,18,20) -176.8191 estimate D2E/DX2 !

! D104 D(16,15,18,20) 1.3449 estimate D2E/DX2 !

! D105 D(15,16,17,12) 176.9588 estimate D2E/DX2 !

! D106 D(15,16,17,13) -1.4182 estimate D2E/DX2 !

! D107 D(25,16,17,12) -16.0591 estimate D2E/DX2 !

! D108 D(25,16,17,13) 165.5639 estimate D2E/DX2 !

! D109 D(15,16,25,2) -173.6149 estimate D2E/DX2 !

! D110 D(15,16,25,8) -97.4231 estimate D2E/DX2 !

! D111 D(15,16,25,19) -21.2313 estimate D2E/DX2 !

! D112 D(17,16,25,2) 21.2313 estimate D2E/DX2 !

! D113 D(17,16,25,8) 97.4231 estimate D2E/DX2 !

! D114 D(17,16,25,19) 173.6149 estimate D2E/DX2 !

! D115 D(15,18,20,19) -4.2138 estimate D2E/DX2 !

! D116 D(15,18,20,21) 174.0897 estimate D2E/DX2 !

! D117 D(23,19,20,18) 177.5772 estimate D2E/DX2 !

! D118 D(23,19,20,21) -0.9301 estimate D2E/DX2 !

! D119 D(25,19,20,18) -10.8063 estimate D2E/DX2 !

! D120 D(25,19,20,21) 170.6864 estimate D2E/DX2 !

! D121 D(20,19,23,22) 0.9301 estimate D2E/DX2 !

! D122 D(20,19,23,24) -177.5772 estimate D2E/DX2 !

! D123 D(25,19,23,22) -170.6864 estimate D2E/DX2 !

! D124 D(25,19,23,24) 10.8063 estimate D2E/DX2 !

! D125 D(20,19,25,2) 94.7834 estimate D2E/DX2 !

! D126 D(20,19,25,8) 170.5979 estimate D2E/DX2 !

! D127 D(20,19,25,16) 18.9689 estimate D2E/DX2 !

! D128 D(23,19,25,2) -94.7834 estimate D2E/DX2 !

! D129 D(23,19,25,8) -18.9689 estimate D2E/DX2 !

! D130 D(23,19,25,16) -170.5979 estimate D2E/DX2 !

! D131 D(18,20,21,22) -178.0266 estimate D2E/DX2 !

! D132 D(18,20,21,33) 1.4029 estimate D2E/DX2 !

! D133 D(19,20,21,22) 0.5536 estimate D2E/DX2 !

! D134 D(19,20,21,33) 179.9832 estimate D2E/DX2 !

! D135 D(20,21,22,23) 0.0 estimate D2E/DX2 !

! D136 D(20,21,22,30) 179.511 estimate D2E/DX2 !

! D137 D(33,21,22,23) -179.511 estimate D2E/DX2 !

! D138 D(33,21,22,30) 0.0 estimate D2E/DX2 !

! D139 D(20,21,33,32) -179.664 estimate D2E/DX2 !

! D140 D(20,21,33,61) 0.3949 estimate D2E/DX2 !

! D141 D(22,21,33,32) -0.3042 estimate D2E/DX2 !

! D142 D(22,21,33,61) 179.7547 estimate D2E/DX2 !

! D143 D(21,22,23,19) -0.5536 estimate D2E/DX2 !

! D144 D(21,22,23,24) 178.0266 estimate D2E/DX2 !

! D145 D(30,22,23,19) -179.9832 estimate D2E/DX2 !

! D146 D(30,22,23,24) -1.4029 estimate D2E/DX2 !

! D147 D(21,22,30,31) 0.3042 estimate D2E/DX2 !

! D148 D(21,22,30,60) -179.7547 estimate D2E/DX2 !

! D149 D(23,22,30,31) 179.664 estimate D2E/DX2 !

! D150 D(23,22,30,60) -0.3949 estimate D2E/DX2 !

! D151 D(19,23,24,9) 4.2138 estimate D2E/DX2 !

! D152 D(22,23,24,9) -174.0897 estimate D2E/DX2 !

! D153 D(13,26,27,28) 0.3382 estimate D2E/DX2 !

! D154 D(13,26,27,49) -179.6882 estimate D2E/DX2 !

! D155 D(58,26,27,28) -179.7222 estimate D2E/DX2 !

! D156 D(58,26,27,49) 0.2514 estimate D2E/DX2 !

! D157 D(26,27,28,29) 0.0 estimate D2E/DX2 !

! D158 D(26,27,28,46) 179.9742 estimate D2E/DX2 !

! D159 D(49,27,28,29) -179.9742 estimate D2E/DX2 !

! D160 D(49,27,28,46) 0.0 estimate D2E/DX2 !

! D161 D(26,27,49,48) 179.9916 estimate D2E/DX2 !

! D162 D(26,27,49,73) 0.002 estimate D2E/DX2 !

! D163 D(28,27,49,48) -0.0346 estimate D2E/DX2 !

! D164 D(28,27,49,73) 179.9759 estimate D2E/DX2 !

! D165 D(27,28,29,14) -0.3382 estimate D2E/DX2 !

! D166 D(27,28,29,59) 179.7222 estimate D2E/DX2 !

! D167 D(46,28,29,14) 179.6882 estimate D2E/DX2 !

! D168 D(46,28,29,59) -0.2514 estimate D2E/DX2 !

! D169 D(27,28,46,47) 0.0346 estimate D2E/DX2 !

! D170 D(27,28,46,70) -179.9759 estimate D2E/DX2 !

! D171 D(29,28,46,47) -179.9916 estimate D2E/DX2 !

! D172 D(29,28,46,70) -0.002 estimate D2E/DX2 !

! D173 D(22,30,31,32) -0.3006 estimate D2E/DX2 !

! D174 D(22,30,31,45) 179.774 estimate D2E/DX2 !

! D175 D(60,30,31,32) 179.7573 estimate D2E/DX2 !

! D176 D(60,30,31,45) -0.1682 estimate D2E/DX2 !

! D177 D(30,31,32,33) 0.0 estimate D2E/DX2 !

! D178 D(30,31,32,42) -179.9274 estimate D2E/DX2 !

! D179 D(45,31,32,33) 179.9274 estimate D2E/DX2 !

! D180 D(45,31,32,42) 0.0 estimate D2E/DX2 !

! D181 D(30,31,45,44) 179.9248 estimate D2E/DX2 !

! D182 D(30,31,45,69) -0.0595 estimate D2E/DX2 !

! D183 D(32,31,45,44) -0.0016 estimate D2E/DX2 !

! D184 D(32,31,45,69) -179.9858 estimate D2E/DX2 !

! D185 D(31,32,33,21) 0.3006 estimate D2E/DX2 !

! D186 D(31,32,33,61) -179.7573 estimate D2E/DX2 !

! D187 D(42,32,33,21) -179.774 estimate D2E/DX2 !

! D188 D(42,32,33,61) 0.1682 estimate D2E/DX2 !

! D189 D(31,32,42,43) 0.0016 estimate D2E/DX2 !

! D190 D(31,32,42,66) 179.9858 estimate D2E/DX2 !

! D191 D(33,32,42,43) -179.9248 estimate D2E/DX2 !

! D192 D(33,32,42,66) 0.0595 estimate D2E/DX2 !

! D193 D(11,34,35,36) -0.3382 estimate D2E/DX2 !

! D194 D(11,34,35,57) 179.6882 estimate D2E/DX2 !

! D195 D(62,34,35,36) 179.7222 estimate D2E/DX2 !

! D196 D(62,34,35,57) -0.2514 estimate D2E/DX2 !

! D197 D(34,35,36,37) 0.0 estimate D2E/DX2 !

! D198 D(34,35,36,54) -179.9742 estimate D2E/DX2 !

! D199 D(57,35,36,37) 179.9742 estimate D2E/DX2 !

! D200 D(57,35,36,54) 0.0 estimate D2E/DX2 !

! D201 D(34,35,57,56) -179.9916 estimate D2E/DX2 !

! D202 D(34,35,57,81) -0.002 estimate D2E/DX2 !

! D203 D(36,35,57,56) 0.0346 estimate D2E/DX2 !

! D204 D(36,35,57,81) -179.9759 estimate D2E/DX2 !

! D205 D(35,36,37,10) 0.3382 estimate D2E/DX2 !

! D206 D(35,36,37,63) -179.7222 estimate D2E/DX2 !

! D207 D(54,36,37,10) -179.6882 estimate D2E/DX2 !

! D208 D(54,36,37,63) 0.2514 estimate D2E/DX2 !

! D209 D(35,36,54,55) -0.0346 estimate D2E/DX2 !

! D210 D(35,36,54,78) 179.9759 estimate D2E/DX2 !

! D211 D(37,36,54,55) 179.9916 estimate D2E/DX2 !

! D212 D(37,36,54,78) 0.002 estimate D2E/DX2 !

! D213 D(5,38,39,40) -0.3006 estimate D2E/DX2 !

! D214 D(5,38,39,53) 179.774 estimate D2E/DX2 !

! D215 D(64,38,39,40) 179.7573 estimate D2E/DX2 !

! D216 D(64,38,39,53) -0.1682 estimate D2E/DX2 !

! D217 D(38,39,40,41) 0.0 estimate D2E/DX2 !

! D218 D(38,39,40,50) -179.9274 estimate D2E/DX2 !

! D219 D(53,39,40,41) 179.9274 estimate D2E/DX2 !

! D220 D(53,39,40,50) 0.0 estimate D2E/DX2 !

! D221 D(38,39,53,52) 179.9248 estimate D2E/DX2 !

! D222 D(38,39,53,77) -0.0595 estimate D2E/DX2 !

! D223 D(40,39,53,52) -0.0016 estimate D2E/DX2 !

! D224 D(40,39,53,77) -179.9858 estimate D2E/DX2 !

! D225 D(39,40,41,4) 0.3006 estimate D2E/DX2 !

! D226 D(39,40,41,65) -179.7573 estimate D2E/DX2 !

! D227 D(50,40,41,4) -179.774 estimate D2E/DX2 !

! D228 D(50,40,41,65) 0.1682 estimate D2E/DX2 !

! D229 D(39,40,50,51) 0.0016 estimate D2E/DX2 !

! D230 D(39,40,50,74) 179.9858 estimate D2E/DX2 !

! D231 D(41,40,50,51) -179.9248 estimate D2E/DX2 !

! D232 D(41,40,50,74) 0.0595 estimate D2E/DX2 !

! D233 D(32,42,43,44) -0.0016 estimate D2E/DX2 !

! D234 D(32,42,43,67) 179.9581 estimate D2E/DX2 !

! D235 D(66,42,43,44) -179.9855 estimate D2E/DX2 !

! D236 D(66,42,43,67) -0.0258 estimate D2E/DX2 !

! D237 D(42,43,44,45) 0.0 estimate D2E/DX2 !

! D238 D(42,43,44,68) 179.9599 estimate D2E/DX2 !

! D239 D(67,43,44,45) -179.9599 estimate D2E/DX2 !

! D240 D(67,43,44,68) 0.0 estimate D2E/DX2 !

! D241 D(43,44,45,31) 0.0016 estimate D2E/DX2 !

! D242 D(43,44,45,69) 179.9855 estimate D2E/DX2 !

! D243 D(68,44,45,31) -179.9581 estimate D2E/DX2 !

! D244 D(68,44,45,69) 0.0258 estimate D2E/DX2 !

! D245 D(28,46,47,48) -0.0351 estimate D2E/DX2 !

! D246 D(28,46,47,71) -179.9995 estimate D2E/DX2 !

! D247 D(70,46,47,48) 179.9756 estimate D2E/DX2 !

! D248 D(70,46,47,71) 0.0111 estimate D2E/DX2 !

! D249 D(46,47,48,49) 0.0 estimate D2E/DX2 !

! D250 D(46,47,48,72) -179.9645 estimate D2E/DX2 !

! D251 D(71,47,48,49) 179.9645 estimate D2E/DX2 !

! D252 D(71,47,48,72) 0.0 estimate D2E/DX2 !

! D253 D(47,48,49,27) 0.0351 estimate D2E/DX2 !

! D254 D(47,48,49,73) -179.9756 estimate D2E/DX2 !

! D255 D(72,48,49,27) 179.9995 estimate D2E/DX2 !

! D256 D(72,48,49,73) -0.0111 estimate D2E/DX2 !

! D257 D(40,50,51,52) -0.0016 estimate D2E/DX2 !

! D258 D(40,50,51,75) 179.9581 estimate D2E/DX2 !

! D259 D(74,50,51,52) -179.9855 estimate D2E/DX2 !

! D260 D(74,50,51,75) -0.0258 estimate D2E/DX2 !

! D261 D(50,51,52,53) 0.0 estimate D2E/DX2 !

! D262 D(50,51,52,76) 179.9599 estimate D2E/DX2 !

! D263 D(75,51,52,53) -179.9599 estimate D2E/DX2 !

! D264 D(75,51,52,76) 0.0 estimate D2E/DX2 !

! D265 D(51,52,53,39) 0.0016 estimate D2E/DX2 !

! D266 D(51,52,53,77) 179.9855 estimate D2E/DX2 !

! D267 D(76,52,53,39) -179.9581 estimate D2E/DX2 !

! D268 D(76,52,53,77) 0.0258 estimate D2E/DX2 !

! D269 D(36,54,55,56) 0.0351 estimate D2E/DX2 !

! D270 D(36,54,55,79) 179.9995 estimate D2E/DX2 !

! D271 D(78,54,55,56) -179.9756 estimate D2E/DX2 !

! D272 D(78,54,55,79) -0.0111 estimate D2E/DX2 !

! D273 D(54,55,56,57) 0.0 estimate D2E/DX2 !

! D274 D(54,55,56,80) 179.9645 estimate D2E/DX2 !

! D275 D(79,55,56,57) -179.9645 estimate D2E/DX2 !

! D276 D(79,55,56,80) 0.0 estimate D2E/DX2 !

! D277 D(55,56,57,35) -0.0351 estimate D2E/DX2 !

! D278 D(55,56,57,81) 179.9756 estimate D2E/DX2 !

! D279 D(80,56,57,35) -179.9995 estimate D2E/DX2 !

! D280 D(80,56,57,81) 0.0111 estimate D2E/DX2 !

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

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

Number of steps in this run= 486 maximum allowed number of steps= 486.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Jun 30 19:49:27 2019, MaxMem= 1342177280 cpu: 0.3

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

Stoichiometry C48H24N8Zn(3)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C48H24N4)]

Deg. of freedom 61

Full point group C2V NOp 4

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 1.122098 2.799610 0.143329

2 7 0 0.000000 2.023672 0.243534

3 6 0 -1.122098 2.799610 0.143329

4 6 0 -0.719051 4.187993 -0.013436

5 6 0 0.719051 4.187993 -0.013436

6 7 0 -2.415638 2.389563 0.150456

7 6 0 -2.799037 1.128368 0.179488

8 7 0 -2.010819 0.000000 0.233123

9 6 0 -2.799037 -1.128368 0.179488

10 6 0 -4.214374 -0.713830 0.117869

11 6 0 -4.214374 0.713830 0.117869

12 7 0 2.415638 2.389563 0.150456

13 6 0 4.214374 0.713830 0.117869

14 6 0 4.214374 -0.713830 0.117869

15 6 0 2.799037 -1.128368 0.179488

16 7 0 2.010819 0.000000 0.233123

17 6 0 2.799037 1.128368 0.179488

18 7 0 2.415638 -2.389563 0.150456

19 7 0 0.000000 -2.023672 0.243534

20 6 0 1.122098 -2.799610 0.143329

21 6 0 0.719051 -4.187993 -0.013436

22 6 0 -0.719051 -4.187993 -0.013436

23 6 0 -1.122098 -2.799610 0.143329

24 7 0 -2.415638 -2.389563 0.150456

25 30 0 0.000000 0.000000 0.757537

26 6 0 5.382867 1.430187 0.057677

27 6 0 6.620182 0.720248 0.001469

28 6 0 6.620182 -0.720248 0.001469

29 6 0 5.382867 -1.430187 0.057677

30 6 0 -1.432168 -5.360765 -0.156002

31 6 0 -0.722616 -6.583261 -0.297962

32 6 0 0.722616 -6.583261 -0.297962

33 6 0 1.432168 -5.360765 -0.156002

34 6 0 -5.382867 1.430187 0.057677

35 6 0 -6.620182 0.720248 0.001469

36 6 0 -6.620182 -0.720248 0.001469

37 6 0 -5.382867 -1.430187 0.057677

38 6 0 1.432168 5.360765 -0.156002

39 6 0 0.722616 6.583261 -0.297962

40 6 0 -0.722616 6.583261 -0.297962

41 6 0 -1.432168 5.360765 -0.156002

42 6 0 1.405965 -7.822982 -0.443515

43 6 0 0.709758 -9.005334 -0.582365

44 6 0 -0.709758 -9.005334 -0.582365

45 6 0 -1.405965 -7.822982 -0.443515

46 6 0 7.861980 -1.405053 -0.055502

47 6 0 9.053768 -0.707732 -0.109462

48 6 0 9.053768 0.707732 -0.109462

49 6 0 7.861980 1.405053 -0.055502

50 6 0 -1.405965 7.822982 -0.443515

51 6 0 -0.709758 9.005334 -0.582365

52 6 0 0.709758 9.005334 -0.582365

53 6 0 1.405965 7.822982 -0.443515

54 6 0 -7.861980 -1.405053 -0.055502

55 6 0 -9.053768 -0.707732 -0.109462

56 6 0 -9.053768 0.707732 -0.109462

57 6 0 -7.861980 1.405053 -0.055502

58 1 0 5.385060 2.516433 0.052998

59 1 0 5.385060 -2.516433 0.052998

60 1 0 -2.518555 -5.365820 -0.160615

61 1 0 2.518555 -5.365820 -0.160615

62 1 0 -5.385060 2.516433 0.052998

63 1 0 -5.385060 -2.516433 0.052998

64 1 0 2.518555 5.365820 -0.160615

65 1 0 -2.518555 5.365820 -0.160615

66 1 0 2.492795 -7.819422 -0.443335

67 1 0 1.246479 -9.943003 -0.693146

68 1 0 -1.246479 -9.943003 -0.693146

69 1 0 -2.492795 -7.819422 -0.443335

70 1 0 7.858142 -2.491702 -0.055728

71 1 0 9.996231 -1.245593 -0.152718

72 1 0 9.996231 1.245593 -0.152718

73 1 0 7.858142 2.491702 -0.055728

74 1 0 -2.492795 7.819422 -0.443335

75 1 0 -1.246479 9.943003 -0.693146

76 1 0 1.246479 9.943003 -0.693146

77 1 0 2.492795 7.819422 -0.443335

78 1 0 -7.858142 -2.491702 -0.055728

79 1 0 -9.996231 -1.245593 -0.152718

80 1 0 -9.996231 1.245593 -0.152718

81 1 0 -7.858142 2.491702 -0.055728

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

Rotational constants (GHZ): 0.0383820 0.0380061 0.0192116

Leave Link 202 at Sun Jun 30 19:49:27 2019, MaxMem= 1342177280 cpu: 0.5

(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: 58 59 60 61 62 63 64 65 66 67

Centers: 68 69 70 71 72 73 74 75 76 77

Centers: 78 79 80 81 1 3 4 5 7 9

Centers: 10 11 13 14 15 17 20 21 22 23

Centers: 26 27 28 29 30 31 32 33 34 35

Centers: 36 37 38 39 40 41 42 43 44 45

Centers: 46 47 48 49 50 51 52 53 54 55

Centers: 56 57 2 6 8 12 16 18 19 24

6-311G\*

\*\*\*\*

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

Pseudopotential Parameters

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

Center Atomic Valence Angular Power

Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

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

1 6

No pseudopotential on this center.

2 7

No pseudopotential on this center.

3 6

No pseudopotential on this center.

4 6

No pseudopotential on this center.

5 6

No pseudopotential on this center.

6 7

No pseudopotential on this center.

7 6

No pseudopotential on this center.

8 7

No pseudopotential on this center.

9 6

No pseudopotential on this center.

10 6

No pseudopotential on this center.

11 6

No pseudopotential on this center.

12 7

No pseudopotential on this center.

13 6

No pseudopotential on this center.

14 6

No pseudopotential on this center.

15 6

No pseudopotential on this center.

16 7

No pseudopotential on this center.

17 6

No pseudopotential on this center.

18 7

No pseudopotential on this center.

19 7

No pseudopotential on this center.

20 6

No pseudopotential on this center.

21 6

No pseudopotential on this center.

22 6

No pseudopotential on this center.

23 6

No pseudopotential on this center.

24 7

No pseudopotential on this center.

25 30 12

F and up

1 386.7379660 -18.00000000 0.00000000

2 72.8587359 -124.35274030 0.00000000

2 15.9066170 -30.66018220 0.00000000

2 4.3502340 -10.63589890 0.00000000

2 1.2842199 -0.76836230 0.00000000

S - F

0 19.0867858 3.00000000 0.00000000

1 5.0231080 22.52342250 0.00000000

2 1.2701744 48.44659420 0.00000000

2 1.0671287 -44.55601190 0.00000000

2 0.9264190 12.99839580 0.00000000

P - F

0 43.4927750 5.00000000 0.00000000

1 20.8692669 20.74355890 0.00000000

2 21.7118378 90.30271580 0.00000000

2 6.3616915 74.66103160 0.00000000

2 1.2291195 9.88944240 0.00000000

D - F

2 13.5851800 -4.84903590 0.00000000

2 9.8373050 3.69133790 0.00000000

2 0.8373113 -0.50373190 0.00000000

26 6

No pseudopotential on this center.

27 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 6

No pseudopotential on this center.

43 6

No pseudopotential on this center.

44 6

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45 6

No pseudopotential on this center.

46 6

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47 6

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48 6

No pseudopotential on this center.

49 6

No pseudopotential on this center.

50 6

No pseudopotential on this center.

51 6

No pseudopotential on this center.

52 6

No pseudopotential on this center.

53 6

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54 6

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55 6

No pseudopotential on this center.

56 6

No pseudopotential on this center.

57 6

No pseudopotential on this center.

58 1

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 1

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 1

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 1

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 1

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 1

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.

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

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

There are 307 symmetry adapted cartesian basis functions of A1 symmetry.

There are 278 symmetry adapted cartesian basis functions of A2 symmetry.

There are 289 symmetry adapted cartesian basis functions of B1 symmetry.

There are 289 symmetry adapted cartesian basis functions of B2 symmetry.

There are 289 symmetry adapted basis functions of A1 symmetry.

There are 265 symmetry adapted basis functions of A2 symmetry.

There are 275 symmetry adapted basis functions of B1 symmetry.

There are 275 symmetry adapted basis functions of B2 symmetry.

1104 basis functions, 1951 primitive gaussians, 1163 cartesian basis functions

191 alpha electrons 189 beta electrons

nuclear repulsion energy 6873.6130570138 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= 81 NActive= 81 NUniq= 22 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= -0.2357670630 Hartrees.

Nuclear repulsion after empirical dispersion term = 6873.3772899508 Hartrees.

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

Polarizable Continuum Model (PCM)

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 81.

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 = 81

GePol: Total number of spheres = 81

GePol: Number of exposed spheres = 81 (100.00%)

GePol: Number of points = 6398

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.57D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 336

GePol: Fraction of low-weight points (<1% of avg) = 5.25%

GePol: Cavity surface area = 673.789 Ang\*\*2

GePol: Cavity volume = 696.795 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0166906258 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 6873.3605993250 Hartrees.

Leave Link 301 at Sun Jun 30 19:49:28 2019, MaxMem= 1342177280 cpu: 2.1

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36581 LenP2D= 94878.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1104 RedAO= T EigKep= 2.94D-05 NBF= 289 265 275 275

NBsUse= 1104 1.00D-06 EigRej= -1.00D+00 NBFU= 289 265 275 275

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= 1060 1060 1060 1060 1060 MxSgAt= 81 MxSgA2= 81.

Leave Link 302 at Sun Jun 30 19:49:42 2019, MaxMem= 1342177280 cpu: 146.2

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Jun 30 19:49:43 2019, MaxMem= 1342177280 cpu: 3.4

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

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2348.34533507917

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

Alpha Orbitals:

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The electronic state of the initial guess is 3-B2.

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

Leave Link 401 at Sun Jun 30 19:49:53 2019, MaxMem= 1342177280 cpu: 113.6

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4103221 IEndB= 4103221 NGot= 1342177280 MDV= 1339444432

LenX= 1339444432 LenY= 1338090700

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= 420000000 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= 122803212.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.99D-15 for 6398.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.16D-15 for 6379 6292.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.99D-15 for 6398.

Iteration 1 A^-1\*A deviation from orthogonality is 8.07D-11 for 1290 1268.

E= -2347.03988166301

DIIS: error= 8.85D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2347.03988166301 IErMin= 1 ErrMin= 8.85D-02

ErrMax= 8.85D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.51D+00 BMatP= 5.51D+00

IDIUse=3 WtCom= 1.15D-01 WtEn= 8.85D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.020 Goal= None Shift= 0.000

GapD= 0.020 DampG=0.250 DampE=0.250 DampFc=0.1250 IDamp=-1.

Damping current iteration by 1.25D-01

RMSDP=2.17D-03 MaxDP=8.96D-02 OVMax= 4.35D-01

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.71D-04 CP: 9.98D-01

E= -2347.26393836850 Delta-E= -0.224056705496 Rises=F Damp=T

DIIS: error= 6.33D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2347.26393836850 IErMin= 2 ErrMin= 6.33D-02

ErrMax= 6.33D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.23D+00 BMatP= 5.51D+00

IDIUse=3 WtCom= 3.67D-01 WtEn= 6.33D-01

Coeff-Com: -0.296D+01 0.396D+01

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

Coeff: -0.109D+01 0.209D+01

Gap= 0.037 Goal= None Shift= 0.000

Gap= 0.058 Goal= None Shift= 0.000

RMSDP=1.32D-03 MaxDP=5.62D-02 DE=-2.24D-01 OVMax= 2.65D-01

Cycle 3 Pass 1 IDiag 1:

RMSU= 8.10D-04 CP: 9.82D-01 3.00D+00

E= -2347.94104624622 Delta-E= -0.677107877715 Rises=F Damp=F

DIIS: error= 4.12D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2347.94104624622 IErMin= 3 ErrMin= 4.12D-02

ErrMax= 4.12D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.06D-01 BMatP= 3.23D+00

IDIUse=3 WtCom= 5.88D-01 WtEn= 4.12D-01

Coeff-Com: 0.186D+01-0.191D+01 0.105D+01

Coeff-En: 0.388D-01 0.000D+00 0.961D+00

Coeff: 0.111D+01-0.113D+01 0.102D+01

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.087 Goal= None Shift= 0.000

RMSDP=6.57D-04 MaxDP=3.00D-02 DE=-6.77D-01 OVMax= 1.52D-01

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.80D-04 CP: 9.84D-01 3.00D+00 3.39D-01

E= -2348.09621386183 Delta-E= -0.155167615609 Rises=F Damp=F

DIIS: error= 1.70D-02 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2348.09621386183 IErMin= 4 ErrMin= 1.70D-02

ErrMax= 1.70D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.69D-01 BMatP= 9.06D-01

IDIUse=3 WtCom= 8.30D-01 WtEn= 1.70D-01

Coeff-Com: -0.255D+00 0.327D+00 0.255D+00 0.673D+00

Coeff-En: 0.000D+00 0.000D+00 0.948D-01 0.905D+00

Coeff: -0.212D+00 0.272D+00 0.228D+00 0.712D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.080 Goal= None Shift= 0.000

RMSDP=1.97D-04 MaxDP=1.17D-02 DE=-1.55D-01 OVMax= 3.78D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 5.57D-05 CP: 9.84D-01 3.00D+00 5.28D-01 7.11D-01

E= -2348.12753193508 Delta-E= -0.031318073252 Rises=F Damp=F

DIIS: error= 2.28D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2348.12753193508 IErMin= 5 ErrMin= 2.28D-03

ErrMax= 2.28D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-02 BMatP= 1.69D-01

IDIUse=3 WtCom= 9.77D-01 WtEn= 2.28D-02

Coeff-Com: -0.220D+00 0.257D+00 0.946D-01 0.441D+00 0.427D+00

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

Coeff: -0.215D+00 0.251D+00 0.925D-01 0.431D+00 0.440D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.082 Goal= None Shift= 0.000

RMSDP=3.81D-05 MaxDP=3.61D-03 DE=-3.13D-02 OVMax= 8.07D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.23D-05 CP: 9.84D-01 3.00D+00 5.11D-01 7.43D-01 5.60D-01

E= -2348.12972207388 Delta-E= -0.002190138805 Rises=F Damp=F

DIIS: error= 6.02D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2348.12972207388 IErMin= 6 ErrMin= 6.02D-04

ErrMax= 6.02D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.40D-04 BMatP= 1.03D-02

IDIUse=3 WtCom= 9.94D-01 WtEn= 6.02D-03

Coeff-Com: -0.110D+00 0.126D+00 0.167D-01 0.152D+00 0.212D+00 0.604D+00

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

Coeff: -0.109D+00 0.125D+00 0.166D-01 0.151D+00 0.210D+00 0.606D+00

Gap= 0.041 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=1.11D-05 MaxDP=1.08D-03 DE=-2.19D-03 OVMax= 3.41D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 8.85D-06 CP: 9.84D-01 3.00D+00 5.12D-01 7.50D-01 6.40D-01

CP: 8.10D-01

E= -2348.12981106191 Delta-E= -0.000088988030 Rises=F Damp=F

DIIS: error= 2.17D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2348.12981106191 IErMin= 7 ErrMin= 2.17D-04

ErrMax= 2.17D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.88D-05 BMatP= 3.40D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.17D-03

Coeff-Com: -0.341D-01 0.380D-01-0.693D-02 0.160D-01 0.445D-01 0.343D+00

Coeff-Com: 0.599D+00

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

Coeff-En: 0.100D+01

Coeff: -0.340D-01 0.379D-01-0.691D-02 0.159D-01 0.444D-01 0.342D+00

Coeff: 0.600D+00

Gap= 0.041 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=5.52D-06 MaxDP=5.50D-04 DE=-8.90D-05 OVMax= 2.30D-03

Cycle 8 Pass 1 IDiag 1:

RMSU= 4.16D-06 CP: 9.84D-01 3.00D+00 5.14D-01 7.49D-01 6.54D-01

CP: 9.46D-01 9.49D-01

E= -2348.12984205966 Delta-E= -0.000030997748 Rises=F Damp=F

DIIS: error= 1.09D-04 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2348.12984205966 IErMin= 8 ErrMin= 1.09D-04

ErrMax= 1.09D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.50D-05 BMatP= 7.88D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.09D-03

Coeff-Com: 0.387D-01-0.446D-01-0.108D-01-0.670D-01-0.855D-01-0.148D+00

Coeff-Com: 0.237D+00 0.108D+01

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

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

Coeff: 0.387D-01-0.446D-01-0.108D-01-0.669D-01-0.854D-01-0.147D+00

Coeff: 0.237D+00 0.108D+01

Gap= 0.041 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=5.19D-06 MaxDP=5.74D-04 DE=-3.10D-05 OVMax= 2.64D-03

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.36D-06 CP: 9.84D-01 3.00D+00 5.13D-01 7.51D-01 6.80D-01

CP: 1.06D+00 1.31D+00 1.22D+00

E= -2348.12985547773 Delta-E= -0.000013418074 Rises=F Damp=F

DIIS: error= 4.60D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2348.12985547773 IErMin= 9 ErrMin= 4.60D-05

ErrMax= 4.60D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.61D-06 BMatP= 1.50D-05

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

Coeff-Com: 0.275D-01-0.316D-01-0.517D-02-0.401D-01-0.527D-01-0.134D+00

Coeff-Com: 0.450D-01 0.633D+00 0.558D+00

Coeff: 0.275D-01-0.316D-01-0.517D-02-0.401D-01-0.527D-01-0.134D+00

Coeff: 0.450D-01 0.633D+00 0.558D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=2.02D-06 MaxDP=1.41D-04 DE=-1.34D-05 OVMax= 7.95D-04

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.43D-06 CP: 9.84D-01 3.00D+00 5.14D-01 7.50D-01 6.84D-01

CP: 1.06D+00 1.34D+00 1.48D+00 8.70D-01

E= -2348.12985749814 Delta-E= -0.000002020404 Rises=F Damp=F

DIIS: error= 2.02D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -2348.12985749814 IErMin=10 ErrMin= 2.02D-05

ErrMax= 2.02D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.81D-07 BMatP= 5.61D-06

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

Coeff-Com: 0.335D-02-0.376D-02 0.617D-03-0.704D-03-0.122D-03-0.234D-01

Coeff-Com: -0.386D-01 0.116D-01 0.245D+00 0.806D+00

Coeff: 0.335D-02-0.376D-02 0.617D-03-0.704D-03-0.122D-03-0.234D-01

Coeff: -0.386D-01 0.116D-01 0.245D+00 0.806D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=6.66D-07 MaxDP=7.50D-05 DE=-2.02D-06 OVMax= 2.11D-04

Cycle 11 Pass 1 IDiag 1:

RMSU= 4.18D-07 CP: 9.84D-01 3.00D+00 5.14D-01 7.50D-01 6.84D-01

CP: 1.07D+00 1.35D+00 1.52D+00 1.05D+00 1.00D+00

E= -2348.12985775133 Delta-E= -0.000000253189 Rises=F Damp=F

DIIS: error= 1.04D-05 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -2348.12985775133 IErMin=11 ErrMin= 1.04D-05

ErrMax= 1.04D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.82D-07 BMatP= 6.81D-07

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

Coeff-Com: -0.113D-02 0.134D-02 0.816D-03 0.369D-02 0.523D-02 0.678D-05

Coeff-Com: -0.237D-01-0.585D-01 0.766D-01 0.448D+00 0.548D+00

Coeff: -0.113D-02 0.134D-02 0.816D-03 0.369D-02 0.523D-02 0.678D-05

Coeff: -0.237D-01-0.585D-01 0.766D-01 0.448D+00 0.548D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=2.67D-07 MaxDP=2.37D-05 DE=-2.53D-07 OVMax= 1.28D-04

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.43D-07 CP: 9.84D-01 3.00D+00 5.14D-01 7.50D-01 6.84D-01

CP: 1.07D+00 1.35D+00 1.53D+00 1.08D+00 1.05D+00

CP: 9.00D-01

E= -2348.12985780575 Delta-E= -0.000000054426 Rises=F Damp=F

DIIS: error= 5.30D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -2348.12985780575 IErMin=12 ErrMin= 5.30D-06

ErrMax= 5.30D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.56D-08 BMatP= 1.82D-07

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

Coeff-Com: -0.127D-02 0.146D-02 0.228D-03 0.179D-02 0.223D-02 0.438D-02

Coeff-Com: -0.132D-02-0.315D-01-0.177D-01 0.237D-01 0.306D+00 0.712D+00

Coeff: -0.127D-02 0.146D-02 0.228D-03 0.179D-02 0.223D-02 0.438D-02

Coeff: -0.132D-02-0.315D-01-0.177D-01 0.237D-01 0.306D+00 0.712D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=1.41D-07 MaxDP=1.39D-05 DE=-5.44D-08 OVMax= 5.50D-05

Cycle 13 Pass 1 IDiag 1:

RMSU= 8.50D-08 CP: 9.84D-01 3.00D+00 5.14D-01 7.50D-01 6.84D-01

CP: 1.07D+00 1.36D+00 1.53D+00 1.10D+00 1.07D+00

CP: 1.11D+00 9.91D-01

E= -2348.12985781834 Delta-E= -0.000000012587 Rises=F Damp=F

DIIS: error= 1.92D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -2348.12985781834 IErMin=13 ErrMin= 1.92D-06

ErrMax= 1.92D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.98D-09 BMatP= 3.56D-08

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

Coeff-Com: -0.544D-03 0.618D-03 0.135D-04 0.472D-03 0.448D-03 0.267D-02

Coeff-Com: 0.325D-02-0.940D-02-0.214D-01-0.642D-01 0.920D-01 0.426D+00

Coeff-Com: 0.570D+00

Coeff: -0.544D-03 0.618D-03 0.135D-04 0.472D-03 0.448D-03 0.267D-02

Coeff: 0.325D-02-0.940D-02-0.214D-01-0.642D-01 0.920D-01 0.426D+00

Coeff: 0.570D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=5.98D-08 MaxDP=4.91D-06 DE=-1.26D-08 OVMax= 3.52D-05

Cycle 14 Pass 1 IDiag 1:

RMSU= 4.07D-08 CP: 9.84D-01 3.00D+00 5.14D-01 7.50D-01 6.84D-01

CP: 1.07D+00 1.35D+00 1.53D+00 1.10D+00 1.08D+00

CP: 1.15D+00 1.11D+00 8.10D-01

E= -2348.12985782107 Delta-E= -0.000000002730 Rises=F Damp=F

DIIS: error= 1.01D-06 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -2348.12985782107 IErMin=14 ErrMin= 1.01D-06

ErrMax= 1.01D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-09 BMatP= 8.98D-09

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

Coeff-Com: 0.125D-03-0.148D-03-0.274D-04-0.208D-03-0.303D-03 0.178D-03

Coeff-Com: 0.134D-02 0.285D-02-0.268D-02-0.314D-01-0.417D-01-0.209D-01

Coeff-Com: 0.245D+00 0.848D+00

Coeff: 0.125D-03-0.148D-03-0.274D-04-0.208D-03-0.303D-03 0.178D-03

Coeff: 0.134D-02 0.285D-02-0.268D-02-0.314D-01-0.417D-01-0.209D-01

Coeff: 0.245D+00 0.848D+00

Gap= 0.041 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=3.01D-08 MaxDP=2.13D-06 DE=-2.73D-09 OVMax= 1.42D-05

Cycle 15 Pass 1 IDiag 1:

RMSU= 1.49D-08 CP: 9.84D-01 3.00D+00 5.14D-01 7.50D-01 6.84D-01

CP: 1.07D+00 1.35D+00 1.53D+00 1.11D+00 1.08D+00

CP: 1.18D+00 1.16D+00 9.75D-01 1.03D+00

E= -2348.12985782170 Delta-E= -0.000000000624 Rises=F Damp=F

DIIS: error= 1.63D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -2348.12985782170 IErMin=15 ErrMin= 1.63D-07

ErrMax= 1.63D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.56D-11 BMatP= 1.05D-09

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

Coeff-Com: 0.828D-04-0.960D-04-0.936D-05-0.970D-04-0.106D-03-0.162D-03

Coeff-Com: 0.113D-03 0.141D-02 0.898D-03-0.396D-02-0.189D-01-0.408D-01

Coeff-Com: 0.249D-01 0.261D+00 0.776D+00

Coeff: 0.828D-04-0.960D-04-0.936D-05-0.970D-04-0.106D-03-0.162D-03

Coeff: 0.113D-03 0.141D-02 0.898D-03-0.396D-02-0.189D-01-0.408D-01

Coeff: 0.249D-01 0.261D+00 0.776D+00

Gap= 0.041 Goal= None Shift= 0.000

Gap= 0.083 Goal= None Shift= 0.000

RMSDP=8.08D-09 MaxDP=7.61D-07 DE=-6.24D-10 OVMax= 4.14D-06

Error on total polarization charges = 0.08852

SCF Done: E(UB3LYP) = -2348.12985782 A.U. after 15 cycles

NFock= 15 Conv=0.81D-08 -V/T= 1.9832

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0222 S= 1.0074

<L.S>= 0.000000000000E+00

KE= 2.388162461931D+03 PE=-1.928967771397D+04 EE= 7.680024794896D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -10.47

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0222, after 2.0003

Leave Link 502 at Sun Jun 30 20:01:40 2019, MaxMem= 1342177280 cpu: 7725.9

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

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

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Population analysis using the SCF density.

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Orbital symmetries:

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The electronic state is 3-B2.

Alpha occ. eigenvalues -- -14.31855 -14.31854 -14.30947 -14.30947 -14.30880

Alpha occ. eigenvalues -- -14.30880 -14.30880 -14.30879 -10.25712 -10.25712

Alpha occ. eigenvalues -- -10.25711 -10.25711 -10.24862 -10.24862 -10.24860

Alpha occ. eigenvalues -- -10.24860 -10.19527 -10.19527 -10.19488 -10.19488

Alpha occ. eigenvalues -- -10.19171 -10.19171 -10.19133 -10.19133 -10.19012

Alpha occ. eigenvalues -- -10.19012 -10.19012 -10.19012 -10.18809 -10.18809

Alpha occ. eigenvalues -- -10.18767 -10.18767 -10.18705 -10.18705 -10.18704

Alpha occ. eigenvalues -- -10.18704 -10.18264 -10.18264 -10.18224 -10.18224

Alpha occ. eigenvalues -- -10.18035 -10.18035 -10.18033 -10.18033 -10.17957

Alpha occ. eigenvalues -- -10.17957 -10.17915 -10.17915 -10.17842 -10.17842

Alpha occ. eigenvalues -- -10.17842 -10.17842 -10.17732 -10.17732 -10.17691

Alpha occ. eigenvalues -- -10.17691 -1.00332 -0.99021 -0.98930 -0.96293

Alpha occ. eigenvalues -- -0.94082 -0.90388 -0.89813 -0.88396 -0.88041

Alpha occ. eigenvalues -- -0.87933 -0.87818 -0.86388 -0.82969 -0.82905

Alpha occ. eigenvalues -- -0.82538 -0.82532 -0.79141 -0.78635 -0.78462

Alpha occ. eigenvalues -- -0.78411 -0.75603 -0.75590 -0.75579 -0.75272

Alpha occ. eigenvalues -- -0.75171 -0.73646 -0.73613 -0.72930 -0.70734

Alpha occ. eigenvalues -- -0.69453 -0.68779 -0.65954 -0.65647 -0.65271

Alpha occ. eigenvalues -- -0.65024 -0.63057 -0.62498 -0.60977 -0.60881

Alpha occ. eigenvalues -- -0.60478 -0.60430 -0.60429 -0.60156 -0.60088

Alpha occ. eigenvalues -- -0.59764 -0.58029 -0.56852 -0.56637 -0.56589

Alpha occ. eigenvalues -- -0.55937 -0.54507 -0.54403 -0.54134 -0.53574

Alpha occ. eigenvalues -- -0.53501 -0.53278 -0.51787 -0.51712 -0.51611

Alpha occ. eigenvalues -- -0.51588 -0.51380 -0.51117 -0.50785 -0.50718

Alpha occ. eigenvalues -- -0.49083 -0.46458 -0.45842 -0.45827 -0.45713

Alpha occ. eigenvalues -- -0.45634 -0.45460 -0.45105 -0.45021 -0.45003

Alpha occ. eigenvalues -- -0.44876 -0.44377 -0.44065 -0.43786 -0.43639

Alpha occ. eigenvalues -- -0.43464 -0.43305 -0.42987 -0.42939 -0.42590

Alpha occ. eigenvalues -- -0.42558 -0.42214 -0.42122 -0.42035 -0.41405

Alpha occ. eigenvalues -- -0.39777 -0.39753 -0.39560 -0.38948 -0.38943

Alpha occ. eigenvalues -- -0.38621 -0.37866 -0.37645 -0.37225 -0.36707

Alpha occ. eigenvalues -- -0.35757 -0.35627 -0.35492 -0.35317 -0.34509

Alpha occ. eigenvalues -- -0.34374 -0.34286 -0.34168 -0.33962 -0.33659

Alpha occ. eigenvalues -- -0.33228 -0.32774 -0.32663 -0.32084 -0.31688

Alpha occ. eigenvalues -- -0.31639 -0.30749 -0.30713 -0.29840 -0.29464

Alpha occ. eigenvalues -- -0.29301 -0.27972 -0.27869 -0.26674 -0.26305

Alpha occ. eigenvalues -- -0.25450 -0.25349 -0.25257 -0.25194 -0.24795

Alpha occ. eigenvalues -- -0.24722 -0.23026 -0.23005 -0.22921 -0.18580

Alpha occ. eigenvalues -- -0.14242

Alpha virt. eigenvalues -- -0.10092 -0.06726 -0.06312 -0.06035 -0.05817

Alpha virt. eigenvalues -- -0.05018 -0.00459 -0.00442 -0.00334 0.00262

Alpha virt. eigenvalues -- 0.00449 0.00883 0.01098 0.02001 0.02322

Alpha virt. eigenvalues -- 0.04221 0.04970 0.04990 0.05914 0.06241

Alpha virt. eigenvalues -- 0.06267 0.06285 0.06356 0.07092 0.07316

Alpha virt. eigenvalues -- 0.07335 0.07716 0.08318 0.08693 0.08733

Alpha virt. eigenvalues -- 0.09656 0.09657 0.10522 0.10867 0.10928

Alpha virt. eigenvalues -- 0.11601 0.11615 0.11805 0.11879 0.12259

Alpha virt. eigenvalues -- 0.12419 0.12442 0.12495 0.13275 0.13304

Alpha virt. eigenvalues -- 0.14338 0.14529 0.16285 0.16367 0.17795

Alpha virt. eigenvalues -- 0.18067 0.18180 0.18252 0.18444 0.18462

Alpha virt. eigenvalues -- 0.18613 0.18639 0.18685 0.19244 0.20326

Alpha virt. eigenvalues -- 0.21188 0.21498 0.22103 0.22321 0.22798

Alpha virt. eigenvalues -- 0.22857 0.22949 0.23991 0.24256 0.24585

Alpha virt. eigenvalues -- 0.25461 0.25689 0.25962 0.26237 0.26487

Alpha virt. eigenvalues -- 0.27426 0.27648 0.27682 0.27711 0.27855

Alpha virt. eigenvalues -- 0.28054 0.28214 0.28451 0.28532 0.28912

Alpha virt. eigenvalues -- 0.28953 0.29448 0.30320 0.30486 0.30518

Alpha virt. eigenvalues -- 0.30615 0.30878 0.31008 0.31058 0.31750

Alpha virt. eigenvalues -- 0.31753 0.32562 0.32634 0.32953 0.34412

Alpha virt. eigenvalues -- 0.34563 0.34845 0.34904 0.35499 0.35786

Alpha virt. eigenvalues -- 0.35995 0.36476 0.36802 0.37003 0.37191

Alpha virt. eigenvalues -- 0.37260 0.37456 0.37694 0.37747 0.37873

Alpha virt. eigenvalues -- 0.38214 0.38233 0.38371 0.38587 0.39031

Alpha virt. eigenvalues -- 0.39066 0.39080 0.39627 0.39698 0.39989

Alpha virt. eigenvalues -- 0.40065 0.40137 0.40165 0.40667 0.40672

Alpha virt. eigenvalues -- 0.40968 0.41027 0.41379 0.41593 0.41893

Alpha virt. eigenvalues -- 0.42364 0.42604 0.42737 0.42831 0.42852

Alpha virt. eigenvalues -- 0.42993 0.43011 0.43167 0.43303 0.43367

Alpha virt. eigenvalues -- 0.43385 0.43416 0.43855 0.43930 0.44193

Alpha virt. eigenvalues -- 0.44286 0.44456 0.44641 0.44783 0.44955

Alpha virt. eigenvalues -- 0.45160 0.45972 0.46055 0.46082 0.46195

Alpha virt. eigenvalues -- 0.46422 0.46474 0.46581 0.46873 0.47054

Alpha virt. eigenvalues -- 0.47058 0.47382 0.47535 0.47603 0.47875

Alpha virt. eigenvalues -- 0.48344 0.48684 0.48763 0.48999 0.49325

Alpha virt. eigenvalues -- 0.49574 0.50140 0.50471 0.50635 0.50689

Alpha virt. eigenvalues -- 0.51154 0.51413 0.51414 0.51954 0.52105

Alpha virt. eigenvalues -- 0.52998 0.53112 0.53189 0.53210 0.53531

Alpha virt. eigenvalues -- 0.53562 0.54400 0.54805 0.55186 0.55567

Alpha virt. eigenvalues -- 0.56272 0.56284 0.56407 0.57784 0.58023

Alpha virt. eigenvalues -- 0.58624 0.58815 0.59251 0.59929 0.60152

Alpha virt. eigenvalues -- 0.60409 0.60577 0.60788 0.60852 0.61197

Alpha virt. eigenvalues -- 0.61433 0.61609 0.61624 0.61962 0.62041

Alpha virt. eigenvalues -- 0.62421 0.62525 0.62736 0.62758 0.62923

Alpha virt. eigenvalues -- 0.62986 0.63346 0.63352 0.64235 0.64351

Alpha virt. eigenvalues -- 0.64365 0.64481 0.65236 0.65569 0.65587

Alpha virt. eigenvalues -- 0.66143 0.67003 0.67413 0.67429 0.67936

Alpha virt. eigenvalues -- 0.67963 0.68116 0.68295 0.68759 0.68760

Alpha virt. eigenvalues -- 0.69060 0.69090 0.69148 0.69699 0.69811

Alpha virt. eigenvalues -- 0.70548 0.70561 0.70918 0.71898 0.72644

Alpha virt. eigenvalues -- 0.72925 0.73019 0.73096 0.73246 0.73315

Alpha virt. eigenvalues -- 0.73742 0.74251 0.74626 0.75114 0.75152

Alpha virt. eigenvalues -- 0.75906 0.75960 0.76393 0.76442 0.76746

Alpha virt. eigenvalues -- 0.78198 0.78398 0.78502 0.78556 0.78677

Alpha virt. eigenvalues -- 0.79074 0.79106 0.79416 0.80052 0.80080

Alpha virt. eigenvalues -- 0.80159 0.80215 0.80555 0.81134 0.81153

Alpha virt. eigenvalues -- 0.81338 0.81671 0.82054 0.82286 0.82376

Alpha virt. eigenvalues -- 0.82672 0.83862 0.83965 0.84122 0.84631

Alpha virt. eigenvalues -- 0.84943 0.85200 0.85454 0.85658 0.85995

Alpha virt. eigenvalues -- 0.87515 0.87557 0.87870 0.88058 0.88534

Alpha virt. eigenvalues -- 0.88660 0.89744 0.91481 0.91574 0.91938

Alpha virt. eigenvalues -- 0.92213 0.93117 0.93440 0.94502 0.94591

Alpha virt. eigenvalues -- 0.94597 0.95598 0.95785 0.96125 0.96861

Alpha virt. eigenvalues -- 0.97009 0.97326 0.97336 0.97426 0.97757

Alpha virt. eigenvalues -- 0.97813 0.98015 0.98374 0.98498 0.98588

Alpha virt. eigenvalues -- 0.99460 0.99646 0.99734 1.00164 1.01124

Alpha virt. eigenvalues -- 1.01954 1.02168 1.02399 1.02635 1.03459

Alpha virt. eigenvalues -- 1.03804 1.03873 1.05429 1.05442 1.06009

Alpha virt. eigenvalues -- 1.06117 1.06404 1.06936 1.07014 1.08624

Alpha virt. eigenvalues -- 1.09679 1.09728 1.09880 1.10315 1.10493

Alpha virt. eigenvalues -- 1.10797 1.11102 1.11176 1.11362 1.11480

Alpha virt. eigenvalues -- 1.11582 1.12113 1.12179 1.12208 1.12366

Alpha virt. eigenvalues -- 1.12390 1.13376 1.13884 1.13968 1.14422

Alpha virt. eigenvalues -- 1.14456 1.16379 1.16495 1.16557 1.16879

Alpha virt. eigenvalues -- 1.17045 1.17301 1.17570 1.18202 1.18680

Alpha virt. eigenvalues -- 1.19011 1.19224 1.20616 1.21302 1.21308

Alpha virt. eigenvalues -- 1.21505 1.21512 1.21860 1.22240 1.22257

Alpha virt. eigenvalues -- 1.22475 1.22951 1.24482 1.24509 1.25199

Alpha virt. eigenvalues -- 1.25438 1.25699 1.26638 1.26784 1.27260

Alpha virt. eigenvalues -- 1.27570 1.27758 1.28122 1.28155 1.29040

Alpha virt. eigenvalues -- 1.29880 1.30324 1.30377 1.30607 1.33201

Alpha virt. eigenvalues -- 1.33849 1.34345 1.34988 1.35177 1.35422

Alpha virt. eigenvalues -- 1.36182 1.37724 1.38331 1.38449 1.39096

Alpha virt. eigenvalues -- 1.39200 1.39637 1.39866 1.40090 1.42635

Alpha virt. eigenvalues -- 1.42867 1.43077 1.44283 1.44382 1.44502

Alpha virt. eigenvalues -- 1.44504 1.44829 1.45588 1.45593 1.46069

Alpha virt. eigenvalues -- 1.46880 1.48065 1.48352 1.48546 1.51036

Alpha virt. eigenvalues -- 1.51255 1.51269 1.51357 1.51500 1.51549

Alpha virt. eigenvalues -- 1.51594 1.51709 1.51774 1.51893 1.52242

Alpha virt. eigenvalues -- 1.52278 1.52714 1.52813 1.52918 1.52926

Alpha virt. eigenvalues -- 1.53920 1.54181 1.54182 1.54700 1.55973

Alpha virt. eigenvalues -- 1.56144 1.56468 1.57422 1.57902 1.60555

Alpha virt. eigenvalues -- 1.60650 1.63897 1.64542 1.64606 1.64790

Alpha virt. eigenvalues -- 1.64826 1.65064 1.66487 1.67975 1.68020

Alpha virt. eigenvalues -- 1.68901 1.69250 1.69322 1.70359 1.70377

Alpha virt. eigenvalues -- 1.71183 1.71292 1.71879 1.72166 1.73470

Alpha virt. eigenvalues -- 1.73771 1.74186 1.75085 1.75418 1.76468

Alpha virt. eigenvalues -- 1.76546 1.76724 1.77402 1.77602 1.77661

Alpha virt. eigenvalues -- 1.78788 1.79877 1.79969 1.80864 1.81606

Alpha virt. eigenvalues -- 1.81734 1.81754 1.81873 1.82345 1.82585

Alpha virt. eigenvalues -- 1.82988 1.83311 1.84241 1.84686 1.85640

Alpha virt. eigenvalues -- 1.86046 1.86078 1.86174 1.86832 1.86917

Alpha virt. eigenvalues -- 1.87804 1.88290 1.88437 1.88523 1.88720

Alpha virt. eigenvalues -- 1.89138 1.89297 1.89655 1.89981 1.90896

Alpha virt. eigenvalues -- 1.91054 1.91195 1.91775 1.91783 1.91788

Alpha virt. eigenvalues -- 1.92058 1.92177 1.92237 1.92242 1.92400

Alpha virt. eigenvalues -- 1.93849 1.94198 1.94443 1.94448 1.94686

Alpha virt. eigenvalues -- 1.94757 1.94824 1.95295 1.95809 1.96045

Alpha virt. eigenvalues -- 1.96680 1.96754 1.96984 1.97263 1.97352

Alpha virt. eigenvalues -- 1.97610 1.98847 1.99195 1.99397 2.01793

Alpha virt. eigenvalues -- 2.02369 2.03412 2.04218 2.04308 2.04561

Alpha virt. eigenvalues -- 2.06499 2.06829 2.08161 2.08762 2.12078

Alpha virt. eigenvalues -- 2.12748 2.13543 2.14366 2.14702 2.14951

Alpha virt. eigenvalues -- 2.15328 2.18329 2.18560 2.18841 2.19393

Alpha virt. eigenvalues -- 2.20987 2.21114 2.21413 2.21797 2.21809

Alpha virt. eigenvalues -- 2.22015 2.22031 2.22545 2.22624 2.24082

Alpha virt. eigenvalues -- 2.24401 2.24452 2.24516 2.25796 2.25883

Alpha virt. eigenvalues -- 2.25885 2.26872 2.27446 2.27810 2.28056

Alpha virt. eigenvalues -- 2.29707 2.30607 2.31188 2.31266 2.31466

Alpha virt. eigenvalues -- 2.31481 2.32100 2.33166 2.33611 2.34473

Alpha virt. eigenvalues -- 2.34694 2.34771 2.34772 2.35517 2.35796

Alpha virt. eigenvalues -- 2.35860 2.38031 2.38463 2.39832 2.39846

Alpha virt. eigenvalues -- 2.42244 2.43385 2.43571 2.43909 2.44264

Alpha virt. eigenvalues -- 2.44861 2.45071 2.45117 2.45856 2.47438

Alpha virt. eigenvalues -- 2.49509 2.50231 2.50948 2.51441 2.51627

Alpha virt. eigenvalues -- 2.52177 2.52492 2.52755 2.52805 2.52831

Alpha virt. eigenvalues -- 2.53348 2.54468 2.54524 2.54749 2.54974

Alpha virt. eigenvalues -- 2.55491 2.55540 2.55662 2.56744 2.57180

Alpha virt. eigenvalues -- 2.57198 2.57213 2.58634 2.60671 2.62618

Alpha virt. eigenvalues -- 2.64335 2.64550 2.64638 2.64873 2.65342

Alpha virt. eigenvalues -- 2.67437 2.68299 2.69006 2.69113 2.69210

Alpha virt. eigenvalues -- 2.70270 2.70407 2.70709 2.70743 2.71403

Alpha virt. eigenvalues -- 2.71593 2.71900 2.72698 2.72868 2.73088

Alpha virt. eigenvalues -- 2.73170 2.73237 2.73462 2.73932 2.74138

Alpha virt. eigenvalues -- 2.74501 2.74674 2.75021 2.75203 2.77212

Alpha virt. eigenvalues -- 2.79653 2.80161 2.80200 2.80395 2.81150

Alpha virt. eigenvalues -- 2.81464 2.81581 2.81896 2.82030 2.82098

Alpha virt. eigenvalues -- 2.82243 2.84043 2.86010 2.86211 2.86471

Alpha virt. eigenvalues -- 2.86489 2.86590 2.86687 2.86834 2.87374

Alpha virt. eigenvalues -- 2.87676 2.88586 2.89076 2.89102 2.90637

Alpha virt. eigenvalues -- 2.91761 2.92213 2.92821 2.93353 2.95992

Alpha virt. eigenvalues -- 2.96373 2.98173 3.02027 3.02676 3.02821

Alpha virt. eigenvalues -- 3.03503 3.03549 3.04561 3.05024 3.05202

Alpha virt. eigenvalues -- 3.07146 3.07702 3.08038 3.14294 3.14751

Alpha virt. eigenvalues -- 3.14843 3.15063 3.15774 3.16489 3.16807

Alpha virt. eigenvalues -- 3.17720 3.17778 3.19029 3.19055 3.19279

Alpha virt. eigenvalues -- 3.19352 3.20517 3.20609 3.21654 3.22310

Alpha virt. eigenvalues -- 3.22319 3.23127 3.23802 3.23971 3.25826

Alpha virt. eigenvalues -- 3.26278 3.26483 3.26899 3.27481 3.27514

Alpha virt. eigenvalues -- 3.27684 3.27710 3.27729 3.27836 3.28640

Alpha virt. eigenvalues -- 3.28653 3.30667 3.30693 3.31520 3.31697

Alpha virt. eigenvalues -- 3.31732 3.33068 3.33156 3.33294 3.34144

Alpha virt. eigenvalues -- 3.34224 3.34438 3.36814 3.39069 3.40622

Alpha virt. eigenvalues -- 3.40662 3.41769 3.41910 3.42271 3.42419

Alpha virt. eigenvalues -- 3.42818 3.46125 3.46467 3.46508 3.47103

Alpha virt. eigenvalues -- 3.51126 3.51135 3.51262 3.51752 3.52180

Alpha virt. eigenvalues -- 3.52365 3.52369 3.52942 3.54844 3.59118

Alpha virt. eigenvalues -- 3.59793 3.61475 3.61860 3.62260 3.62524

Alpha virt. eigenvalues -- 3.70078 3.70386 3.70831 3.71562 3.74039

Alpha virt. eigenvalues -- 3.74208 3.74584 3.75889 3.82674 3.82817

Alpha virt. eigenvalues -- 3.83758 3.83847 3.87226 3.87868 3.88464

Alpha virt. eigenvalues -- 3.88829 3.88885 3.89882 3.89989 3.90213

Alpha virt. eigenvalues -- 3.90418 4.00089 4.00389 4.00420 4.01689

Alpha virt. eigenvalues -- 4.02248 4.02720 4.02801 4.05304 4.10623

Alpha virt. eigenvalues -- 4.11722 4.12435 4.20106 4.24191 4.27748

Alpha virt. eigenvalues -- 4.29037 4.38071 4.41161 4.42677 4.44614

Alpha virt. eigenvalues -- 4.44862 4.47087 4.52712 4.53723 4.54466

Alpha virt. eigenvalues -- 4.75138 4.75152 4.75162 4.75178 4.78141

Alpha virt. eigenvalues -- 4.78211 4.78222 4.78361 5.11101 5.11714

Alpha virt. eigenvalues -- 5.12316 5.15182 5.21492 5.34839 5.35521

Alpha virt. eigenvalues -- 5.50268 7.82882 7.87397 7.88224 7.88703

Alpha virt. eigenvalues -- 8.10390 11.10367 23.20453 23.21908 23.22374

Alpha virt. eigenvalues -- 23.23089 23.55515 23.57398 23.57714 23.58575

Alpha virt. eigenvalues -- 23.71302 23.71352 23.72313 23.72343 23.79982

Alpha virt. eigenvalues -- 23.80223 23.80277 23.81068 23.81184 23.81357

Alpha virt. eigenvalues -- 23.81533 23.83018 23.86839 23.87722 23.88317

Alpha virt. eigenvalues -- 23.88883 23.89997 23.90082 23.91927 23.92019

Alpha virt. eigenvalues -- 23.97044 23.97117 23.97203 23.97359 24.04155

Alpha virt. eigenvalues -- 24.04157 24.04940 24.04943 24.08451 24.08494

Alpha virt. eigenvalues -- 24.09133 24.09181 24.11936 24.11939 24.12187

Alpha virt. eigenvalues -- 24.12213 24.12598 24.12654 24.13828 24.14133

Alpha virt. eigenvalues -- 35.56368 35.59647 35.60174 35.61065 35.69004

Alpha virt. eigenvalues -- 35.69667 35.69681 35.69769

Beta occ. eigenvalues -- -14.32025 -14.32025 -14.30885 -14.30885 -14.30885

Beta occ. eigenvalues -- -14.30884 -14.30803 -14.30803 -10.25513 -10.25513

Beta occ. eigenvalues -- -10.25512 -10.25512 -10.24431 -10.24431 -10.24430

Beta occ. eigenvalues -- -10.24430 -10.19526 -10.19526 -10.19487 -10.19487

Beta occ. eigenvalues -- -10.19153 -10.19153 -10.19116 -10.19116 -10.18950

Beta occ. eigenvalues -- -10.18950 -10.18949 -10.18949 -10.18836 -10.18836

Beta occ. eigenvalues -- -10.18795 -10.18795 -10.18596 -10.18596 -10.18595

Beta occ. eigenvalues -- -10.18595 -10.18281 -10.18281 -10.18242 -10.18242

Beta occ. eigenvalues -- -10.18022 -10.18022 -10.18019 -10.18019 -10.17945

Beta occ. eigenvalues -- -10.17945 -10.17903 -10.17903 -10.17823 -10.17823

Beta occ. eigenvalues -- -10.17823 -10.17823 -10.17705 -10.17705 -10.17663

Beta occ. eigenvalues -- -10.17663 -0.99954 -0.98648 -0.98558 -0.95966

Beta occ. eigenvalues -- -0.93717 -0.90172 -0.89552 -0.88331 -0.87923

Beta occ. eigenvalues -- -0.87822 -0.87712 -0.86280 -0.82896 -0.82829

Beta occ. eigenvalues -- -0.82472 -0.82464 -0.78912 -0.78537 -0.78252

Beta occ. eigenvalues -- -0.78246 -0.75529 -0.75492 -0.75199 -0.75194

Beta occ. eigenvalues -- -0.75101 -0.73516 -0.73385 -0.72810 -0.70319

Beta occ. eigenvalues -- -0.68834 -0.68443 -0.65770 -0.65477 -0.65133

Beta occ. eigenvalues -- -0.64880 -0.62874 -0.62243 -0.60897 -0.60762

Beta occ. eigenvalues -- -0.60381 -0.60372 -0.60369 -0.60094 -0.60017

Beta occ. eigenvalues -- -0.59543 -0.58010 -0.56830 -0.56600 -0.56594

Beta occ. eigenvalues -- -0.55841 -0.54285 -0.54163 -0.54031 -0.53445

Beta occ. eigenvalues -- -0.53357 -0.53132 -0.51727 -0.51679 -0.51561

Beta occ. eigenvalues -- -0.51529 -0.51221 -0.51056 -0.50656 -0.50632

Beta occ. eigenvalues -- -0.48929 -0.45795 -0.45788 -0.45627 -0.45560

Beta occ. eigenvalues -- -0.45436 -0.45424 -0.45040 -0.44833 -0.44268

Beta occ. eigenvalues -- -0.44174 -0.44029 -0.43883 -0.43740 -0.43585

Beta occ. eigenvalues -- -0.43386 -0.43259 -0.42930 -0.42812 -0.42506

Beta occ. eigenvalues -- -0.42172 -0.42077 -0.41949 -0.41873 -0.41259

Beta occ. eigenvalues -- -0.39471 -0.39470 -0.39160 -0.38894 -0.38096

Beta occ. eigenvalues -- -0.37813 -0.37649 -0.37607 -0.37184 -0.36662

Beta occ. eigenvalues -- -0.35706 -0.35588 -0.35401 -0.35230 -0.34248

Beta occ. eigenvalues -- -0.34151 -0.33957 -0.33810 -0.33721 -0.33622

Beta occ. eigenvalues -- -0.32977 -0.32634 -0.32542 -0.31686 -0.31218

Beta occ. eigenvalues -- -0.30754 -0.30612 -0.30164 -0.29380 -0.29073

Beta occ. eigenvalues -- -0.28559 -0.27913 -0.27750 -0.26608 -0.26256

Beta occ. eigenvalues -- -0.25322 -0.25057 -0.25048 -0.24827 -0.24515

Beta occ. eigenvalues -- -0.24276 -0.22705 -0.22431 -0.22310

Beta virt. eigenvalues -- -0.13967 -0.09327 -0.09093 -0.06092 -0.05745

Beta virt. eigenvalues -- -0.05552 -0.05263 -0.04220 0.00095 0.00102

Beta virt. eigenvalues -- 0.00296 0.00555 0.00896 0.01276 0.01464

Beta virt. eigenvalues -- 0.02107 0.03338 0.05030 0.05080 0.05635

Beta virt. eigenvalues -- 0.05946 0.06252 0.06277 0.06304 0.06377

Beta virt. eigenvalues -- 0.07151 0.07344 0.07361 0.07751 0.08329

Beta virt. eigenvalues -- 0.09565 0.09604 0.09727 0.09742 0.10535

Beta virt. eigenvalues -- 0.10889 0.11350 0.11619 0.11630 0.12277

Beta virt. eigenvalues -- 0.12340 0.12500 0.12881 0.13245 0.13291

Beta virt. eigenvalues -- 0.13382 0.13433 0.14357 0.14589 0.16338

Beta virt. eigenvalues -- 0.16415 0.17823 0.18172 0.18353 0.18520

Beta virt. eigenvalues -- 0.18662 0.18687 0.18795 0.19020 0.19147

Beta virt. eigenvalues -- 0.19610 0.20426 0.21649 0.21700 0.22528

Beta virt. eigenvalues -- 0.22617 0.22947 0.22950 0.23180 0.24148

Beta virt. eigenvalues -- 0.24396 0.24886 0.25655 0.25907 0.26263

Beta virt. eigenvalues -- 0.26336 0.26707 0.27483 0.27691 0.27719

Beta virt. eigenvalues -- 0.27775 0.28016 0.28207 0.28314 0.28577

Beta virt. eigenvalues -- 0.28632 0.29064 0.29136 0.29516 0.30485

Beta virt. eigenvalues -- 0.30635 0.30734 0.30843 0.30942 0.31124

Beta virt. eigenvalues -- 0.31130 0.31801 0.31805 0.32842 0.32852

Beta virt. eigenvalues -- 0.33096 0.34582 0.34753 0.34927 0.35344

Beta virt. eigenvalues -- 0.35879 0.36079 0.36144 0.36641 0.36980

Beta virt. eigenvalues -- 0.37138 0.37381 0.37394 0.37572 0.37851

Beta virt. eigenvalues -- 0.37910 0.38059 0.38316 0.38360 0.38566

Beta virt. eigenvalues -- 0.38879 0.39176 0.39273 0.39289 0.39822

Beta virt. eigenvalues -- 0.40114 0.40172 0.40221 0.40336 0.40420

Beta virt. eigenvalues -- 0.40899 0.40997 0.41126 0.41310 0.41570

Beta virt. eigenvalues -- 0.41730 0.41937 0.42445 0.42697 0.42877

Beta virt. eigenvalues -- 0.42905 0.42968 0.43087 0.43130 0.43273

Beta virt. eigenvalues -- 0.43375 0.43510 0.43556 0.43775 0.43951

Beta virt. eigenvalues -- 0.44047 0.44387 0.44554 0.44675 0.44914

Beta virt. eigenvalues -- 0.45054 0.45088 0.45675 0.46013 0.46138

Beta virt. eigenvalues -- 0.46302 0.46438 0.46503 0.46542 0.46809

Beta virt. eigenvalues -- 0.46992 0.47160 0.47180 0.47472 0.47637

Beta virt. eigenvalues -- 0.47756 0.48087 0.48489 0.48791 0.49088

Beta virt. eigenvalues -- 0.49174 0.49572 0.49778 0.50229 0.50591

Beta virt. eigenvalues -- 0.50779 0.50837 0.51365 0.51480 0.51488

Beta virt. eigenvalues -- 0.52277 0.52302 0.53220 0.53300 0.53414

Beta virt. eigenvalues -- 0.53442 0.53611 0.53849 0.54461 0.54907

Beta virt. eigenvalues -- 0.55363 0.55734 0.56415 0.56415 0.56589

Beta virt. eigenvalues -- 0.57968 0.58144 0.58751 0.58888 0.59320

Beta virt. eigenvalues -- 0.59994 0.60215 0.60497 0.60808 0.60906

Beta virt. eigenvalues -- 0.60919 0.61245 0.61669 0.61709 0.61809

Beta virt. eigenvalues -- 0.62006 0.62112 0.62612 0.62678 0.62832

Beta virt. eigenvalues -- 0.62919 0.63116 0.63130 0.63497 0.63547

Beta virt. eigenvalues -- 0.64296 0.64401 0.64417 0.64536 0.65390

Beta virt. eigenvalues -- 0.65712 0.65717 0.66207 0.67103 0.67545

Beta virt. eigenvalues -- 0.67729 0.68039 0.68194 0.68261 0.68460

Beta virt. eigenvalues -- 0.68833 0.68876 0.69161 0.69187 0.69262

Beta virt. eigenvalues -- 0.69842 0.69893 0.70574 0.70775 0.71005

Beta virt. eigenvalues -- 0.72104 0.72760 0.73050 0.73090 0.73179

Beta virt. eigenvalues -- 0.73280 0.73471 0.73805 0.74420 0.74707

Beta virt. eigenvalues -- 0.75167 0.75228 0.75943 0.76173 0.76545

Beta virt. eigenvalues -- 0.76688 0.76883 0.78327 0.78493 0.78612

Beta virt. eigenvalues -- 0.78746 0.78830 0.79143 0.79154 0.79479

Beta virt. eigenvalues -- 0.80116 0.80240 0.80251 0.80365 0.80684

Beta virt. eigenvalues -- 0.81207 0.81258 0.81451 0.81774 0.82157

Beta virt. eigenvalues -- 0.82358 0.82470 0.82799 0.83924 0.84052

Beta virt. eigenvalues -- 0.84211 0.84736 0.85016 0.85330 0.85588

Beta virt. eigenvalues -- 0.85737 0.86124 0.87613 0.87624 0.87957

Beta virt. eigenvalues -- 0.88283 0.88653 0.88725 0.89843 0.91561

Beta virt. eigenvalues -- 0.91627 0.91989 0.92359 0.93189 0.93486

Beta virt. eigenvalues -- 0.94677 0.94691 0.94713 0.95799 0.95939

Beta virt. eigenvalues -- 0.96261 0.96949 0.97118 0.97396 0.97442

Beta virt. eigenvalues -- 0.97617 0.97858 0.97919 0.98114 0.98541

Beta virt. eigenvalues -- 0.98544 0.98631 0.99562 0.99766 0.99885

Beta virt. eigenvalues -- 1.00259 1.01218 1.02000 1.02190 1.02508

Beta virt. eigenvalues -- 1.02736 1.03770 1.04070 1.04076 1.05514

Beta virt. eigenvalues -- 1.05589 1.06173 1.06385 1.06642 1.07090

Beta virt. eigenvalues -- 1.07138 1.08848 1.10014 1.10181 1.10388

Beta virt. eigenvalues -- 1.10614 1.10931 1.11048 1.11259 1.11319

Beta virt. eigenvalues -- 1.11558 1.11676 1.11767 1.12193 1.12315

Beta virt. eigenvalues -- 1.12346 1.12625 1.12650 1.13500 1.13972

Beta virt. eigenvalues -- 1.14080 1.14500 1.14510 1.16620 1.16634

Beta virt. eigenvalues -- 1.16986 1.17092 1.17132 1.17536 1.17715

Beta virt. eigenvalues -- 1.18364 1.18805 1.19367 1.19492 1.20777

Beta virt. eigenvalues -- 1.21376 1.21383 1.21651 1.21658 1.21991

Beta virt. eigenvalues -- 1.22374 1.22418 1.22613 1.23062 1.24581

Beta virt. eigenvalues -- 1.24649 1.25701 1.25750 1.25807 1.26723

Beta virt. eigenvalues -- 1.26893 1.27343 1.27717 1.27859 1.28206

Beta virt. eigenvalues -- 1.28553 1.29113 1.29965 1.30403 1.30507

Beta virt. eigenvalues -- 1.30706 1.33342 1.34089 1.34536 1.35400

Beta virt. eigenvalues -- 1.35412 1.35656 1.36328 1.38026 1.38485

Beta virt. eigenvalues -- 1.39013 1.39239 1.39472 1.40035 1.40381

Beta virt. eigenvalues -- 1.40402 1.42782 1.42958 1.43229 1.44325

Beta virt. eigenvalues -- 1.44448 1.44534 1.44567 1.44873 1.45611

Beta virt. eigenvalues -- 1.45622 1.46098 1.47016 1.48106 1.48415

Beta virt. eigenvalues -- 1.48592 1.51215 1.51408 1.51412 1.51483

Beta virt. eigenvalues -- 1.51740 1.51745 1.51813 1.51886 1.51929

Beta virt. eigenvalues -- 1.52081 1.52443 1.52714 1.52967 1.53009

Beta virt. eigenvalues -- 1.53362 1.53504 1.54052 1.54251 1.54312

Beta virt. eigenvalues -- 1.55031 1.56420 1.56538 1.56985 1.57855

Beta virt. eigenvalues -- 1.58091 1.60903 1.61048 1.64024 1.64680

Beta virt. eigenvalues -- 1.64714 1.64877 1.64903 1.65314 1.66629

Beta virt. eigenvalues -- 1.68098 1.68227 1.69118 1.69495 1.69516

Beta virt. eigenvalues -- 1.70602 1.70619 1.71501 1.71636 1.72182

Beta virt. eigenvalues -- 1.72438 1.73548 1.73965 1.74329 1.75218

Beta virt. eigenvalues -- 1.75656 1.76630 1.76733 1.76868 1.77584

Beta virt. eigenvalues -- 1.77671 1.77790 1.78902 1.80023 1.80138

Beta virt. eigenvalues -- 1.80968 1.81672 1.81778 1.81864 1.81988

Beta virt. eigenvalues -- 1.82458 1.82694 1.83103 1.83484 1.84394

Beta virt. eigenvalues -- 1.84973 1.85796 1.86141 1.86193 1.86331

Beta virt. eigenvalues -- 1.86940 1.87192 1.87944 1.88487 1.88541

Beta virt. eigenvalues -- 1.88699 1.88935 1.89290 1.89437 1.89858

Beta virt. eigenvalues -- 1.90134 1.91053 1.91148 1.91371 1.91886

Beta virt. eigenvalues -- 1.91910 1.91914 1.92132 1.92338 1.92480

Beta virt. eigenvalues -- 1.92485 1.92529 1.93973 1.94320 1.94534

Beta virt. eigenvalues -- 1.94557 1.94753 1.94933 1.94986 1.95332

Beta virt. eigenvalues -- 1.96005 1.96325 1.96914 1.96955 1.97137

Beta virt. eigenvalues -- 1.97465 1.97797 1.98109 1.99249 1.99359

Beta virt. eigenvalues -- 1.99546 2.01972 2.02570 2.03619 2.04443

Beta virt. eigenvalues -- 2.04699 2.04883 2.07153 2.07728 2.08580

Beta virt. eigenvalues -- 2.09395 2.12140 2.13005 2.13983 2.14419

Beta virt. eigenvalues -- 2.14756 2.15026 2.15432 2.18429 2.18719

Beta virt. eigenvalues -- 2.18985 2.19459 2.21057 2.21121 2.21484

Beta virt. eigenvalues -- 2.21842 2.22013 2.22103 2.22127 2.22621

Beta virt. eigenvalues -- 2.22902 2.24251 2.24446 2.24560 2.24569

Beta virt. eigenvalues -- 2.25955 2.26012 2.26031 2.27035 2.27470

Beta virt. eigenvalues -- 2.27837 2.28086 2.29746 2.30994 2.31273

Beta virt. eigenvalues -- 2.31333 2.31526 2.31532 2.32228 2.33429

Beta virt. eigenvalues -- 2.33750 2.34552 2.34743 2.34826 2.34830

Beta virt. eigenvalues -- 2.35555 2.35820 2.35900 2.38128 2.39058

Beta virt. eigenvalues -- 2.40096 2.40383 2.42698 2.43517 2.43901

Beta virt. eigenvalues -- 2.44296 2.44483 2.44976 2.45158 2.45210

Beta virt. eigenvalues -- 2.46302 2.47577 2.49632 2.50351 2.51137

Beta virt. eigenvalues -- 2.51563 2.51846 2.52350 2.52529 2.52831

Beta virt. eigenvalues -- 2.52848 2.52858 2.53375 2.54502 2.54573

Beta virt. eigenvalues -- 2.54797 2.54864 2.55529 2.55815 2.56091

Beta virt. eigenvalues -- 2.56966 2.57281 2.57435 2.57532 2.58929

Beta virt. eigenvalues -- 2.60845 2.63013 2.64439 2.64752 2.64842

Beta virt. eigenvalues -- 2.65117 2.65543 2.67524 2.68565 2.69385

Beta virt. eigenvalues -- 2.69554 2.69669 2.70586 2.70650 2.70799

Beta virt. eigenvalues -- 2.71248 2.71667 2.71785 2.72003 2.72951

Beta virt. eigenvalues -- 2.72983 2.73275 2.73288 2.73503 2.73572

Beta virt. eigenvalues -- 2.74030 2.74208 2.74732 2.74924 2.75404

Beta virt. eigenvalues -- 2.75477 2.77597 2.80265 2.80648 2.80664

Beta virt. eigenvalues -- 2.80876 2.81578 2.81624 2.81738 2.82178

Beta virt. eigenvalues -- 2.82285 2.82369 2.82581 2.84105 2.86242

Beta virt. eigenvalues -- 2.86390 2.86648 2.86798 2.86810 2.86814

Beta virt. eigenvalues -- 2.86901 2.87509 2.87925 2.88624 2.89378

Beta virt. eigenvalues -- 2.89472 2.91118 2.91903 2.92337 2.92912

Beta virt. eigenvalues -- 2.93972 2.96626 2.97301 2.98846 3.02140

Beta virt. eigenvalues -- 3.02778 3.03048 3.03650 3.03702 3.04701

Beta virt. eigenvalues -- 3.05106 3.05458 3.07530 3.07822 3.08123

Beta virt. eigenvalues -- 3.14322 3.14777 3.14866 3.15084 3.15820

Beta virt. eigenvalues -- 3.16526 3.16869 3.17822 3.17843 3.19116

Beta virt. eigenvalues -- 3.19159 3.19359 3.19436 3.20614 3.20703

Beta virt. eigenvalues -- 3.21774 3.22378 3.22496 3.23208 3.23863

Beta virt. eigenvalues -- 3.24045 3.25849 3.26331 3.26538 3.26980

Beta virt. eigenvalues -- 3.27506 3.27528 3.27714 3.27745 3.27757

Beta virt. eigenvalues -- 3.27873 3.28707 3.28722 3.30699 3.30722

Beta virt. eigenvalues -- 3.31585 3.31724 3.31790 3.33094 3.33181

Beta virt. eigenvalues -- 3.33353 3.34188 3.34294 3.34482 3.36865

Beta virt. eigenvalues -- 3.39137 3.40679 3.40715 3.41814 3.41983

Beta virt. eigenvalues -- 3.42322 3.42493 3.42861 3.46156 3.46508

Beta virt. eigenvalues -- 3.46529 3.47138 3.51207 3.51216 3.51337

Beta virt. eigenvalues -- 3.51825 3.52253 3.52438 3.52461 3.53027

Beta virt. eigenvalues -- 3.55037 3.59235 3.59925 3.61513 3.61894

Beta virt. eigenvalues -- 3.62308 3.62643 3.70176 3.70513 3.70914

Beta virt. eigenvalues -- 3.71645 3.74191 3.74376 3.74745 3.76088

Beta virt. eigenvalues -- 3.82823 3.82915 3.83688 3.84128 3.87343

Beta virt. eigenvalues -- 3.87925 3.88618 3.88915 3.88921 3.89825

Beta virt. eigenvalues -- 3.90023 3.90477 3.90660 4.00132 4.00428

Beta virt. eigenvalues -- 4.00495 4.01750 4.02362 4.02865 4.02876

Beta virt. eigenvalues -- 4.05447 4.10657 4.11798 4.12499 4.20225

Beta virt. eigenvalues -- 4.24248 4.27867 4.29120 4.38189 4.41432

Beta virt. eigenvalues -- 4.42865 4.44889 4.45082 4.47289 4.52930

Beta virt. eigenvalues -- 4.53827 4.54591 4.75208 4.75223 4.75232

Beta virt. eigenvalues -- 4.75245 4.78208 4.78265 4.78319 4.78445

Beta virt. eigenvalues -- 5.11326 5.12015 5.12548 5.15475 5.21791

Beta virt. eigenvalues -- 5.35156 5.35838 5.50594 7.82881 7.87389

Beta virt. eigenvalues -- 7.88246 7.88705 8.10391 11.10371 23.20484

Beta virt. eigenvalues -- 23.21927 23.22419 23.23122 23.55584 23.57427

Beta virt. eigenvalues -- 23.57807 23.58630 23.71354 23.71405 23.72338

Beta virt. eigenvalues -- 23.72368 23.80286 23.80303 23.80385 23.81160

Beta virt. eigenvalues -- 23.81392 23.81521 23.81741 23.83324 23.87211

Beta virt. eigenvalues -- 23.88130 23.88543 23.89183 23.90006 23.90108

Beta virt. eigenvalues -- 23.91981 23.92080 23.97059 23.97119 23.97234

Beta virt. eigenvalues -- 23.97379 24.04170 24.04172 24.04968 24.04971

Beta virt. eigenvalues -- 24.08513 24.08556 24.09158 24.09205 24.11951

Beta virt. eigenvalues -- 24.11953 24.12219 24.12244 24.12641 24.12695

Beta virt. eigenvalues -- 24.13838 24.14146 35.56368 35.59776 35.60017

Beta virt. eigenvalues -- 35.61037 35.69002 35.69671 35.69703 35.69750

Condensed to atoms (all electrons):

Atomic-Atomic Spin Densities.

Mulliken charges and spin densities:

1 2

1 C 0.378796 0.265533

2 N -0.635497 -0.091757

3 C 0.378796 0.265533

4 C -0.076201 -0.018837

5 C -0.076201 -0.018837

6 N -0.423821 -0.016920

7 C 0.407008 0.124817

8 N -0.680644 0.061973

9 C 0.407008 0.124817

10 C -0.072672 -0.023522

11 C -0.072672 -0.023522

12 N -0.423821 -0.016920

13 C -0.072672 -0.023522

14 C -0.072672 -0.023522

15 C 0.407008 0.124817

16 N -0.680644 0.061973

17 C 0.407008 0.124817

18 N -0.423821 -0.016920

19 N -0.635497 -0.091757

20 C 0.378796 0.265533

21 C -0.076201 -0.018837

22 C -0.076201 -0.018837

23 C 0.378796 0.265533

24 N -0.423821 -0.016920

25 Zn 1.391737 0.000460

26 C -0.200698 0.047921

27 C 0.010149 -0.000301

28 C 0.010149 -0.000301

29 C -0.200698 0.047921

30 C -0.210135 0.081568

31 C 0.007111 0.011190

32 C 0.007111 0.011190

33 C -0.210135 0.081568

34 C -0.200698 0.047921

35 C 0.010149 -0.000301

36 C 0.010149 -0.000301

37 C -0.200698 0.047921

38 C -0.210135 0.081568

39 C 0.007111 0.011190

40 C 0.007111 0.011190

41 C -0.210135 0.081568

42 C -0.228662 0.013946

43 C -0.223520 0.020097

44 C -0.223520 0.020097

45 C -0.228662 0.013946

46 C -0.226477 0.010202

47 C -0.218821 0.008411

48 C -0.218821 0.008411

49 C -0.226477 0.010202

50 C -0.228662 0.013946

51 C -0.223520 0.020097

52 C -0.223520 0.020097

53 C -0.228662 0.013946

54 C -0.226477 0.010202

55 C -0.218821 0.008411

56 C -0.218821 0.008411

57 C -0.226477 0.010202

58 H 0.233672 -0.002308

59 H 0.233672 -0.002308

60 H 0.230583 -0.004084

61 H 0.230583 -0.004084

62 H 0.233672 -0.002308

63 H 0.233672 -0.002308

64 H 0.230583 -0.004084

65 H 0.230583 -0.004084

66 H 0.230567 -0.000576

67 H 0.228992 -0.001324

68 H 0.228992 -0.001324

69 H 0.230567 -0.000576

70 H 0.233023 -0.000481

71 H 0.231242 -0.000554

72 H 0.231242 -0.000554

73 H 0.233023 -0.000481

74 H 0.230567 -0.000576

75 H 0.228992 -0.001324

76 H 0.228992 -0.001324

77 H 0.230567 -0.000576

78 H 0.233023 -0.000481

79 H 0.231242 -0.000554

80 H 0.231242 -0.000554

81 H 0.233023 -0.000481

Sum of Mulliken charges = 0.00000 2.00000

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

1 2

1 C 0.378796 0.265533

2 N -0.635497 -0.091757

3 C 0.378796 0.265533

4 C -0.076201 -0.018837

5 C -0.076201 -0.018837

6 N -0.423821 -0.016920

7 C 0.407008 0.124817

8 N -0.680644 0.061973

9 C 0.407008 0.124817

10 C -0.072672 -0.023522

11 C -0.072672 -0.023522

12 N -0.423821 -0.016920

13 C -0.072672 -0.023522

14 C -0.072672 -0.023522

15 C 0.407008 0.124817

16 N -0.680644 0.061973

17 C 0.407008 0.124817

18 N -0.423821 -0.016920

19 N -0.635497 -0.091757

20 C 0.378796 0.265533

21 C -0.076201 -0.018837

22 C -0.076201 -0.018837

23 C 0.378796 0.265533

24 N -0.423821 -0.016920

25 Zn 1.391737 0.000460

26 C 0.032974 0.045613

27 C 0.010149 -0.000301

28 C 0.010149 -0.000301

29 C 0.032974 0.045613

30 C 0.020448 0.077484

31 C 0.007111 0.011190

32 C 0.007111 0.011190

33 C 0.020448 0.077484

34 C 0.032974 0.045613

35 C 0.010149 -0.000301

36 C 0.010149 -0.000301

37 C 0.032974 0.045613

38 C 0.020448 0.077484

39 C 0.007111 0.011190

40 C 0.007111 0.011190

41 C 0.020448 0.077484

42 C 0.001905 0.013370

43 C 0.005472 0.018773

44 C 0.005472 0.018773

45 C 0.001905 0.013370

46 C 0.006546 0.009722

47 C 0.012421 0.007857

48 C 0.012421 0.007857

49 C 0.006546 0.009722

50 C 0.001905 0.013370

51 C 0.005472 0.018773

52 C 0.005472 0.018773

53 C 0.001905 0.013370

54 C 0.006546 0.009722

55 C 0.012421 0.007857

56 C 0.012421 0.007857

57 C 0.006546 0.009722

Electronic spatial extent (au): <R\*\*2>= 50597.5331

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0000 Y= 0.0000 Z= 2.4572 Tot= 2.4572

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

XX= -242.3208 YY= -270.8596 ZZ= -338.1910

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XX= 41.4697 YY= 12.9308 ZZ= -54.4005

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XXX= 0.0000 YYY= 0.0000 ZZZ= 58.1740 XYY= 0.0000

XXY= 0.0000 XXZ= -19.4770 XZZ= 0.0000 YZZ= 0.0000

YYZ= -62.8369 XYZ= 0.0000

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

XXXX= -26678.9608 YYYY= -28278.7572 ZZZZ= -520.6303 XXXY= 0.0000

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

ZZZY= 0.0000 XXYY= -10288.4511 XXZZ= -6675.9961 YYZZ= -6584.1664

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 6.873360599325D+03 E-N=-1.928967763355D+04 KE= 2.388162461931D+03

Symmetry A1 KE= 6.739687259112D+02

Symmetry A2 KE= 5.315915090687D+02

Symmetry B1 KE= 5.921305843396D+02

Symmetry B2 KE= 5.904716426114D+02

Isotropic Fermi Contact Couplings

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

1 C(13) 0.01978 11.11546 3.96627 3.70772

2 N(14) -0.01713 -2.76766 -0.98757 -0.92319

3 C(13) 0.01978 11.11546 3.96627 3.70772

4 C(13) -0.00961 -5.40250 -1.92775 -1.80208

5 C(13) -0.00961 -5.40250 -1.92775 -1.80208

6 N(14) -0.00567 -0.91631 -0.32696 -0.30565

7 C(13) 0.00768 4.31646 1.54022 1.43982

8 N(14) 0.00584 0.94339 0.33663 0.31468

9 C(13) 0.00768 4.31646 1.54022 1.43982

10 C(13) -0.00565 -3.17497 -1.13291 -1.05906

11 C(13) -0.00565 -3.17497 -1.13291 -1.05906

12 N(14) -0.00567 -0.91631 -0.32696 -0.30565

13 C(13) -0.00565 -3.17497 -1.13291 -1.05906

14 C(13) -0.00565 -3.17497 -1.13291 -1.05906

15 C(13) 0.00768 4.31646 1.54022 1.43982

16 N(14) 0.00584 0.94339 0.33663 0.31468

17 C(13) 0.00768 4.31646 1.54022 1.43982

18 N(14) -0.00567 -0.91631 -0.32696 -0.30565

19 N(14) -0.01713 -2.76766 -0.98757 -0.92319

20 C(13) 0.01978 11.11546 3.96627 3.70772

21 C(13) -0.00961 -5.40250 -1.92775 -1.80208

22 C(13) -0.00961 -5.40250 -1.92775 -1.80208

23 C(13) 0.01978 11.11546 3.96627 3.70772

24 N(14) -0.00567 -0.91631 -0.32696 -0.30565

25 Zn(67) 0.00000 0.00000 0.00000 0.00000

26 C(13) 0.00256 1.44160 0.51440 0.48087

27 C(13) -0.00144 -0.80741 -0.28810 -0.26932

28 C(13) -0.00144 -0.80741 -0.28810 -0.26932

29 C(13) 0.00256 1.44160 0.51440 0.48087

30 C(13) 0.00332 1.86411 0.66516 0.62180

31 C(13) -0.00211 -1.18412 -0.42252 -0.39498

32 C(13) -0.00211 -1.18412 -0.42252 -0.39498

33 C(13) 0.00332 1.86411 0.66516 0.62180

34 C(13) 0.00256 1.44160 0.51440 0.48087

35 C(13) -0.00144 -0.80741 -0.28810 -0.26932

36 C(13) -0.00144 -0.80741 -0.28810 -0.26932

37 C(13) 0.00256 1.44160 0.51440 0.48087

38 C(13) 0.00332 1.86411 0.66516 0.62180

39 C(13) -0.00211 -1.18412 -0.42252 -0.39498

40 C(13) -0.00211 -1.18412 -0.42252 -0.39498

41 C(13) 0.00332 1.86411 0.66516 0.62180

42 C(13) -0.00031 -0.17387 -0.06204 -0.05800

43 C(13) 0.00014 0.07782 0.02777 0.02596

44 C(13) 0.00014 0.07782 0.02777 0.02596

45 C(13) -0.00031 -0.17387 -0.06204 -0.05800

46 C(13) 0.00018 0.09839 0.03511 0.03282

47 C(13) -0.00005 -0.02596 -0.00926 -0.00866

48 C(13) -0.00005 -0.02596 -0.00926 -0.00866

49 C(13) 0.00018 0.09839 0.03511 0.03282

50 C(13) -0.00031 -0.17387 -0.06204 -0.05800

51 C(13) 0.00014 0.07782 0.02777 0.02596

52 C(13) 0.00014 0.07782 0.02777 0.02596

53 C(13) -0.00031 -0.17387 -0.06204 -0.05800

54 C(13) 0.00018 0.09839 0.03511 0.03282

55 C(13) -0.00005 -0.02596 -0.00926 -0.00866

56 C(13) -0.00005 -0.02596 -0.00926 -0.00866

57 C(13) 0.00018 0.09839 0.03511 0.03282

58 H(1) -0.00068 -1.51551 -0.54077 -0.50552

59 H(1) -0.00068 -1.51551 -0.54077 -0.50552

60 H(1) -0.00119 -2.65132 -0.94606 -0.88439

61 H(1) -0.00119 -2.65132 -0.94606 -0.88439

62 H(1) -0.00068 -1.51551 -0.54077 -0.50552

63 H(1) -0.00068 -1.51551 -0.54077 -0.50552

64 H(1) -0.00119 -2.65132 -0.94606 -0.88439

65 H(1) -0.00119 -2.65132 -0.94606 -0.88439

66 H(1) -0.00023 -0.50543 -0.18035 -0.16859

67 H(1) -0.00034 -0.75708 -0.27015 -0.25254

68 H(1) -0.00034 -0.75708 -0.27015 -0.25254

69 H(1) -0.00023 -0.50543 -0.18035 -0.16859

70 H(1) -0.00015 -0.34545 -0.12326 -0.11523

71 H(1) -0.00014 -0.32348 -0.11542 -0.10790

72 H(1) -0.00014 -0.32348 -0.11542 -0.10790

73 H(1) -0.00015 -0.34545 -0.12326 -0.11523

74 H(1) -0.00023 -0.50543 -0.18035 -0.16859

75 H(1) -0.00034 -0.75708 -0.27015 -0.25254

76 H(1) -0.00034 -0.75708 -0.27015 -0.25254

77 H(1) -0.00023 -0.50543 -0.18035 -0.16859

78 H(1) -0.00015 -0.34545 -0.12326 -0.11523

79 H(1) -0.00014 -0.32348 -0.11542 -0.10790

80 H(1) -0.00014 -0.32348 -0.11542 -0.10790

81 H(1) -0.00015 -0.34545 -0.12326 -0.11523

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

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

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

1 Atom -0.174145 -0.164797 0.338942

2 Atom 0.080431 0.067408 -0.147839

3 Atom -0.174145 -0.164797 0.338942

4 Atom -0.006791 0.005903 0.000888

5 Atom -0.006791 0.005903 0.000888

6 Atom -0.014773 -0.009164 0.023937

7 Atom -0.081338 -0.077131 0.158469

8 Atom -0.089342 -0.084764 0.174106

9 Atom -0.081338 -0.077131 0.158469

10 Atom 0.012968 0.005605 -0.018573

11 Atom 0.012968 0.005605 -0.018573

12 Atom -0.014773 -0.009164 0.023937

13 Atom 0.012968 0.005605 -0.018573

14 Atom 0.012968 0.005605 -0.018573

15 Atom -0.081338 -0.077131 0.158469

16 Atom -0.089342 -0.084764 0.174106

17 Atom -0.081338 -0.077131 0.158469

18 Atom -0.014773 -0.009164 0.023937

19 Atom 0.080431 0.067408 -0.147839

20 Atom -0.174145 -0.164797 0.338942

21 Atom -0.006791 0.005903 0.000888

22 Atom -0.006791 0.005903 0.000888

23 Atom -0.174145 -0.164797 0.338942

24 Atom -0.014773 -0.009164 0.023937

25 Atom 0.013040 -0.010406 -0.002634

26 Atom -0.024498 -0.027361 0.051858

27 Atom 0.000162 -0.002537 0.002374

28 Atom 0.000162 -0.002537 0.002374

29 Atom -0.024498 -0.027361 0.051858

30 Atom -0.046665 -0.040494 0.087159

31 Atom -0.010902 -0.006783 0.017685

32 Atom -0.010902 -0.006783 0.017685

33 Atom -0.046665 -0.040494 0.087159

34 Atom -0.024498 -0.027361 0.051858

35 Atom 0.000162 -0.002537 0.002374

36 Atom 0.000162 -0.002537 0.002374

37 Atom -0.024498 -0.027361 0.051858

38 Atom -0.046665 -0.040494 0.087159

39 Atom -0.010902 -0.006783 0.017685

40 Atom -0.010902 -0.006783 0.017685

41 Atom -0.046665 -0.040494 0.087159

42 Atom -0.010120 -0.005705 0.015826

43 Atom -0.012724 -0.010990 0.023714

44 Atom -0.012724 -0.010990 0.023714

45 Atom -0.010120 -0.005705 0.015826

46 Atom -0.004436 -0.006647 0.011083

47 Atom -0.004563 -0.005570 0.010133

48 Atom -0.004563 -0.005570 0.010133

49 Atom -0.004436 -0.006647 0.011083

50 Atom -0.010120 -0.005705 0.015826

51 Atom -0.012724 -0.010990 0.023714

52 Atom -0.012724 -0.010990 0.023714

53 Atom -0.010120 -0.005705 0.015826

54 Atom -0.004436 -0.006647 0.011083

55 Atom -0.004563 -0.005570 0.010133

56 Atom -0.004563 -0.005570 0.010133

57 Atom -0.004436 -0.006647 0.011083

58 Atom -0.000892 0.003079 -0.002187

59 Atom -0.000892 0.003079 -0.002187

60 Atom 0.006127 -0.003134 -0.002994

61 Atom 0.006127 -0.003134 -0.002994

62 Atom -0.000892 0.003079 -0.002187

63 Atom -0.000892 0.003079 -0.002187

64 Atom 0.006127 -0.003134 -0.002994

65 Atom 0.006127 -0.003134 -0.002994

66 Atom 0.001113 0.000502 -0.001615

67 Atom -0.001529 0.002381 -0.000852

68 Atom -0.001529 0.002381 -0.000852

69 Atom 0.001113 0.000502 -0.001615

70 Atom 0.000415 0.000604 -0.001019

71 Atom 0.001272 -0.000694 -0.000578

72 Atom 0.001272 -0.000694 -0.000578

73 Atom 0.000415 0.000604 -0.001019

74 Atom 0.001113 0.000502 -0.001615

75 Atom -0.001529 0.002381 -0.000852

76 Atom -0.001529 0.002381 -0.000852

77 Atom 0.001113 0.000502 -0.001615

78 Atom 0.000415 0.000604 -0.001019

79 Atom 0.001272 -0.000694 -0.000578

80 Atom 0.001272 -0.000694 -0.000578

81 Atom 0.000415 0.000604 -0.001019

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XY XZ YZ

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

1 Atom -0.001905 0.014614 0.057288

2 Atom 0.000000 0.000000 -0.036473

3 Atom 0.001905 -0.014614 0.057288

4 Atom -0.002584 0.000160 0.000490

5 Atom 0.002584 -0.000160 0.000490

6 Atom 0.007301 -0.006803 0.010765

7 Atom -0.000105 -0.014370 0.001971

8 Atom 0.000000 -0.029378 0.000000

9 Atom 0.000105 -0.014370 -0.001971

10 Atom 0.001580 0.001141 0.000195

11 Atom -0.001580 0.001141 -0.000195

12 Atom -0.007301 0.006803 0.010765

13 Atom 0.001580 -0.001141 -0.000195

14 Atom -0.001580 -0.001141 0.000195

15 Atom -0.000105 0.014370 -0.001971

16 Atom 0.000000 0.029378 0.000000

17 Atom 0.000105 0.014370 0.001971

18 Atom 0.007301 0.006803 -0.010765

19 Atom 0.000000 0.000000 0.036473

20 Atom 0.001905 0.014614 -0.057288

21 Atom -0.002584 -0.000160 -0.000490

22 Atom 0.002584 0.000160 -0.000490

23 Atom -0.001905 -0.014614 -0.057288

24 Atom -0.007301 -0.006803 -0.010765

25 Atom 0.000000 0.000000 0.000000

26 Atom -0.000146 0.003320 0.000749

27 Atom -0.000394 0.000117 0.000095

28 Atom 0.000394 0.000117 -0.000095

29 Atom 0.000146 0.003320 -0.000749

30 Atom 0.000183 -0.000377 -0.015525

31 Atom -0.000807 -0.000127 -0.002973

32 Atom 0.000807 0.000127 -0.002973

33 Atom -0.000183 0.000377 -0.015525

34 Atom 0.000146 -0.003320 0.000749

35 Atom 0.000394 -0.000117 0.000095

36 Atom -0.000394 -0.000117 -0.000095

37 Atom -0.000146 -0.003320 -0.000749

38 Atom 0.000183 0.000377 0.015525

39 Atom -0.000807 0.000127 0.002973

40 Atom 0.000807 -0.000127 0.002973

41 Atom -0.000183 -0.000377 0.015525

42 Atom 0.000089 0.000022 -0.002537

43 Atom 0.000048 -0.000005 -0.004192

44 Atom -0.000048 0.000005 -0.004192

45 Atom -0.000089 -0.000022 -0.002537

46 Atom 0.000018 0.000773 -0.000062

47 Atom 0.000062 0.000721 -0.000002

48 Atom -0.000062 0.000721 0.000002

49 Atom -0.000018 0.000773 0.000062

50 Atom 0.000089 -0.000022 0.002537

51 Atom 0.000048 0.000005 0.004192

52 Atom -0.000048 -0.000005 0.004192

53 Atom -0.000089 0.000022 0.002537

54 Atom -0.000018 -0.000773 -0.000062

55 Atom -0.000062 -0.000721 -0.000002

56 Atom 0.000062 -0.000721 0.000002

57 Atom 0.000018 -0.000773 0.000062

58 Atom 0.000523 0.000020 -0.000143

59 Atom -0.000523 0.000020 0.000143

60 Atom 0.000603 0.000061 -0.000088

61 Atom -0.000603 -0.000061 -0.000088

62 Atom -0.000523 -0.000020 -0.000143

63 Atom 0.000523 -0.000020 0.000143

64 Atom 0.000603 -0.000061 0.000088

65 Atom -0.000603 0.000061 0.000088

66 Atom -0.000389 -0.000046 0.000226

67 Atom -0.001460 -0.000171 0.000373

68 Atom 0.001460 0.000171 0.000373

69 Atom 0.000389 0.000046 0.000226

70 Atom -0.000295 -0.000043 0.000016

71 Atom -0.000710 -0.000073 0.000033

72 Atom 0.000710 -0.000073 -0.000033

73 Atom 0.000295 -0.000043 -0.000016

74 Atom -0.000389 0.000046 -0.000226

75 Atom -0.001460 0.000171 -0.000373

76 Atom 0.001460 -0.000171 -0.000373

77 Atom 0.000389 -0.000046 -0.000226

78 Atom 0.000295 0.000043 0.000016

79 Atom 0.000710 0.000073 0.000033

80 Atom -0.000710 0.000073 -0.000033

81 Atom -0.000295 0.000043 -0.000016

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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 -0.1768 -23.722 -8.464 -7.913 0.8438 0.5302 -0.0828

1 C(13) Bbb -0.1690 -22.677 -8.092 -7.564 -0.5359 0.8405 -0.0794

Bcc 0.3458 46.399 16.556 15.477 0.0275 0.1114 0.9934

Baa -0.1539 -5.934 -2.117 -1.979 0.0000 0.1626 0.9867

2 N(14) Bbb 0.0734 2.832 1.010 0.945 0.0000 0.9867 -0.1626

Bcc 0.0804 3.102 1.107 1.035 1.0000 0.0000 0.0000

Baa -0.1768 -23.722 -8.464 -7.913 0.8438 -0.5302 0.0828

3 C(13) Bbb -0.1690 -22.677 -8.092 -7.564 0.5359 0.8405 -0.0794

Bcc 0.3458 46.399 16.556 15.477 -0.0275 0.1114 0.9934

Baa -0.0073 -0.980 -0.350 -0.327 0.9807 0.1930 -0.0307

4 C(13) Bbb 0.0009 0.115 0.041 0.038 0.0457 -0.0733 0.9963

Bcc 0.0064 0.865 0.309 0.289 -0.1900 0.9785 0.0807

Baa -0.0073 -0.980 -0.350 -0.327 0.9807 -0.1930 0.0307

5 C(13) Bbb 0.0009 0.115 0.041 0.038 -0.0457 -0.0733 0.9963

Bcc 0.0064 0.865 0.309 0.289 0.1900 0.9785 0.0807

Baa -0.0228 -0.880 -0.314 -0.293 0.7584 -0.6024 0.2491

6 N(14) Bbb -0.0048 -0.186 -0.066 -0.062 0.6426 0.7550 -0.1306

Bcc 0.0276 1.065 0.380 0.355 -0.1094 0.2591 0.9596

Baa -0.0822 -11.030 -3.936 -3.679 0.9982 -0.0025 0.0596

7 C(13) Bbb -0.0771 -10.352 -3.694 -3.453 0.0030 1.0000 -0.0082

Bcc 0.1593 21.382 7.630 7.132 -0.0596 0.0083 0.9982

Baa -0.0926 -3.571 -1.274 -1.191 0.9940 0.0000 0.1095

8 N(14) Bbb -0.0848 -3.269 -1.167 -1.090 0.0000 1.0000 0.0000

Bcc 0.1773 6.840 2.441 2.281 -0.1095 0.0000 0.9940

Baa -0.0822 -11.030 -3.936 -3.679 0.9982 0.0025 0.0596

9 C(13) Bbb -0.0771 -10.352 -3.694 -3.453 -0.0030 1.0000 0.0082

Bcc 0.1593 21.382 7.630 7.132 -0.0596 -0.0083 0.9982

Baa -0.0186 -2.498 -0.891 -0.833 -0.0358 -0.0057 0.9993

10 C(13) Bbb 0.0053 0.709 0.253 0.236 -0.2011 0.9796 -0.0016

Bcc 0.0133 1.789 0.639 0.597 0.9789 0.2010 0.0362

Baa -0.0186 -2.498 -0.891 -0.833 -0.0358 0.0057 0.9993

11 C(13) Bbb 0.0053 0.709 0.253 0.236 0.2011 0.9796 0.0016

Bcc 0.0133 1.789 0.639 0.597 0.9789 -0.2010 0.0362

Baa -0.0228 -0.880 -0.314 -0.293 0.7584 0.6024 -0.2491

12 N(14) Bbb -0.0048 -0.186 -0.066 -0.062 -0.6426 0.7550 -0.1306

Bcc 0.0276 1.065 0.380 0.355 0.1094 0.2591 0.9596

Baa -0.0186 -2.498 -0.891 -0.833 0.0358 0.0057 0.9993

13 C(13) Bbb 0.0053 0.709 0.253 0.236 -0.2011 0.9796 0.0016

Bcc 0.0133 1.789 0.639 0.597 0.9789 0.2010 -0.0362

Baa -0.0186 -2.498 -0.891 -0.833 0.0358 -0.0057 0.9993

14 C(13) Bbb 0.0053 0.709 0.253 0.236 0.2011 0.9796 -0.0016

Bcc 0.0133 1.789 0.639 0.597 0.9789 -0.2010 -0.0362

Baa -0.0822 -11.030 -3.936 -3.679 0.9982 -0.0025 -0.0596

15 C(13) Bbb -0.0771 -10.352 -3.694 -3.453 0.0030 1.0000 0.0082

Bcc 0.1593 21.382 7.630 7.132 0.0596 -0.0083 0.9982

Baa -0.0926 -3.571 -1.274 -1.191 0.9940 0.0000 -0.1095

16 N(14) Bbb -0.0848 -3.269 -1.167 -1.090 0.0000 1.0000 0.0000

Bcc 0.1773 6.840 2.441 2.281 0.1095 0.0000 0.9940

Baa -0.0822 -11.030 -3.936 -3.679 0.9982 0.0025 -0.0596

17 C(13) Bbb -0.0771 -10.352 -3.694 -3.453 -0.0030 1.0000 -0.0082

Bcc 0.1593 21.382 7.630 7.132 0.0596 0.0083 0.9982

Baa -0.0228 -0.880 -0.314 -0.293 0.7584 -0.6024 -0.2491

18 N(14) Bbb -0.0048 -0.186 -0.066 -0.062 0.6426 0.7550 0.1306

Bcc 0.0276 1.065 0.380 0.355 0.1094 -0.2591 0.9596

Baa -0.1539 -5.934 -2.117 -1.979 0.0000 -0.1626 0.9867

19 N(14) Bbb 0.0734 2.832 1.010 0.945 0.0000 0.9867 0.1626

Bcc 0.0804 3.102 1.107 1.035 1.0000 0.0000 0.0000

Baa -0.1768 -23.722 -8.464 -7.913 0.8438 -0.5302 -0.0828

20 C(13) Bbb -0.1690 -22.677 -8.092 -7.564 0.5359 0.8405 0.0794

Bcc 0.3458 46.399 16.556 15.477 0.0275 -0.1114 0.9934

Baa -0.0073 -0.980 -0.350 -0.327 0.9807 0.1930 0.0307

21 C(13) Bbb 0.0009 0.115 0.041 0.038 -0.0457 0.0733 0.9963

Bcc 0.0064 0.865 0.309 0.289 -0.1900 0.9785 -0.0807

Baa -0.0073 -0.980 -0.350 -0.327 0.9807 -0.1930 -0.0307

22 C(13) Bbb 0.0009 0.115 0.041 0.038 0.0457 0.0733 0.9963

Bcc 0.0064 0.865 0.309 0.289 0.1900 0.9785 -0.0807

Baa -0.1768 -23.722 -8.464 -7.913 0.8438 0.5302 0.0828

23 C(13) Bbb -0.1690 -22.677 -8.092 -7.564 -0.5359 0.8405 0.0794

Bcc 0.3458 46.399 16.556 15.477 -0.0275 -0.1114 0.9934

Baa -0.0228 -0.880 -0.314 -0.293 0.7584 0.6024 0.2491

24 N(14) Bbb -0.0048 -0.186 -0.066 -0.062 -0.6426 0.7550 0.1306

Bcc 0.0276 1.065 0.380 0.355 -0.1094 -0.2591 0.9596

Baa -0.0104 -0.348 -0.124 -0.116 0.0000 1.0000 0.0000

25 Zn(67) Bbb -0.0026 -0.088 -0.031 -0.029 0.0000 0.0000 1.0000

Bcc 0.0130 0.436 0.156 0.145 1.0000 0.0000 0.0000

Baa -0.0274 -3.674 -1.311 -1.226 0.0647 0.9978 -0.0121

26 C(13) Bbb -0.0246 -3.305 -1.179 -1.102 0.9970 -0.0652 -0.0426

Bcc 0.0520 6.979 2.490 2.328 0.0433 0.0094 0.9990

Baa -0.0026 -0.348 -0.124 -0.116 0.1422 0.9896 -0.0223

27 C(13) Bbb 0.0002 0.029 0.010 0.010 0.9886 -0.1431 -0.0471

Bcc 0.0024 0.320 0.114 0.107 0.0498 0.0154 0.9986

Baa -0.0026 -0.348 -0.124 -0.116 -0.1422 0.9896 0.0223

28 C(13) Bbb 0.0002 0.029 0.010 0.010 0.9886 0.1431 -0.0471

Bcc 0.0024 0.320 0.114 0.107 0.0498 -0.0154 0.9986

Baa -0.0274 -3.674 -1.311 -1.226 -0.0647 0.9978 0.0121

29 C(13) Bbb -0.0246 -3.305 -1.179 -1.102 0.9970 0.0652 -0.0426

Bcc 0.0520 6.979 2.490 2.328 0.0433 -0.0094 0.9990

Baa -0.0467 -6.263 -2.235 -2.089 0.9995 -0.0319 -0.0009

30 C(13) Bbb -0.0424 -5.683 -2.028 -1.896 0.0318 0.9924 0.1191

Bcc 0.0890 11.946 4.263 3.985 -0.0029 -0.1190 0.9929

Baa -0.0111 -1.486 -0.530 -0.496 0.9791 0.2018 0.0252

31 C(13) Bbb -0.0070 -0.935 -0.334 -0.312 -0.2034 0.9722 0.1162

Bcc 0.0180 2.421 0.864 0.808 -0.0010 -0.1189 0.9929

Baa -0.0111 -1.486 -0.530 -0.496 0.9791 -0.2018 -0.0252

32 C(13) Bbb -0.0070 -0.935 -0.334 -0.312 0.2034 0.9722 0.1162

Bcc 0.0180 2.421 0.864 0.808 0.0010 -0.1189 0.9929

Baa -0.0467 -6.263 -2.235 -2.089 0.9995 0.0319 0.0009

33 C(13) Bbb -0.0424 -5.683 -2.028 -1.896 -0.0318 0.9924 0.1191

Bcc 0.0890 11.946 4.263 3.985 0.0029 -0.1190 0.9929

Baa -0.0274 -3.674 -1.311 -1.226 -0.0647 0.9978 -0.0121

34 C(13) Bbb -0.0246 -3.305 -1.179 -1.102 0.9970 0.0652 0.0426

Bcc 0.0520 6.979 2.490 2.328 -0.0433 0.0094 0.9990

Baa -0.0026 -0.348 -0.124 -0.116 -0.1422 0.9896 -0.0223

35 C(13) Bbb 0.0002 0.029 0.010 0.010 0.9886 0.1431 0.0471

Bcc 0.0024 0.320 0.114 0.107 -0.0498 0.0154 0.9986

Baa -0.0026 -0.348 -0.124 -0.116 0.1422 0.9896 0.0223

36 C(13) Bbb 0.0002 0.029 0.010 0.010 0.9886 -0.1431 0.0471

Bcc 0.0024 0.320 0.114 0.107 -0.0498 -0.0154 0.9986

Baa -0.0274 -3.674 -1.311 -1.226 0.0647 0.9978 0.0121

37 C(13) Bbb -0.0246 -3.305 -1.179 -1.102 0.9970 -0.0652 0.0426

Bcc 0.0520 6.979 2.490 2.328 -0.0433 -0.0094 0.9990

Baa -0.0467 -6.263 -2.235 -2.089 0.9995 -0.0319 0.0009

38 C(13) Bbb -0.0424 -5.683 -2.028 -1.896 0.0318 0.9924 -0.1191

Bcc 0.0890 11.946 4.263 3.985 0.0029 0.1190 0.9929

Baa -0.0111 -1.486 -0.530 -0.496 0.9791 0.2018 -0.0252

39 C(13) Bbb -0.0070 -0.935 -0.334 -0.312 -0.2034 0.9722 -0.1162

Bcc 0.0180 2.421 0.864 0.808 0.0010 0.1189 0.9929

Baa -0.0111 -1.486 -0.530 -0.496 0.9791 -0.2018 0.0252

40 C(13) Bbb -0.0070 -0.935 -0.334 -0.312 0.2034 0.9722 -0.1162

Bcc 0.0180 2.421 0.864 0.808 -0.0010 0.1189 0.9929

Baa -0.0467 -6.263 -2.235 -2.089 0.9995 0.0319 -0.0009

41 C(13) Bbb -0.0424 -5.683 -2.028 -1.896 -0.0318 0.9924 -0.1191

Bcc 0.0890 11.946 4.263 3.985 -0.0029 0.1190 0.9929

Baa -0.0101 -1.358 -0.485 -0.453 0.9998 -0.0220 -0.0030

42 C(13) Bbb -0.0060 -0.805 -0.287 -0.268 0.0222 0.9931 0.1154

Bcc 0.0161 2.163 0.772 0.722 0.0005 -0.1154 0.9933

Baa -0.0127 -1.708 -0.609 -0.570 0.9993 -0.0380 -0.0042

43 C(13) Bbb -0.0115 -1.541 -0.550 -0.514 0.0382 0.9923 0.1182

Bcc 0.0242 3.249 1.159 1.084 -0.0003 -0.1182 0.9930

Baa -0.0127 -1.708 -0.609 -0.570 0.9993 0.0380 0.0042

44 C(13) Bbb -0.0115 -1.541 -0.550 -0.514 -0.0382 0.9923 0.1182

Bcc 0.0242 3.249 1.159 1.084 0.0003 -0.1182 0.9930

Baa -0.0101 -1.358 -0.485 -0.453 0.9998 0.0220 0.0030

45 C(13) Bbb -0.0060 -0.805 -0.287 -0.268 -0.0222 0.9931 0.1154

Bcc 0.0161 2.163 0.772 0.722 -0.0005 -0.1154 0.9933

Baa -0.0066 -0.892 -0.318 -0.298 -0.0093 0.9999 0.0039

46 C(13) Bbb -0.0045 -0.600 -0.214 -0.200 0.9987 0.0095 -0.0496

Bcc 0.0111 1.492 0.533 0.498 0.0497 -0.0034 0.9988

Baa -0.0056 -0.748 -0.267 -0.249 -0.0635 0.9980 0.0030

47 C(13) Bbb -0.0046 -0.617 -0.220 -0.206 0.9968 0.0636 -0.0488

Bcc 0.0102 1.364 0.487 0.455 0.0489 0.0001 0.9988

Baa -0.0056 -0.748 -0.267 -0.249 0.0635 0.9980 -0.0030

48 C(13) Bbb -0.0046 -0.617 -0.220 -0.206 0.9968 -0.0636 -0.0488

Bcc 0.0102 1.364 0.487 0.455 0.0489 -0.0001 0.9988

Baa -0.0066 -0.892 -0.318 -0.298 0.0093 0.9999 -0.0039

49 C(13) Bbb -0.0045 -0.600 -0.214 -0.200 0.9987 -0.0095 -0.0496

Bcc 0.0111 1.492 0.533 0.498 0.0497 0.0034 0.9988

Baa -0.0101 -1.358 -0.485 -0.453 0.9998 -0.0220 0.0030

50 C(13) Bbb -0.0060 -0.805 -0.287 -0.268 0.0222 0.9931 -0.1154

Bcc 0.0161 2.163 0.772 0.722 -0.0005 0.1154 0.9933

Baa -0.0127 -1.708 -0.609 -0.570 0.9993 -0.0380 0.0042

51 C(13) Bbb -0.0115 -1.541 -0.550 -0.514 0.0382 0.9923 -0.1182

Bcc 0.0242 3.249 1.159 1.084 0.0003 0.1182 0.9930

Baa -0.0127 -1.708 -0.609 -0.570 0.9993 0.0380 -0.0042

52 C(13) Bbb -0.0115 -1.541 -0.550 -0.514 -0.0382 0.9923 -0.1182

Bcc 0.0242 3.249 1.159 1.084 -0.0003 0.1182 0.9930

Baa -0.0101 -1.358 -0.485 -0.453 0.9998 0.0220 -0.0030

53 C(13) Bbb -0.0060 -0.805 -0.287 -0.268 -0.0222 0.9931 -0.1154

Bcc 0.0161 2.163 0.772 0.722 0.0005 0.1154 0.9933

Baa -0.0066 -0.892 -0.318 -0.298 0.0093 0.9999 0.0039

54 C(13) Bbb -0.0045 -0.600 -0.214 -0.200 0.9987 -0.0095 0.0496

Bcc 0.0111 1.492 0.533 0.498 -0.0497 -0.0034 0.9988

Baa -0.0056 -0.748 -0.267 -0.249 0.0635 0.9980 0.0030

55 C(13) Bbb -0.0046 -0.617 -0.220 -0.206 0.9968 -0.0636 0.0488

Bcc 0.0102 1.364 0.487 0.455 -0.0489 0.0001 0.9988

Baa -0.0056 -0.748 -0.267 -0.249 -0.0635 0.9980 -0.0030

56 C(13) Bbb -0.0046 -0.617 -0.220 -0.206 0.9968 0.0636 0.0488

Bcc 0.0102 1.364 0.487 0.455 -0.0489 -0.0001 0.9988

Baa -0.0066 -0.892 -0.318 -0.298 -0.0093 0.9999 -0.0039

57 C(13) Bbb -0.0045 -0.600 -0.214 -0.200 0.9987 0.0095 0.0496

Bcc 0.0111 1.492 0.533 0.498 -0.0497 0.0034 0.9988

Baa -0.0022 -1.169 -0.417 -0.390 -0.0271 0.0298 0.9992

58 H(1) Bbb -0.0010 -0.511 -0.183 -0.171 0.9914 -0.1274 0.0307

Bcc 0.0032 1.681 0.600 0.561 0.1282 0.9914 -0.0261

Baa -0.0022 -1.169 -0.417 -0.390 -0.0271 -0.0298 0.9992

59 H(1) Bbb -0.0010 -0.511 -0.183 -0.171 0.9914 0.1274 0.0307

Bcc 0.0032 1.681 0.600 0.561 -0.1282 0.9914 0.0261

Baa -0.0032 -1.713 -0.611 -0.571 -0.0618 0.9195 0.3881

60 H(1) Bbb -0.0030 -1.577 -0.563 -0.526 0.0196 -0.3876 0.9216

Bcc 0.0062 3.290 1.174 1.098 0.9979 0.0646 0.0060

Baa -0.0032 -1.713 -0.611 -0.571 0.0618 0.9195 0.3881

61 H(1) Bbb -0.0030 -1.577 -0.563 -0.526 -0.0196 -0.3876 0.9216

Bcc 0.0062 3.290 1.174 1.098 0.9979 -0.0646 -0.0060

Baa -0.0022 -1.169 -0.417 -0.390 0.0271 0.0298 0.9992

62 H(1) Bbb -0.0010 -0.511 -0.183 -0.171 0.9914 0.1274 -0.0307

Bcc 0.0032 1.681 0.600 0.561 -0.1282 0.9914 -0.0261

Baa -0.0022 -1.169 -0.417 -0.390 0.0271 -0.0298 0.9992

63 H(1) Bbb -0.0010 -0.511 -0.183 -0.171 0.9914 -0.1274 -0.0307

Bcc 0.0032 1.681 0.600 0.561 0.1282 0.9914 0.0261

Baa -0.0032 -1.713 -0.611 -0.571 -0.0618 0.9195 -0.3881

64 H(1) Bbb -0.0030 -1.577 -0.563 -0.526 -0.0196 0.3876 0.9216

Bcc 0.0062 3.290 1.174 1.098 0.9979 0.0646 -0.0060

Baa -0.0032 -1.713 -0.611 -0.571 0.0618 0.9195 -0.3881

65 H(1) Bbb -0.0030 -1.577 -0.563 -0.526 0.0196 0.3876 0.9216

Bcc 0.0062 3.290 1.174 1.098 0.9979 -0.0646 0.0060

Baa -0.0016 -0.875 -0.312 -0.292 0.0018 -0.1045 0.9945

66 H(1) Bbb 0.0003 0.176 0.063 0.059 0.4470 0.8897 0.0927

Bcc 0.0013 0.698 0.249 0.233 0.8945 -0.4444 -0.0483

Baa -0.0020 -1.076 -0.384 -0.359 0.9493 0.3119 0.0399

67 H(1) Bbb -0.0009 -0.477 -0.170 -0.159 -0.0040 -0.1149 0.9934

Bcc 0.0029 1.553 0.554 0.518 -0.3144 0.9431 0.1078

Baa -0.0020 -1.076 -0.384 -0.359 0.9493 -0.3119 -0.0399

68 H(1) Bbb -0.0009 -0.477 -0.170 -0.159 0.0040 -0.1149 0.9934

Bcc 0.0029 1.553 0.554 0.518 0.3144 0.9431 0.1078

Baa -0.0016 -0.875 -0.312 -0.292 -0.0018 -0.1045 0.9945

69 H(1) Bbb 0.0003 0.176 0.063 0.059 -0.4470 0.8897 0.0927

Bcc 0.0013 0.698 0.249 0.233 0.8945 0.4444 0.0483

Baa -0.0010 -0.544 -0.194 -0.182 0.0290 -0.0044 0.9996

70 H(1) Bbb 0.0002 0.106 0.038 0.036 0.8070 0.5902 -0.0209

Bcc 0.0008 0.438 0.156 0.146 -0.5899 0.8072 0.0207

Baa -0.0009 -0.493 -0.176 -0.164 0.3068 0.9514 -0.0249

71 H(1) Bbb -0.0006 -0.310 -0.111 -0.103 0.0439 0.0119 0.9990

Bcc 0.0015 0.803 0.286 0.268 0.9507 -0.3076 -0.0381

Baa -0.0009 -0.493 -0.176 -0.164 -0.3068 0.9514 0.0249

72 H(1) Bbb -0.0006 -0.310 -0.111 -0.103 0.0439 -0.0119 0.9990

Bcc 0.0015 0.803 0.286 0.268 0.9507 0.3076 -0.0381

Baa -0.0010 -0.544 -0.194 -0.182 0.0290 0.0044 0.9996

73 H(1) Bbb 0.0002 0.106 0.038 0.036 0.8070 -0.5902 -0.0209

Bcc 0.0008 0.438 0.156 0.146 0.5899 0.8072 -0.0207

Baa -0.0016 -0.875 -0.312 -0.292 -0.0018 0.1045 0.9945

74 H(1) Bbb 0.0003 0.176 0.063 0.059 0.4470 0.8897 -0.0927

Bcc 0.0013 0.698 0.249 0.233 0.8945 -0.4444 0.0483

Baa -0.0020 -1.076 -0.384 -0.359 0.9493 0.3119 -0.0399

75 H(1) Bbb -0.0009 -0.477 -0.170 -0.159 0.0040 0.1149 0.9934

Bcc 0.0029 1.553 0.554 0.518 -0.3144 0.9431 -0.1078

Baa -0.0020 -1.076 -0.384 -0.359 0.9493 -0.3119 0.0399

76 H(1) Bbb -0.0009 -0.477 -0.170 -0.159 -0.0040 0.1149 0.9934

Bcc 0.0029 1.553 0.554 0.518 0.3144 0.9431 -0.1078

Baa -0.0016 -0.875 -0.312 -0.292 0.0018 0.1045 0.9945

77 H(1) Bbb 0.0003 0.176 0.063 0.059 -0.4470 0.8897 -0.0927

Bcc 0.0013 0.698 0.249 0.233 0.8945 0.4444 -0.0483

Baa -0.0010 -0.544 -0.194 -0.182 -0.0290 -0.0044 0.9996

78 H(1) Bbb 0.0002 0.106 0.038 0.036 0.8070 -0.5902 0.0209

Bcc 0.0008 0.438 0.156 0.146 0.5899 0.8072 0.0207

Baa -0.0009 -0.493 -0.176 -0.164 -0.3068 0.9514 -0.0249

79 H(1) Bbb -0.0006 -0.310 -0.111 -0.103 -0.0439 0.0119 0.9990

Bcc 0.0015 0.803 0.286 0.268 0.9507 0.3076 0.0381

Baa -0.0009 -0.493 -0.176 -0.164 0.3068 0.9514 0.0249

80 H(1) Bbb -0.0006 -0.310 -0.111 -0.103 -0.0439 -0.0119 0.9990

Bcc 0.0015 0.803 0.286 0.268 0.9507 -0.3076 0.0381

Baa -0.0010 -0.544 -0.194 -0.182 -0.0290 0.0044 0.9996

81 H(1) Bbb 0.0002 0.106 0.038 0.036 0.8070 0.5902 0.0209

Bcc 0.0008 0.438 0.156 0.146 -0.5899 0.8072 -0.0207

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

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Sun Jun 30 20:02:07 2019, MaxMem= 1342177280 cpu: 265.0

(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.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36581 LenP2D= 94878.

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 = 193

Leave Link 701 at Sun Jun 30 20:02:45 2019, MaxMem= 1342177280 cpu: 378.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sun Jun 30 20:02:45 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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 Sun Jun 30 20:03:34 2019, MaxMem= 1342177280 cpu: 488.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-4.60076421D-13 5.08038056D-13 9.66740697D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000873120 -0.001682621 -0.000239899

2 7 0.000000000 0.004286255 -0.000036850

3 6 -0.000873120 -0.001682621 -0.000239899

4 6 -0.000110634 0.001264938 -0.000337645

5 6 0.000110634 0.001264938 -0.000337645

6 7 0.000411622 -0.002517510 0.000093866

7 6 0.002349264 0.002325156 -0.000023456

8 7 -0.003820212 0.000000000 0.000541680

9 6 0.002349264 -0.002325156 -0.000023456

10 6 -0.001638040 0.000106278 -0.000308159

11 6 -0.001638040 -0.000106278 -0.000308159

12 7 -0.000411622 -0.002517510 0.000093866

13 6 0.001638040 -0.000106278 -0.000308159

14 6 0.001638040 0.000106278 -0.000308159

15 6 -0.002349264 -0.002325156 -0.000023456

16 7 0.003820212 0.000000000 0.000541680

17 6 -0.002349264 0.002325156 -0.000023456

18 7 -0.000411622 0.002517510 0.000093866

19 7 0.000000000 -0.004286255 -0.000036850

20 6 0.000873120 0.001682621 -0.000239899

21 6 0.000110634 -0.001264938 -0.000337645

22 6 -0.000110634 -0.001264938 -0.000337645

23 6 -0.000873120 0.001682621 -0.000239899

24 7 0.000411622 0.002517510 0.000093866

25 30 0.000000000 0.000000000 -0.000396854

26 6 -0.001004897 -0.002541493 0.000014749

27 6 0.000334502 0.000300583 0.000008958

28 6 0.000334502 -0.000300583 0.000008958

29 6 -0.001004897 0.002541493 0.000014749

30 6 0.002547301 0.000568990 0.000093880

31 6 -0.000650744 0.000077782 0.000029968

32 6 0.000650744 0.000077782 0.000029968

33 6 -0.002547301 0.000568990 0.000093880

34 6 0.001004897 -0.002541493 0.000014749

35 6 -0.000334502 0.000300583 0.000008958

36 6 -0.000334502 -0.000300583 0.000008958

37 6 0.001004897 0.002541493 0.000014749

38 6 -0.002547301 -0.000568990 0.000093880

39 6 0.000650744 -0.000077782 0.000029968

40 6 -0.000650744 -0.000077782 0.000029968

41 6 0.002547301 -0.000568990 0.000093880

42 6 -0.002810842 -0.001465897 -0.000171355

43 6 -0.000336882 0.003307752 0.000387980

44 6 0.000336882 0.003307752 0.000387980

45 6 0.002810842 -0.001465897 -0.000171355

46 6 0.001191834 0.002783955 -0.000005560

47 6 -0.003180828 0.000618312 0.000133723

48 6 -0.003180828 -0.000618312 0.000133723

49 6 0.001191834 -0.002783955 -0.000005560

50 6 0.002810842 0.001465897 -0.000171355

51 6 0.000336882 -0.003307752 0.000387980

52 6 -0.000336882 -0.003307752 0.000387980

53 6 -0.002810842 0.001465897 -0.000171355

54 6 -0.001191834 0.002783955 -0.000005560

55 6 0.003180828 0.000618312 0.000133723

56 6 0.003180828 -0.000618312 0.000133723

57 6 -0.001191834 -0.002783955 -0.000005560

58 1 -0.000199240 -0.001038139 0.000047996

59 1 -0.000199240 0.001038139 0.000047996

60 1 0.001038124 0.000183994 0.000001980

61 1 -0.001038124 0.000183994 0.000001980

62 1 0.000199240 -0.001038139 0.000047996

63 1 0.000199240 0.001038139 0.000047996

64 1 -0.001038124 -0.000183994 0.000001980

65 1 0.001038124 -0.000183994 0.000001980

66 1 -0.001006430 -0.000198422 -0.000007171

67 1 -0.000506002 0.000852958 0.000105615

68 1 0.000506002 0.000852958 0.000105615

69 1 0.001006430 -0.000198422 -0.000007171

70 1 0.000200448 0.001022384 -0.000012596

71 1 -0.000870364 0.000522392 0.000033925

72 1 -0.000870364 -0.000522392 0.000033925

73 1 0.000200448 -0.001022384 -0.000012596

74 1 0.001006430 0.000198422 -0.000007171

75 1 0.000506002 -0.000852958 0.000105615

76 1 -0.000506002 -0.000852958 0.000105615

77 1 -0.001006430 0.000198422 -0.000007171

78 1 -0.000200448 0.001022384 -0.000012596

79 1 0.000870364 0.000522392 0.000033925

80 1 0.000870364 -0.000522392 0.000033925

81 1 -0.000200448 -0.001022384 -0.000012596

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

Cartesian Forces: Max 0.004286255 RMS 0.001311993

Leave Link 716 at Sun Jun 30 20:03:34 2019, MaxMem= 1342177280 cpu: 2.3

(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 0.004779867 RMS 0.001179041

Search for a local minimum.

Step number 1 out of a maximum of 486

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .11790D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Second derivative matrix not updated -- first step.

ITU= 0

Eigenvalues --- 0.01437 0.01496 0.01503 0.01542 0.01575

Eigenvalues --- 0.01602 0.01628 0.01657 0.01688 0.01695

Eigenvalues --- 0.01698 0.01709 0.01713 0.01715 0.01725

Eigenvalues --- 0.01730 0.01730 0.01732 0.01736 0.01738

Eigenvalues --- 0.01754 0.01760 0.01764 0.01791 0.01802

Eigenvalues --- 0.01826 0.01829 0.01830 0.01851 0.01854

Eigenvalues --- 0.01869 0.01870 0.01900 0.01928 0.01968

Eigenvalues --- 0.01968 0.01972 0.01972 0.01976 0.01992

Eigenvalues --- 0.01992 0.01993 0.01993 0.02043 0.02080

Eigenvalues --- 0.02080 0.02086 0.02086 0.02090 0.02090

Eigenvalues --- 0.02095 0.02095 0.02099 0.02099 0.02103

Eigenvalues --- 0.02103 0.02106 0.02106 0.02124 0.02125

Eigenvalues --- 0.02137 0.02141 0.02144 0.02144 0.02148

Eigenvalues --- 0.02148 0.02172 0.02173 0.02214 0.02214

Eigenvalues --- 0.02224 0.02225 0.02276 0.02283 0.02341

Eigenvalues --- 0.02346 0.03235 0.05442 0.05622 0.08008

Eigenvalues --- 0.14669 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 --- 0.16144 0.16208 0.16845 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22501 0.22501 0.22505

Eigenvalues --- 0.22505 0.23234 0.23234 0.23234 0.23239

Eigenvalues --- 0.23482 0.23936 0.23941 0.23942 0.23950

Eigenvalues --- 0.24057 0.24278 0.24459 0.24555 0.24556

Eigenvalues --- 0.24557 0.24558 0.24734 0.24901 0.24901

Eigenvalues --- 0.24909 0.24983 0.24990 0.24991 0.24991

Eigenvalues --- 0.24992 0.24998 0.24998 0.24998 0.24998

Eigenvalues --- 0.32875 0.32956 0.33683 0.33699 0.33773

Eigenvalues --- 0.33852 0.35037 0.35058 0.35181 0.35181

Eigenvalues --- 0.35181 0.35181 0.35202 0.35202 0.35202

Eigenvalues --- 0.35202 0.35231 0.35231 0.35231 0.35231

Eigenvalues --- 0.35249 0.35249 0.35249 0.35249 0.35270

Eigenvalues --- 0.35270 0.35270 0.35270 0.35279 0.35279

Eigenvalues --- 0.35279 0.35279 0.35404 0.35421 0.36320

Eigenvalues --- 0.36363 0.37406 0.37464 0.37970 0.37981

Eigenvalues --- 0.39288 0.39288 0.39625 0.39625 0.40201

Eigenvalues --- 0.40201 0.40268 0.40268 0.40856 0.40907

Eigenvalues --- 0.41004 0.41012 0.41602 0.41606 0.41821

Eigenvalues --- 0.41877 0.42215 0.42215 0.42294 0.42806

Eigenvalues --- 0.42807 0.42930 0.42967 0.45592 0.47071

Eigenvalues --- 0.47127 0.47127 0.47388 0.47390 0.47583

Eigenvalues --- 0.47584 0.48142 0.48221 0.48222 0.48442

Eigenvalues --- 0.48466 0.48475 0.48633 0.48683 0.48687

Eigenvalues --- 0.48712 0.48736 0.49087 0.49899 0.49907

Eigenvalues --- 0.50371 0.50932 0.52482 0.58738 0.59251

Eigenvalues --- 0.59815 0.60898

RFO step: Lambda=-1.73267220D-03 EMin= 1.43730065D-02

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.01543408 RMS(Int)= 0.00001192

Iteration 2 RMS(Cart)= 0.00004931 RMS(Int)= 0.00000378

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000378

ITry= 1 IFail=0 DXMaxC= 5.46D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.20D-08 for atom 77.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58501 -0.00255 0.00000 -0.00474 -0.00474 2.58027

R2 2.74800 -0.00196 0.00000 -0.00536 -0.00536 2.74264

R3 2.56435 -0.00212 0.00000 -0.00519 -0.00520 2.55915

R4 2.58501 -0.00255 0.00000 -0.00474 -0.00474 2.58027

R5 3.94561 -0.00135 0.00000 -0.00186 -0.00186 3.94375

R6 2.74800 -0.00196 0.00000 -0.00536 -0.00536 2.74264

R7 2.56435 -0.00212 0.00000 -0.00519 -0.00520 2.55915

R8 2.71762 -0.00181 0.00000 -0.00526 -0.00526 2.71236

R9 2.60772 -0.00391 0.00000 -0.00797 -0.00797 2.59975

R10 2.60772 -0.00391 0.00000 -0.00797 -0.00797 2.59975

R11 2.49161 -0.00372 0.00000 -0.00707 -0.00707 2.48454

R12 2.60301 -0.00244 0.00000 -0.00489 -0.00488 2.59813

R13 2.78939 -0.00181 0.00000 -0.00532 -0.00532 2.78407

R14 2.60301 -0.00244 0.00000 -0.00489 -0.00488 2.59813

R15 3.92700 -0.00160 0.00000 -0.00524 -0.00522 3.92177

R16 2.78939 -0.00181 0.00000 -0.00532 -0.00532 2.78407

R17 2.49161 -0.00372 0.00000 -0.00707 -0.00707 2.48454

R18 2.69789 -0.00220 0.00000 -0.00605 -0.00606 2.69183

R19 2.59255 -0.00411 0.00000 -0.00818 -0.00818 2.58438

R20 2.59255 -0.00411 0.00000 -0.00818 -0.00818 2.58438

R21 2.49161 -0.00372 0.00000 -0.00707 -0.00707 2.48454

R22 2.69789 -0.00220 0.00000 -0.00605 -0.00606 2.69183

R23 2.78939 -0.00181 0.00000 -0.00532 -0.00532 2.78407

R24 2.59255 -0.00411 0.00000 -0.00818 -0.00818 2.58438

R25 2.78939 -0.00181 0.00000 -0.00532 -0.00532 2.78407

R26 2.59255 -0.00411 0.00000 -0.00818 -0.00818 2.58438

R27 2.60301 -0.00244 0.00000 -0.00489 -0.00488 2.59813

R28 2.49161 -0.00372 0.00000 -0.00707 -0.00707 2.48454

R29 2.60301 -0.00244 0.00000 -0.00489 -0.00488 2.59813

R30 3.92700 -0.00160 0.00000 -0.00524 -0.00522 3.92177

R31 2.56435 -0.00212 0.00000 -0.00519 -0.00520 2.55915

R32 2.58501 -0.00255 0.00000 -0.00474 -0.00474 2.58027

R33 2.58501 -0.00255 0.00000 -0.00474 -0.00474 2.58027

R34 3.94561 -0.00135 0.00000 -0.00186 -0.00186 3.94375

R35 2.74800 -0.00196 0.00000 -0.00536 -0.00536 2.74264

R36 2.71762 -0.00181 0.00000 -0.00526 -0.00526 2.71236

R37 2.60772 -0.00391 0.00000 -0.00797 -0.00797 2.59975

R38 2.74800 -0.00196 0.00000 -0.00536 -0.00536 2.74264

R39 2.60772 -0.00391 0.00000 -0.00797 -0.00797 2.59975

R40 2.56435 -0.00212 0.00000 -0.00519 -0.00520 2.55915

R41 2.69783 -0.00276 0.00000 -0.00655 -0.00655 2.69128

R42 2.05273 -0.00104 0.00000 -0.00293 -0.00293 2.04980

R43 2.72214 -0.00275 0.00000 -0.00645 -0.00645 2.71569

R44 2.68199 -0.00309 0.00000 -0.00710 -0.00710 2.67489

R45 2.69783 -0.00276 0.00000 -0.00655 -0.00655 2.69128

R46 2.68199 -0.00309 0.00000 -0.00710 -0.00710 2.67489

R47 2.05273 -0.00104 0.00000 -0.00293 -0.00293 2.04980

R48 2.68455 -0.00304 0.00000 -0.00710 -0.00710 2.67745

R49 2.05301 -0.00104 0.00000 -0.00293 -0.00293 2.05008

R50 2.73109 -0.00245 0.00000 -0.00585 -0.00585 2.72524

R51 2.68917 -0.00293 0.00000 -0.00682 -0.00682 2.68235

R52 2.68455 -0.00304 0.00000 -0.00710 -0.00710 2.67745

R53 2.68917 -0.00293 0.00000 -0.00682 -0.00682 2.68235

R54 2.05301 -0.00104 0.00000 -0.00293 -0.00293 2.05008

R55 2.69783 -0.00276 0.00000 -0.00655 -0.00655 2.69128

R56 2.05273 -0.00104 0.00000 -0.00293 -0.00293 2.04980

R57 2.72214 -0.00275 0.00000 -0.00645 -0.00645 2.71569

R58 2.68199 -0.00309 0.00000 -0.00710 -0.00710 2.67489

R59 2.69783 -0.00276 0.00000 -0.00655 -0.00655 2.69128

R60 2.68199 -0.00309 0.00000 -0.00710 -0.00710 2.67489

R61 2.05273 -0.00104 0.00000 -0.00293 -0.00293 2.04980

R62 2.68455 -0.00304 0.00000 -0.00710 -0.00710 2.67745

R63 2.05301 -0.00104 0.00000 -0.00293 -0.00293 2.05008

R64 2.73109 -0.00245 0.00000 -0.00585 -0.00585 2.72524

R65 2.68917 -0.00293 0.00000 -0.00682 -0.00682 2.68235

R66 2.68455 -0.00304 0.00000 -0.00710 -0.00710 2.67745

R67 2.68917 -0.00293 0.00000 -0.00682 -0.00682 2.68235

R68 2.05301 -0.00104 0.00000 -0.00293 -0.00293 2.05008

R69 2.60614 -0.00478 0.00000 -0.00979 -0.00979 2.59634

R70 2.05382 -0.00101 0.00000 -0.00285 -0.00285 2.05097

R71 2.68250 -0.00315 0.00000 -0.00766 -0.00765 2.67484

R72 2.05239 -0.00100 0.00000 -0.00281 -0.00281 2.04958

R73 2.60614 -0.00478 0.00000 -0.00979 -0.00979 2.59634

R74 2.05239 -0.00100 0.00000 -0.00281 -0.00281 2.04958

R75 2.05382 -0.00101 0.00000 -0.00285 -0.00285 2.05097

R76 2.61133 -0.00463 0.00000 -0.00957 -0.00957 2.60176

R77 2.05348 -0.00102 0.00000 -0.00289 -0.00289 2.05059

R78 2.67484 -0.00337 0.00000 -0.00805 -0.00805 2.66679

R79 2.05225 -0.00102 0.00000 -0.00286 -0.00286 2.04938

R80 2.61133 -0.00463 0.00000 -0.00957 -0.00957 2.60176

R81 2.05225 -0.00102 0.00000 -0.00286 -0.00286 2.04938

R82 2.05348 -0.00102 0.00000 -0.00289 -0.00289 2.05059

R83 2.60614 -0.00478 0.00000 -0.00979 -0.00979 2.59634

R84 2.05382 -0.00101 0.00000 -0.00285 -0.00285 2.05097

R85 2.68250 -0.00315 0.00000 -0.00766 -0.00765 2.67484

R86 2.05239 -0.00100 0.00000 -0.00281 -0.00281 2.04958

R87 2.60614 -0.00478 0.00000 -0.00979 -0.00979 2.59634

R88 2.05239 -0.00100 0.00000 -0.00281 -0.00281 2.04958

R89 2.05382 -0.00101 0.00000 -0.00285 -0.00285 2.05097

R90 2.61133 -0.00463 0.00000 -0.00957 -0.00957 2.60176

R91 2.05348 -0.00102 0.00000 -0.00289 -0.00289 2.05059

R92 2.67484 -0.00337 0.00000 -0.00805 -0.00805 2.66679

R93 2.05225 -0.00102 0.00000 -0.00286 -0.00286 2.04938

R94 2.61133 -0.00463 0.00000 -0.00957 -0.00957 2.60176

R95 2.05225 -0.00102 0.00000 -0.00286 -0.00286 2.04938

R96 2.05348 -0.00102 0.00000 -0.00289 -0.00289 2.05059

A1 1.89876 -0.00103 0.00000 -0.00277 -0.00276 1.89599

A2 2.22704 0.00076 0.00000 0.00318 0.00318 2.23022

A3 2.15708 0.00027 0.00000 -0.00039 -0.00039 2.15669

A4 1.92384 0.00163 0.00000 0.00340 0.00339 1.92723

A5 2.17464 -0.00081 0.00000 -0.00109 -0.00110 2.17354

A6 2.17464 -0.00081 0.00000 -0.00109 -0.00110 2.17354

A7 1.89876 -0.00103 0.00000 -0.00277 -0.00276 1.89599

A8 2.22704 0.00076 0.00000 0.00318 0.00318 2.23022

A9 2.15708 0.00027 0.00000 -0.00039 -0.00039 2.15669

A10 1.85164 0.00021 0.00000 0.00104 0.00104 1.85268

A11 2.31763 -0.00024 0.00000 -0.00096 -0.00096 2.31667

A12 2.11387 0.00003 0.00000 -0.00006 -0.00006 2.11381

A13 1.85164 0.00021 0.00000 0.00104 0.00104 1.85268

A14 2.31763 -0.00024 0.00000 -0.00096 -0.00096 2.31667

A15 2.11387 0.00003 0.00000 -0.00006 -0.00006 2.11381

A16 2.17286 -0.00021 0.00000 -0.00317 -0.00316 2.16970

A17 2.23703 0.00097 0.00000 0.00363 0.00363 2.24066

A18 2.14901 -0.00003 0.00000 -0.00119 -0.00120 2.14781

A19 1.89679 -0.00094 0.00000 -0.00255 -0.00255 1.89425

A20 1.91992 0.00139 0.00000 0.00296 0.00294 1.92286

A21 2.16945 -0.00068 0.00000 -0.00046 -0.00048 2.16898

A22 2.16945 -0.00068 0.00000 -0.00046 -0.00048 2.16898

A23 1.89679 -0.00094 0.00000 -0.00255 -0.00255 1.89425

A24 2.23703 0.00097 0.00000 0.00363 0.00363 2.24066

A25 2.14901 -0.00003 0.00000 -0.00119 -0.00120 2.14781

A26 1.85546 0.00024 0.00000 0.00102 0.00102 1.85648

A27 2.30751 -0.00033 0.00000 -0.00103 -0.00103 2.30648

A28 2.12017 0.00009 0.00000 0.00002 0.00003 2.12020

A29 1.85546 0.00024 0.00000 0.00102 0.00102 1.85648

A30 2.30751 -0.00033 0.00000 -0.00103 -0.00103 2.30648

A31 2.12017 0.00009 0.00000 0.00002 0.00003 2.12020

A32 2.17286 -0.00021 0.00000 -0.00317 -0.00316 2.16970

A33 1.85546 0.00024 0.00000 0.00102 0.00102 1.85648

A34 2.12017 0.00009 0.00000 0.00002 0.00003 2.12020

A35 2.30751 -0.00033 0.00000 -0.00103 -0.00103 2.30648

A36 1.85546 0.00024 0.00000 0.00102 0.00102 1.85648

A37 2.12017 0.00009 0.00000 0.00002 0.00003 2.12020

A38 2.30751 -0.00033 0.00000 -0.00103 -0.00103 2.30648

A39 1.89679 -0.00094 0.00000 -0.00255 -0.00255 1.89425

A40 2.14901 -0.00003 0.00000 -0.00119 -0.00120 2.14781

A41 2.23703 0.00097 0.00000 0.00363 0.00363 2.24066

A42 1.91992 0.00139 0.00000 0.00296 0.00294 1.92286

A43 2.16945 -0.00068 0.00000 -0.00046 -0.00048 2.16898

A44 2.16945 -0.00068 0.00000 -0.00046 -0.00048 2.16898

A45 2.14901 -0.00003 0.00000 -0.00119 -0.00120 2.14781

A46 2.23703 0.00097 0.00000 0.00363 0.00363 2.24066

A47 1.89679 -0.00094 0.00000 -0.00255 -0.00255 1.89425

A48 2.17286 -0.00021 0.00000 -0.00317 -0.00316 2.16970

A49 1.92384 0.00163 0.00000 0.00340 0.00339 1.92723

A50 2.17464 -0.00081 0.00000 -0.00109 -0.00110 2.17354

A51 2.17464 -0.00081 0.00000 -0.00109 -0.00110 2.17354

A52 2.22704 0.00076 0.00000 0.00318 0.00318 2.23022

A53 2.15708 0.00027 0.00000 -0.00039 -0.00039 2.15669

A54 1.89876 -0.00103 0.00000 -0.00277 -0.00276 1.89599

A55 1.85164 0.00021 0.00000 0.00104 0.00104 1.85268

A56 2.31763 -0.00024 0.00000 -0.00096 -0.00096 2.31667

A57 2.11387 0.00003 0.00000 -0.00006 -0.00006 2.11381

A58 1.85164 0.00021 0.00000 0.00104 0.00104 1.85268

A59 2.11387 0.00003 0.00000 -0.00006 -0.00006 2.11381

A60 2.31763 -0.00024 0.00000 -0.00096 -0.00096 2.31667

A61 1.89876 -0.00103 0.00000 -0.00277 -0.00276 1.89599

A62 2.22704 0.00076 0.00000 0.00318 0.00318 2.23022

A63 2.15708 0.00027 0.00000 -0.00039 -0.00039 2.15669

A64 2.17286 -0.00021 0.00000 -0.00317 -0.00316 2.16970

A65 1.50863 -0.00013 0.00000 -0.00061 -0.00061 1.50803

A66 1.50863 -0.00013 0.00000 -0.00061 -0.00061 1.50803

A67 2.64412 -0.00064 0.00000 -0.00519 -0.00519 2.63894

A68 2.63137 -0.00044 0.00000 0.00024 0.00024 2.63160

A69 1.50863 -0.00013 0.00000 -0.00061 -0.00061 1.50803

A70 1.50863 -0.00013 0.00000 -0.00061 -0.00061 1.50803

A71 2.07173 0.00004 0.00000 0.00030 0.00029 2.07203

A72 2.12241 -0.00023 0.00000 -0.00141 -0.00141 2.12099

A73 2.08905 0.00018 0.00000 0.00111 0.00111 2.09016

A74 2.09126 -0.00013 0.00000 -0.00033 -0.00033 2.09094

A75 2.11760 0.00035 0.00000 0.00069 0.00069 2.11830

A76 2.07432 -0.00022 0.00000 -0.00036 -0.00036 2.07395

A77 2.09126 -0.00013 0.00000 -0.00033 -0.00033 2.09094

A78 2.07432 -0.00022 0.00000 -0.00036 -0.00036 2.07395

A79 2.11760 0.00035 0.00000 0.00069 0.00069 2.11830

A80 2.07173 0.00004 0.00000 0.00030 0.00029 2.07203

A81 2.12241 -0.00023 0.00000 -0.00141 -0.00141 2.12099

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D5 -0.00966 -0.00003 0.00000 -0.00188 -0.00187 -0.01154

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D7 3.10715 -0.00001 0.00000 -0.00071 -0.00071 3.10644

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D46 -0.03222 -0.00015 0.00000 -0.00711 -0.00710 -0.03932

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D197 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D198 -3.14114 0.00000 0.00000 -0.00024 -0.00024 -3.14138

D199 3.14114 0.00000 0.00000 0.00024 0.00024 3.14138

D200 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D201 -3.14145 -0.00001 0.00000 -0.00033 -0.00033 3.14141

D202 -0.00004 0.00000 0.00000 0.00025 0.00025 0.00021

D203 0.00060 -0.00001 0.00000 -0.00057 -0.00057 0.00004

D204 -3.14117 0.00000 0.00000 0.00001 0.00001 -3.14116

D205 0.00590 0.00004 0.00000 0.00128 0.00128 0.00718

D206 -3.13674 -0.00001 0.00000 -0.00095 -0.00095 -3.13770

D207 -3.13615 0.00004 0.00000 0.00152 0.00152 -3.13463

D208 0.00439 -0.00001 0.00000 -0.00071 -0.00071 0.00368

D209 -0.00060 0.00001 0.00000 0.00057 0.00057 -0.00004

D210 3.14117 0.00000 0.00000 -0.00001 -0.00001 3.14116

D211 3.14145 0.00001 0.00000 0.00033 0.00033 -3.14141

D212 0.00004 0.00000 0.00000 -0.00025 -0.00025 -0.00021

D213 -0.00525 -0.00003 0.00000 -0.00144 -0.00144 -0.00669

D214 3.13765 -0.00004 0.00000 -0.00199 -0.00199 3.13565

D215 3.13736 0.00000 0.00000 0.00008 0.00008 3.13743

D216 -0.00293 -0.00001 0.00000 -0.00047 -0.00047 -0.00341

D217 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D218 -3.14033 -0.00001 0.00000 -0.00054 -0.00054 -3.14086

D219 3.14033 0.00001 0.00000 0.00054 0.00054 3.14086

D220 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D221 3.14028 0.00001 0.00000 0.00056 0.00056 3.14084

D222 -0.00104 0.00000 0.00000 0.00003 0.00003 -0.00101

D223 -0.00003 0.00000 0.00000 0.00001 0.00001 -0.00002

D224 -3.14135 -0.00001 0.00000 -0.00051 -0.00051 3.14133

D225 0.00525 0.00003 0.00000 0.00144 0.00144 0.00669

D226 -3.13736 0.00000 0.00000 -0.00008 -0.00008 -3.13743

D227 -3.13765 0.00004 0.00000 0.00199 0.00199 -3.13565

D228 0.00293 0.00001 0.00000 0.00047 0.00047 0.00341

D229 0.00003 0.00000 0.00000 -0.00001 -0.00001 0.00002

D230 3.14135 0.00001 0.00000 0.00051 0.00051 -3.14133

D231 -3.14028 -0.00001 0.00000 -0.00056 -0.00056 -3.14084

D232 0.00104 0.00000 0.00000 -0.00003 -0.00003 0.00101

D233 -0.00003 0.00000 0.00000 0.00001 0.00001 -0.00002

D234 3.14086 0.00001 0.00000 0.00032 0.00032 3.14118

D235 -3.14134 -0.00001 0.00000 -0.00052 -0.00052 3.14132

D236 -0.00045 0.00000 0.00000 -0.00022 -0.00022 -0.00067

D237 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D238 3.14089 0.00001 0.00000 0.00030 0.00030 3.14120

D239 -3.14089 -0.00001 0.00000 -0.00030 -0.00030 -3.14120

D240 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D241 0.00003 0.00000 0.00000 -0.00001 -0.00001 0.00002

D242 3.14134 0.00001 0.00000 0.00052 0.00052 -3.14132

D243 -3.14086 -0.00001 0.00000 -0.00032 -0.00032 -3.14118

D244 0.00045 0.00000 0.00000 0.00022 0.00022 0.00067

D245 -0.00061 0.00001 0.00000 0.00058 0.00058 -0.00004

D246 -3.14158 0.00001 0.00000 0.00053 0.00053 -3.14106

D247 3.14117 0.00000 0.00000 -0.00001 -0.00001 3.14116

D248 0.00019 0.00000 0.00000 -0.00006 -0.00006 0.00014

D249 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D250 -3.14097 0.00000 0.00000 -0.00005 -0.00005 -3.14102

D251 3.14097 0.00000 0.00000 0.00005 0.00005 3.14102

D252 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D253 0.00061 -0.00001 0.00000 -0.00058 -0.00058 0.00004

D254 -3.14117 0.00000 0.00000 0.00001 0.00001 -3.14116

D255 3.14158 -0.00001 0.00000 -0.00053 -0.00053 3.14106

D256 -0.00019 0.00000 0.00000 0.00006 0.00006 -0.00014

D257 -0.00003 0.00000 0.00000 0.00001 0.00001 -0.00002

D258 3.14086 0.00001 0.00000 0.00032 0.00032 3.14118

D259 -3.14134 -0.00001 0.00000 -0.00052 -0.00052 3.14132

D260 -0.00045 0.00000 0.00000 -0.00022 -0.00022 -0.00067

D261 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D262 3.14089 0.00001 0.00000 0.00030 0.00030 3.14120

D263 -3.14089 -0.00001 0.00000 -0.00030 -0.00030 -3.14120

D264 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D265 0.00003 0.00000 0.00000 -0.00001 -0.00001 0.00002

D266 3.14134 0.00001 0.00000 0.00052 0.00052 -3.14132

D267 -3.14086 -0.00001 0.00000 -0.00032 -0.00032 -3.14118

D268 0.00045 0.00000 0.00000 0.00022 0.00022 0.00067

D269 0.00061 -0.00001 0.00000 -0.00058 -0.00058 0.00004

D270 3.14158 -0.00001 0.00000 -0.00053 -0.00053 3.14106

D271 -3.14117 0.00000 0.00000 0.00001 0.00001 -3.14116

D272 -0.00019 0.00000 0.00000 0.00006 0.00006 -0.00014

D273 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D274 3.14097 0.00000 0.00000 0.00005 0.00005 3.14102

D275 -3.14097 0.00000 0.00000 -0.00005 -0.00005 -3.14102

D276 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D277 -0.00061 0.00001 0.00000 0.00058 0.00058 -0.00004

D278 3.14117 0.00000 0.00000 -0.00001 -0.00001 3.14116

D279 -3.14158 0.00001 0.00000 0.00053 0.00053 -3.14106

D280 0.00019 0.00000 0.00000 -0.00006 -0.00006 0.00014

Item Value Threshold Converged?

Maximum Force 0.004780 0.000450 NO

RMS Force 0.001179 0.000300 NO

Maximum Displacement 0.054604 0.001800 NO

RMS Displacement 0.015445 0.001200 NO

Predicted change in Energy=-8.717029D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Jun 30 20:03:43 2019, MaxMem= 1342177280 cpu: 84.1

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

Stoichiometry C48H24N8Zn(3)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C48H24N4)]

Deg. of freedom 61

Full point group C2V NOp 4

RotChk: IX=0 Diff= 4.29D-14

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 1.121365 2.793002 0.147996

2 7 0 0.000000 2.021379 0.255295

3 6 0 -1.121365 2.793002 0.147996

4 6 0 -0.717658 4.177205 -0.017517

5 6 0 0.717658 4.177205 -0.017517

6 7 0 -2.412836 2.385566 0.156776

7 6 0 -2.792874 1.127409 0.191547

8 7 0 -2.008207 0.000000 0.250819

9 6 0 -2.792874 -1.127409 0.191547

10 6 0 -4.204870 -0.712227 0.125205

11 6 0 -4.204870 0.712227 0.125205

12 7 0 2.412836 2.385566 0.156776

13 6 0 4.204870 0.712227 0.125205

14 6 0 4.204870 -0.712227 0.125205

15 6 0 2.792874 -1.127409 0.191547

16 7 0 2.008207 0.000000 0.250819

17 6 0 2.792874 1.127409 0.191547

18 7 0 2.412836 -2.385566 0.156776

19 7 0 0.000000 -2.021379 0.255295

20 6 0 1.121365 -2.793002 0.147996

21 6 0 0.717658 -4.177205 -0.017517

22 6 0 -0.717658 -4.177205 -0.017517

23 6 0 -1.121365 -2.793002 0.147996

24 7 0 -2.412836 -2.385566 0.156776

25 30 0 0.000000 0.000000 0.774298

26 6 0 5.369487 1.426354 0.061953

27 6 0 6.603947 0.718542 0.004048

28 6 0 6.603947 -0.718542 0.004048

29 6 0 5.369487 -1.426354 0.061953

30 6 0 -1.428520 -5.345648 -0.166008

31 6 0 -0.721068 -6.564467 -0.312440

32 6 0 0.721068 -6.564467 -0.312440

33 6 0 1.428520 -5.345648 -0.166008

34 6 0 -5.369487 1.426354 0.061953

35 6 0 -6.603947 0.718542 0.004048

36 6 0 -6.603947 -0.718542 0.004048

37 6 0 -5.369487 -1.426354 0.061953

38 6 0 1.428520 5.345648 -0.166008

39 6 0 0.721068 6.564467 -0.312440

40 6 0 -0.721068 6.564467 -0.312440

41 6 0 -1.428520 5.345648 -0.166008

42 6 0 1.402088 -7.800865 -0.461901

43 6 0 0.707733 -8.977851 -0.604198

44 6 0 -0.707733 -8.977851 -0.604198

45 6 0 -1.402088 -7.800865 -0.461901

46 6 0 7.842632 -1.401082 -0.054317

47 6 0 9.029536 -0.705603 -0.110201

48 6 0 9.029536 0.705603 -0.110201

49 6 0 7.842632 1.401082 -0.054317

50 6 0 -1.402088 7.800865 -0.461901

51 6 0 -0.707733 8.977851 -0.604198

52 6 0 0.707733 8.977851 -0.604198

53 6 0 1.402088 7.800865 -0.461901

54 6 0 -7.842632 -1.401082 -0.054317

55 6 0 -9.029536 -0.705603 -0.110201

56 6 0 -9.029536 0.705603 -0.110201

57 6 0 -7.842632 1.401082 -0.054317

58 1 0 5.370153 2.511054 0.058249

59 1 0 5.370153 -2.511054 0.058249

60 1 0 -2.513360 -5.349407 -0.170405

61 1 0 2.513360 -5.349407 -0.170405

62 1 0 -5.370153 2.511054 0.058249

63 1 0 -5.370153 -2.511054 0.058249

64 1 0 2.513360 5.349407 -0.170405

65 1 0 -2.513360 5.349407 -0.170405

66 1 0 2.487415 -7.799306 -0.461458

67 1 0 1.243323 -9.914108 -0.717768

68 1 0 -1.243323 -9.914108 -0.717768

69 1 0 -2.487415 -7.799306 -0.461458

70 1 0 7.840679 -2.486206 -0.054633

71 1 0 9.970844 -1.242296 -0.155059

72 1 0 9.970844 1.242296 -0.155059

73 1 0 7.840679 2.486206 -0.054633

74 1 0 -2.487415 7.799306 -0.461458

75 1 0 -1.243323 9.914108 -0.717768

76 1 0 1.243323 9.914108 -0.717768

77 1 0 2.487415 7.799306 -0.461458

78 1 0 -7.840679 -2.486206 -0.054633

79 1 0 -9.970844 -1.242296 -0.155059

80 1 0 -9.970844 1.242296 -0.155059

81 1 0 -7.840679 2.486206 -0.054633

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

Rotational constants (GHZ): 0.0385814 0.0381769 0.0193131

Leave Link 202 at Sun Jun 30 20:03:43 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 307 symmetry adapted cartesian basis functions of A1 symmetry.

There are 278 symmetry adapted cartesian basis functions of A2 symmetry.

There are 289 symmetry adapted cartesian basis functions of B1 symmetry.

There are 289 symmetry adapted cartesian basis functions of B2 symmetry.

There are 289 symmetry adapted basis functions of A1 symmetry.

There are 265 symmetry adapted basis functions of A2 symmetry.

There are 275 symmetry adapted basis functions of B1 symmetry.

There are 275 symmetry adapted basis functions of B2 symmetry.

1104 basis functions, 1951 primitive gaussians, 1163 cartesian basis functions

191 alpha electrons 189 beta electrons

nuclear repulsion energy 6890.0782616115 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= 81 NActive= 81 NUniq= 22 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= -0.2361849799 Hartrees.

Nuclear repulsion after empirical dispersion term = 6889.8420766316 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= 81.

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 = 81

GePol: Total number of spheres = 81

GePol: Number of exposed spheres = 81 (100.00%)

GePol: Number of points = 6410

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.23D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 356

GePol: Fraction of low-weight points (<1% of avg) = 5.55%

GePol: Cavity surface area = 670.866 Ang\*\*2

GePol: Cavity volume = 694.068 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0169121373 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 6889.8251644943 Hartrees.

Leave Link 301 at Sun Jun 30 20:03:44 2019, MaxMem= 1342177280 cpu: 1.7

(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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36701 LenP2D= 95190.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1104 RedAO= T EigKep= 2.85D-05 NBF= 289 265 275 275

NBsUse= 1104 1.00D-06 EigRej= -1.00D+00 NBFU= 289 265 275 275

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= 1060 1060 1060 1060 1060 MxSgAt= 81 MxSgA2= 81.

Leave Link 302 at Sun Jun 30 20:04:12 2019, MaxMem= 1342177280 cpu: 281.6

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Jun 30 20:04:13 2019, MaxMem= 1342177280 cpu: 4.6

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

Initial guess from the checkpoint file: "ZnNPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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

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The electronic state of the initial guess is 3-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0221 S= 1.0074

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -2348.36483714761

Leave Link 401 at Sun Jun 30 20:04:37 2019, MaxMem= 1342177280 cpu: 241.6

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4103221 IEndB= 4103221 NGot= 1342177280 MDV= 1339444432

LenX= 1339444432 LenY= 1338090700

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= 420000000 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= 123264300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.02D-14 for 1062.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.66D-15 for 1331 484.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.14D-14 for 508.

Iteration 1 A^-1\*A deviation from orthogonality is 4.81D-10 for 1911 1825.

Iteration 2 A\*A^-1 deviation from unit magnitude is 1.67D-14 for 508.

Iteration 2 A\*A^-1 deviation from orthogonality is 1.09D-14 for 1339 486.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.44D-15 for 502.

Iteration 2 A^-1\*A deviation from orthogonality is 5.26D-16 for 4368 2094.

E= -2348.13008797951

DIIS: error= 4.72D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2348.13008797951 IErMin= 1 ErrMin= 4.72D-04

ErrMax= 4.72D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.73D-03 BMatP= 1.73D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.72D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.379 Goal= None Shift= 0.000

Gap= 0.459 Goal= None Shift= 0.000

RMSDP=4.82D-05 MaxDP=1.54D-03 OVMax= 3.69D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.77D-05 CP: 1.00D+00

E= -2348.13061420506 Delta-E= -0.000526225549 Rises=F Damp=F

DIIS: error= 2.15D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2348.13061420506 IErMin= 2 ErrMin= 2.15D-04

ErrMax= 2.15D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.34D-04 BMatP= 1.73D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.15D-03

Coeff-Com: 0.102D+00 0.898D+00

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

Coeff: 0.101D+00 0.899D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.12D-05 MaxDP=5.42D-04 DE=-5.26D-04 OVMax= 2.05D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.09D-05 CP: 1.00D+00 1.05D+00

E= -2348.13062667457 Delta-E= -0.000012469507 Rises=F Damp=F

DIIS: error= 1.54D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2348.13062667457 IErMin= 3 ErrMin= 1.54D-04

ErrMax= 1.54D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.76D-05 BMatP= 1.34D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.54D-03

Coeff-Com: -0.114D-01 0.458D+00 0.553D+00

Coeff-En: 0.000D+00 0.389D+00 0.611D+00

Coeff: -0.114D-01 0.458D+00 0.553D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=5.37D-06 MaxDP=2.35D-04 DE=-1.25D-05 OVMax= 1.72D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.22D-06 CP: 1.00D+00 1.04D+00 6.10D-01

E= -2348.13064869926 Delta-E= -0.000022024693 Rises=F Damp=F

DIIS: error= 6.52D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2348.13064869926 IErMin= 4 ErrMin= 6.52D-05

ErrMax= 6.52D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.33D-05 BMatP= 9.76D-05

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

Coeff-Com: -0.134D-01 0.222D+00 0.341D+00 0.451D+00

Coeff: -0.134D-01 0.222D+00 0.341D+00 0.451D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.65D-06 MaxDP=1.54D-04 DE=-2.20D-05 OVMax= 4.73D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.01D-06 CP: 1.00D+00 1.05D+00 6.34D-01 6.11D-01

E= -2348.13065179296 Delta-E= -0.000003093703 Rises=F Damp=F

DIIS: error= 1.45D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2348.13065179296 IErMin= 5 ErrMin= 1.45D-05

ErrMax= 1.45D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.02D-07 BMatP= 1.33D-05

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

Coeff-Com: -0.500D-02 0.567D-01 0.105D+00 0.215D+00 0.628D+00

Coeff: -0.500D-02 0.567D-01 0.105D+00 0.215D+00 0.628D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=4.33D-07 MaxDP=3.54D-05 DE=-3.09D-06 OVMax= 1.16D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.90D-07 CP: 1.00D+00 1.05D+00 6.24D-01 6.25D-01 8.98D-01

E= -2348.13065190406 Delta-E= -0.000000111097 Rises=F Damp=F

DIIS: error= 8.04D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2348.13065190406 IErMin= 6 ErrMin= 8.04D-06

ErrMax= 8.04D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.12D-07 BMatP= 6.02D-07

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

Coeff-Com: -0.628D-03-0.280D-02 0.573D-02 0.499D-01 0.344D+00 0.604D+00

Coeff: -0.628D-03-0.280D-02 0.573D-02 0.499D-01 0.344D+00 0.604D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.18D-07 MaxDP=9.83D-06 DE=-1.11D-07 OVMax= 5.88D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.21D-07 CP: 1.00D+00 1.05D+00 6.33D-01 6.34D-01 9.09D-01

CP: 6.80D-01

E= -2348.13065192990 Delta-E= -0.000000025841 Rises=F Damp=F

DIIS: error= 1.77D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2348.13065192990 IErMin= 7 ErrMin= 1.77D-06

ErrMax= 1.77D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.20D-09 BMatP= 1.12D-07

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

Coeff-Com: 0.758D-05-0.547D-02-0.446D-02 0.997D-02 0.126D+00 0.296D+00

Coeff-Com: 0.579D+00

Coeff: 0.758D-05-0.547D-02-0.446D-02 0.997D-02 0.126D+00 0.296D+00

Coeff: 0.579D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=5.61D-08 MaxDP=2.97D-06 DE=-2.58D-08 OVMax= 2.06D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 3.94D-08 CP: 1.00D+00 1.05D+00 6.33D-01 6.40D-01 9.26D-01

CP: 7.17D-01 7.86D-01

E= -2348.13065193195 Delta-E= -0.000000002048 Rises=F Damp=F

DIIS: error= 7.61D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2348.13065193195 IErMin= 8 ErrMin= 7.61D-07

ErrMax= 7.61D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.56D-09 BMatP= 8.20D-09

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

Coeff-Com: 0.121D-03-0.292D-02-0.393D-02-0.348D-02 0.130D-01 0.644D-01

Coeff-Com: 0.317D+00 0.616D+00

Coeff: 0.121D-03-0.292D-02-0.393D-02-0.348D-02 0.130D-01 0.644D-01

Coeff: 0.317D+00 0.616D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.97D-08 MaxDP=1.45D-06 DE=-2.05D-09 OVMax= 6.92D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.55D-08 CP: 1.00D+00 1.05D+00 6.33D-01 6.40D-01 9.29D-01

CP: 7.31D-01 8.68D-01 8.88D-01

E= -2348.13065193262 Delta-E= -0.000000000668 Rises=F Damp=F

DIIS: error= 2.30D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2348.13065193262 IErMin= 9 ErrMin= 2.30D-07

ErrMax= 2.30D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.08D-10 BMatP= 1.56D-09

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

Coeff-Com: 0.264D-04 0.166D-03-0.171D-03-0.217D-02-0.147D-01-0.284D-01

Coeff-Com: -0.991D-02 0.142D+00 0.913D+00

Coeff: 0.264D-04 0.166D-03-0.171D-03-0.217D-02-0.147D-01-0.284D-01

Coeff: -0.991D-02 0.142D+00 0.913D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.17D-08 MaxDP=9.08D-07 DE=-6.68D-10 OVMax= 8.42D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 7.60D-09 CP: 1.00D+00 1.05D+00 6.33D-01 6.40D-01 9.31D-01

CP: 7.35D-01 8.93D-01 1.06D+00 1.23D+00

E= -2348.13065193222 Delta-E= 0.000000000397 Rises=F Damp=F

DIIS: error= 2.24D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin= 9 EnMin= -2348.13065193262 IErMin=10 ErrMin= 2.24D-07

ErrMax= 2.24D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.13D-11 BMatP= 1.08D-10

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

Coeff-Com: -0.401D-05 0.654D-03 0.622D-03-0.810D-03-0.122D-01-0.311D-01

Coeff-Com: -0.657D-01-0.280D-01 0.607D+00 0.529D+00

Coeff: -0.401D-05 0.654D-03 0.622D-03-0.810D-03-0.122D-01-0.311D-01

Coeff: -0.657D-01-0.280D-01 0.607D+00 0.529D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=5.70D-09 MaxDP=5.09D-07 DE= 3.97D-10 OVMax= 2.07D-06

Error on total polarization charges = 0.08838

SCF Done: E(UB3LYP) = -2348.13065193 A.U. after 10 cycles

NFock= 10 Conv=0.57D-08 -V/T= 1.9830

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

<L.S>= 0.000000000000E+00

KE= 2.388806243299D+03 PE=-1.932311462173D+04 EE= 7.696352562001D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -10.61

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0219, after 2.0003

Leave Link 502 at Sun Jun 30 20:15:49 2019, MaxMem= 1342177280 cpu: 7107.0

(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.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36701 LenP2D= 95190.

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 = 193

Leave Link 701 at Sun Jun 30 20:16:23 2019, MaxMem= 1342177280 cpu: 366.6

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sun Jun 30 20:16:23 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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 Sun Jun 30 20:17:09 2019, MaxMem= 1342177280 cpu: 489.8

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 2.38031816D-13 5.89750471D-13 9.69930275D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000084217 -0.000232456 -0.000102841

2 7 0.000000000 0.000264778 0.000307153

3 6 0.000084217 -0.000232456 -0.000102841

4 6 -0.000088563 0.000152644 -0.000205006

5 6 0.000088563 0.000152644 -0.000205006

6 7 0.000177008 -0.000500427 0.000185443

7 6 0.000409354 0.000430357 -0.000151400

8 7 -0.000175570 0.000000000 0.000617855

9 6 0.000409354 -0.000430357 -0.000151400

10 6 -0.000314711 0.000025865 -0.000121098

11 6 -0.000314711 -0.000025865 -0.000121098

12 7 -0.000177008 -0.000500427 0.000185443

13 6 0.000314711 -0.000025865 -0.000121098

14 6 0.000314711 0.000025865 -0.000121098

15 6 -0.000409354 -0.000430357 -0.000151400

16 7 0.000175570 0.000000000 0.000617855

17 6 -0.000409354 0.000430357 -0.000151400

18 7 -0.000177008 0.000500427 0.000185443

19 7 0.000000000 -0.000264778 0.000307153

20 6 -0.000084217 0.000232456 -0.000102841

21 6 0.000088563 -0.000152644 -0.000205006

22 6 -0.000088563 -0.000152644 -0.000205006

23 6 0.000084217 0.000232456 -0.000102841

24 7 0.000177008 0.000500427 0.000185443

25 30 0.000000000 0.000000000 -0.000353739

26 6 -0.000069232 -0.000043768 0.000080908

27 6 0.000031574 0.000317851 -0.000010852

28 6 0.000031574 -0.000317851 -0.000010852

29 6 -0.000069232 0.000043768 0.000080908

30 6 0.000101396 -0.000000331 0.000087002

31 6 -0.000382410 0.000014635 -0.000009538

32 6 0.000382410 0.000014635 -0.000009538

33 6 -0.000101396 -0.000000331 0.000087002

34 6 0.000069232 -0.000043768 0.000080908

35 6 -0.000031574 0.000317851 -0.000010852

36 6 -0.000031574 -0.000317851 -0.000010852

37 6 0.000069232 0.000043768 0.000080908

38 6 -0.000101396 0.000000331 0.000087002

39 6 0.000382410 -0.000014635 -0.000009538

40 6 -0.000382410 -0.000014635 -0.000009538

41 6 0.000101396 0.000000331 0.000087002

42 6 0.000066942 -0.000157708 -0.000028664

43 6 0.000298380 -0.000217733 -0.000020762

44 6 -0.000298380 -0.000217733 -0.000020762

45 6 -0.000066942 -0.000157708 -0.000028664

46 6 0.000108123 -0.000108979 -0.000013379

47 6 0.000236814 -0.000258946 -0.000005354

48 6 0.000236814 0.000258946 -0.000005354

49 6 0.000108123 0.000108979 -0.000013379

50 6 -0.000066942 0.000157708 -0.000028664

51 6 -0.000298380 0.000217733 -0.000020762

52 6 0.000298380 0.000217733 -0.000020762

53 6 0.000066942 0.000157708 -0.000028664

54 6 -0.000108123 -0.000108979 -0.000013379

55 6 -0.000236814 -0.000258946 -0.000005354

56 6 -0.000236814 0.000258946 -0.000005354

57 6 -0.000108123 0.000108979 -0.000013379

58 1 -0.000046041 0.000109590 -0.000012418

59 1 -0.000046041 -0.000109590 -0.000012418

60 1 -0.000107593 0.000061463 -0.000027166

61 1 0.000107593 0.000061463 -0.000027166

62 1 0.000046041 0.000109590 -0.000012418

63 1 0.000046041 -0.000109590 -0.000012418

64 1 0.000107593 -0.000061463 -0.000027166

65 1 -0.000107593 -0.000061463 -0.000027166

66 1 0.000097141 -0.000009033 -0.000000469

67 1 0.000024611 -0.000120139 -0.000013492

68 1 -0.000024611 -0.000120139 -0.000013492

69 1 -0.000097141 -0.000009033 -0.000000469

70 1 0.000014885 -0.000094833 0.000000694

71 1 0.000117710 -0.000028495 -0.000005679

72 1 0.000117710 0.000028495 -0.000005679

73 1 0.000014885 0.000094833 0.000000694

74 1 -0.000097141 0.000009033 -0.000000469

75 1 -0.000024611 0.000120139 -0.000013492

76 1 0.000024611 0.000120139 -0.000013492

77 1 0.000097141 0.000009033 -0.000000469

78 1 -0.000014885 -0.000094833 0.000000694

79 1 -0.000117710 -0.000028495 -0.000005679

80 1 -0.000117710 0.000028495 -0.000005679

81 1 -0.000014885 0.000094833 0.000000694

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

Cartesian Forces: Max 0.000617855 RMS 0.000178870

Leave Link 716 at Sun Jun 30 20:17:09 2019, MaxMem= 1342177280 cpu: 4.6

(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 0.000729409 RMS 0.000163828

Search for a local minimum.

Step number 2 out of a maximum of 486

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .16383D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 1 2

DE= -7.94D-04 DEPred=-8.72D-04 R= 9.11D-01

TightC=F SS= 1.41D+00 RLast= 7.93D-02 DXNew= 5.0454D-01 2.3778D-01

Trust test= 9.11D-01 RLast= 7.93D-02 DXMaxT set to 3.00D-01

ITU= 1 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.01437 0.01493 0.01503 0.01518 0.01575

Eigenvalues --- 0.01601 0.01628 0.01657 0.01686 0.01695

Eigenvalues --- 0.01698 0.01708 0.01713 0.01715 0.01725

Eigenvalues --- 0.01730 0.01730 0.01731 0.01736 0.01738

Eigenvalues --- 0.01753 0.01759 0.01761 0.01791 0.01801

Eigenvalues --- 0.01827 0.01829 0.01830 0.01851 0.01854

Eigenvalues --- 0.01870 0.01870 0.01902 0.01931 0.01968

Eigenvalues --- 0.01968 0.01972 0.01972 0.01977 0.01992

Eigenvalues --- 0.01992 0.01993 0.01993 0.02043 0.02080

Eigenvalues --- 0.02080 0.02086 0.02086 0.02090 0.02090

Eigenvalues --- 0.02095 0.02095 0.02099 0.02099 0.02103

Eigenvalues --- 0.02103 0.02105 0.02106 0.02124 0.02124

Eigenvalues --- 0.02137 0.02141 0.02144 0.02144 0.02147

Eigenvalues --- 0.02148 0.02172 0.02173 0.02214 0.02214

Eigenvalues --- 0.02225 0.02225 0.02275 0.02283 0.02333

Eigenvalues --- 0.02345 0.03205 0.05508 0.05605 0.08027

Eigenvalues --- 0.14680 0.15967 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 0.16003

Eigenvalues --- 0.16156 0.16242 0.16937 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22500 0.22500 0.22504

Eigenvalues --- 0.22506 0.23155 0.23233 0.23234 0.23234

Eigenvalues --- 0.23551 0.23937 0.23940 0.23941 0.23950

Eigenvalues --- 0.24090 0.24303 0.24479 0.24554 0.24556

Eigenvalues --- 0.24557 0.24557 0.24751 0.24900 0.24901

Eigenvalues --- 0.24981 0.24988 0.24989 0.24992 0.24992

Eigenvalues --- 0.24998 0.24998 0.24998 0.24998 0.25184

Eigenvalues --- 0.32870 0.32952 0.33665 0.33686 0.33832

Eigenvalues --- 0.33859 0.35035 0.35057 0.35133 0.35181

Eigenvalues --- 0.35181 0.35181 0.35191 0.35202 0.35202

Eigenvalues --- 0.35202 0.35219 0.35231 0.35231 0.35231

Eigenvalues --- 0.35241 0.35249 0.35249 0.35249 0.35263

Eigenvalues --- 0.35270 0.35270 0.35270 0.35275 0.35279

Eigenvalues --- 0.35279 0.35279 0.35411 0.35676 0.36347

Eigenvalues --- 0.36624 0.37452 0.37497 0.37969 0.38038

Eigenvalues --- 0.39276 0.39277 0.39612 0.39612 0.40187

Eigenvalues --- 0.40187 0.40258 0.40258 0.40903 0.40904

Eigenvalues --- 0.41000 0.41049 0.41591 0.41603 0.41874

Eigenvalues --- 0.41919 0.42215 0.42285 0.42486 0.42806

Eigenvalues --- 0.42919 0.42961 0.44034 0.45610 0.47124

Eigenvalues --- 0.47124 0.47168 0.47384 0.47386 0.47579

Eigenvalues --- 0.47580 0.48133 0.48218 0.48226 0.48328

Eigenvalues --- 0.48464 0.48466 0.48645 0.48680 0.48706

Eigenvalues --- 0.48729 0.49088 0.49444 0.49897 0.50383

Eigenvalues --- 0.50952 0.51936 0.52483 0.58369 0.59247

Eigenvalues --- 0.59820 0.60898

RFO step: Lambda=-4.61227197D-05 EMin= 1.43665845D-02

Quartic linear search produced a step of -0.07953.

Iteration 1 RMS(Cart)= 0.01320928 RMS(Int)= 0.00001100

Iteration 2 RMS(Cart)= 0.00005680 RMS(Int)= 0.00000098

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000098

ITry= 1 IFail=0 DXMaxC= 7.46D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.29D-08 for atom 68.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58027 -0.00003 0.00038 -0.00057 -0.00019 2.58008

R2 2.74264 0.00060 0.00043 0.00091 0.00134 2.74398

R3 2.55915 0.00013 0.00041 -0.00027 0.00014 2.55929

R4 2.58027 -0.00003 0.00038 -0.00057 -0.00019 2.58008

R5 3.94375 0.00037 0.00015 0.00283 0.00298 3.94673

R6 2.74264 0.00060 0.00043 0.00091 0.00134 2.74398

R7 2.55915 0.00013 0.00041 -0.00027 0.00014 2.55929

R8 2.71236 0.00014 0.00042 -0.00017 0.00024 2.71260

R9 2.59975 0.00036 0.00063 -0.00017 0.00047 2.60022

R10 2.59975 0.00036 0.00063 -0.00017 0.00047 2.60022

R11 2.48454 -0.00014 0.00056 -0.00093 -0.00037 2.48417

R12 2.59813 0.00009 0.00039 -0.00044 -0.00005 2.59808

R13 2.78407 0.00073 0.00042 0.00139 0.00182 2.78588

R14 2.59813 0.00009 0.00039 -0.00044 -0.00005 2.59808

R15 3.92177 0.00029 0.00042 0.00109 0.00151 3.92328

R16 2.78407 0.00073 0.00042 0.00139 0.00182 2.78588

R17 2.48454 -0.00014 0.00056 -0.00093 -0.00037 2.48417

R18 2.69183 0.00016 0.00048 -0.00020 0.00029 2.69211

R19 2.58438 0.00034 0.00065 -0.00024 0.00041 2.58478

R20 2.58438 0.00034 0.00065 -0.00024 0.00041 2.58478

R21 2.48454 -0.00014 0.00056 -0.00093 -0.00037 2.48417

R22 2.69183 0.00016 0.00048 -0.00020 0.00029 2.69211

R23 2.78407 0.00073 0.00042 0.00139 0.00182 2.78588

R24 2.58438 0.00034 0.00065 -0.00024 0.00041 2.58478

R25 2.78407 0.00073 0.00042 0.00139 0.00182 2.78588

R26 2.58438 0.00034 0.00065 -0.00024 0.00041 2.58478

R27 2.59813 0.00009 0.00039 -0.00044 -0.00005 2.59808

R28 2.48454 -0.00014 0.00056 -0.00093 -0.00037 2.48417

R29 2.59813 0.00009 0.00039 -0.00044 -0.00005 2.59808

R30 3.92177 0.00029 0.00042 0.00109 0.00151 3.92328

R31 2.55915 0.00013 0.00041 -0.00027 0.00014 2.55929

R32 2.58027 -0.00003 0.00038 -0.00057 -0.00019 2.58008

R33 2.58027 -0.00003 0.00038 -0.00057 -0.00019 2.58008

R34 3.94375 0.00037 0.00015 0.00283 0.00298 3.94673

R35 2.74264 0.00060 0.00043 0.00091 0.00134 2.74398

R36 2.71236 0.00014 0.00042 -0.00017 0.00024 2.71260

R37 2.59975 0.00036 0.00063 -0.00017 0.00047 2.60022

R38 2.74264 0.00060 0.00043 0.00091 0.00134 2.74398

R39 2.59975 0.00036 0.00063 -0.00017 0.00047 2.60022

R40 2.55915 0.00013 0.00041 -0.00027 0.00014 2.55929

R41 2.69128 0.00047 0.00052 0.00036 0.00088 2.69216

R42 2.04980 0.00011 0.00023 -0.00002 0.00021 2.05001

R43 2.71569 0.00047 0.00051 0.00042 0.00094 2.71663

R44 2.67489 0.00047 0.00057 0.00026 0.00083 2.67571

R45 2.69128 0.00047 0.00052 0.00036 0.00088 2.69216

R46 2.67489 0.00047 0.00057 0.00026 0.00083 2.67571

R47 2.04980 0.00011 0.00023 -0.00002 0.00021 2.05001

R48 2.67745 0.00044 0.00056 0.00021 0.00077 2.67822

R49 2.05008 0.00011 0.00023 -0.00003 0.00020 2.05028

R50 2.72524 0.00048 0.00047 0.00054 0.00101 2.72625

R51 2.68235 0.00049 0.00054 0.00035 0.00089 2.68324

R52 2.67745 0.00044 0.00056 0.00021 0.00077 2.67822

R53 2.68235 0.00049 0.00054 0.00035 0.00089 2.68324

R54 2.05008 0.00011 0.00023 -0.00003 0.00020 2.05028

R55 2.69128 0.00047 0.00052 0.00036 0.00088 2.69216

R56 2.04980 0.00011 0.00023 -0.00002 0.00021 2.05001

R57 2.71569 0.00047 0.00051 0.00042 0.00094 2.71663

R58 2.67489 0.00047 0.00057 0.00026 0.00083 2.67571

R59 2.69128 0.00047 0.00052 0.00036 0.00088 2.69216

R60 2.67489 0.00047 0.00057 0.00026 0.00083 2.67571

R61 2.04980 0.00011 0.00023 -0.00002 0.00021 2.05001

R62 2.67745 0.00044 0.00056 0.00021 0.00077 2.67822

R63 2.05008 0.00011 0.00023 -0.00003 0.00020 2.05028

R64 2.72524 0.00048 0.00047 0.00054 0.00101 2.72625

R65 2.68235 0.00049 0.00054 0.00035 0.00089 2.68324

R66 2.67745 0.00044 0.00056 0.00021 0.00077 2.67822

R67 2.68235 0.00049 0.00054 0.00035 0.00089 2.68324

R68 2.05008 0.00011 0.00023 -0.00003 0.00020 2.05028

R69 2.59634 0.00033 0.00078 -0.00041 0.00037 2.59672

R70 2.05097 0.00010 0.00023 -0.00005 0.00018 2.05115

R71 2.67484 0.00040 0.00061 0.00007 0.00067 2.67552

R72 2.04958 0.00012 0.00022 0.00001 0.00023 2.04981

R73 2.59634 0.00033 0.00078 -0.00041 0.00037 2.59672

R74 2.04958 0.00012 0.00022 0.00001 0.00023 2.04981

R75 2.05097 0.00010 0.00023 -0.00005 0.00018 2.05115

R76 2.60176 0.00036 0.00076 -0.00033 0.00043 2.60219

R77 2.05059 0.00009 0.00023 -0.00006 0.00017 2.05076

R78 2.66679 0.00039 0.00064 -0.00001 0.00063 2.66742

R79 2.04938 0.00012 0.00023 0.00000 0.00023 2.04961

R80 2.60176 0.00036 0.00076 -0.00033 0.00043 2.60219

R81 2.04938 0.00012 0.00023 0.00000 0.00023 2.04961

R82 2.05059 0.00009 0.00023 -0.00006 0.00017 2.05076

R83 2.59634 0.00033 0.00078 -0.00041 0.00037 2.59672

R84 2.05097 0.00010 0.00023 -0.00005 0.00018 2.05115

R85 2.67484 0.00040 0.00061 0.00007 0.00067 2.67552

R86 2.04958 0.00012 0.00022 0.00001 0.00023 2.04981

R87 2.59634 0.00033 0.00078 -0.00041 0.00037 2.59672

R88 2.04958 0.00012 0.00022 0.00001 0.00023 2.04981

R89 2.05097 0.00010 0.00023 -0.00005 0.00018 2.05115

R90 2.60176 0.00036 0.00076 -0.00033 0.00043 2.60219

R91 2.05059 0.00009 0.00023 -0.00006 0.00017 2.05076

R92 2.66679 0.00039 0.00064 -0.00001 0.00063 2.66742

R93 2.04938 0.00012 0.00023 0.00000 0.00023 2.04961

R94 2.60176 0.00036 0.00076 -0.00033 0.00043 2.60219

R95 2.04938 0.00012 0.00023 0.00000 0.00023 2.04961

R96 2.05059 0.00009 0.00023 -0.00006 0.00017 2.05076

A1 1.89599 0.00012 0.00022 -0.00001 0.00021 1.89621

A2 2.23022 -0.00021 -0.00025 -0.00027 -0.00052 2.22970

A3 2.15669 0.00009 0.00003 0.00025 0.00028 2.15697

A4 1.92723 -0.00002 -0.00027 0.00033 0.00005 1.92728

A5 2.17354 0.00002 0.00009 0.00028 0.00037 2.17391

A6 2.17354 0.00002 0.00009 0.00028 0.00037 2.17391

A7 1.89599 0.00012 0.00022 -0.00001 0.00021 1.89621

A8 2.23022 -0.00021 -0.00025 -0.00027 -0.00052 2.22970

A9 2.15669 0.00009 0.00003 0.00025 0.00028 2.15697

A10 1.85268 -0.00011 -0.00008 -0.00015 -0.00023 1.85244

A11 2.31667 0.00017 0.00008 0.00048 0.00056 2.31723

A12 2.11381 -0.00006 0.00001 -0.00033 -0.00032 2.11349

A13 1.85268 -0.00011 -0.00008 -0.00015 -0.00023 1.85244

A14 2.31667 0.00017 0.00008 0.00048 0.00056 2.31723

A15 2.11381 -0.00006 0.00001 -0.00033 -0.00032 2.11349

A16 2.16970 0.00038 0.00025 0.00123 0.00148 2.17118

A17 2.24066 -0.00017 -0.00029 -0.00018 -0.00047 2.24019

A18 2.14781 0.00012 0.00010 0.00046 0.00055 2.14836

A19 1.89425 0.00005 0.00020 -0.00033 -0.00013 1.89411

A20 1.92286 0.00003 -0.00023 0.00066 0.00042 1.92328

A21 2.16898 0.00000 0.00004 0.00044 0.00047 2.16945

A22 2.16898 0.00000 0.00004 0.00044 0.00047 2.16945

A23 1.89425 0.00005 0.00020 -0.00033 -0.00013 1.89411

A24 2.24066 -0.00017 -0.00029 -0.00018 -0.00047 2.24019

A25 2.14781 0.00012 0.00010 0.00046 0.00055 2.14836

A26 1.85648 -0.00007 -0.00008 -0.00006 -0.00014 1.85633

A27 2.30648 0.00012 0.00008 0.00033 0.00041 2.30689

A28 2.12020 -0.00005 0.00000 -0.00027 -0.00027 2.11993

A29 1.85648 -0.00007 -0.00008 -0.00006 -0.00014 1.85633

A30 2.30648 0.00012 0.00008 0.00033 0.00041 2.30689

A31 2.12020 -0.00005 0.00000 -0.00027 -0.00027 2.11993

A32 2.16970 0.00038 0.00025 0.00123 0.00148 2.17118

A33 1.85648 -0.00007 -0.00008 -0.00006 -0.00014 1.85633

A34 2.12020 -0.00005 0.00000 -0.00027 -0.00027 2.11993

A35 2.30648 0.00012 0.00008 0.00033 0.00041 2.30689

A36 1.85648 -0.00007 -0.00008 -0.00006 -0.00014 1.85633

A37 2.12020 -0.00005 0.00000 -0.00027 -0.00027 2.11993

A38 2.30648 0.00012 0.00008 0.00033 0.00041 2.30689

A39 1.89425 0.00005 0.00020 -0.00033 -0.00013 1.89411

A40 2.14781 0.00012 0.00010 0.00046 0.00055 2.14836

A41 2.24066 -0.00017 -0.00029 -0.00018 -0.00047 2.24019

A42 1.92286 0.00003 -0.00023 0.00066 0.00042 1.92328

A43 2.16898 0.00000 0.00004 0.00044 0.00047 2.16945

A44 2.16898 0.00000 0.00004 0.00044 0.00047 2.16945

A45 2.14781 0.00012 0.00010 0.00046 0.00055 2.14836

A46 2.24066 -0.00017 -0.00029 -0.00018 -0.00047 2.24019

A47 1.89425 0.00005 0.00020 -0.00033 -0.00013 1.89411

A48 2.16970 0.00038 0.00025 0.00123 0.00148 2.17118

A49 1.92723 -0.00002 -0.00027 0.00033 0.00005 1.92728

A50 2.17354 0.00002 0.00009 0.00028 0.00037 2.17391

A51 2.17354 0.00002 0.00009 0.00028 0.00037 2.17391

A52 2.23022 -0.00021 -0.00025 -0.00027 -0.00052 2.22970

A53 2.15669 0.00009 0.00003 0.00025 0.00028 2.15697

A54 1.89599 0.00012 0.00022 -0.00001 0.00021 1.89621

A55 1.85268 -0.00011 -0.00008 -0.00015 -0.00023 1.85244

A56 2.31667 0.00017 0.00008 0.00048 0.00056 2.31723

A57 2.11381 -0.00006 0.00001 -0.00033 -0.00032 2.11349

A58 1.85268 -0.00011 -0.00008 -0.00015 -0.00023 1.85244

A59 2.11381 -0.00006 0.00001 -0.00033 -0.00032 2.11349

A60 2.31667 0.00017 0.00008 0.00048 0.00056 2.31723

A61 1.89599 0.00012 0.00022 -0.00001 0.00021 1.89621

A62 2.23022 -0.00021 -0.00025 -0.00027 -0.00052 2.22970

A63 2.15669 0.00009 0.00003 0.00025 0.00028 2.15697

A64 2.16970 0.00038 0.00025 0.00123 0.00148 2.17118

A65 1.50803 0.00001 0.00005 -0.00003 0.00002 1.50804

A66 1.50803 0.00001 0.00005 -0.00003 0.00002 1.50804

A67 2.63894 -0.00005 0.00041 -0.00256 -0.00215 2.63679

A68 2.63160 0.00010 -0.00002 0.00233 0.00232 2.63392

A69 1.50803 0.00001 0.00005 -0.00003 0.00002 1.50804

A70 1.50803 0.00001 0.00005 -0.00003 0.00002 1.50804

A71 2.07203 0.00019 -0.00002 0.00078 0.00076 2.07279

A72 2.12099 -0.00014 0.00011 -0.00079 -0.00068 2.12031

A73 2.09016 -0.00005 -0.00009 0.00001 -0.00008 2.09008

A74 2.09094 -0.00014 0.00003 -0.00052 -0.00049 2.09045

A75 2.11830 0.00020 -0.00005 0.00080 0.00074 2.11904

A76 2.07395 -0.00006 0.00003 -0.00028 -0.00025 2.07370

A77 2.09094 -0.00014 0.00003 -0.00052 -0.00049 2.09045

A78 2.07395 -0.00006 0.00003 -0.00028 -0.00025 2.07370

A79 2.11830 0.00020 -0.00005 0.00080 0.00074 2.11904

A80 2.07203 0.00019 -0.00002 0.00078 0.00076 2.07279

A81 2.12099 -0.00014 0.00011 -0.00079 -0.00068 2.12031

A82 2.09016 -0.00005 -0.00009 0.00001 -0.00008 2.09008

A83 2.07575 0.00021 -0.00002 0.00088 0.00086 2.07661

A84 2.11775 -0.00016 0.00010 -0.00090 -0.00080 2.11695

A85 2.08968 -0.00004 -0.00008 0.00003 -0.00005 2.08962

A86 2.09360 -0.00015 0.00001 -0.00055 -0.00053 2.09307

A87 2.11838 0.00022 -0.00005 0.00089 0.00084 2.11922

A88 2.07120 -0.00008 0.00004 -0.00034 -0.00031 2.07090

A89 2.09360 -0.00015 0.00001 -0.00055 -0.00053 2.09307

A90 2.07120 -0.00008 0.00004 -0.00034 -0.00031 2.07090

A91 2.11838 0.00022 -0.00005 0.00089 0.00084 2.11922

A92 2.07575 0.00021 -0.00002 0.00088 0.00086 2.07661

A93 2.11775 -0.00016 0.00010 -0.00090 -0.00080 2.11695

A94 2.08968 -0.00004 -0.00008 0.00003 -0.00005 2.08962

A95 2.07203 0.00019 -0.00002 0.00078 0.00076 2.07279

A96 2.12099 -0.00014 0.00011 -0.00079 -0.00068 2.12031

A97 2.09016 -0.00005 -0.00009 0.00001 -0.00008 2.09008

A98 2.09094 -0.00014 0.00003 -0.00052 -0.00049 2.09045

A99 2.11830 0.00020 -0.00005 0.00080 0.00074 2.11904

A100 2.07395 -0.00006 0.00003 -0.00028 -0.00025 2.07370

A101 2.09094 -0.00014 0.00003 -0.00052 -0.00049 2.09045

A102 2.07395 -0.00006 0.00003 -0.00028 -0.00025 2.07370

A103 2.11830 0.00020 -0.00005 0.00080 0.00074 2.11904

A104 2.07203 0.00019 -0.00002 0.00078 0.00076 2.07279

A105 2.12099 -0.00014 0.00011 -0.00079 -0.00068 2.12031

A106 2.09016 -0.00005 -0.00009 0.00001 -0.00008 2.09008

A107 2.07575 0.00021 -0.00002 0.00088 0.00086 2.07661

A108 2.11775 -0.00016 0.00010 -0.00090 -0.00080 2.11695

A109 2.08968 -0.00004 -0.00008 0.00003 -0.00005 2.08962

A110 2.09360 -0.00015 0.00001 -0.00055 -0.00053 2.09307

A111 2.11838 0.00022 -0.00005 0.00089 0.00084 2.11922

A112 2.07120 -0.00008 0.00004 -0.00034 -0.00031 2.07090

A113 2.09360 -0.00015 0.00001 -0.00055 -0.00053 2.09307

A114 2.07120 -0.00008 0.00004 -0.00034 -0.00031 2.07090

A115 2.11838 0.00022 -0.00005 0.00089 0.00084 2.11922

A116 2.07575 0.00021 -0.00002 0.00088 0.00086 2.07661

A117 2.11775 -0.00016 0.00010 -0.00090 -0.00080 2.11695

A118 2.08968 -0.00004 -0.00008 0.00003 -0.00005 2.08962

A119 2.11136 0.00011 0.00001 0.00043 0.00045 2.11181

A120 2.06973 -0.00005 -0.00010 -0.00003 -0.00014 2.06959

A121 2.10209 -0.00006 0.00009 -0.00040 -0.00031 2.10178

A122 2.10062 -0.00003 -0.00005 -0.00009 -0.00014 2.10048

A123 2.09529 0.00006 0.00002 0.00028 0.00030 2.09559

A124 2.08727 -0.00002 0.00003 -0.00019 -0.00016 2.08711

A125 2.10062 -0.00003 -0.00005 -0.00009 -0.00014 2.10048

A126 2.08727 -0.00002 0.00003 -0.00019 -0.00016 2.08711

A127 2.09529 0.00006 0.00002 0.00028 0.00030 2.09559

A128 2.11136 0.00011 0.00001 0.00043 0.00045 2.11181

A129 2.06973 -0.00005 -0.00010 -0.00003 -0.00014 2.06959

A130 2.10209 -0.00006 0.00009 -0.00040 -0.00031 2.10178

A131 2.10889 0.00009 0.00002 0.00035 0.00037 2.10926

A132 2.07217 -0.00003 -0.00011 0.00005 -0.00006 2.07211

A133 2.10213 -0.00006 0.00009 -0.00040 -0.00031 2.10182

A134 2.10035 -0.00003 -0.00005 -0.00007 -0.00012 2.10023

A135 2.09434 0.00005 0.00001 0.00025 0.00026 2.09460

A136 2.08850 -0.00002 0.00004 -0.00018 -0.00014 2.08835

A137 2.10035 -0.00003 -0.00005 -0.00007 -0.00012 2.10023

A138 2.08850 -0.00002 0.00004 -0.00018 -0.00014 2.08835

A139 2.09434 0.00005 0.00001 0.00025 0.00026 2.09460

A140 2.10889 0.00009 0.00002 0.00035 0.00037 2.10926

A141 2.07217 -0.00003 -0.00011 0.00005 -0.00006 2.07211

A142 2.10213 -0.00006 0.00009 -0.00040 -0.00031 2.10182

A143 2.11136 0.00011 0.00001 0.00043 0.00045 2.11181

A144 2.06973 -0.00005 -0.00010 -0.00003 -0.00014 2.06959

A145 2.10209 -0.00006 0.00009 -0.00040 -0.00031 2.10178

A146 2.10062 -0.00003 -0.00005 -0.00009 -0.00014 2.10048

A147 2.09529 0.00006 0.00002 0.00028 0.00030 2.09559

A148 2.08727 -0.00002 0.00003 -0.00019 -0.00016 2.08711

A149 2.10062 -0.00003 -0.00005 -0.00009 -0.00014 2.10048

A150 2.08727 -0.00002 0.00003 -0.00019 -0.00016 2.08711

A151 2.09529 0.00006 0.00002 0.00028 0.00030 2.09559

A152 2.11136 0.00011 0.00001 0.00043 0.00045 2.11181

A153 2.06973 -0.00005 -0.00010 -0.00003 -0.00014 2.06959

A154 2.10209 -0.00006 0.00009 -0.00040 -0.00031 2.10178

A155 2.10889 0.00009 0.00002 0.00035 0.00037 2.10926

A156 2.07217 -0.00003 -0.00011 0.00005 -0.00006 2.07211

A157 2.10213 -0.00006 0.00009 -0.00040 -0.00031 2.10182

A158 2.10035 -0.00003 -0.00005 -0.00007 -0.00012 2.10023

A159 2.09434 0.00005 0.00001 0.00025 0.00026 2.09460

A160 2.08850 -0.00002 0.00004 -0.00018 -0.00014 2.08835

A161 2.10035 -0.00003 -0.00005 -0.00007 -0.00012 2.10023

A162 2.08850 -0.00002 0.00004 -0.00018 -0.00014 2.08835

A163 2.09434 0.00005 0.00001 0.00025 0.00026 2.09460

A164 2.10889 0.00009 0.00002 0.00035 0.00037 2.10926

A165 2.07217 -0.00003 -0.00011 0.00005 -0.00006 2.07211

A166 2.10213 -0.00006 0.00009 -0.00040 -0.00031 2.10182

D1 0.01942 -0.00005 -0.00025 -0.00054 -0.00079 0.01863

D2 -2.98467 -0.00013 0.00045 -0.00744 -0.00700 -2.99166

D3 -3.09727 -0.00004 -0.00016 0.00053 0.00037 -3.09690

D4 0.18182 -0.00012 0.00054 -0.00637 -0.00583 0.17599

D5 -0.01154 0.00003 0.00015 0.00032 0.00047 -0.01106

D6 3.13868 0.00001 0.00026 -0.00036 -0.00010 3.13858

D7 3.10644 0.00002 0.00006 -0.00070 -0.00065 3.10580

D8 -0.02653 0.00000 0.00016 -0.00138 -0.00122 -0.02775

D9 0.07705 0.00008 -0.00028 0.00350 0.00323 0.08027

D10 -3.03623 0.00010 -0.00018 0.00473 0.00455 -3.03168

D11 -0.01942 0.00005 0.00025 0.00054 0.00079 -0.01863

D12 3.09727 0.00004 0.00016 -0.00053 -0.00037 3.09690

D13 2.98467 0.00013 -0.00045 0.00744 0.00700 2.99166

D14 -0.18182 0.00012 -0.00054 0.00637 0.00583 -0.17599

D15 -2.97257 -0.00001 -0.00039 0.00272 0.00233 -2.97024

D16 -0.32560 0.00009 -0.00044 0.00515 0.00471 -0.32089

D17 -1.64908 0.00004 -0.00041 0.00393 0.00352 -1.64556

D18 0.32560 -0.00009 0.00044 -0.00515 -0.00471 0.32089

D19 2.97257 0.00001 0.00039 -0.00272 -0.00233 2.97024

D20 1.64908 -0.00004 0.00041 -0.00393 -0.00352 1.64556

D21 0.01154 -0.00003 -0.00015 -0.00032 -0.00047 0.01106

D22 -3.13868 -0.00001 -0.00026 0.00036 0.00010 -3.13858

D23 -3.10644 -0.00002 -0.00006 0.00070 0.00065 -3.10580

D24 0.02653 0.00000 -0.00016 0.00138 0.00122 0.02775

D25 -0.07705 -0.00008 0.00028 -0.00350 -0.00323 -0.08027

D26 3.03623 -0.00010 0.00018 -0.00473 -0.00455 3.03168

D27 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D28 3.13419 0.00002 -0.00009 0.00059 0.00050 3.13469

D29 -3.13419 -0.00002 0.00009 -0.00059 -0.00050 -3.13469

D30 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D31 -3.13869 -0.00001 0.00024 -0.00054 -0.00030 -3.13899

D32 0.00548 -0.00003 0.00011 -0.00124 -0.00113 0.00435

D33 -0.00677 0.00001 0.00012 0.00023 0.00034 -0.00642

D34 3.13740 -0.00001 -0.00001 -0.00048 -0.00048 3.13691

D35 3.13869 0.00001 -0.00024 0.00054 0.00030 3.13899

D36 -0.00548 0.00003 -0.00011 0.00124 0.00113 -0.00435

D37 0.00677 -0.00001 -0.00012 -0.00023 -0.00034 0.00642

D38 -3.13740 0.00001 0.00001 0.00048 0.00048 -3.13691

D39 0.02386 0.00003 -0.00003 0.00079 0.00076 0.02462

D40 -3.08077 0.00006 -0.00042 0.00286 0.00244 -3.07833

D41 -3.08014 0.00011 -0.00067 0.00606 0.00539 -3.07475

D42 0.27935 -0.00002 0.00007 -0.00134 -0.00126 0.27808

D43 0.02878 0.00008 -0.00032 0.00424 0.00392 0.03271

D44 -2.89491 -0.00005 0.00042 -0.00316 -0.00273 -2.89765

D45 3.09387 -0.00008 0.00050 -0.00423 -0.00373 3.09014

D46 -0.03932 -0.00007 0.00056 -0.00460 -0.00404 -0.04336

D47 -0.01717 -0.00005 0.00019 -0.00252 -0.00233 -0.01950

D48 3.13283 -0.00004 0.00025 -0.00289 -0.00264 3.13019

D49 -0.02878 -0.00008 0.00032 -0.00424 -0.00392 -0.03271

D50 3.08014 -0.00011 0.00067 -0.00606 -0.00539 3.07475

D51 2.89491 0.00005 -0.00042 0.00316 0.00273 2.89765

D52 -0.27935 0.00002 -0.00007 0.00134 0.00126 -0.27808

D53 -0.36757 0.00005 -0.00024 0.00291 0.00267 -0.36490

D54 -1.69484 0.00007 -0.00044 0.00422 0.00379 -1.69105

D55 -3.02211 0.00010 -0.00064 0.00554 0.00490 -3.01721

D56 3.02211 -0.00010 0.00064 -0.00554 -0.00490 3.01721

D57 1.69484 -0.00007 0.00044 -0.00422 -0.00379 1.69105

D58 0.36757 -0.00005 0.00024 -0.00291 -0.00267 0.36490

D59 0.01717 0.00005 -0.00019 0.00252 0.00233 0.01950

D60 -3.13283 0.00004 -0.00025 0.00289 0.00264 -3.13019

D61 -3.09387 0.00008 -0.00050 0.00423 0.00373 -3.09014

D62 0.03932 0.00007 -0.00056 0.00460 0.00404 0.04336

D63 -0.02386 -0.00003 0.00003 -0.00079 -0.00076 -0.02462

D64 3.08077 -0.00006 0.00042 -0.00286 -0.00244 3.07833

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13428 -0.00001 -0.00005 0.00032 0.00027 3.13456

D67 -3.13428 0.00001 0.00005 -0.00032 -0.00027 -3.13456

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 -3.13944 0.00001 0.00017 -0.00030 -0.00013 -3.13957

D70 0.00550 0.00000 -0.00001 -0.00046 -0.00047 0.00502

D71 -0.00731 0.00000 0.00010 0.00011 0.00022 -0.00709

D72 3.13763 -0.00001 -0.00008 -0.00005 -0.00013 3.13751

D73 3.13944 -0.00001 -0.00017 0.00030 0.00013 3.13957

D74 -0.00550 0.00000 0.00001 0.00046 0.00047 -0.00502

D75 0.00731 0.00000 -0.00010 -0.00011 -0.00022 0.00709

D76 -3.13763 0.00001 0.00008 0.00005 0.00013 -3.13751

D77 3.08077 -0.00006 0.00042 -0.00286 -0.00244 3.07833

D78 -0.02386 -0.00003 0.00003 -0.00079 -0.00076 -0.02462

D79 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D80 3.13428 -0.00001 -0.00005 0.00032 0.00027 3.13456

D81 -3.13428 0.00001 0.00005 -0.00032 -0.00027 -3.13456

D82 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D83 -3.09387 0.00008 -0.00050 0.00423 0.00373 -3.09014

D84 0.01717 0.00005 -0.00019 0.00252 0.00233 0.01950

D85 0.03932 0.00007 -0.00056 0.00460 0.00404 0.04336

D86 -3.13283 0.00004 -0.00025 0.00289 0.00264 -3.13019

D87 -0.00731 0.00000 0.00010 0.00011 0.00022 -0.00709

D88 3.13763 -0.00001 -0.00008 -0.00005 -0.00013 3.13751

D89 -3.13944 0.00001 0.00017 -0.00030 -0.00013 -3.13957

D90 0.00550 0.00000 -0.00001 -0.00046 -0.00047 0.00502

D91 -0.01717 -0.00005 0.00019 -0.00252 -0.00233 -0.01950

D92 3.09387 -0.00008 0.00050 -0.00423 -0.00373 3.09014

D93 3.13283 -0.00004 0.00025 -0.00289 -0.00264 3.13019

D94 -0.03932 -0.00007 0.00056 -0.00460 -0.00404 -0.04336

D95 0.00731 0.00000 -0.00010 -0.00011 -0.00022 0.00709

D96 -3.13763 0.00001 0.00008 0.00005 0.00013 -3.13751

D97 3.13944 -0.00001 -0.00017 0.00030 0.00013 3.13957

D98 -0.00550 0.00000 0.00001 0.00046 0.00047 -0.00502

D99 0.02878 0.00008 -0.00032 0.00424 0.00392 0.03271

D100 -2.89491 -0.00005 0.00042 -0.00316 -0.00273 -2.89765

D101 -3.08014 0.00011 -0.00067 0.00606 0.00539 -3.07475

D102 0.27935 -0.00002 0.00007 -0.00134 -0.00126 0.27808

D103 -3.08077 0.00006 -0.00042 0.00286 0.00244 -3.07833

D104 0.02386 0.00003 -0.00003 0.00079 0.00076 0.02462

D105 3.08014 -0.00011 0.00067 -0.00606 -0.00539 3.07475

D106 -0.02878 -0.00008 0.00032 -0.00424 -0.00392 -0.03271

D107 -0.27935 0.00002 -0.00007 0.00134 0.00126 -0.27808

D108 2.89491 0.00005 -0.00042 0.00316 0.00273 2.89765

D109 -3.02211 0.00010 -0.00064 0.00554 0.00490 -3.01721

D110 -1.69484 0.00007 -0.00044 0.00422 0.00379 -1.69105

D111 -0.36757 0.00005 -0.00024 0.00291 0.00267 -0.36490

D112 0.36757 -0.00005 0.00024 -0.00291 -0.00267 0.36490

D113 1.69484 -0.00007 0.00044 -0.00422 -0.00379 1.69105

D114 3.02211 -0.00010 0.00064 -0.00554 -0.00490 3.01721

D115 -0.07705 -0.00008 0.00028 -0.00350 -0.00323 -0.08027

D116 3.03623 -0.00010 0.00018 -0.00473 -0.00455 3.03168

D117 3.09727 0.00004 0.00016 -0.00053 -0.00037 3.09690

D118 -0.01942 0.00005 0.00025 0.00054 0.00079 -0.01863

D119 -0.18182 0.00012 -0.00054 0.00637 0.00583 -0.17599

D120 2.98467 0.00013 -0.00045 0.00744 0.00700 2.99166

D121 0.01942 -0.00005 -0.00025 -0.00054 -0.00079 0.01863

D122 -3.09727 -0.00004 -0.00016 0.00053 0.00037 -3.09690

D123 -2.98467 -0.00013 0.00045 -0.00744 -0.00700 -2.99166

D124 0.18182 -0.00012 0.00054 -0.00637 -0.00583 0.17599

D125 1.64908 -0.00004 0.00041 -0.00393 -0.00352 1.64556

D126 2.97257 0.00001 0.00039 -0.00272 -0.00233 2.97024

D127 0.32560 -0.00009 0.00044 -0.00515 -0.00471 0.32089

D128 -1.64908 0.00004 -0.00041 0.00393 0.00352 -1.64556

D129 -0.32560 0.00009 -0.00044 0.00515 0.00471 -0.32089

D130 -2.97257 -0.00001 -0.00039 0.00272 0.00233 -2.97024

D131 -3.10644 -0.00002 -0.00006 0.00070 0.00065 -3.10580

D132 0.02653 0.00000 -0.00016 0.00138 0.00122 0.02775

D133 0.01154 -0.00003 -0.00015 -0.00032 -0.00047 0.01106

D134 -3.13868 -0.00001 -0.00026 0.00036 0.00010 -3.13858

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.13419 0.00002 -0.00009 0.00059 0.00050 3.13469

D137 -3.13419 -0.00002 0.00009 -0.00059 -0.00050 -3.13469

D138 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D139 -3.13869 -0.00001 0.00024 -0.00054 -0.00030 -3.13899

D140 0.00548 -0.00003 0.00011 -0.00124 -0.00113 0.00435

D141 -0.00677 0.00001 0.00012 0.00023 0.00034 -0.00642

D142 3.13740 -0.00001 -0.00001 -0.00048 -0.00048 3.13691

D143 -0.01154 0.00003 0.00015 0.00032 0.00047 -0.01106

D144 3.10644 0.00002 0.00006 -0.00070 -0.00065 3.10580

D145 3.13868 0.00001 0.00026 -0.00036 -0.00010 3.13858

D146 -0.02653 0.00000 0.00016 -0.00138 -0.00122 -0.02775

D147 0.00677 -0.00001 -0.00012 -0.00023 -0.00034 0.00642

D148 -3.13740 0.00001 0.00001 0.00048 0.00048 -3.13691

D149 3.13869 0.00001 -0.00024 0.00054 0.00030 3.13899

D150 -0.00548 0.00003 -0.00011 0.00124 0.00113 -0.00435

D151 0.07705 0.00008 -0.00028 0.00350 0.00323 0.08027

D152 -3.03623 0.00010 -0.00018 0.00473 0.00455 -3.03168

D153 0.00718 0.00000 -0.00010 -0.00011 -0.00021 0.00697

D154 -3.13463 0.00000 -0.00012 0.00003 -0.00010 -3.13472

D155 -3.13770 0.00001 0.00008 0.00005 0.00012 -3.13757

D156 0.00368 0.00001 0.00006 0.00018 0.00024 0.00392

D157 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D158 3.14138 0.00000 -0.00002 0.00013 0.00011 3.14150

D159 -3.14138 0.00000 0.00002 -0.00013 -0.00011 -3.14150

D160 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D161 -3.14141 0.00000 -0.00003 -0.00019 -0.00021 3.14156

D162 -0.00021 0.00000 0.00002 -0.00009 -0.00007 -0.00029

D163 -0.00004 0.00000 -0.00005 -0.00005 -0.00010 -0.00013

D164 3.14116 0.00000 0.00000 0.00004 0.00004 3.14121

D165 -0.00718 0.00000 0.00010 0.00011 0.00021 -0.00697

D166 3.13770 -0.00001 -0.00008 -0.00005 -0.00012 3.13757

D167 3.13463 0.00000 0.00012 -0.00003 0.00010 3.13472

D168 -0.00368 -0.00001 -0.00006 -0.00018 -0.00024 -0.00392

D169 0.00004 0.00000 0.00005 0.00005 0.00010 0.00013

D170 -3.14116 0.00000 0.00000 -0.00004 -0.00004 -3.14121

D171 3.14141 0.00000 0.00003 0.00019 0.00021 -3.14156

D172 0.00021 0.00000 -0.00002 0.00009 0.00007 0.00029

D173 -0.00669 0.00001 0.00011 0.00023 0.00034 -0.00635

D174 3.13565 0.00001 0.00016 0.00009 0.00025 3.13590

D175 3.13743 -0.00001 -0.00001 -0.00047 -0.00047 3.13696

D176 -0.00341 -0.00001 0.00004 -0.00060 -0.00057 -0.00397

D177 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D178 -3.14086 0.00000 0.00004 -0.00013 -0.00009 -3.14095

D179 3.14086 0.00000 -0.00004 0.00013 0.00009 3.14095

D180 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D181 3.14084 0.00001 -0.00004 0.00031 0.00026 3.14110

D182 -0.00101 0.00000 0.00000 0.00005 0.00005 -0.00095

D183 -0.00002 0.00000 0.00000 0.00017 0.00017 0.00016

D184 3.14133 0.00000 0.00004 -0.00008 -0.00004 3.14129

D185 0.00669 -0.00001 -0.00011 -0.00023 -0.00034 0.00635

D186 -3.13743 0.00001 0.00001 0.00047 0.00047 -3.13696

D187 -3.13565 -0.00001 -0.00016 -0.00009 -0.00025 -3.13590

D188 0.00341 0.00001 -0.00004 0.00060 0.00057 0.00397

D189 0.00002 0.00000 0.00000 -0.00017 -0.00017 -0.00016

D190 -3.14133 0.00000 -0.00004 0.00008 0.00004 -3.14129

D191 -3.14084 -0.00001 0.00004 -0.00031 -0.00026 -3.14110

D192 0.00101 0.00000 0.00000 -0.00005 -0.00005 0.00095

D193 -0.00718 0.00000 0.00010 0.00011 0.00021 -0.00697

D194 3.13463 0.00000 0.00012 -0.00003 0.00010 3.13472

D195 3.13770 -0.00001 -0.00008 -0.00005 -0.00012 3.13757

D196 -0.00368 -0.00001 -0.00006 -0.00018 -0.00024 -0.00392

D197 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D198 -3.14138 0.00000 0.00002 -0.00013 -0.00011 -3.14150

D199 3.14138 0.00000 -0.00002 0.00013 0.00011 3.14150

D200 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D201 3.14141 0.00000 0.00003 0.00019 0.00021 -3.14156

D202 0.00021 0.00000 -0.00002 0.00009 0.00007 0.00029

D203 0.00004 0.00000 0.00005 0.00005 0.00010 0.00013

D204 -3.14116 0.00000 0.00000 -0.00004 -0.00004 -3.14121

D205 0.00718 0.00000 -0.00010 -0.00011 -0.00021 0.00697

D206 -3.13770 0.00001 0.00008 0.00005 0.00012 -3.13757

D207 -3.13463 0.00000 -0.00012 0.00003 -0.00010 -3.13472

D208 0.00368 0.00001 0.00006 0.00018 0.00024 0.00392

D209 -0.00004 0.00000 -0.00005 -0.00005 -0.00010 -0.00013

D210 3.14116 0.00000 0.00000 0.00004 0.00004 3.14121

D211 -3.14141 0.00000 -0.00003 -0.00019 -0.00021 3.14156

D212 -0.00021 0.00000 0.00002 -0.00009 -0.00007 -0.00029

D213 -0.00669 0.00001 0.00011 0.00023 0.00034 -0.00635

D214 3.13565 0.00001 0.00016 0.00009 0.00025 3.13590

D215 3.13743 -0.00001 -0.00001 -0.00047 -0.00047 3.13696

D216 -0.00341 -0.00001 0.00004 -0.00060 -0.00057 -0.00397

D217 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D218 -3.14086 0.00000 0.00004 -0.00013 -0.00009 -3.14095

D219 3.14086 0.00000 -0.00004 0.00013 0.00009 3.14095

D220 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D221 3.14084 0.00001 -0.00004 0.00031 0.00026 3.14110

D222 -0.00101 0.00000 0.00000 0.00005 0.00005 -0.00095

D223 -0.00002 0.00000 0.00000 0.00017 0.00017 0.00016

D224 3.14133 0.00000 0.00004 -0.00008 -0.00004 3.14129

D225 0.00669 -0.00001 -0.00011 -0.00023 -0.00034 0.00635

D226 -3.13743 0.00001 0.00001 0.00047 0.00047 -3.13696

D227 -3.13565 -0.00001 -0.00016 -0.00009 -0.00025 -3.13590

D228 0.00341 0.00001 -0.00004 0.00060 0.00057 0.00397

D229 0.00002 0.00000 0.00000 -0.00017 -0.00017 -0.00016

D230 -3.14133 0.00000 -0.00004 0.00008 0.00004 -3.14129

D231 -3.14084 -0.00001 0.00004 -0.00031 -0.00026 -3.14110

D232 0.00101 0.00000 0.00000 -0.00005 -0.00005 0.00095

D233 -0.00002 0.00000 0.00000 0.00018 0.00018 0.00016

D234 3.14118 0.00000 -0.00003 0.00018 0.00016 3.14134

D235 3.14132 0.00000 0.00004 -0.00008 -0.00004 3.14128

D236 -0.00067 0.00000 0.00002 -0.00007 -0.00006 -0.00073

D237 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D238 3.14120 0.00000 -0.00002 0.00001 -0.00002 3.14118

D239 -3.14120 0.00000 0.00002 -0.00001 0.00002 -3.14118

D240 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D241 0.00002 0.00000 0.00000 -0.00018 -0.00018 -0.00016

D242 -3.14132 0.00000 -0.00004 0.00008 0.00004 -3.14128

D243 -3.14118 0.00000 0.00003 -0.00018 -0.00016 -3.14134

D244 0.00067 0.00000 -0.00002 0.00007 0.00006 0.00073

D245 -0.00004 0.00000 -0.00005 -0.00005 -0.00010 -0.00013

D246 -3.14106 0.00000 -0.00004 -0.00003 -0.00007 -3.14113

D247 3.14116 0.00000 0.00000 0.00004 0.00004 3.14120

D248 0.00014 0.00000 0.00000 0.00007 0.00007 0.00021

D249 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D250 -3.14102 0.00000 0.00000 0.00002 0.00003 -3.14100

D251 3.14102 0.00000 0.00000 -0.00002 -0.00003 3.14100

D252 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D253 0.00004 0.00000 0.00005 0.00005 0.00010 0.00013

D254 -3.14116 0.00000 0.00000 -0.00004 -0.00004 -3.14120

D255 3.14106 0.00000 0.00004 0.00003 0.00007 3.14113

D256 -0.00014 0.00000 0.00000 -0.00007 -0.00007 -0.00021

D257 -0.00002 0.00000 0.00000 0.00018 0.00018 0.00016

D258 3.14118 0.00000 -0.00003 0.00018 0.00016 3.14134

D259 3.14132 0.00000 0.00004 -0.00008 -0.00004 3.14128

D260 -0.00067 0.00000 0.00002 -0.00007 -0.00006 -0.00073

D261 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D262 3.14120 0.00000 -0.00002 0.00001 -0.00002 3.14118

D263 -3.14120 0.00000 0.00002 -0.00001 0.00002 -3.14118

D264 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D265 0.00002 0.00000 0.00000 -0.00018 -0.00018 -0.00016

D266 -3.14132 0.00000 -0.00004 0.00008 0.00004 -3.14128

D267 -3.14118 0.00000 0.00003 -0.00018 -0.00016 -3.14134

D268 0.00067 0.00000 -0.00002 0.00007 0.00006 0.00073

D269 0.00004 0.00000 0.00005 0.00005 0.00010 0.00013

D270 3.14106 0.00000 0.00004 0.00003 0.00007 3.14113

D271 -3.14116 0.00000 0.00000 -0.00004 -0.00004 -3.14120

D272 -0.00014 0.00000 0.00000 -0.00007 -0.00007 -0.00021

D273 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D274 3.14102 0.00000 0.00000 -0.00002 -0.00003 3.14100

D275 -3.14102 0.00000 0.00000 0.00002 0.00003 -3.14100

D276 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D277 -0.00004 0.00000 -0.00005 -0.00005 -0.00010 -0.00013

D278 3.14116 0.00000 0.00000 0.00004 0.00004 3.14120

D279 -3.14106 0.00000 -0.00004 -0.00003 -0.00007 -3.14113

D280 0.00014 0.00000 0.00000 0.00007 0.00007 0.00021

Item Value Threshold Converged?

Maximum Force 0.000729 0.000450 NO

RMS Force 0.000164 0.000300 YES

Maximum Displacement 0.074588 0.001800 NO

RMS Displacement 0.013224 0.001200 NO

Predicted change in Energy=-2.877028D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Jun 30 20:17:17 2019, MaxMem= 1342177280 cpu: 85.1

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

Stoichiometry C48H24N8Zn(3)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C48H24N4)]

Deg. of freedom 61

Full point group C2V NOp 4

RotChk: IX=0 Diff= 5.50D-16

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 1.121303 2.793204 0.153717

2 7 0 0.000000 2.022346 0.265783

3 6 0 -1.121303 2.793204 0.153717

4 6 0 -0.717723 4.176985 -0.021556

5 6 0 0.717723 4.176985 -0.021556

6 7 0 -2.412612 2.385062 0.164712

7 6 0 -2.793737 1.127551 0.203331

8 7 0 -2.009583 0.000000 0.266002

9 6 0 -2.793737 -1.127551 0.203331

10 6 0 -4.206682 -0.712302 0.136263

11 6 0 -4.206682 0.712302 0.136263

12 7 0 2.412612 2.385062 0.164712

13 6 0 4.206682 0.712302 0.136263

14 6 0 4.206682 -0.712302 0.136263

15 6 0 2.793737 -1.127551 0.203331

16 7 0 2.009583 0.000000 0.266002

17 6 0 2.793737 1.127551 0.203331

18 7 0 2.412612 -2.385062 0.164712

19 7 0 0.000000 -2.022346 0.265783

20 6 0 1.121303 -2.793204 0.153717

21 6 0 0.717723 -4.176985 -0.021556

22 6 0 -0.717723 -4.176985 -0.021556

23 6 0 -1.121303 -2.793204 0.153717

24 7 0 -2.412612 -2.385062 0.164712

25 30 0 0.000000 0.000000 0.787354

26 6 0 5.371660 1.426228 0.072747

27 6 0 6.606845 0.718790 0.014273

28 6 0 6.606845 -0.718790 0.014273

29 6 0 5.371660 -1.426228 0.072747

30 6 0 -1.428335 -5.344876 -0.177679

31 6 0 -0.721334 -6.563391 -0.332533

32 6 0 0.721334 -6.563391 -0.332533

33 6 0 1.428335 -5.344876 -0.177679

34 6 0 -5.371660 1.426228 0.072747

35 6 0 -6.606845 0.718790 0.014273

36 6 0 -6.606845 -0.718790 0.014273

37 6 0 -5.371660 -1.426228 0.072747

38 6 0 1.428335 5.344876 -0.177679

39 6 0 0.721334 6.563391 -0.332533

40 6 0 -0.721334 6.563391 -0.332533

41 6 0 -1.428335 5.344876 -0.177679

42 6 0 1.402199 -7.799369 -0.490412

43 6 0 0.707911 -8.975659 -0.640480

44 6 0 -0.707911 -8.975659 -0.640480

45 6 0 -1.402199 -7.799369 -0.490412

46 6 0 7.846067 -1.401226 -0.044513

47 6 0 9.033235 -0.705769 -0.100673

48 6 0 9.033235 0.705769 -0.100673

49 6 0 7.846067 1.401226 -0.044513

50 6 0 -1.402199 7.799369 -0.490412

51 6 0 -0.707911 8.975659 -0.640480

52 6 0 0.707911 8.975659 -0.640480

53 6 0 1.402199 7.799369 -0.490412

54 6 0 -7.846067 -1.401226 -0.044513

55 6 0 -9.033235 -0.705769 -0.100673

56 6 0 -9.033235 0.705769 -0.100673

57 6 0 -7.846067 1.401226 -0.044513

58 1 0 5.371872 2.511039 0.068948

59 1 0 5.371872 -2.511039 0.068948

60 1 0 -2.513284 -5.348031 -0.182479

61 1 0 2.513284 -5.348031 -0.182479

62 1 0 -5.371872 2.511039 0.068948

63 1 0 -5.371872 -2.511039 0.068948

64 1 0 2.513284 5.348031 -0.182479

65 1 0 -2.513284 5.348031 -0.182479

66 1 0 2.487622 -7.798001 -0.489947

67 1 0 1.243414 -9.911337 -0.760245

68 1 0 -1.243414 -9.911337 -0.760245

69 1 0 -2.487622 -7.798001 -0.489947

70 1 0 7.844323 -2.486441 -0.044799

71 1 0 9.974715 -1.242386 -0.145774

72 1 0 9.974715 1.242386 -0.145774

73 1 0 7.844323 2.486441 -0.044799

74 1 0 -2.487622 7.798001 -0.489947

75 1 0 -1.243414 9.911337 -0.760245

76 1 0 1.243414 9.911337 -0.760245

77 1 0 2.487622 7.798001 -0.489947

78 1 0 -7.844323 -2.486441 -0.044799

79 1 0 -9.974715 -1.242386 -0.145774

80 1 0 -9.974715 1.242386 -0.145774

81 1 0 -7.844323 2.486441 -0.044799

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Rotational constants (GHZ): 0.0385743 0.0381270 0.0193087

Leave Link 202 at Sun Jun 30 20:17:17 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 307 symmetry adapted cartesian basis functions of A1 symmetry.

There are 278 symmetry adapted cartesian basis functions of A2 symmetry.

There are 289 symmetry adapted cartesian basis functions of B1 symmetry.

There are 289 symmetry adapted cartesian basis functions of B2 symmetry.

There are 289 symmetry adapted basis functions of A1 symmetry.

There are 265 symmetry adapted basis functions of A2 symmetry.

There are 275 symmetry adapted basis functions of B1 symmetry.

There are 275 symmetry adapted basis functions of B2 symmetry.

1104 basis functions, 1951 primitive gaussians, 1163 cartesian basis functions

191 alpha electrons 189 beta electrons

nuclear repulsion energy 6888.1660698656 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= 81 NActive= 81 NUniq= 22 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= -0.2361250180 Hartrees.

Nuclear repulsion after empirical dispersion term = 6887.9299448476 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= 81.

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 = 81

GePol: Total number of spheres = 81

GePol: Number of exposed spheres = 81 (100.00%)

GePol: Number of points = 6422

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.15D-10

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 376

GePol: Fraction of low-weight points (<1% of avg) = 5.85%

GePol: Cavity surface area = 670.899 Ang\*\*2

GePol: Cavity volume = 694.213 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0169275959 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 6887.9130172518 Hartrees.

Leave Link 301 at Sun Jun 30 20:17:18 2019, MaxMem= 1342177280 cpu: 1.8

(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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36689 LenP2D= 95162.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1104 RedAO= T EigKep= 2.86D-05 NBF= 289 265 275 275

NBsUse= 1104 1.00D-06 EigRej= -1.00D+00 NBFU= 289 265 275 275

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= 1060 1060 1060 1060 1060 MxSgAt= 81 MxSgA2= 81.

Leave Link 302 at Sun Jun 30 20:17:40 2019, MaxMem= 1342177280 cpu: 246.5

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Jun 30 20:17:40 2019, MaxMem= 1342177280 cpu: 2.6

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

Initial guess from the checkpoint file: "ZnNPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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The electronic state of the initial guess is 3-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -2348.36353345186

Leave Link 401 at Sun Jun 30 20:18:11 2019, MaxMem= 1342177280 cpu: 303.4

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4103221 IEndB= 4103221 NGot= 1342177280 MDV= 1339444432

LenX= 1339444432 LenY= 1338090700

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= 420000000 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= 123726252.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.11D-15 for 6415.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.54D-15 for 1586 1521.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.66D-15 for 6415.

Iteration 1 A^-1\*A deviation from orthogonality is 2.53D-08 for 1293 1269.

Iteration 2 A\*A^-1 deviation from unit magnitude is 4.66D-15 for 1562.

Iteration 2 A\*A^-1 deviation from orthogonality is 4.78D-15 for 5334 921.

Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 553.

Iteration 2 A^-1\*A deviation from orthogonality is 5.49D-16 for 3090 2596.

E= -2348.13029994000

DIIS: error= 5.83D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2348.13029994000 IErMin= 1 ErrMin= 5.83D-04

ErrMax= 5.83D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.87D-04 BMatP= 7.87D-04

IDIUse=3 WtCom= 9.94D-01 WtEn= 5.83D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.379 Goal= None Shift= 0.000

Gap= 0.459 Goal= None Shift= 0.000

RMSDP=1.99D-05 MaxDP=6.39D-04 OVMax= 3.47D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.98D-05 CP: 1.00D+00

E= -2348.13068538855 Delta-E= -0.000385448551 Rises=F Damp=F

DIIS: error= 8.05D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2348.13068538855 IErMin= 2 ErrMin= 8.05D-05

ErrMax= 8.05D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.83D-06 BMatP= 7.87D-04

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

Coeff-Com: -0.678D-01 0.107D+01

Coeff: -0.678D-01 0.107D+01

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.95D-06 MaxDP=1.30D-04 DE=-3.85D-04 OVMax= 5.43D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.57D-06 CP: 1.00D+00 1.07D+00

E= -2348.13069039706 Delta-E= -0.000005008515 Rises=F Damp=F

DIIS: error= 5.68D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2348.13069039706 IErMin= 3 ErrMin= 5.68D-05

ErrMax= 5.68D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.56D-06 BMatP= 9.83D-06

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

Coeff-Com: -0.350D-01 0.472D+00 0.563D+00

Coeff: -0.350D-01 0.472D+00 0.563D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.33D-06 MaxDP=7.96D-05 DE=-5.01D-06 OVMax= 2.41D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.16D-06 CP: 1.00D+00 1.08D+00 7.83D-01

E= -2348.13069110291 Delta-E= -0.000000705850 Rises=F Damp=F

DIIS: error= 2.07D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2348.13069110291 IErMin= 4 ErrMin= 2.07D-05

ErrMax= 2.07D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.44D-06 BMatP= 4.56D-06

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

Coeff-Com: -0.843D-02 0.876D-01 0.357D+00 0.564D+00

Coeff: -0.843D-02 0.876D-01 0.357D+00 0.564D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=6.70D-07 MaxDP=3.46D-05 DE=-7.06D-07 OVMax= 1.38D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.00D-07 CP: 1.00D+00 1.08D+00 8.61D-01 5.83D-01

E= -2348.13069138945 Delta-E= -0.000000286534 Rises=F Damp=F

DIIS: error= 8.27D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2348.13069138945 IErMin= 5 ErrMin= 8.27D-06

ErrMax= 8.27D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D-07 BMatP= 1.44D-06

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

Coeff-Com: -0.717D-03-0.594D-02 0.130D+00 0.297D+00 0.579D+00

Coeff: -0.717D-03-0.594D-02 0.130D+00 0.297D+00 0.579D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.05D-07 MaxDP=1.25D-05 DE=-2.87D-07 OVMax= 5.40D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.36D-07 CP: 1.00D+00 1.08D+00 8.70D-01 6.58D-01 6.97D-01

E= -2348.13069141070 Delta-E= -0.000000021248 Rises=F Damp=F

DIIS: error= 4.19D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2348.13069141070 IErMin= 6 ErrMin= 4.19D-06

ErrMax= 4.19D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.03D-08 BMatP= 1.13D-07

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

Coeff-Com: 0.746D-03-0.169D-01 0.274D-01 0.961D-01 0.347D+00 0.546D+00

Coeff: 0.746D-03-0.169D-01 0.274D-01 0.961D-01 0.347D+00 0.546D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=6.62D-08 MaxDP=6.89D-06 DE=-2.12D-08 OVMax= 1.96D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.66D-08 CP: 1.00D+00 1.08D+00 8.77D-01 6.65D-01 7.21D-01

CP: 6.28D-01

E= -2348.13069141485 Delta-E= -0.000000004155 Rises=F Damp=F

DIIS: error= 1.05D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2348.13069141485 IErMin= 7 ErrMin= 1.05D-06

ErrMax= 1.05D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.29D-09 BMatP= 2.03D-08

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

Coeff-Com: 0.454D-03-0.889D-02 0.640D-02 0.326D-01 0.151D+00 0.290D+00

Coeff-Com: 0.529D+00

Coeff: 0.454D-03-0.889D-02 0.640D-02 0.326D-01 0.151D+00 0.290D+00

Coeff: 0.529D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.87D-08 MaxDP=2.02D-06 DE=-4.15D-09 OVMax= 4.84D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.55D-08 CP: 1.00D+00 1.08D+00 8.78D-01 6.64D-01 7.29D-01

CP: 6.46D-01 7.47D-01

E= -2348.13069141589 Delta-E= -0.000000001042 Rises=F Damp=F

DIIS: error= 4.97D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2348.13069141589 IErMin= 8 ErrMin= 4.97D-07

ErrMax= 4.97D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.09D-10 BMatP= 1.29D-09

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

Coeff-Com: 0.994D-04-0.141D-02-0.185D-02-0.165D-02 0.124D-01 0.472D-01

Coeff-Com: 0.286D+00 0.659D+00

Coeff: 0.994D-04-0.141D-02-0.185D-02-0.165D-02 0.124D-01 0.472D-01

Coeff: 0.286D+00 0.659D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=7.94D-09 MaxDP=9.37D-07 DE=-1.04D-09 OVMax= 3.03D-06

Error on total polarization charges = 0.08840

SCF Done: E(UB3LYP) = -2348.13069142 A.U. after 8 cycles

NFock= 8 Conv=0.79D-08 -V/T= 1.9830

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

<L.S>= 0.000000000000E+00

KE= 2.388751779606D+03 PE=-1.931923931451D+04 EE= 7.694443826239D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -10.62

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0219, after 2.0003

Leave Link 502 at Sun Jun 30 20:23:29 2019, MaxMem= 1342177280 cpu: 3546.1

(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.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36689 LenP2D= 95162.

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 = 194

Leave Link 701 at Sun Jun 30 20:24:06 2019, MaxMem= 1342177280 cpu: 377.8

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sun Jun 30 20:24:06 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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 Sun Jun 30 20:24:47 2019, MaxMem= 1342177280 cpu: 445.6

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-1.77635684D-13 7.56728014D-13 9.59325302D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000032614 -0.000112428 -0.000267904

2 7 0.000000000 0.000248300 0.000427206

3 6 -0.000032614 -0.000112428 -0.000267904

4 6 -0.000034357 0.000020692 -0.000042143

5 6 0.000034357 0.000020692 -0.000042143

6 7 0.000023409 -0.000167666 0.000151121

7 6 0.000187830 0.000262051 -0.000054925

8 7 -0.000097609 0.000000000 0.000345834

9 6 0.000187830 -0.000262051 -0.000054925

10 6 -0.000117402 0.000048125 -0.000078084

11 6 -0.000117402 -0.000048125 -0.000078084

12 7 -0.000023409 -0.000167666 0.000151121

13 6 0.000117402 -0.000048125 -0.000078084

14 6 0.000117402 0.000048125 -0.000078084

15 6 -0.000187830 -0.000262051 -0.000054925

16 7 0.000097609 0.000000000 0.000345834

17 6 -0.000187830 0.000262051 -0.000054925

18 7 -0.000023409 0.000167666 0.000151121

19 7 0.000000000 -0.000248300 0.000427206

20 6 0.000032614 0.000112428 -0.000267904

21 6 0.000034357 -0.000020692 -0.000042143

22 6 -0.000034357 -0.000020692 -0.000042143

23 6 -0.000032614 0.000112428 -0.000267904

24 7 0.000023409 0.000167666 0.000151121

25 30 0.000000000 0.000000000 -0.000425190

26 6 0.000020992 -0.000028844 0.000017939

27 6 -0.000019704 0.000094289 0.000005074

28 6 -0.000019704 -0.000094289 0.000005074

29 6 0.000020992 0.000028844 0.000017939

30 6 0.000048836 -0.000054597 0.000018227

31 6 -0.000129056 0.000036285 -0.000001118

32 6 0.000129056 0.000036285 -0.000001118

33 6 -0.000048836 -0.000054597 0.000018227

34 6 -0.000020992 -0.000028844 0.000017939

35 6 0.000019704 0.000094289 0.000005074

36 6 0.000019704 -0.000094289 0.000005074

37 6 -0.000020992 0.000028844 0.000017939

38 6 -0.000048836 0.000054597 0.000018227

39 6 0.000129056 -0.000036285 -0.000001118

40 6 -0.000129056 -0.000036285 -0.000001118

41 6 0.000048836 0.000054597 0.000018227

42 6 0.000012840 0.000018677 -0.000012897

43 6 0.000103767 -0.000032737 -0.000002313

44 6 -0.000103767 -0.000032737 -0.000002313

45 6 -0.000012840 0.000018677 -0.000012897

46 6 -0.000022951 -0.000026178 0.000004943

47 6 0.000040476 -0.000088372 -0.000002109

48 6 0.000040476 0.000088372 -0.000002109

49 6 -0.000022951 0.000026178 0.000004943

50 6 -0.000012840 -0.000018677 -0.000012897

51 6 -0.000103767 0.000032737 -0.000002313

52 6 0.000103767 0.000032737 -0.000002313

53 6 0.000012840 -0.000018677 -0.000012897

54 6 0.000022951 -0.000026178 0.000004943

55 6 -0.000040476 -0.000088372 -0.000002109

56 6 -0.000040476 0.000088372 -0.000002109

57 6 0.000022951 0.000026178 0.000004943

58 1 -0.000006131 0.000049058 -0.000007925

59 1 -0.000006131 -0.000049058 -0.000007925

60 1 -0.000052256 0.000014713 -0.000007784

61 1 0.000052256 0.000014713 -0.000007784

62 1 0.000006131 0.000049058 -0.000007925

63 1 0.000006131 -0.000049058 -0.000007925

64 1 0.000052256 -0.000014713 -0.000007784

65 1 -0.000052256 -0.000014713 -0.000007784

66 1 0.000039252 0.000008644 0.000001933

67 1 0.000008070 -0.000022341 -0.000000783

68 1 -0.000008070 -0.000022341 -0.000000783

69 1 -0.000039252 0.000008644 0.000001933

70 1 -0.000003622 -0.000037582 -0.000000138

71 1 0.000021368 -0.000009746 -0.000001335

72 1 0.000021368 0.000009746 -0.000001335

73 1 -0.000003622 0.000037582 -0.000000138

74 1 -0.000039252 -0.000008644 0.000001933

75 1 -0.000008070 0.000022341 -0.000000783

76 1 0.000008070 0.000022341 -0.000000783

77 1 0.000039252 -0.000008644 0.000001933

78 1 0.000003622 -0.000037582 -0.000000138

79 1 -0.000021368 -0.000009746 -0.000001335

80 1 -0.000021368 0.000009746 -0.000001335

81 1 0.000003622 0.000037582 -0.000000138

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

Cartesian Forces: Max 0.000427206 RMS 0.000096764

Leave Link 716 at Sun Jun 30 20:24:47 2019, MaxMem= 1342177280 cpu: 2.2

(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 0.000162246 RMS 0.000037904

Search for a local minimum.

Step number 3 out of a maximum of 486

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .37904D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3

DE= -3.95D-05 DEPred=-2.88D-05 R= 1.37D+00

TightC=F SS= 1.41D+00 RLast= 3.67D-02 DXNew= 5.0454D-01 1.1011D-01

Trust test= 1.37D+00 RLast= 3.67D-02 DXMaxT set to 3.00D-01

ITU= 1 1 0

Eigenvalues --- 0.00902 0.01435 0.01491 0.01502 0.01574

Eigenvalues --- 0.01599 0.01627 0.01656 0.01667 0.01695

Eigenvalues --- 0.01698 0.01707 0.01713 0.01715 0.01717

Eigenvalues --- 0.01725 0.01730 0.01730 0.01736 0.01738

Eigenvalues --- 0.01746 0.01752 0.01759 0.01791 0.01816

Eigenvalues --- 0.01827 0.01829 0.01829 0.01851 0.01854

Eigenvalues --- 0.01870 0.01870 0.01899 0.01932 0.01968

Eigenvalues --- 0.01968 0.01970 0.01972 0.01977 0.01992

Eigenvalues --- 0.01992 0.01993 0.01993 0.01994 0.02080

Eigenvalues --- 0.02080 0.02086 0.02086 0.02088 0.02089

Eigenvalues --- 0.02095 0.02095 0.02098 0.02100 0.02103

Eigenvalues --- 0.02103 0.02105 0.02106 0.02124 0.02124

Eigenvalues --- 0.02137 0.02144 0.02144 0.02147 0.02148

Eigenvalues --- 0.02150 0.02172 0.02173 0.02214 0.02214

Eigenvalues --- 0.02225 0.02225 0.02275 0.02276 0.02283

Eigenvalues --- 0.02346 0.03071 0.05539 0.05569 0.08035

Eigenvalues --- 0.14670 0.15983 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 0.16014

Eigenvalues --- 0.16152 0.16254 0.16976 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22500 0.22502 0.22504

Eigenvalues --- 0.22524 0.23233 0.23234 0.23234 0.23597

Eigenvalues --- 0.23719 0.23938 0.23940 0.23941 0.23951

Eigenvalues --- 0.24118 0.24319 0.24496 0.24554 0.24556

Eigenvalues --- 0.24557 0.24557 0.24763 0.24898 0.24900

Eigenvalues --- 0.24979 0.24986 0.24988 0.24992 0.24992

Eigenvalues --- 0.24998 0.24998 0.24998 0.24998 0.25849

Eigenvalues --- 0.32870 0.32952 0.33670 0.33695 0.33836

Eigenvalues --- 0.33843 0.35036 0.35058 0.35175 0.35181

Eigenvalues --- 0.35181 0.35181 0.35192 0.35202 0.35202

Eigenvalues --- 0.35202 0.35202 0.35231 0.35231 0.35231

Eigenvalues --- 0.35241 0.35249 0.35249 0.35249 0.35257

Eigenvalues --- 0.35270 0.35270 0.35270 0.35275 0.35279

Eigenvalues --- 0.35279 0.35279 0.35413 0.35439 0.36350

Eigenvalues --- 0.36526 0.37455 0.37551 0.37969 0.38309

Eigenvalues --- 0.39276 0.39276 0.39611 0.39611 0.40187

Eigenvalues --- 0.40187 0.40257 0.40257 0.40906 0.40983

Eigenvalues --- 0.41001 0.41019 0.41603 0.41633 0.41875

Eigenvalues --- 0.41987 0.42215 0.42253 0.42598 0.42806

Eigenvalues --- 0.42918 0.42966 0.44741 0.45630 0.47088

Eigenvalues --- 0.47124 0.47124 0.47384 0.47386 0.47579

Eigenvalues --- 0.47580 0.48132 0.48159 0.48218 0.48287

Eigenvalues --- 0.48465 0.48466 0.48657 0.48680 0.48706

Eigenvalues --- 0.48729 0.49088 0.49489 0.49898 0.50387

Eigenvalues --- 0.50960 0.52483 0.53985 0.58128 0.59247

Eigenvalues --- 0.59827 0.60901

En-DIIS/RFO-DIIS IScMMF= 0 using points: 3 2

RFO step: Lambda=-3.65316099D-06.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 3.95D-05 SmlDif= 1.00D-05

RMS Error= 0.2371761324D-03 NUsed= 2 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.58089 -0.58089

Iteration 1 RMS(Cart)= 0.02046474 RMS(Int)= 0.00002856

Iteration 2 RMS(Cart)= 0.00013843 RMS(Int)= 0.00000381

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000381

ITry= 1 IFail=0 DXMaxC= 1.18D-01 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.21D-08 for atom 69.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58008 -0.00004 -0.00011 -0.00017 -0.00028 2.57981

R2 2.74398 0.00006 0.00078 -0.00024 0.00054 2.74451

R3 2.55929 -0.00002 0.00008 -0.00032 -0.00024 2.55905

R4 2.58008 -0.00004 -0.00011 -0.00017 -0.00028 2.57981

R5 3.94673 0.00007 0.00173 0.00111 0.00284 3.94957

R6 2.74398 0.00006 0.00078 -0.00024 0.00054 2.74451

R7 2.55929 -0.00002 0.00008 -0.00032 -0.00024 2.55905

R8 2.71260 0.00006 0.00014 0.00002 0.00015 2.71275

R9 2.60022 0.00003 0.00027 -0.00022 0.00005 2.60027

R10 2.60022 0.00003 0.00027 -0.00022 0.00005 2.60027

R11 2.48417 -0.00015 -0.00022 -0.00056 -0.00078 2.48339

R12 2.59808 0.00002 -0.00003 -0.00008 -0.00011 2.59797

R13 2.78588 0.00016 0.00105 0.00014 0.00120 2.78708

R14 2.59808 0.00002 -0.00003 -0.00008 -0.00011 2.59797

R15 3.92328 0.00000 0.00088 -0.00014 0.00074 3.92402

R16 2.78588 0.00016 0.00105 0.00014 0.00120 2.78708

R17 2.48417 -0.00015 -0.00022 -0.00056 -0.00078 2.48339

R18 2.69211 0.00003 0.00017 -0.00010 0.00006 2.69217

R19 2.58478 0.00003 0.00024 -0.00020 0.00003 2.58481

R20 2.58478 0.00003 0.00024 -0.00020 0.00003 2.58481

R21 2.48417 -0.00015 -0.00022 -0.00056 -0.00078 2.48339

R22 2.69211 0.00003 0.00017 -0.00010 0.00006 2.69217

R23 2.78588 0.00016 0.00105 0.00014 0.00120 2.78708

R24 2.58478 0.00003 0.00024 -0.00020 0.00003 2.58481

R25 2.78588 0.00016 0.00105 0.00014 0.00120 2.78708

R26 2.58478 0.00003 0.00024 -0.00020 0.00003 2.58481

R27 2.59808 0.00002 -0.00003 -0.00008 -0.00011 2.59797

R28 2.48417 -0.00015 -0.00022 -0.00056 -0.00078 2.48339

R29 2.59808 0.00002 -0.00003 -0.00008 -0.00011 2.59797

R30 3.92328 0.00000 0.00088 -0.00014 0.00074 3.92402

R31 2.55929 -0.00002 0.00008 -0.00032 -0.00024 2.55905

R32 2.58008 -0.00004 -0.00011 -0.00017 -0.00028 2.57981

R33 2.58008 -0.00004 -0.00011 -0.00017 -0.00028 2.57981

R34 3.94673 0.00007 0.00173 0.00111 0.00284 3.94957

R35 2.74398 0.00006 0.00078 -0.00024 0.00054 2.74451

R36 2.71260 0.00006 0.00014 0.00002 0.00015 2.71275

R37 2.60022 0.00003 0.00027 -0.00022 0.00005 2.60027

R38 2.74398 0.00006 0.00078 -0.00024 0.00054 2.74451

R39 2.60022 0.00003 0.00027 -0.00022 0.00005 2.60027

R40 2.55929 -0.00002 0.00008 -0.00032 -0.00024 2.55905

R41 2.69216 0.00002 0.00051 -0.00034 0.00017 2.69233

R42 2.05001 0.00005 0.00012 0.00010 0.00022 2.05023

R43 2.71663 0.00012 0.00054 0.00009 0.00064 2.71727

R44 2.67571 0.00004 0.00048 -0.00024 0.00024 2.67595

R45 2.69216 0.00002 0.00051 -0.00034 0.00017 2.69233

R46 2.67571 0.00004 0.00048 -0.00024 0.00024 2.67595

R47 2.05001 0.00005 0.00012 0.00010 0.00022 2.05023

R48 2.67822 -0.00001 0.00045 -0.00041 0.00004 2.67826

R49 2.05028 0.00005 0.00012 0.00011 0.00023 2.05052

R50 2.72625 0.00014 0.00058 0.00017 0.00076 2.72700

R51 2.68324 0.00003 0.00052 -0.00028 0.00024 2.68348

R52 2.67822 -0.00001 0.00045 -0.00041 0.00004 2.67826

R53 2.68324 0.00003 0.00052 -0.00028 0.00024 2.68348

R54 2.05028 0.00005 0.00012 0.00011 0.00023 2.05052

R55 2.69216 0.00002 0.00051 -0.00034 0.00017 2.69233

R56 2.05001 0.00005 0.00012 0.00010 0.00022 2.05023

R57 2.71663 0.00012 0.00054 0.00009 0.00064 2.71727

R58 2.67571 0.00004 0.00048 -0.00024 0.00024 2.67595

R59 2.69216 0.00002 0.00051 -0.00034 0.00017 2.69233

R60 2.67571 0.00004 0.00048 -0.00024 0.00024 2.67595

R61 2.05001 0.00005 0.00012 0.00010 0.00022 2.05023

R62 2.67822 -0.00001 0.00045 -0.00041 0.00004 2.67826

R63 2.05028 0.00005 0.00012 0.00011 0.00023 2.05052

R64 2.72625 0.00014 0.00058 0.00017 0.00076 2.72700

R65 2.68324 0.00003 0.00052 -0.00028 0.00024 2.68348

R66 2.67822 -0.00001 0.00045 -0.00041 0.00004 2.67826

R67 2.68324 0.00003 0.00052 -0.00028 0.00024 2.68348

R68 2.05028 0.00005 0.00012 0.00011 0.00023 2.05052

R69 2.59672 0.00007 0.00022 -0.00012 0.00009 2.59681

R70 2.05115 0.00004 0.00010 0.00006 0.00017 2.05132

R71 2.67552 0.00015 0.00039 0.00020 0.00059 2.67611

R72 2.04981 0.00002 0.00014 -0.00002 0.00011 2.04992

R73 2.59672 0.00007 0.00022 -0.00012 0.00009 2.59681

R74 2.04981 0.00002 0.00014 -0.00002 0.00011 2.04992

R75 2.05115 0.00004 0.00010 0.00006 0.00017 2.05132

R76 2.60219 0.00007 0.00025 -0.00010 0.00015 2.60234

R77 2.05076 0.00004 0.00010 0.00006 0.00016 2.05092

R78 2.66742 0.00014 0.00036 0.00016 0.00052 2.66794

R79 2.04961 0.00002 0.00013 -0.00002 0.00011 2.04972

R80 2.60219 0.00007 0.00025 -0.00010 0.00015 2.60234

R81 2.04961 0.00002 0.00013 -0.00002 0.00011 2.04972

R82 2.05076 0.00004 0.00010 0.00006 0.00016 2.05092

R83 2.59672 0.00007 0.00022 -0.00012 0.00009 2.59681

R84 2.05115 0.00004 0.00010 0.00006 0.00017 2.05132

R85 2.67552 0.00015 0.00039 0.00020 0.00059 2.67611

R86 2.04981 0.00002 0.00014 -0.00002 0.00011 2.04992

R87 2.59672 0.00007 0.00022 -0.00012 0.00009 2.59681

R88 2.04981 0.00002 0.00014 -0.00002 0.00011 2.04992

R89 2.05115 0.00004 0.00010 0.00006 0.00017 2.05132

R90 2.60219 0.00007 0.00025 -0.00010 0.00015 2.60234

R91 2.05076 0.00004 0.00010 0.00006 0.00016 2.05092

R92 2.66742 0.00014 0.00036 0.00016 0.00052 2.66794

R93 2.04961 0.00002 0.00013 -0.00002 0.00011 2.04972

R94 2.60219 0.00007 0.00025 -0.00010 0.00015 2.60234

R95 2.04961 0.00002 0.00013 -0.00002 0.00011 2.04972

R96 2.05076 0.00004 0.00010 0.00006 0.00016 2.05092

A1 1.89621 -0.00001 0.00012 -0.00017 -0.00004 1.89617

A2 2.22970 -0.00001 -0.00030 0.00036 0.00005 2.22975

A3 2.15697 0.00002 0.00016 -0.00016 0.00000 2.15697

A4 1.92728 0.00005 0.00003 0.00023 0.00025 1.92753

A5 2.17391 -0.00002 0.00021 0.00040 0.00058 2.17448

A6 2.17391 -0.00002 0.00021 0.00040 0.00058 2.17448

A7 1.89621 -0.00001 0.00012 -0.00017 -0.00004 1.89617

A8 2.22970 -0.00001 -0.00030 0.00036 0.00005 2.22975

A9 2.15697 0.00002 0.00016 -0.00016 0.00000 2.15697

A10 1.85244 -0.00002 -0.00013 0.00003 -0.00010 1.85234

A11 2.31723 0.00001 0.00032 -0.00013 0.00019 2.31742

A12 2.11349 0.00000 -0.00019 0.00009 -0.00009 2.11339

A13 1.85244 -0.00002 -0.00013 0.00003 -0.00010 1.85234

A14 2.31723 0.00001 0.00032 -0.00013 0.00019 2.31742

A15 2.11349 0.00000 -0.00019 0.00009 -0.00009 2.11339

A16 2.17118 0.00006 0.00086 -0.00011 0.00075 2.17193

A17 2.24019 0.00000 -0.00027 0.00024 -0.00003 2.24016

A18 2.14836 0.00002 0.00032 -0.00008 0.00023 2.14859

A19 1.89411 -0.00002 -0.00008 -0.00024 -0.00031 1.89380

A20 1.92328 0.00005 0.00024 0.00028 0.00050 1.92378

A21 2.16945 -0.00002 0.00027 0.00035 0.00060 2.17005

A22 2.16945 -0.00002 0.00027 0.00035 0.00060 2.17005

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A27 2.30689 0.00000 0.00024 -0.00015 0.00009 2.30699

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A51 2.17391 -0.00002 0.00021 0.00040 0.00058 2.17448

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A66 1.50804 0.00000 0.00001 0.00006 0.00007 1.50812

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D3 -3.09690 -0.00002 0.00021 0.00045 0.00066 -3.09625

D4 0.17599 -0.00011 -0.00339 -0.00788 -0.01127 0.16472

D5 -0.01106 0.00000 0.00027 -0.00098 -0.00071 -0.01177

D6 3.13858 0.00001 -0.00006 -0.00004 -0.00010 3.13848

D7 3.10580 0.00002 -0.00037 0.00018 -0.00020 3.10560

D8 -0.02775 0.00002 -0.00071 0.00112 0.00041 -0.02734

D9 0.08027 0.00007 0.00187 0.00465 0.00653 0.08680

D10 -3.03168 0.00006 0.00264 0.00327 0.00592 -3.02576

D11 -0.01863 0.00001 0.00046 -0.00166 -0.00120 -0.01982

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D13 2.99166 0.00009 0.00406 0.00667 0.01074 3.00240

D14 -0.17599 0.00011 0.00339 0.00788 0.01127 -0.16472

D15 -2.97024 0.00003 0.00135 0.00388 0.00524 -2.96500

D16 -0.32089 0.00007 0.00274 0.00559 0.00833 -0.31255

D17 -1.64556 0.00005 0.00204 0.00474 0.00678 -1.63878

D18 0.32089 -0.00007 -0.00274 -0.00559 -0.00833 0.31255

D19 2.97024 -0.00003 -0.00135 -0.00388 -0.00524 2.96500

D20 1.64556 -0.00005 -0.00204 -0.00474 -0.00678 1.63878

D21 0.01106 0.00000 -0.00027 0.00098 0.00071 0.01177

D22 -3.13858 -0.00001 0.00006 0.00004 0.00010 -3.13848

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D24 0.02775 -0.00002 0.00071 -0.00112 -0.00041 0.02734

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D29 -3.13469 0.00000 -0.00029 0.00081 0.00052 -3.13417

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D33 -0.00642 0.00001 0.00020 0.00052 0.00072 -0.00570

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D41 -3.07475 0.00007 0.00313 0.00483 0.00797 -3.06678

D42 0.27808 0.00000 -0.00073 -0.00003 -0.00076 0.27732

D43 0.03271 0.00004 0.00228 0.00213 0.00441 0.03712

D44 -2.89765 -0.00004 -0.00159 -0.00273 -0.00432 -2.90197

D45 3.09014 -0.00006 -0.00217 -0.00379 -0.00596 3.08418

D46 -0.04336 -0.00005 -0.00235 -0.00372 -0.00606 -0.04942

D47 -0.01950 -0.00002 -0.00136 -0.00127 -0.00262 -0.02212

D48 3.13019 -0.00001 -0.00153 -0.00119 -0.00273 3.12746

D49 -0.03271 -0.00004 -0.00228 -0.00213 -0.00441 -0.03712

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D54 -1.69105 0.00004 0.00220 0.00276 0.00496 -1.68609

D55 -3.01721 0.00007 0.00285 0.00338 0.00623 -3.01098

D56 3.01721 -0.00007 -0.00285 -0.00338 -0.00623 3.01098

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D69 -3.13957 0.00000 -0.00008 -0.00047 -0.00055 -3.14013

D70 0.00502 0.00000 -0.00028 -0.00015 -0.00042 0.00460

D71 -0.00709 -0.00001 0.00013 -0.00056 -0.00043 -0.00752

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D74 -0.00502 0.00000 0.00028 0.00015 0.00042 -0.00460

D75 0.00709 0.00001 -0.00013 0.00056 0.00043 0.00752

D76 -3.13751 0.00001 0.00007 0.00023 0.00030 -3.13720

D77 3.07833 -0.00006 -0.00142 -0.00342 -0.00484 3.07349

D78 -0.02462 -0.00002 -0.00044 -0.00036 -0.00080 -0.02542

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D83 -3.09014 0.00006 0.00217 0.00379 0.00596 -3.08418

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D87 -0.00709 -0.00001 0.00013 -0.00056 -0.00043 -0.00752

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D91 -0.01950 -0.00002 -0.00136 -0.00127 -0.00262 -0.02212

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D93 3.13019 -0.00001 -0.00153 -0.00119 -0.00273 3.12746

D94 -0.04336 -0.00005 -0.00235 -0.00372 -0.00606 -0.04942

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D110 -1.69105 0.00004 0.00220 0.00276 0.00496 -1.68609

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D130 -2.97024 0.00003 0.00135 0.00388 0.00524 -2.96500

D131 -3.10580 -0.00002 0.00037 -0.00018 0.00020 -3.10560

D132 0.02775 -0.00002 0.00071 -0.00112 -0.00041 0.02734

D133 0.01106 0.00000 -0.00027 0.00098 0.00071 0.01177

D134 -3.13858 -0.00001 0.00006 0.00004 0.00010 -3.13848

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.13469 0.00000 0.00029 -0.00081 -0.00052 3.13417

D137 -3.13469 0.00000 -0.00029 0.00081 0.00052 -3.13417

D138 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D139 -3.13899 0.00001 -0.00018 0.00158 0.00141 -3.13758

D140 0.00435 0.00000 -0.00066 0.00053 -0.00013 0.00422

D141 -0.00642 0.00001 0.00020 0.00052 0.00072 -0.00570

D142 3.13691 -0.00001 -0.00028 -0.00053 -0.00081 3.13610

D143 -0.01106 0.00000 0.00027 -0.00098 -0.00071 -0.01177

D144 3.10580 0.00002 -0.00037 0.00018 -0.00020 3.10560

D145 3.13858 0.00001 -0.00006 -0.00004 -0.00010 3.13848

D146 -0.02775 0.00002 -0.00071 0.00112 0.00041 -0.02734

D147 0.00642 -0.00001 -0.00020 -0.00052 -0.00072 0.00570

D148 -3.13691 0.00001 0.00028 0.00053 0.00081 -3.13610

D149 3.13899 -0.00001 0.00018 -0.00158 -0.00141 3.13758

D150 -0.00435 0.00000 0.00066 -0.00053 0.00013 -0.00422

D151 0.08027 0.00007 0.00187 0.00465 0.00653 0.08680

D152 -3.03168 0.00006 0.00264 0.00327 0.00592 -3.02576

D153 0.00697 0.00001 -0.00012 0.00055 0.00042 0.00739

D154 -3.13472 0.00001 -0.00006 0.00047 0.00042 -3.13430

D155 -3.13757 0.00001 0.00007 0.00023 0.00030 -3.13728

D156 0.00392 0.00000 0.00014 0.00015 0.00029 0.00421

D157 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D158 3.14150 0.00000 0.00007 -0.00007 -0.00001 3.14149

D159 -3.14150 0.00000 -0.00007 0.00007 0.00001 -3.14149

D160 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D161 3.14156 0.00000 -0.00012 0.00013 0.00001 3.14157

D162 -0.00029 0.00000 -0.00004 0.00004 -0.00001 -0.00030

D163 -0.00013 0.00000 -0.00006 0.00006 0.00001 -0.00013

D164 3.14121 0.00000 0.00002 -0.00004 -0.00001 3.14119

D165 -0.00697 -0.00001 0.00012 -0.00055 -0.00042 -0.00739

D166 3.13757 -0.00001 -0.00007 -0.00023 -0.00030 3.13728

D167 3.13472 -0.00001 0.00006 -0.00047 -0.00042 3.13430

D168 -0.00392 0.00000 -0.00014 -0.00015 -0.00029 -0.00421

D169 0.00013 0.00000 0.00006 -0.00006 -0.00001 0.00013

D170 -3.14121 0.00000 -0.00002 0.00004 0.00001 -3.14119

D171 -3.14156 0.00000 0.00012 -0.00013 -0.00001 -3.14157

D172 0.00029 0.00000 0.00004 -0.00004 0.00001 0.00030

D173 -0.00635 0.00001 0.00020 0.00052 0.00071 -0.00563

D174 3.13590 0.00001 0.00014 0.00082 0.00097 3.13687

D175 3.13696 -0.00001 -0.00028 -0.00052 -0.00079 3.13617

D176 -0.00397 0.00000 -0.00033 -0.00021 -0.00054 -0.00451

D177 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D178 -3.14095 0.00000 -0.00005 0.00030 0.00024 -3.14071

D179 3.14095 0.00000 0.00005 -0.00030 -0.00024 3.14071

D180 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D181 3.14110 0.00000 0.00015 -0.00004 0.00012 3.14122

D182 -0.00095 0.00000 0.00003 -0.00026 -0.00023 -0.00119

D183 0.00016 0.00000 0.00010 0.00027 0.00037 0.00052

D184 3.14129 0.00000 -0.00002 0.00004 0.00002 3.14131

D185 0.00635 -0.00001 -0.00020 -0.00052 -0.00071 0.00563

D186 -3.13696 0.00001 0.00028 0.00052 0.00079 -3.13617

D187 -3.13590 -0.00001 -0.00014 -0.00082 -0.00097 -3.13687

D188 0.00397 0.00000 0.00033 0.00021 0.00054 0.00451

D189 -0.00016 0.00000 -0.00010 -0.00027 -0.00037 -0.00052

D190 -3.14129 0.00000 0.00002 -0.00004 -0.00002 -3.14131

D191 -3.14110 0.00000 -0.00015 0.00004 -0.00012 -3.14122

D192 0.00095 0.00000 -0.00003 0.00026 0.00023 0.00119

D193 -0.00697 -0.00001 0.00012 -0.00055 -0.00042 -0.00739

D194 3.13472 -0.00001 0.00006 -0.00047 -0.00042 3.13430

D195 3.13757 -0.00001 -0.00007 -0.00023 -0.00030 3.13728

D196 -0.00392 0.00000 -0.00014 -0.00015 -0.00029 -0.00421

D197 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D198 -3.14150 0.00000 -0.00007 0.00007 0.00001 -3.14149

D199 3.14150 0.00000 0.00007 -0.00007 -0.00001 3.14149

D200 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D201 -3.14156 0.00000 0.00012 -0.00013 -0.00001 -3.14157

D202 0.00029 0.00000 0.00004 -0.00004 0.00001 0.00030

D203 0.00013 0.00000 0.00006 -0.00006 -0.00001 0.00013

D204 -3.14121 0.00000 -0.00002 0.00004 0.00001 -3.14119

D205 0.00697 0.00001 -0.00012 0.00055 0.00042 0.00739

D206 -3.13757 0.00001 0.00007 0.00023 0.00030 -3.13728

D207 -3.13472 0.00001 -0.00006 0.00047 0.00042 -3.13430

D208 0.00392 0.00000 0.00014 0.00015 0.00029 0.00421

D209 -0.00013 0.00000 -0.00006 0.00006 0.00001 -0.00013

D210 3.14121 0.00000 0.00002 -0.00004 -0.00001 3.14119

D211 3.14156 0.00000 -0.00012 0.00013 0.00001 3.14157

D212 -0.00029 0.00000 -0.00004 0.00004 -0.00001 -0.00030

D213 -0.00635 0.00001 0.00020 0.00052 0.00071 -0.00563

D214 3.13590 0.00001 0.00014 0.00082 0.00097 3.13687

D215 3.13696 -0.00001 -0.00028 -0.00052 -0.00079 3.13617

D216 -0.00397 0.00000 -0.00033 -0.00021 -0.00054 -0.00451

D217 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D218 -3.14095 0.00000 -0.00005 0.00030 0.00024 -3.14071

D219 3.14095 0.00000 0.00005 -0.00030 -0.00024 3.14071

D220 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D221 3.14110 0.00000 0.00015 -0.00004 0.00012 3.14122

D222 -0.00095 0.00000 0.00003 -0.00026 -0.00023 -0.00119

D223 0.00016 0.00000 0.00010 0.00027 0.00037 0.00052

D224 3.14129 0.00000 -0.00002 0.00004 0.00002 3.14131

D225 0.00635 -0.00001 -0.00020 -0.00052 -0.00071 0.00563

D226 -3.13696 0.00001 0.00028 0.00052 0.00079 -3.13617

D227 -3.13590 -0.00001 -0.00014 -0.00082 -0.00097 -3.13687

D228 0.00397 0.00000 0.00033 0.00021 0.00054 0.00451

D229 -0.00016 0.00000 -0.00010 -0.00027 -0.00037 -0.00052

D230 -3.14129 0.00000 0.00002 -0.00004 -0.00002 -3.14131

D231 -3.14110 0.00000 -0.00015 0.00004 -0.00012 -3.14122

D232 0.00095 0.00000 -0.00003 0.00026 0.00023 0.00119

D233 0.00016 0.00000 0.00010 0.00027 0.00037 0.00053

D234 3.14134 0.00000 0.00009 0.00024 0.00034 -3.14151

D235 3.14128 0.00000 -0.00002 0.00004 0.00002 3.14130

D236 -0.00073 0.00000 -0.00003 0.00001 -0.00002 -0.00074

D237 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D238 3.14118 0.00000 -0.00001 -0.00003 -0.00004 3.14114

D239 -3.14118 0.00000 0.00001 0.00003 0.00004 -3.14114

D240 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D241 -0.00016 0.00000 -0.00010 -0.00027 -0.00037 -0.00053

D242 -3.14128 0.00000 0.00002 -0.00004 -0.00002 -3.14130

D243 -3.14134 0.00000 -0.00009 -0.00024 -0.00034 3.14151

D244 0.00073 0.00000 0.00003 -0.00001 0.00002 0.00074

D245 -0.00013 0.00000 -0.00006 0.00006 0.00001 -0.00013

D246 -3.14113 0.00000 -0.00004 0.00007 0.00003 -3.14110

D247 3.14120 0.00000 0.00002 -0.00004 -0.00001 3.14119

D248 0.00021 0.00000 0.00004 -0.00003 0.00001 0.00022

D249 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D250 -3.14100 0.00000 0.00002 0.00001 0.00002 -3.14097

D251 3.14100 0.00000 -0.00002 -0.00001 -0.00002 3.14097

D252 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D253 0.00013 0.00000 0.00006 -0.00006 -0.00001 0.00013

D254 -3.14120 0.00000 -0.00002 0.00004 0.00001 -3.14119

D255 3.14113 0.00000 0.00004 -0.00007 -0.00003 3.14110

D256 -0.00021 0.00000 -0.00004 0.00003 -0.00001 -0.00022

D257 0.00016 0.00000 0.00010 0.00027 0.00037 0.00053

D258 3.14134 0.00000 0.00009 0.00024 0.00034 -3.14151

D259 3.14128 0.00000 -0.00002 0.00004 0.00002 3.14130

D260 -0.00073 0.00000 -0.00003 0.00001 -0.00002 -0.00074

D261 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D262 3.14118 0.00000 -0.00001 -0.00003 -0.00004 3.14114

D263 -3.14118 0.00000 0.00001 0.00003 0.00004 -3.14114

D264 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D265 -0.00016 0.00000 -0.00010 -0.00027 -0.00037 -0.00053

D266 -3.14128 0.00000 0.00002 -0.00004 -0.00002 -3.14130

D267 -3.14134 0.00000 -0.00009 -0.00024 -0.00034 3.14151

D268 0.00073 0.00000 0.00003 -0.00001 0.00002 0.00074

D269 0.00013 0.00000 0.00006 -0.00006 -0.00001 0.00013

D270 3.14113 0.00000 0.00004 -0.00007 -0.00003 3.14110

D271 -3.14120 0.00000 -0.00002 0.00004 0.00001 -3.14119

D272 -0.00021 0.00000 -0.00004 0.00003 -0.00001 -0.00022

D273 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D274 3.14100 0.00000 -0.00002 -0.00001 -0.00002 3.14097

D275 -3.14100 0.00000 0.00002 0.00001 0.00002 -3.14097

D276 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D277 -0.00013 0.00000 -0.00006 0.00006 0.00001 -0.00013

D278 3.14120 0.00000 0.00002 -0.00004 -0.00001 3.14119

D279 -3.14113 0.00000 -0.00004 0.00007 0.00003 -3.14110

D280 0.00021 0.00000 0.00004 -0.00003 0.00001 0.00022

Item Value Threshold Converged?

Maximum Force 0.000162 0.000450 YES

RMS Force 0.000038 0.000300 YES

Maximum Displacement 0.118221 0.001800 NO

RMS Displacement 0.020482 0.001200 NO

Predicted change in Energy=-1.525260D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Jun 30 20:25:01 2019, MaxMem= 1342177280 cpu: 153.4

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

Stoichiometry C48H24N8Zn(3)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C48H24N4)]

Deg. of freedom 61

Full point group C2V NOp 4

RotChk: IX=0 Diff= 9.19D-15

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 1.121281 2.792517 0.162995

2 7 0 0.000000 2.023166 0.283540

3 6 0 -1.121281 2.792517 0.162995

4 6 0 -0.717764 4.174812 -0.025975

5 6 0 0.717764 4.174812 -0.025975

6 7 0 -2.412420 2.384384 0.177816

7 6 0 -2.794219 1.127704 0.222417

8 7 0 -2.010751 0.000000 0.289539

9 6 0 -2.794219 -1.127704 0.222417

10 6 0 -4.207691 -0.712317 0.153407

11 6 0 -4.207691 0.712317 0.153407

12 7 0 2.412420 2.384384 0.177816

13 6 0 4.207691 0.712317 0.153407

14 6 0 4.207691 -0.712317 0.153407

15 6 0 2.794219 -1.127704 0.222417

16 7 0 2.010751 0.000000 0.289539

17 6 0 2.794219 1.127704 0.222417

18 7 0 2.412420 -2.384384 0.177816

19 7 0 0.000000 -2.023166 0.283540

20 6 0 1.121281 -2.792517 0.162995

21 6 0 0.717764 -4.174812 -0.025975

22 6 0 -0.717764 -4.174812 -0.025975

23 6 0 -1.121281 -2.792517 0.162995

24 7 0 -2.412420 -2.384384 0.177816

25 30 0 0.000000 0.000000 0.807939

26 6 0 5.372646 1.426179 0.088421

27 6 0 6.608013 0.718958 0.028916

28 6 0 6.608013 -0.718958 0.028916

29 6 0 5.372646 -1.426179 0.088421

30 6 0 -1.428282 -5.341104 -0.194242

31 6 0 -0.721534 -6.557987 -0.362666

32 6 0 0.721534 -6.557987 -0.362666

33 6 0 1.428282 -5.341104 -0.194242

34 6 0 -5.372646 1.426179 0.088421

35 6 0 -6.608013 0.718958 0.028916

36 6 0 -6.608013 -0.718958 0.028916

37 6 0 -5.372646 -1.426179 0.088421

38 6 0 1.428282 5.341104 -0.194242

39 6 0 0.721534 6.557987 -0.362666

40 6 0 -0.721534 6.557987 -0.362666

41 6 0 -1.428282 5.341104 -0.194242

42 6 0 1.402352 -7.792258 -0.534611

43 6 0 0.708068 -8.966883 -0.697624

44 6 0 -0.708068 -8.966883 -0.697624

45 6 0 -1.402352 -7.792258 -0.534611

46 6 0 7.847336 -1.401387 -0.030906

47 6 0 9.034533 -0.705908 -0.088061

48 6 0 9.034533 0.705908 -0.088061

49 6 0 7.847336 1.401387 -0.030906

50 6 0 -1.402352 7.792258 -0.534611

51 6 0 -0.708068 8.966883 -0.697624

52 6 0 0.708068 8.966883 -0.697624

53 6 0 1.402352 7.792258 -0.534611

54 6 0 -7.847336 -1.401387 -0.030906

55 6 0 -9.034533 -0.705908 -0.088061

56 6 0 -9.034533 0.705908 -0.088061

57 6 0 -7.847336 1.401387 -0.030906

58 1 0 5.372555 2.511106 0.084357

59 1 0 5.372555 -2.511106 0.084357

60 1 0 -2.513352 -5.343726 -0.199765

61 1 0 2.513352 -5.343726 -0.199765

62 1 0 -5.372555 2.511106 0.084357

63 1 0 -5.372555 -2.511106 0.084357

64 1 0 2.513352 5.343726 -0.199765

65 1 0 -2.513352 5.343726 -0.199765

66 1 0 2.487864 -7.790891 -0.534146

67 1 0 1.243501 -9.901287 -0.827727

68 1 0 -1.243501 -9.901287 -0.827727

69 1 0 -2.487864 -7.790891 -0.534146

70 1 0 7.845650 -2.486685 -0.031205

71 1 0 9.976067 -1.242476 -0.133976

72 1 0 9.976067 1.242476 -0.133976

73 1 0 7.845650 2.486685 -0.031205

74 1 0 -2.487864 7.790891 -0.534146

75 1 0 -1.243501 9.901287 -0.827727

76 1 0 1.243501 9.901287 -0.827727

77 1 0 2.487864 7.790891 -0.534146

78 1 0 -7.845650 -2.486685 -0.031205

79 1 0 -9.976067 -1.242476 -0.133976

80 1 0 -9.976067 1.242476 -0.133976

81 1 0 -7.845650 2.486685 -0.031205

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

Rotational constants (GHZ): 0.0386014 0.0380818 0.0193209

Leave Link 202 at Sun Jun 30 20:25:01 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 307 symmetry adapted cartesian basis functions of A1 symmetry.

There are 278 symmetry adapted cartesian basis functions of A2 symmetry.

There are 289 symmetry adapted cartesian basis functions of B1 symmetry.

There are 289 symmetry adapted cartesian basis functions of B2 symmetry.

There are 289 symmetry adapted basis functions of A1 symmetry.

There are 265 symmetry adapted basis functions of A2 symmetry.

There are 275 symmetry adapted basis functions of B1 symmetry.

There are 275 symmetry adapted basis functions of B2 symmetry.

1104 basis functions, 1951 primitive gaussians, 1163 cartesian basis functions

191 alpha electrons 189 beta electrons

nuclear repulsion energy 6887.8538277670 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= 81 NActive= 81 NUniq= 22 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= -0.2361027034 Hartrees.

Nuclear repulsion after empirical dispersion term = 6887.6177250637 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= 81.

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 = 81

GePol: Total number of spheres = 81

GePol: Number of exposed spheres = 81 (100.00%)

GePol: Number of points = 6422

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.28D-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) = 5.64%

GePol: Cavity surface area = 670.649 Ang\*\*2

GePol: Cavity volume = 694.174 Ang\*\*3

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

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

PCM non-electrostatic energy = -0.0169625197 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 6887.6007625439 Hartrees.

Leave Link 301 at Sun Jun 30 20:25:02 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.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36693 LenP2D= 95166.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1104 RedAO= T EigKep= 2.88D-05 NBF= 289 265 275 275

NBsUse= 1104 1.00D-06 EigRej= -1.00D+00 NBFU= 289 265 275 275

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= 1060 1060 1060 1060 1060 MxSgAt= 81 MxSgA2= 81.

Leave Link 302 at Sun Jun 30 20:25:19 2019, MaxMem= 1342177280 cpu: 185.4

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Jun 30 20:25:20 2019, MaxMem= 1342177280 cpu: 3.8

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

Initial guess from the checkpoint file: "ZnNPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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

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

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

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

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The electronic state of the initial guess is 3-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -2348.36315126925

Leave Link 401 at Sun Jun 30 20:25:47 2019, MaxMem= 1342177280 cpu: 296.6

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4103221 IEndB= 4103221 NGot= 1342177280 MDV= 1339444432

LenX= 1339444432 LenY= 1338090700

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= 420000000 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= 123726252.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.44D-15 for 6408.

Iteration 1 A\*A^-1 deviation from orthogonality is 9.40D-15 for 6407 1188.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.77D-15 for 6407.

Iteration 1 A^-1\*A deviation from orthogonality is 4.32D-09 for 5118 5094.

Iteration 2 A\*A^-1 deviation from unit magnitude is 4.77D-15 for 139.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.98D-15 for 5182 187.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 6388.

Iteration 2 A^-1\*A deviation from orthogonality is 5.57D-16 for 6144 1286.

E= -2348.12971119391

DIIS: error= 9.47D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2348.12971119391 IErMin= 1 ErrMin= 9.47D-04

ErrMax= 9.47D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.97D-03 BMatP= 1.97D-03

IDIUse=3 WtCom= 9.91D-01 WtEn= 9.47D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.378 Goal= None Shift= 0.000

Gap= 0.459 Goal= None Shift= 0.000

RMSDP=2.89D-05 MaxDP=9.66D-04 OVMax= 5.71D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.88D-05 CP: 1.00D+00

E= -2348.13069641700 Delta-E= -0.000985223094 Rises=F Damp=F

DIIS: error= 1.28D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2348.13069641700 IErMin= 2 ErrMin= 1.28D-04

ErrMax= 1.28D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.27D-05 BMatP= 1.97D-03

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.28D-03

Coeff-Com: -0.730D-01 0.107D+01

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

Coeff: -0.729D-01 0.107D+01

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=4.45D-06 MaxDP=1.99D-04 DE=-9.85D-04 OVMax= 8.93D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.66D-06 CP: 1.00D+00 1.09D+00

E= -2348.13070984991 Delta-E= -0.000013432909 Rises=F Damp=F

DIIS: error= 4.62D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2348.13070984991 IErMin= 3 ErrMin= 4.62D-05

ErrMax= 4.62D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.85D-06 BMatP= 2.27D-05

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

Coeff-Com: -0.317D-01 0.414D+00 0.618D+00

Coeff: -0.317D-01 0.414D+00 0.618D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.00D-06 MaxDP=1.37D-04 DE=-1.34D-05 OVMax= 3.55D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.80D-06 CP: 1.00D+00 1.10D+00 7.91D-01

E= -2348.13071049643 Delta-E= -0.000000646522 Rises=F Damp=F

DIIS: error= 3.76D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2348.13071049643 IErMin= 4 ErrMin= 3.76D-05

ErrMax= 3.76D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.15D-06 BMatP= 6.85D-06

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

Coeff-Com: -0.636D-02 0.599D-01 0.431D+00 0.516D+00

Coeff: -0.636D-02 0.599D-01 0.431D+00 0.516D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=9.76D-07 MaxDP=7.11D-05 DE=-6.47D-07 OVMax= 1.91D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.55D-07 CP: 1.00D+00 1.10D+00 8.94D-01 5.76D-01

E= -2348.13071135515 Delta-E= -0.000000858714 Rises=F Damp=F

DIIS: error= 8.63D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2348.13071135515 IErMin= 5 ErrMin= 8.63D-06

ErrMax= 8.63D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.18D-07 BMatP= 4.15D-06

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

Coeff-Com: 0.273D-03-0.166D-01 0.124D+00 0.216D+00 0.677D+00

Coeff: 0.273D-03-0.166D-01 0.124D+00 0.216D+00 0.677D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.02D-07 MaxDP=1.93D-05 DE=-8.59D-07 OVMax= 5.45D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.51D-07 CP: 1.00D+00 1.10D+00 9.06D-01 6.19D-01 7.84D-01

E= -2348.13071137399 Delta-E= -0.000000018841 Rises=F Damp=F

DIIS: error= 5.90D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2348.13071137399 IErMin= 6 ErrMin= 5.90D-06

ErrMax= 5.90D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.96D-08 BMatP= 1.18D-07

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

Coeff-Com: 0.852D-03-0.175D-01 0.320D-01 0.802D-01 0.427D+00 0.477D+00

Coeff: 0.852D-03-0.175D-01 0.320D-01 0.802D-01 0.427D+00 0.477D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=8.46D-08 MaxDP=1.02D-05 DE=-1.88D-08 OVMax= 2.30D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.97D-08 CP: 1.00D+00 1.10D+00 9.11D-01 6.23D-01 8.11D-01

CP: 5.26D-01

E= -2348.13071138227 Delta-E= -0.000000008282 Rises=F Damp=F

DIIS: error= 1.13D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2348.13071138227 IErMin= 7 ErrMin= 1.13D-06

ErrMax= 1.13D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.32D-09 BMatP= 3.96D-08

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

Coeff-Com: 0.395D-03-0.745D-02 0.864D-02 0.263D-01 0.168D+00 0.230D+00

Coeff-Com: 0.575D+00

Coeff: 0.395D-03-0.745D-02 0.864D-02 0.263D-01 0.168D+00 0.230D+00

Coeff: 0.575D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.04D-08 MaxDP=2.00D-06 DE=-8.28D-09 OVMax= 6.77D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.89D-08 CP: 1.00D+00 1.10D+00 9.11D-01 6.24D-01 8.11D-01

CP: 5.53D-01 8.67D-01

E= -2348.13071138251 Delta-E= -0.000000000240 Rises=F Damp=F

DIIS: error= 6.10D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2348.13071138251 IErMin= 8 ErrMin= 6.10D-07

ErrMax= 6.10D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.99D-10 BMatP= 1.32D-09

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

Coeff-Com: -0.366D-05 0.558D-03-0.393D-02-0.743D-02-0.216D-01 0.271D-02

Coeff-Com: 0.366D+00 0.664D+00

Coeff: -0.366D-05 0.558D-03-0.393D-02-0.743D-02-0.216D-01 0.271D-02

Coeff: 0.366D+00 0.664D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.04D-08 MaxDP=1.02D-06 DE=-2.40D-10 OVMax= 3.51D-06

Cycle 9 Pass 1 IDiag 1:

RMSU= 6.44D-09 CP: 1.00D+00 1.10D+00 9.11D-01 6.24D-01 8.14D-01

CP: 5.65D-01 1.02D+00 7.68D-01

E= -2348.13071138254 Delta-E= -0.000000000029 Rises=F Damp=F

DIIS: error= 1.25D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2348.13071138254 IErMin= 9 ErrMin= 1.25D-07

ErrMax= 1.25D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.12D-11 BMatP= 3.99D-10

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

Coeff-Com: -0.397D-04 0.999D-03-0.277D-02-0.633D-02-0.269D-01-0.199D-01

Coeff-Com: 0.134D+00 0.341D+00 0.580D+00

Coeff: -0.397D-04 0.999D-03-0.277D-02-0.633D-02-0.269D-01-0.199D-01

Coeff: 0.134D+00 0.341D+00 0.580D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=4.09D-09 MaxDP=3.30D-07 DE=-2.91D-11 OVMax= 1.39D-06

Error on total polarization charges = 0.08840

SCF Done: E(UB3LYP) = -2348.13071138 A.U. after 9 cycles

NFock= 9 Conv=0.41D-08 -V/T= 1.9830

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

<L.S>= 0.000000000000E+00

KE= 2.388734593916D+03 PE=-1.931860028421D+04 EE= 7.694134216368D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -10.64

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0219, after 2.0003

Leave Link 502 at Sun Jun 30 20:31:43 2019, MaxMem= 1342177280 cpu: 3923.6

(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.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36693 LenP2D= 95166.

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 = 195

Leave Link 701 at Sun Jun 30 20:32:18 2019, MaxMem= 1342177280 cpu: 353.0

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sun Jun 30 20:32:18 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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 Sun Jun 30 20:33:08 2019, MaxMem= 1342177280 cpu: 491.2

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 4.45865567D-13 4.93827201D-13 9.38087519D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000026375 0.000106370 -0.000159654

2 7 0.000000000 -0.000083982 0.000323563

3 6 0.000026375 0.000106370 -0.000159654

4 6 0.000041685 -0.000102258 0.000057186

5 6 -0.000041685 -0.000102258 0.000057186

6 7 -0.000068896 0.000144599 0.000093236

7 6 -0.000128049 -0.000105178 -0.000070007

8 7 0.000126235 0.000000000 0.000078134

9 6 -0.000128049 0.000105178 -0.000070007

10 6 0.000096685 0.000056923 0.000021658

11 6 0.000096685 -0.000056923 0.000021658

12 7 0.000068896 0.000144599 0.000093236

13 6 -0.000096685 -0.000056923 0.000021658

14 6 -0.000096685 0.000056923 0.000021658

15 6 0.000128049 0.000105178 -0.000070007

16 7 -0.000126235 0.000000000 0.000078134

17 6 0.000128049 -0.000105178 -0.000070007

18 7 0.000068896 -0.000144599 0.000093236

19 7 0.000000000 0.000083982 0.000323563

20 6 -0.000026375 -0.000106370 -0.000159654

21 6 -0.000041685 0.000102258 0.000057186

22 6 0.000041685 0.000102258 0.000057186

23 6 0.000026375 -0.000106370 -0.000159654

24 7 -0.000068896 -0.000144599 0.000093236

25 30 0.000000000 0.000000000 -0.000366329

26 6 0.000044428 0.000061845 -0.000001626

27 6 -0.000023514 -0.000097437 -0.000003846

28 6 -0.000023514 0.000097437 -0.000003846

29 6 0.000044428 -0.000061845 -0.000001626

30 6 -0.000069415 -0.000024759 -0.000078807

31 6 0.000106867 -0.000003310 0.000004856

32 6 -0.000106867 -0.000003310 0.000004856

33 6 0.000069415 -0.000024759 -0.000078807

34 6 -0.000044428 0.000061845 -0.000001626

35 6 0.000023514 -0.000097437 -0.000003846

36 6 0.000023514 0.000097437 -0.000003846

37 6 -0.000044428 -0.000061845 -0.000001626

38 6 0.000069415 0.000024759 -0.000078807

39 6 -0.000106867 0.000003310 0.000004856

40 6 0.000106867 0.000003310 0.000004856

41 6 -0.000069415 0.000024759 -0.000078807

42 6 0.000009920 0.000068501 0.000006678

43 6 -0.000088530 0.000008531 -0.000005594

44 6 0.000088530 0.000008531 -0.000005594

45 6 -0.000009920 0.000068501 0.000006678

46 6 -0.000041969 -0.000002883 0.000004569

47 6 -0.000017451 0.000071458 0.000000707

48 6 -0.000017451 -0.000071458 0.000000707

49 6 -0.000041969 0.000002883 0.000004569

50 6 -0.000009920 -0.000068501 0.000006678

51 6 0.000088530 -0.000008531 -0.000005594

52 6 -0.000088530 -0.000008531 -0.000005594

53 6 0.000009920 -0.000068501 0.000006678

54 6 0.000041969 -0.000002883 0.000004569

55 6 0.000017451 0.000071458 0.000000707

56 6 0.000017451 -0.000071458 0.000000707

57 6 0.000041969 0.000002883 0.000004569

58 1 0.000017240 -0.000021453 -0.000003788

59 1 0.000017240 0.000021453 -0.000003788

60 1 0.000019587 -0.000018966 0.000017396

61 1 -0.000019587 -0.000018966 0.000017396

62 1 -0.000017240 -0.000021453 -0.000003788

63 1 -0.000017240 0.000021453 -0.000003788

64 1 -0.000019587 0.000018966 0.000017396

65 1 0.000019587 0.000018966 0.000017396

66 1 -0.000017946 0.000009230 0.000002390

67 1 -0.000004754 0.000018389 0.000003734

68 1 0.000004754 0.000018389 0.000003734

69 1 0.000017946 0.000009230 0.000002390

70 1 -0.000008900 0.000016920 0.000000468

71 1 -0.000019667 0.000005787 0.000001177

72 1 -0.000019667 -0.000005787 0.000001177

73 1 -0.000008900 -0.000016920 0.000000468

74 1 0.000017946 -0.000009230 0.000002390

75 1 0.000004754 -0.000018389 0.000003734

76 1 -0.000004754 -0.000018389 0.000003734

77 1 -0.000017946 -0.000009230 0.000002390

78 1 0.000008900 0.000016920 0.000000468

79 1 0.000019667 0.000005787 0.000001177

80 1 0.000019667 -0.000005787 0.000001177

81 1 0.000008900 -0.000016920 0.000000468

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

Cartesian Forces: Max 0.000366329 RMS 0.000069744

Leave Link 716 at Sun Jun 30 20:33:08 2019, MaxMem= 1342177280 cpu: 1.6

(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 0.000161233 RMS 0.000037405

Search for a local minimum.

Step number 4 out of a maximum of 486

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .37405D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4

DE= -2.00D-05 DEPred=-1.53D-05 R= 1.31D+00

TightC=F SS= 1.41D+00 RLast= 5.57D-02 DXNew= 5.0454D-01 1.6725D-01

Trust test= 1.31D+00 RLast= 5.57D-02 DXMaxT set to 3.00D-01

ITU= 1 1 1 0

Eigenvalues --- 0.00491 0.01434 0.01487 0.01501 0.01574

Eigenvalues --- 0.01595 0.01627 0.01656 0.01661 0.01694

Eigenvalues --- 0.01698 0.01705 0.01713 0.01715 0.01725

Eigenvalues --- 0.01730 0.01730 0.01733 0.01736 0.01737

Eigenvalues --- 0.01751 0.01751 0.01759 0.01791 0.01816

Eigenvalues --- 0.01827 0.01828 0.01829 0.01851 0.01854

Eigenvalues --- 0.01869 0.01869 0.01900 0.01934 0.01968

Eigenvalues --- 0.01968 0.01970 0.01972 0.01977 0.01992

Eigenvalues --- 0.01992 0.01993 0.01993 0.01999 0.02080

Eigenvalues --- 0.02080 0.02086 0.02086 0.02089 0.02096

Eigenvalues --- 0.02096 0.02098 0.02098 0.02103 0.02103

Eigenvalues --- 0.02103 0.02105 0.02106 0.02124 0.02124

Eigenvalues --- 0.02137 0.02144 0.02144 0.02147 0.02147

Eigenvalues --- 0.02152 0.02171 0.02173 0.02214 0.02214

Eigenvalues --- 0.02225 0.02225 0.02277 0.02284 0.02318

Eigenvalues --- 0.02346 0.03152 0.05520 0.05574 0.08092

Eigenvalues --- 0.14690 0.15997 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 0.16066

Eigenvalues --- 0.16149 0.16269 0.17488 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22500 0.22502 0.22504

Eigenvalues --- 0.22527 0.23233 0.23234 0.23234 0.23659

Eigenvalues --- 0.23939 0.23940 0.23941 0.23953 0.24133

Eigenvalues --- 0.24165 0.24340 0.24522 0.24554 0.24557

Eigenvalues --- 0.24557 0.24557 0.24773 0.24895 0.24898

Eigenvalues --- 0.24974 0.24983 0.24987 0.24991 0.24992

Eigenvalues --- 0.24998 0.24998 0.24998 0.24998 0.26284

Eigenvalues --- 0.32869 0.32951 0.33672 0.33736 0.33837

Eigenvalues --- 0.33897 0.35037 0.35061 0.35181 0.35181

Eigenvalues --- 0.35181 0.35187 0.35202 0.35202 0.35202

Eigenvalues --- 0.35210 0.35231 0.35231 0.35231 0.35240

Eigenvalues --- 0.35249 0.35249 0.35249 0.35268 0.35270

Eigenvalues --- 0.35270 0.35270 0.35276 0.35279 0.35279

Eigenvalues --- 0.35279 0.35401 0.35414 0.35805 0.36350

Eigenvalues --- 0.37056 0.37457 0.37629 0.37969 0.39275

Eigenvalues --- 0.39276 0.39359 0.39612 0.39612 0.40188

Eigenvalues --- 0.40188 0.40257 0.40257 0.40906 0.41001

Eigenvalues --- 0.41074 0.41116 0.41604 0.41754 0.41875

Eigenvalues --- 0.42101 0.42215 0.42365 0.42692 0.42806

Eigenvalues --- 0.42916 0.42969 0.45659 0.46476 0.47124

Eigenvalues --- 0.47124 0.47268 0.47384 0.47386 0.47579

Eigenvalues --- 0.47580 0.48130 0.48218 0.48342 0.48465

Eigenvalues --- 0.48465 0.48669 0.48680 0.48707 0.48729

Eigenvalues --- 0.49090 0.49134 0.49680 0.49898 0.50394

Eigenvalues --- 0.50979 0.52335 0.52485 0.59247 0.59617

Eigenvalues --- 0.59839 0.60907

En-DIIS/RFO-DIIS IScMMF= 0 using points: 4 3 2

RFO step: Lambda=-1.94774564D-06.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=F DC= 3.95D-05 SmlDif= 1.00D-05

RMS Error= 0.1597301675D-03 NUsed= 3 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.62423 -0.78716 0.16294

Iteration 1 RMS(Cart)= 0.02432238 RMS(Int)= 0.00003763

Iteration 2 RMS(Cart)= 0.00017387 RMS(Int)= 0.00000365

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000365

ITry= 1 IFail=0 DXMaxC= 1.40D-01 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.56D-08 for atom 68.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.57981 0.00004 -0.00014 0.00010 -0.00004 2.57977

R2 2.74451 -0.00016 0.00012 -0.00026 -0.00015 2.74437

R3 2.55905 0.00001 -0.00017 0.00005 -0.00013 2.55892

R4 2.57981 0.00004 -0.00014 0.00010 -0.00004 2.57977

R5 3.94957 -0.00010 0.00129 -0.00019 0.00110 3.95067

R6 2.74451 -0.00016 0.00012 -0.00026 -0.00015 2.74437

R7 2.55905 0.00001 -0.00017 0.00005 -0.00013 2.55892

R8 2.71275 -0.00003 0.00006 -0.00020 -0.00015 2.71261

R9 2.60027 -0.00002 -0.00004 0.00003 -0.00001 2.60026

R10 2.60027 -0.00002 -0.00004 0.00003 -0.00001 2.60026

R11 2.48339 0.00007 -0.00042 0.00006 -0.00037 2.48303

R12 2.59797 0.00002 -0.00006 0.00000 -0.00006 2.59792

R13 2.78708 -0.00015 0.00045 -0.00024 0.00021 2.78729

R14 2.59797 0.00002 -0.00006 0.00000 -0.00006 2.59792

R15 3.92402 -0.00009 0.00022 -0.00048 -0.00025 3.92377

R16 2.78708 -0.00015 0.00045 -0.00024 0.00021 2.78729

R17 2.48339 0.00007 -0.00042 0.00006 -0.00037 2.48303

R18 2.69217 -0.00005 -0.00001 -0.00021 -0.00022 2.69195

R19 2.58481 -0.00002 -0.00005 0.00000 -0.00004 2.58477

R20 2.58481 -0.00002 -0.00005 0.00000 -0.00004 2.58477

R21 2.48339 0.00007 -0.00042 0.00006 -0.00037 2.48303

R22 2.69217 -0.00005 -0.00001 -0.00021 -0.00022 2.69195

R23 2.78708 -0.00015 0.00045 -0.00024 0.00021 2.78729

R24 2.58481 -0.00002 -0.00005 0.00000 -0.00004 2.58477

R25 2.78708 -0.00015 0.00045 -0.00024 0.00021 2.78729

R26 2.58481 -0.00002 -0.00005 0.00000 -0.00004 2.58477

R27 2.59797 0.00002 -0.00006 0.00000 -0.00006 2.59792

R28 2.48339 0.00007 -0.00042 0.00006 -0.00037 2.48303

R29 2.59797 0.00002 -0.00006 0.00000 -0.00006 2.59792

R30 3.92402 -0.00009 0.00022 -0.00048 -0.00025 3.92377

R31 2.55905 0.00001 -0.00017 0.00005 -0.00013 2.55892

R32 2.57981 0.00004 -0.00014 0.00010 -0.00004 2.57977

R33 2.57981 0.00004 -0.00014 0.00010 -0.00004 2.57977

R34 3.94957 -0.00010 0.00129 -0.00019 0.00110 3.95067

R35 2.74451 -0.00016 0.00012 -0.00026 -0.00015 2.74437

R36 2.71275 -0.00003 0.00006 -0.00020 -0.00015 2.71261

R37 2.60027 -0.00002 -0.00004 0.00003 -0.00001 2.60026

R38 2.74451 -0.00016 0.00012 -0.00026 -0.00015 2.74437

R39 2.60027 -0.00002 -0.00004 0.00003 -0.00001 2.60026

R40 2.55905 0.00001 -0.00017 0.00005 -0.00013 2.55892

R41 2.69233 -0.00009 -0.00003 -0.00007 -0.00010 2.69223

R42 2.05023 -0.00002 0.00010 -0.00010 0.00000 2.05023

R43 2.71727 -0.00010 0.00024 -0.00026 -0.00001 2.71726

R44 2.67595 -0.00008 0.00002 -0.00007 -0.00005 2.67590

R45 2.69233 -0.00009 -0.00003 -0.00007 -0.00010 2.69223

R46 2.67595 -0.00008 0.00002 -0.00007 -0.00005 2.67590

R47 2.05023 -0.00002 0.00010 -0.00010 0.00000 2.05023

R48 2.67826 -0.00008 -0.00010 -0.00003 -0.00014 2.67812

R49 2.05052 -0.00002 0.00011 -0.00010 0.00001 2.05053

R50 2.72700 -0.00011 0.00031 -0.00028 0.00003 2.72703

R51 2.68348 -0.00010 0.00000 -0.00010 -0.00009 2.68339

R52 2.67826 -0.00008 -0.00010 -0.00003 -0.00014 2.67812

R53 2.68348 -0.00010 0.00000 -0.00010 -0.00009 2.68339

R54 2.05052 -0.00002 0.00011 -0.00010 0.00001 2.05053

R55 2.69233 -0.00009 -0.00003 -0.00007 -0.00010 2.69223

R56 2.05023 -0.00002 0.00010 -0.00010 0.00000 2.05023

R57 2.71727 -0.00010 0.00024 -0.00026 -0.00001 2.71726

R58 2.67595 -0.00008 0.00002 -0.00007 -0.00005 2.67590

R59 2.69233 -0.00009 -0.00003 -0.00007 -0.00010 2.69223

R60 2.67595 -0.00008 0.00002 -0.00007 -0.00005 2.67590

R61 2.05023 -0.00002 0.00010 -0.00010 0.00000 2.05023

R62 2.67826 -0.00008 -0.00010 -0.00003 -0.00014 2.67812

R63 2.05052 -0.00002 0.00011 -0.00010 0.00001 2.05053

R64 2.72700 -0.00011 0.00031 -0.00028 0.00003 2.72703

R65 2.68348 -0.00010 0.00000 -0.00010 -0.00009 2.68339

R66 2.67826 -0.00008 -0.00010 -0.00003 -0.00014 2.67812

R67 2.68348 -0.00010 0.00000 -0.00010 -0.00009 2.68339

R68 2.05052 -0.00002 0.00011 -0.00010 0.00001 2.05053

R69 2.59681 -0.00002 0.00000 -0.00005 -0.00005 2.59676

R70 2.05132 -0.00002 0.00008 -0.00009 -0.00001 2.05131

R71 2.67611 -0.00009 0.00026 -0.00028 -0.00002 2.67609

R72 2.04992 -0.00002 0.00003 -0.00004 -0.00001 2.04991

R73 2.59681 -0.00002 0.00000 -0.00005 -0.00005 2.59676

R74 2.04992 -0.00002 0.00003 -0.00004 -0.00001 2.04991

R75 2.05132 -0.00002 0.00008 -0.00009 -0.00001 2.05131

R76 2.60234 -0.00003 0.00002 -0.00008 -0.00006 2.60228

R77 2.05092 -0.00002 0.00007 -0.00008 -0.00001 2.05091

R78 2.66794 -0.00008 0.00023 -0.00026 -0.00004 2.66791

R79 2.04972 -0.00002 0.00003 -0.00005 -0.00002 2.04970

R80 2.60234 -0.00003 0.00002 -0.00008 -0.00006 2.60228

R81 2.04972 -0.00002 0.00003 -0.00005 -0.00002 2.04970

R82 2.05092 -0.00002 0.00007 -0.00008 -0.00001 2.05091

R83 2.59681 -0.00002 0.00000 -0.00005 -0.00005 2.59676

R84 2.05132 -0.00002 0.00008 -0.00009 -0.00001 2.05131

R85 2.67611 -0.00009 0.00026 -0.00028 -0.00002 2.67609

R86 2.04992 -0.00002 0.00003 -0.00004 -0.00001 2.04991

R87 2.59681 -0.00002 0.00000 -0.00005 -0.00005 2.59676

R88 2.04992 -0.00002 0.00003 -0.00004 -0.00001 2.04991

R89 2.05132 -0.00002 0.00008 -0.00009 -0.00001 2.05131

R90 2.60234 -0.00003 0.00002 -0.00008 -0.00006 2.60228

R91 2.05092 -0.00002 0.00007 -0.00008 -0.00001 2.05091

R92 2.66794 -0.00008 0.00023 -0.00026 -0.00004 2.66791

R93 2.04972 -0.00002 0.00003 -0.00005 -0.00002 2.04970

R94 2.60234 -0.00003 0.00002 -0.00008 -0.00006 2.60228

R95 2.04972 -0.00002 0.00003 -0.00005 -0.00002 2.04970

R96 2.05092 -0.00002 0.00007 -0.00008 -0.00001 2.05091

A1 1.89617 -0.00001 -0.00006 0.00011 0.00006 1.89623

A2 2.22975 0.00003 0.00012 0.00007 0.00018 2.22993

A3 2.15697 -0.00003 -0.00005 -0.00022 -0.00027 2.15670

A4 1.92753 -0.00004 0.00015 -0.00024 -0.00010 1.92743

A5 2.17448 0.00002 0.00030 0.00038 0.00065 2.17513

A6 2.17448 0.00002 0.00030 0.00038 0.00065 2.17513

A7 1.89617 -0.00001 -0.00006 0.00011 0.00006 1.89623

A8 2.22975 0.00003 0.00012 0.00007 0.00018 2.22993

A9 2.15697 -0.00003 -0.00005 -0.00022 -0.00027 2.15670

A10 1.85234 0.00003 -0.00003 0.00003 0.00000 1.85234

A11 2.31742 -0.00004 0.00003 -0.00004 -0.00002 2.31740

A12 2.11339 0.00001 -0.00001 0.00000 0.00000 2.11339

A13 1.85234 0.00003 -0.00003 0.00003 0.00000 1.85234

A14 2.31742 -0.00004 0.00003 -0.00004 -0.00002 2.31740

A15 2.11339 0.00001 -0.00001 0.00000 0.00000 2.11339

A16 2.17193 -0.00010 0.00023 -0.00020 0.00002 2.17195

A17 2.24016 0.00003 0.00006 -0.00003 0.00002 2.24018

A18 2.14859 -0.00003 0.00005 -0.00003 0.00001 2.14860

A19 1.89380 0.00000 -0.00017 0.00007 -0.00010 1.89370

A20 1.92378 -0.00004 0.00025 -0.00023 0.00001 1.92379

A21 2.17005 0.00002 0.00030 0.00024 0.00053 2.17058

A22 2.17005 0.00002 0.00030 0.00024 0.00053 2.17058

A23 1.89380 0.00000 -0.00017 0.00007 -0.00010 1.89370

A24 2.24016 0.00003 0.00006 -0.00003 0.00002 2.24018

A25 2.14859 -0.00003 0.00005 -0.00003 0.00001 2.14860

A26 1.85630 0.00002 0.00001 0.00000 0.00000 1.85631

A27 2.30699 -0.00003 -0.00001 -0.00003 -0.00004 2.30695

A28 2.11987 0.00001 0.00000 0.00003 0.00003 2.11990

A29 1.85630 0.00002 0.00001 0.00000 0.00000 1.85631

A30 2.30699 -0.00003 -0.00001 -0.00003 -0.00004 2.30695

A31 2.11987 0.00001 0.00000 0.00003 0.00003 2.11990

A32 2.17193 -0.00010 0.00023 -0.00020 0.00002 2.17195

A33 1.85630 0.00002 0.00001 0.00000 0.00000 1.85631

A34 2.11987 0.00001 0.00000 0.00003 0.00003 2.11990

A35 2.30699 -0.00003 -0.00001 -0.00003 -0.00004 2.30695

A36 1.85630 0.00002 0.00001 0.00000 0.00000 1.85631

A37 2.11987 0.00001 0.00000 0.00003 0.00003 2.11990

A38 2.30699 -0.00003 -0.00001 -0.00003 -0.00004 2.30695

A39 1.89380 0.00000 -0.00017 0.00007 -0.00010 1.89370

A40 2.14859 -0.00003 0.00005 -0.00003 0.00001 2.14860

A41 2.24016 0.00003 0.00006 -0.00003 0.00002 2.24018

A42 1.92378 -0.00004 0.00025 -0.00023 0.00001 1.92379

A43 2.17005 0.00002 0.00030 0.00024 0.00053 2.17058

A44 2.17005 0.00002 0.00030 0.00024 0.00053 2.17058

A45 2.14859 -0.00003 0.00005 -0.00003 0.00001 2.14860

A46 2.24016 0.00003 0.00006 -0.00003 0.00002 2.24018

A47 1.89380 0.00000 -0.00017 0.00007 -0.00010 1.89370

A48 2.17193 -0.00010 0.00023 -0.00020 0.00002 2.17195

A49 1.92753 -0.00004 0.00015 -0.00024 -0.00010 1.92743

A50 2.17448 0.00002 0.00030 0.00038 0.00065 2.17513

A51 2.17448 0.00002 0.00030 0.00038 0.00065 2.17513

A52 2.22975 0.00003 0.00012 0.00007 0.00018 2.22993

A53 2.15697 -0.00003 -0.00005 -0.00022 -0.00027 2.15670

A54 1.89617 -0.00001 -0.00006 0.00011 0.00006 1.89623

A55 1.85234 0.00003 -0.00003 0.00003 0.00000 1.85234

A56 2.31742 -0.00004 0.00003 -0.00004 -0.00002 2.31740

A57 2.11339 0.00001 -0.00001 0.00000 0.00000 2.11339

A58 1.85234 0.00003 -0.00003 0.00003 0.00000 1.85234

A59 2.11339 0.00001 -0.00001 0.00000 0.00000 2.11339

A60 2.31742 -0.00004 0.00003 -0.00004 -0.00002 2.31740

A61 1.89617 -0.00001 -0.00006 0.00011 0.00006 1.89623

A62 2.22975 0.00003 0.00012 0.00007 0.00018 2.22993

A63 2.15697 -0.00003 -0.00005 -0.00022 -0.00027 2.15670

A64 2.17193 -0.00010 0.00023 -0.00020 0.00002 2.17195

A65 1.50812 0.00000 0.00004 0.00010 0.00014 1.50826

A66 1.50812 0.00000 0.00004 0.00010 0.00014 1.50826

A67 2.63436 0.00001 -0.00116 0.00002 -0.00115 2.63321

A68 2.63695 0.00001 0.00152 0.00078 0.00229 2.63924

A69 1.50812 0.00000 0.00004 0.00010 0.00014 1.50826

A70 1.50812 0.00000 0.00004 0.00010 0.00014 1.50826

A71 2.07306 -0.00005 0.00005 -0.00008 -0.00003 2.07303

A72 2.11999 0.00004 -0.00009 0.00010 0.00001 2.12000

A73 2.09013 0.00001 0.00004 -0.00002 0.00002 2.09016

A74 2.09023 0.00004 -0.00005 0.00005 0.00000 2.09023

A75 2.11931 -0.00006 0.00005 -0.00003 0.00002 2.11932

A76 2.07364 0.00002 0.00001 -0.00002 -0.00002 2.07363

A77 2.09023 0.00004 -0.00005 0.00005 0.00000 2.09023

A78 2.07364 0.00002 0.00001 -0.00002 -0.00002 2.07363

A79 2.11931 -0.00006 0.00005 -0.00003 0.00002 2.11932

A80 2.07306 -0.00005 0.00005 -0.00008 -0.00003 2.07303

A81 2.11999 0.00004 -0.00009 0.00010 0.00001 2.12000

A82 2.09013 0.00001 0.00004 -0.00002 0.00002 2.09016

A83 2.07692 -0.00005 0.00005 -0.00004 0.00002 2.07694

A84 2.11651 0.00004 -0.00015 0.00007 -0.00008 2.11643

A85 2.08976 0.00001 0.00009 -0.00003 0.00006 2.08982

A86 2.09286 0.00004 -0.00005 0.00003 -0.00001 2.09284

A87 2.11952 -0.00006 0.00005 -0.00002 0.00003 2.11955

A88 2.07081 0.00002 0.00000 -0.00002 -0.00002 2.07079

A89 2.09286 0.00004 -0.00005 0.00003 -0.00001 2.09284

A90 2.07081 0.00002 0.00000 -0.00002 -0.00002 2.07079

A91 2.11952 -0.00006 0.00005 -0.00002 0.00003 2.11955

A92 2.07692 -0.00005 0.00005 -0.00004 0.00002 2.07694

A93 2.11651 0.00004 -0.00015 0.00007 -0.00008 2.11643

A94 2.08976 0.00001 0.00009 -0.00003 0.00006 2.08982

A95 2.07306 -0.00005 0.00005 -0.00008 -0.00003 2.07303

A96 2.11999 0.00004 -0.00009 0.00010 0.00001 2.12000

A97 2.09013 0.00001 0.00004 -0.00002 0.00002 2.09016

A98 2.09023 0.00004 -0.00005 0.00005 0.00000 2.09023

A99 2.11931 -0.00006 0.00005 -0.00003 0.00002 2.11932

A100 2.07364 0.00002 0.00001 -0.00002 -0.00002 2.07363

A101 2.09023 0.00004 -0.00005 0.00005 0.00000 2.09023

A102 2.07364 0.00002 0.00001 -0.00002 -0.00002 2.07363

A103 2.11931 -0.00006 0.00005 -0.00003 0.00002 2.11932

A104 2.07306 -0.00005 0.00005 -0.00008 -0.00003 2.07303

A105 2.11999 0.00004 -0.00009 0.00010 0.00001 2.12000

A106 2.09013 0.00001 0.00004 -0.00002 0.00002 2.09016

A107 2.07692 -0.00005 0.00005 -0.00004 0.00002 2.07694

A108 2.11651 0.00004 -0.00015 0.00007 -0.00008 2.11643

A109 2.08976 0.00001 0.00009 -0.00003 0.00006 2.08982

A110 2.09286 0.00004 -0.00005 0.00003 -0.00001 2.09284

A111 2.11952 -0.00006 0.00005 -0.00002 0.00003 2.11955

A112 2.07081 0.00002 0.00000 -0.00002 -0.00002 2.07079

A113 2.09286 0.00004 -0.00005 0.00003 -0.00001 2.09284

A114 2.07081 0.00002 0.00000 -0.00002 -0.00002 2.07079

A115 2.11952 -0.00006 0.00005 -0.00002 0.00003 2.11955

A116 2.07692 -0.00005 0.00005 -0.00004 0.00002 2.07694

A117 2.11651 0.00004 -0.00015 0.00007 -0.00008 2.11643

A118 2.08976 0.00001 0.00009 -0.00003 0.00006 2.08982

A119 2.11192 -0.00002 0.00000 0.00004 0.00004 2.11196

A120 2.06950 0.00000 -0.00003 -0.00004 -0.00007 2.06943

A121 2.10176 0.00002 0.00004 0.00000 0.00004 2.10180

A122 2.10045 0.00000 0.00001 -0.00003 -0.00002 2.10044

A123 2.09572 -0.00001 0.00003 0.00004 0.00007 2.09579

A124 2.08701 0.00000 -0.00004 -0.00002 -0.00005 2.08696

A125 2.10045 0.00000 0.00001 -0.00003 -0.00002 2.10044

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A127 2.09572 -0.00001 0.00003 0.00004 0.00007 2.09579

A128 2.11192 -0.00002 0.00000 0.00004 0.00004 2.11196

A129 2.06950 0.00000 -0.00003 -0.00004 -0.00007 2.06943

A130 2.10176 0.00002 0.00004 0.00000 0.00004 2.10180

A131 2.10932 -0.00002 -0.00002 0.00004 0.00002 2.10935

A132 2.07211 0.00000 0.00001 -0.00004 -0.00003 2.07208

A133 2.10176 0.00002 0.00001 0.00000 0.00001 2.10176

A134 2.10022 0.00000 0.00001 -0.00002 -0.00001 2.10021

A135 2.09470 -0.00001 0.00002 0.00004 0.00006 2.09476

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A137 2.10022 0.00000 0.00001 -0.00002 -0.00001 2.10021

A138 2.08827 0.00000 -0.00003 -0.00002 -0.00005 2.08822

A139 2.09470 -0.00001 0.00002 0.00004 0.00006 2.09476

A140 2.10932 -0.00002 -0.00002 0.00004 0.00002 2.10935

A141 2.07211 0.00000 0.00001 -0.00004 -0.00003 2.07208

A142 2.10176 0.00002 0.00001 0.00000 0.00001 2.10176

A143 2.11192 -0.00002 0.00000 0.00004 0.00004 2.11196

A144 2.06950 0.00000 -0.00003 -0.00004 -0.00007 2.06943

A145 2.10176 0.00002 0.00004 0.00000 0.00004 2.10180

A146 2.10045 0.00000 0.00001 -0.00003 -0.00002 2.10044

A147 2.09572 -0.00001 0.00003 0.00004 0.00007 2.09579

A148 2.08701 0.00000 -0.00004 -0.00002 -0.00005 2.08696

A149 2.10045 0.00000 0.00001 -0.00003 -0.00002 2.10044

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A156 2.07211 0.00000 0.00001 -0.00004 -0.00003 2.07208

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A161 2.10022 0.00000 0.00001 -0.00002 -0.00001 2.10021

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A166 2.10176 0.00002 0.00001 0.00000 0.00001 2.10176

D1 0.01982 -0.00002 0.00088 -0.00186 -0.00098 0.01884

D2 -3.00240 -0.00008 -0.00556 -0.00653 -0.01209 -3.01449

D3 -3.09625 -0.00001 0.00035 0.00000 0.00034 -3.09590

D4 0.16472 -0.00007 -0.00609 -0.00467 -0.01076 0.15396

D5 -0.01177 0.00001 -0.00052 0.00110 0.00058 -0.01119

D6 3.13848 0.00004 -0.00005 0.00282 0.00278 3.14126

D7 3.10560 0.00000 -0.00002 -0.00065 -0.00067 3.10493

D8 -0.02734 0.00002 0.00046 0.00107 0.00152 -0.02581

D9 0.08680 0.00004 0.00355 0.00292 0.00647 0.09327

D10 -3.02576 0.00006 0.00295 0.00503 0.00797 -3.01779

D11 -0.01982 0.00002 -0.00088 0.00186 0.00098 -0.01884

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D13 3.00240 0.00008 0.00556 0.00653 0.01209 3.01449

D14 -0.16472 0.00007 0.00609 0.00467 0.01076 -0.15396

D15 -2.96500 0.00003 0.00289 0.00226 0.00515 -2.95985

D16 -0.31255 0.00004 0.00443 0.00301 0.00745 -0.30510

D17 -1.63878 0.00003 0.00366 0.00264 0.00630 -1.63248

D18 0.31255 -0.00004 -0.00443 -0.00301 -0.00745 0.30510

D19 2.96500 -0.00003 -0.00289 -0.00226 -0.00515 2.95985

D20 1.63878 -0.00003 -0.00366 -0.00264 -0.00630 1.63248

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D23 -3.10560 0.00000 0.00002 0.00065 0.00067 -3.10493

D24 0.02734 -0.00002 -0.00046 -0.00107 -0.00152 0.02581

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D26 3.02576 -0.00006 -0.00295 -0.00503 -0.00797 3.01779

D27 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D28 3.13417 -0.00002 -0.00041 -0.00148 -0.00188 3.13229

D29 -3.13417 0.00002 0.00041 0.00148 0.00188 -3.13229

D30 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D31 -3.13758 0.00003 0.00093 0.00163 0.00256 -3.13503

D32 0.00422 0.00003 0.00010 0.00177 0.00187 0.00609

D33 -0.00570 0.00000 0.00040 -0.00030 0.00009 -0.00561

D34 3.13610 0.00000 -0.00043 -0.00016 -0.00059 3.13552

D35 3.13758 -0.00003 -0.00093 -0.00163 -0.00256 3.13503

D36 -0.00422 -0.00003 -0.00010 -0.00177 -0.00187 -0.00609

D37 0.00570 0.00000 -0.00040 0.00030 -0.00009 0.00561

D38 -3.13610 0.00000 0.00043 0.00016 0.00059 -3.13552

D39 0.02542 0.00000 0.00037 0.00005 0.00042 0.02584

D40 -3.07349 0.00000 0.00262 -0.00010 0.00252 -3.07097

D41 -3.06678 0.00002 0.00409 0.00188 0.00597 -3.06081

D42 0.27732 0.00001 -0.00027 0.00056 0.00029 0.27761

D43 0.03712 0.00002 0.00211 0.00201 0.00412 0.04123

D44 -2.90197 0.00001 -0.00225 0.00068 -0.00157 -2.90354

D45 3.08418 -0.00001 -0.00311 -0.00108 -0.00419 3.07999

D46 -0.04942 0.00000 -0.00313 -0.00075 -0.00388 -0.05330

D47 -0.02212 -0.00001 -0.00126 -0.00120 -0.00245 -0.02457

D48 3.12746 0.00000 -0.00127 -0.00087 -0.00214 3.12532

D49 -0.03712 -0.00002 -0.00211 -0.00201 -0.00412 -0.04123

D50 3.06678 -0.00002 -0.00409 -0.00188 -0.00597 3.06081

D51 2.90197 -0.00001 0.00225 -0.00068 0.00157 2.90354

D52 -0.27732 -0.00001 0.00027 -0.00056 -0.00029 -0.27761

D53 -0.36120 0.00001 0.00187 0.00071 0.00258 -0.35862

D54 -1.68609 0.00000 0.00248 0.00073 0.00321 -1.68288

D55 -3.01098 0.00000 0.00309 0.00074 0.00384 -3.00714

D56 3.01098 0.00000 -0.00309 -0.00074 -0.00384 3.00714

D57 1.68609 0.00000 -0.00248 -0.00073 -0.00321 1.68288

D58 0.36120 -0.00001 -0.00187 -0.00071 -0.00258 0.35862

D59 0.02212 0.00001 0.00126 0.00120 0.00245 0.02457

D60 -3.12746 0.00000 0.00127 0.00087 0.00214 -3.12532

D61 -3.08418 0.00001 0.00311 0.00108 0.00419 -3.07999

D62 0.04942 0.00000 0.00313 0.00075 0.00388 0.05330

D63 -0.02542 0.00000 -0.00037 -0.00005 -0.00042 -0.02584

D64 3.07349 0.00000 -0.00262 0.00010 -0.00252 3.07097

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13465 -0.00001 0.00001 -0.00029 -0.00027 3.13438

D67 -3.13465 0.00001 -0.00001 0.00029 0.00027 -3.13438

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 -3.14013 0.00001 -0.00032 0.00044 0.00012 -3.14001

D70 0.00460 0.00000 -0.00019 0.00017 -0.00001 0.00459

D71 -0.00752 0.00000 -0.00030 0.00007 -0.00024 -0.00776

D72 3.13720 0.00000 -0.00017 -0.00019 -0.00036 3.13684

D73 3.14013 -0.00001 0.00032 -0.00044 -0.00012 3.14001

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D76 -3.13720 0.00000 0.00017 0.00019 0.00036 -3.13684

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D78 -0.02542 0.00000 -0.00037 -0.00005 -0.00042 -0.02584

D79 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D81 -3.13465 0.00001 -0.00001 0.00029 0.00027 -3.13438

D82 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D84 0.02212 0.00001 0.00126 0.00120 0.00245 0.02457

D85 0.04942 0.00000 0.00313 0.00075 0.00388 0.05330

D86 -3.12746 0.00000 0.00127 0.00087 0.00214 -3.12532

D87 -0.00752 0.00000 -0.00030 0.00007 -0.00024 -0.00776

D88 3.13720 0.00000 -0.00017 -0.00019 -0.00036 3.13684

D89 -3.14013 0.00001 -0.00032 0.00044 0.00012 -3.14001

D90 0.00460 0.00000 -0.00019 0.00017 -0.00001 0.00459

D91 -0.02212 -0.00001 -0.00126 -0.00120 -0.00245 -0.02457

D92 3.08418 -0.00001 -0.00311 -0.00108 -0.00419 3.07999

D93 3.12746 0.00000 -0.00127 -0.00087 -0.00214 3.12532

D94 -0.04942 0.00000 -0.00313 -0.00075 -0.00388 -0.05330

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D96 -3.13720 0.00000 0.00017 0.00019 0.00036 -3.13684

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D98 -0.00460 0.00000 0.00019 -0.00017 0.00001 -0.00459

D99 0.03712 0.00002 0.00211 0.00201 0.00412 0.04123

D100 -2.90197 0.00001 -0.00225 0.00068 -0.00157 -2.90354

D101 -3.06678 0.00002 0.00409 0.00188 0.00597 -3.06081

D102 0.27732 0.00001 -0.00027 0.00056 0.00029 0.27761

D103 -3.07349 0.00000 0.00262 -0.00010 0.00252 -3.07097

D104 0.02542 0.00000 0.00037 0.00005 0.00042 0.02584

D105 3.06678 -0.00002 -0.00409 -0.00188 -0.00597 3.06081

D106 -0.03712 -0.00002 -0.00211 -0.00201 -0.00412 -0.04123

D107 -0.27732 -0.00001 0.00027 -0.00056 -0.00029 -0.27761

D108 2.90197 -0.00001 0.00225 -0.00068 0.00157 2.90354

D109 -3.01098 0.00000 0.00309 0.00074 0.00384 -3.00714

D110 -1.68609 0.00000 0.00248 0.00073 0.00321 -1.68288

D111 -0.36120 0.00001 0.00187 0.00071 0.00258 -0.35862

D112 0.36120 -0.00001 -0.00187 -0.00071 -0.00258 0.35862

D113 1.68609 0.00000 -0.00248 -0.00073 -0.00321 1.68288

D114 3.01098 0.00000 -0.00309 -0.00074 -0.00384 3.00714

D115 -0.08680 -0.00004 -0.00355 -0.00292 -0.00647 -0.09327

D116 3.02576 -0.00006 -0.00295 -0.00503 -0.00797 3.01779

D117 3.09625 0.00001 -0.00035 0.00000 -0.00034 3.09590

D118 -0.01982 0.00002 -0.00088 0.00186 0.00098 -0.01884

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D120 3.00240 0.00008 0.00556 0.00653 0.01209 3.01449

D121 0.01982 -0.00002 0.00088 -0.00186 -0.00098 0.01884

D122 -3.09625 -0.00001 0.00035 0.00000 0.00034 -3.09590

D123 -3.00240 -0.00008 -0.00556 -0.00653 -0.01209 -3.01449

D124 0.16472 -0.00007 -0.00609 -0.00467 -0.01076 0.15396

D125 1.63878 -0.00003 -0.00366 -0.00264 -0.00630 1.63248

D126 2.96500 -0.00003 -0.00289 -0.00226 -0.00515 2.95985

D127 0.31255 -0.00004 -0.00443 -0.00301 -0.00745 0.30510

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D129 -0.31255 0.00004 0.00443 0.00301 0.00745 -0.30510

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D131 -3.10560 0.00000 0.00002 0.00065 0.00067 -3.10493

D132 0.02734 -0.00002 -0.00046 -0.00107 -0.00152 0.02581

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D134 -3.13848 -0.00004 0.00005 -0.00282 -0.00278 -3.14126

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D140 0.00422 0.00003 0.00010 0.00177 0.00187 0.00609

D141 -0.00570 0.00000 0.00040 -0.00030 0.00009 -0.00561

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D143 -0.01177 0.00001 -0.00052 0.00110 0.00058 -0.01119

D144 3.10560 0.00000 -0.00002 -0.00065 -0.00067 3.10493

D145 3.13848 0.00004 -0.00005 0.00282 0.00278 3.14126

D146 -0.02734 0.00002 0.00046 0.00107 0.00152 -0.02581

D147 0.00570 0.00000 -0.00040 0.00030 -0.00009 0.00561

D148 -3.13610 0.00000 0.00043 0.00016 0.00059 -3.13552

D149 3.13758 -0.00003 -0.00093 -0.00163 -0.00256 3.13503

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D160 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D162 -0.00030 0.00000 0.00001 -0.00007 -0.00006 -0.00036

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D164 3.14119 0.00000 -0.00001 0.00004 0.00003 3.14122

D165 -0.00739 0.00000 -0.00030 0.00007 -0.00023 -0.00762

D166 3.13728 0.00000 -0.00017 -0.00019 -0.00036 3.13692

D167 3.13430 0.00000 -0.00028 -0.00004 -0.00032 3.13399

D168 -0.00421 0.00000 -0.00014 -0.00030 -0.00044 -0.00465

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D171 -3.14157 0.00000 -0.00004 0.00015 0.00011 -3.14146

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D196 -0.00421 0.00000 -0.00014 -0.00030 -0.00044 -0.00465

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D199 3.14149 0.00000 -0.00002 0.00011 0.00009 3.14158

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D235 3.14130 0.00000 0.00002 0.00003 0.00005 3.14135

D236 -0.00074 0.00000 0.00000 0.00010 0.00010 -0.00065

D237 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D238 3.14114 0.00000 -0.00002 0.00006 0.00004 3.14119

D239 -3.14114 0.00000 0.00002 -0.00006 -0.00004 -3.14119

D240 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D241 -0.00053 0.00000 -0.00020 0.00012 -0.00008 -0.00062

D242 -3.14130 0.00000 -0.00002 -0.00003 -0.00005 -3.14135

D243 3.14151 0.00000 -0.00018 0.00006 -0.00013 3.14138

D244 0.00074 0.00000 0.00000 -0.00010 -0.00010 0.00065

D245 -0.00013 0.00000 0.00002 -0.00004 -0.00002 -0.00015

D246 -3.14110 0.00000 0.00003 -0.00005 -0.00002 -3.14112

D247 3.14119 0.00000 -0.00002 0.00004 0.00003 3.14121

D248 0.00022 0.00000 0.00000 0.00003 0.00003 0.00024

D249 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D250 -3.14097 0.00000 0.00001 -0.00001 0.00000 -3.14097

D251 3.14097 0.00000 -0.00001 0.00001 0.00000 3.14097

D252 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D253 0.00013 0.00000 -0.00002 0.00004 0.00002 0.00015

D254 -3.14119 0.00000 0.00002 -0.00004 -0.00003 -3.14121

D255 3.14110 0.00000 -0.00003 0.00005 0.00002 3.14112

D256 -0.00022 0.00000 0.00000 -0.00003 -0.00003 -0.00024

D257 0.00053 0.00000 0.00020 -0.00012 0.00008 0.00062

D258 -3.14151 0.00000 0.00018 -0.00006 0.00013 -3.14138

D259 3.14130 0.00000 0.00002 0.00003 0.00005 3.14135

D260 -0.00074 0.00000 0.00000 0.00010 0.00010 -0.00065

D261 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D262 3.14114 0.00000 -0.00002 0.00006 0.00004 3.14119

D263 -3.14114 0.00000 0.00002 -0.00006 -0.00004 -3.14119

D264 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D265 -0.00053 0.00000 -0.00020 0.00012 -0.00008 -0.00062

D266 -3.14130 0.00000 -0.00002 -0.00003 -0.00005 -3.14135

D267 3.14151 0.00000 -0.00018 0.00006 -0.00013 3.14138

D268 0.00074 0.00000 0.00000 -0.00010 -0.00010 0.00065

D269 0.00013 0.00000 -0.00002 0.00004 0.00002 0.00015

D270 3.14110 0.00000 -0.00003 0.00005 0.00002 3.14112

D271 -3.14119 0.00000 0.00002 -0.00004 -0.00003 -3.14121

D272 -0.00022 0.00000 0.00000 -0.00003 -0.00003 -0.00024

D273 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D274 3.14097 0.00000 -0.00001 0.00001 0.00000 3.14097

D275 -3.14097 0.00000 0.00001 -0.00001 0.00000 -3.14097

D276 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D277 -0.00013 0.00000 0.00002 -0.00004 -0.00002 -0.00015

D278 3.14119 0.00000 -0.00002 0.00004 0.00003 3.14121

D279 -3.14110 0.00000 0.00003 -0.00005 -0.00002 -3.14112

D280 0.00022 0.00000 0.00000 0.00003 0.00003 0.00024

Item Value Threshold Converged?

Maximum Force 0.000161 0.000450 YES

RMS Force 0.000037 0.000300 YES

Maximum Displacement 0.139909 0.001800 NO

RMS Displacement 0.024337 0.001200 NO

Predicted change in Energy=-6.844578D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Jun 30 20:33:23 2019, MaxMem= 1342177280 cpu: 166.5

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

Stoichiometry C48H24N8Zn(3)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C48H24N4)]

Deg. of freedom 61

Full point group C2V NOp 4

RotChk: IX=0 Diff= 1.25D-14

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 1.121223 2.791613 0.173100

2 7 0 0.000000 2.023427 0.301137

3 6 0 -1.121223 2.791613 0.173100

4 6 0 -0.717725 4.171730 -0.030650

5 6 0 0.717725 4.171730 -0.030650

6 7 0 -2.412381 2.383909 0.191485

7 6 0 -2.794414 1.127683 0.240860

8 7 0 -2.011213 0.000000 0.310784

9 6 0 -2.794414 -1.127683 0.240860

10 6 0 -4.208026 -0.712258 0.172541

11 6 0 -4.208026 0.712258 0.172541

12 7 0 2.412381 2.383909 0.191485

13 6 0 4.208026 0.712258 0.172541

14 6 0 4.208026 -0.712258 0.172541

15 6 0 2.794414 -1.127683 0.240860

16 7 0 2.011213 0.000000 0.310784

17 6 0 2.794414 1.127683 0.240860

18 7 0 2.412381 -2.383909 0.191485

19 7 0 0.000000 -2.023427 0.301137

20 6 0 1.121223 -2.791613 0.173100

21 6 0 0.717725 -4.171730 -0.030650

22 6 0 -0.717725 -4.171730 -0.030650

23 6 0 -1.121223 -2.791613 0.173100

24 7 0 -2.412381 -2.383909 0.191485

25 30 0 0.000000 0.000000 0.826847

26 6 0 5.372954 1.426145 0.107813

27 6 0 6.608301 0.718955 0.048878

28 6 0 6.608301 -0.718955 0.048878

29 6 0 5.372954 -1.426145 0.107813

30 6 0 -1.428236 -5.335808 -0.213584

31 6 0 -0.721542 -6.550403 -0.397422

32 6 0 0.721542 -6.550403 -0.397422

33 6 0 1.428236 -5.335808 -0.213584

34 6 0 -5.372954 1.426145 0.107813

35 6 0 -6.608301 0.718955 0.048878

36 6 0 -6.608301 -0.718955 0.048878

37 6 0 -5.372954 -1.426145 0.107813

38 6 0 1.428236 5.335808 -0.213584

39 6 0 0.721542 6.550403 -0.397422

40 6 0 -0.721542 6.550403 -0.397422

41 6 0 -1.428236 5.335808 -0.213584

42 6 0 1.402311 -7.782254 -0.585731

43 6 0 0.708062 -8.954615 -0.764224

44 6 0 -0.708062 -8.954615 -0.764224

45 6 0 -1.402311 -7.782254 -0.585731

46 6 0 7.847642 -1.401351 -0.010269

47 6 0 9.034851 -0.705898 -0.066752

48 6 0 9.034851 0.705898 -0.066752

49 6 0 7.847642 1.401351 -0.010269

50 6 0 -1.402311 7.782254 -0.585731

51 6 0 -0.708062 8.954615 -0.764224

52 6 0 0.708062 8.954615 -0.764224

53 6 0 1.402311 7.782254 -0.585731

54 6 0 -7.847642 -1.401351 -0.010269

55 6 0 -9.034851 -0.705898 -0.066752

56 6 0 -9.034851 0.705898 -0.066752

57 6 0 -7.847642 1.401351 -0.010269

58 1 0 5.372822 2.511070 0.103415

59 1 0 5.372822 -2.511070 0.103415

60 1 0 -2.513308 -5.338197 -0.219666

61 1 0 2.513308 -5.338197 -0.219666

62 1 0 -5.372822 2.511070 0.103415

63 1 0 -5.372822 -2.511070 0.103415

64 1 0 2.513308 5.338197 -0.219666

65 1 0 -2.513308 5.338197 -0.219666

66 1 0 2.487817 -7.780827 -0.585286

67 1 0 1.243441 -9.887252 -0.906606

68 1 0 -1.243441 -9.887252 -0.906606

69 1 0 -2.487817 -7.780827 -0.585286

70 1 0 7.845941 -2.486642 -0.010544

71 1 0 9.976427 -1.242417 -0.112135

72 1 0 9.976427 1.242417 -0.112135

73 1 0 7.845941 2.486642 -0.010544

74 1 0 -2.487817 7.780827 -0.585286

75 1 0 -1.243441 9.887252 -0.906606

76 1 0 1.243441 9.887252 -0.906606

77 1 0 2.487817 7.780827 -0.585286

78 1 0 -7.845941 -2.486642 -0.010544

79 1 0 -9.976427 -1.242417 -0.112135

80 1 0 -9.976427 1.242417 -0.112135

81 1 0 -7.845941 2.486642 -0.010544

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

Rotational constants (GHZ): 0.0386469 0.0380393 0.0193416

Leave Link 202 at Sun Jun 30 20:33:23 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 307 symmetry adapted cartesian basis functions of A1 symmetry.

There are 278 symmetry adapted cartesian basis functions of A2 symmetry.

There are 289 symmetry adapted cartesian basis functions of B1 symmetry.

There are 289 symmetry adapted cartesian basis functions of B2 symmetry.

There are 289 symmetry adapted basis functions of A1 symmetry.

There are 265 symmetry adapted basis functions of A2 symmetry.

There are 275 symmetry adapted basis functions of B1 symmetry.

There are 275 symmetry adapted basis functions of B2 symmetry.

1104 basis functions, 1951 primitive gaussians, 1163 cartesian basis functions

191 alpha electrons 189 beta electrons

nuclear repulsion energy 6888.5083384167 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= 81 NActive= 81 NUniq= 22 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= -0.2361045435 Hartrees.

Nuclear repulsion after empirical dispersion term = 6888.2722338731 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= 81.

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 = 81

GePol: Total number of spheres = 81

GePol: Number of exposed spheres = 81 (100.00%)

GePol: Number of points = 6438

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.15D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 378

GePol: Fraction of low-weight points (<1% of avg) = 5.87%

GePol: Cavity surface area = 670.429 Ang\*\*2

GePol: Cavity volume = 694.146 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0169907444 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 6888.2552431287 Hartrees.

Leave Link 301 at Sun Jun 30 20:33:24 2019, MaxMem= 1342177280 cpu: 1.8

(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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36705 LenP2D= 95190.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1104 RedAO= T EigKep= 2.88D-05 NBF= 289 265 275 275

NBsUse= 1104 1.00D-06 EigRej= -1.00D+00 NBFU= 289 265 275 275

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= 1060 1060 1060 1060 1060 MxSgAt= 81 MxSgA2= 81.

Leave Link 302 at Sun Jun 30 20:33:50 2019, MaxMem= 1342177280 cpu: 262.7

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Jun 30 20:33:51 2019, MaxMem= 1342177280 cpu: 4.0

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

Initial guess from the checkpoint file: "ZnNPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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The electronic state of the initial guess is 3-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -2348.36333809759

Leave Link 401 at Sun Jun 30 20:34:18 2019, MaxMem= 1342177280 cpu: 274.8

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4103221 IEndB= 4103221 NGot= 1342177280 MDV= 1339444432

LenX= 1339444432 LenY= 1338090700

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= 420000000 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= 124343532.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.19D-14 for 484.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.31D-15 for 4359 2113.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.77D-15 for 2652.

Iteration 1 A^-1\*A deviation from orthogonality is 2.92D-08 for 1538 1449.

Iteration 2 A\*A^-1 deviation from unit magnitude is 1.68D-14 for 484.

Iteration 2 A\*A^-1 deviation from orthogonality is 1.26D-14 for 1336 485.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.78D-15 for 1605.

Iteration 2 A^-1\*A deviation from orthogonality is 5.30D-16 for 3194 506.

E= -2348.12948909788

DIIS: error= 1.09D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2348.12948909788 IErMin= 1 ErrMin= 1.09D-03

ErrMax= 1.09D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.40D-03 BMatP= 2.40D-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= 0.378 Goal= None Shift= 0.000

Gap= 0.459 Goal= None Shift= 0.000

GapD= 0.378 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

RMSDP=2.94D-05 MaxDP=1.14D-03 OVMax= 6.71D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.94D-05 CP: 1.00D+00

E= -2348.13070383968 Delta-E= -0.001214741804 Rises=F Damp=F

DIIS: error= 1.49D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2348.13070383968 IErMin= 2 ErrMin= 1.49D-04

ErrMax= 1.49D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.53D-05 BMatP= 2.40D-03

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.49D-03

Coeff-Com: -0.745D-01 0.107D+01

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

Coeff: -0.744D-01 0.107D+01

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=4.53D-06 MaxDP=1.98D-04 DE=-1.21D-03 OVMax= 1.05D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.49D-06 CP: 1.00D+00 1.10D+00

E= -2348.13072139148 Delta-E= -0.000017551796 Rises=F Damp=F

DIIS: error= 3.06D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2348.13072139148 IErMin= 3 ErrMin= 3.06D-05

ErrMax= 3.06D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.42D-06 BMatP= 2.53D-05

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

Coeff-Com: -0.194D-01 0.233D+00 0.787D+00

Coeff: -0.194D-01 0.233D+00 0.787D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.27D-06 MaxDP=1.17D-04 DE=-1.76D-05 OVMax= 3.00D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.23D-06 CP: 1.00D+00 1.11D+00 9.47D-01

E= -2348.13072150625 Delta-E= -0.000000114778 Rises=F Damp=F

DIIS: error= 3.87D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2348.13072150625 IErMin= 3 ErrMin= 3.06D-05

ErrMax= 3.87D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.45D-06 BMatP= 2.42D-06

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

Coeff-Com: -0.466D-02 0.357D-01 0.501D+00 0.468D+00

Coeff: -0.466D-02 0.357D-01 0.501D+00 0.468D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=6.82D-07 MaxDP=8.54D-05 DE=-1.15D-07 OVMax= 1.90D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.03D-07 CP: 1.00D+00 1.11D+00 1.00D+00 5.83D-01

E= -2348.13072203139 Delta-E= -0.000000525137 Rises=F Damp=F

DIIS: error= 7.71D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2348.13072203139 IErMin= 5 ErrMin= 7.71D-06

ErrMax= 7.71D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.21D-07 BMatP= 2.42D-06

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

Coeff-Com: 0.109D-02-0.253D-01 0.102D+00 0.219D+00 0.703D+00

Coeff: 0.109D-02-0.253D-01 0.102D+00 0.219D+00 0.703D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.62D-07 MaxDP=1.90D-05 DE=-5.25D-07 OVMax= 4.10D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.18D-08 CP: 1.00D+00 1.11D+00 1.02D+00 6.32D-01 7.42D-01

E= -2348.13072205505 Delta-E= -0.000000023663 Rises=F Damp=F

DIIS: error= 1.93D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2348.13072205505 IErMin= 6 ErrMin= 1.93D-06

ErrMax= 1.93D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.42D-08 BMatP= 1.21D-07

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

Coeff-Com: 0.802D-03-0.163D-01 0.435D-01 0.114D+00 0.417D+00 0.441D+00

Coeff: 0.802D-03-0.163D-01 0.435D-01 0.114D+00 0.417D+00 0.441D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=5.74D-08 MaxDP=4.19D-06 DE=-2.37D-08 OVMax= 1.38D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.81D-08 CP: 1.00D+00 1.11D+00 1.02D+00 6.35D-01 7.58D-01

CP: 5.45D-01

E= -2348.13072205873 Delta-E= -0.000000003673 Rises=F Damp=F

DIIS: error= 4.69D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2348.13072205873 IErMin= 7 ErrMin= 4.69D-07

ErrMax= 4.69D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.94D-10 BMatP= 1.42D-08

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

Coeff-Com: 0.152D-03-0.244D-02 0.717D-03 0.101D-01 0.559D-01 0.185D+00

Coeff-Com: 0.751D+00

Coeff: 0.152D-03-0.244D-02 0.717D-03 0.101D-01 0.559D-01 0.185D+00

Coeff: 0.751D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.73D-08 MaxDP=8.59D-07 DE=-3.67D-09 OVMax= 4.59D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.29D-08 CP: 1.00D+00 1.11D+00 1.02D+00 6.37D-01 7.56D-01

CP: 6.56D-01 9.04D-01

E= -2348.13072205940 Delta-E= -0.000000000675 Rises=F Damp=F

DIIS: error= 2.10D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2348.13072205940 IErMin= 8 ErrMin= 2.10D-07

ErrMax= 2.10D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.65D-10 BMatP= 6.94D-10

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

Coeff-Com: -0.251D-04 0.866D-03-0.532D-02-0.979D-02-0.249D-01 0.403D-01

Coeff-Com: 0.405D+00 0.594D+00

Coeff: -0.251D-04 0.866D-03-0.532D-02-0.979D-02-0.249D-01 0.403D-01

Coeff: 0.405D+00 0.594D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=6.87D-09 MaxDP=5.97D-07 DE=-6.75D-10 OVMax= 2.96D-06

Error on total polarization charges = 0.08838

SCF Done: E(UB3LYP) = -2348.13072206 A.U. after 8 cycles

NFock= 8 Conv=0.69D-08 -V/T= 1.9830

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

<L.S>= 0.000000000000E+00

KE= 2.388741189003D+03 PE=-1.931991942784D+04 EE= 7.694792273647D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -10.66

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0219, after 2.0003

Leave Link 502 at Sun Jun 30 20:44:50 2019, MaxMem= 1342177280 cpu: 6782.0

(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.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36705 LenP2D= 95190.

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 = 195

Leave Link 701 at Sun Jun 30 20:45:27 2019, MaxMem= 1342177280 cpu: 365.4

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sun Jun 30 20:45:27 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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 Sun Jun 30 20:46:13 2019, MaxMem= 1342177280 cpu: 496.4

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-9.64561764D-13-4.65405492D-13 9.13928869D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000029335 0.000132946 -0.000239207

2 7 0.000000000 -0.000162643 0.000376111

3 6 0.000029335 0.000132946 -0.000239207

4 6 0.000035114 -0.000097011 0.000133361

5 6 -0.000035114 -0.000097011 0.000133361

6 7 -0.000084010 0.000208954 0.000047204

7 6 -0.000225943 -0.000198199 0.000056712

8 7 0.000187874 0.000000000 -0.000237133

9 6 -0.000225943 0.000198199 0.000056712

10 6 0.000151799 -0.000010537 0.000044167

11 6 0.000151799 0.000010537 0.000044167

12 7 0.000084010 0.000208954 0.000047204

13 6 -0.000151799 0.000010537 0.000044167

14 6 -0.000151799 -0.000010537 0.000044167

15 6 0.000225943 0.000198199 0.000056712

16 7 -0.000187874 0.000000000 -0.000237133

17 6 0.000225943 -0.000198199 0.000056712

18 7 0.000084010 -0.000208954 0.000047204

19 7 0.000000000 0.000162643 0.000376111

20 6 -0.000029335 -0.000132946 -0.000239207

21 6 -0.000035114 0.000097011 0.000133361

22 6 0.000035114 0.000097011 0.000133361

23 6 0.000029335 -0.000132946 -0.000239207

24 7 -0.000084010 -0.000208954 0.000047204

25 30 0.000000000 0.000000000 -0.000168255

26 6 0.000033159 0.000087618 -0.000030530

27 6 -0.000013379 -0.000115876 0.000005600

28 6 -0.000013379 0.000115876 0.000005600

29 6 0.000033159 -0.000087618 -0.000030530

30 6 -0.000100186 -0.000000731 -0.000060872

31 6 0.000136283 -0.000013231 -0.000010116

32 6 -0.000136283 -0.000013231 -0.000010116

33 6 0.000100186 -0.000000731 -0.000060872

34 6 -0.000033159 0.000087618 -0.000030530

35 6 0.000013379 -0.000115876 0.000005600

36 6 0.000013379 0.000115876 0.000005600

37 6 -0.000033159 -0.000087618 -0.000030530

38 6 0.000100186 0.000000731 -0.000060872

39 6 -0.000136283 0.000013231 -0.000010116

40 6 0.000136283 0.000013231 -0.000010116

41 6 -0.000100186 0.000000731 -0.000060872

42 6 0.000045363 0.000065714 0.000002271

43 6 -0.000095643 -0.000004689 -0.000008911

44 6 0.000095643 -0.000004689 -0.000008911

45 6 -0.000045363 0.000065714 0.000002271

46 6 -0.000035534 -0.000031476 0.000003254

47 6 -0.000003580 0.000069675 -0.000002027

48 6 -0.000003580 -0.000069675 -0.000002027

49 6 -0.000035534 0.000031476 0.000003254

50 6 -0.000045363 -0.000065714 0.000002271

51 6 0.000095643 0.000004689 -0.000008911

52 6 -0.000095643 0.000004689 -0.000008911

53 6 0.000045363 -0.000065714 0.000002271

54 6 0.000035534 -0.000031476 0.000003254

55 6 0.000003580 0.000069675 -0.000002027

56 6 0.000003580 -0.000069675 -0.000002027

57 6 0.000035534 0.000031476 0.000003254

58 1 0.000017322 -0.000019857 0.000002513

59 1 0.000017322 0.000019857 0.000002513

60 1 0.000018732 -0.000027228 0.000020809

61 1 -0.000018732 -0.000027228 0.000020809

62 1 -0.000017322 -0.000019857 0.000002513

63 1 -0.000017322 0.000019857 0.000002513

64 1 -0.000018732 0.000027228 0.000020809

65 1 0.000018732 0.000027228 0.000020809

66 1 -0.000012307 0.000006019 0.000002888

67 1 0.000006879 0.000015601 0.000004608

68 1 -0.000006879 0.000015601 0.000004608

69 1 0.000012307 0.000006019 0.000002888

70 1 -0.000006653 0.000010830 -0.000000345

71 1 -0.000016106 -0.000003400 0.000001196

72 1 -0.000016106 0.000003400 0.000001196

73 1 -0.000006653 -0.000010830 -0.000000345

74 1 0.000012307 -0.000006019 0.000002888

75 1 -0.000006879 -0.000015601 0.000004608

76 1 0.000006879 -0.000015601 0.000004608

77 1 -0.000012307 -0.000006019 0.000002888

78 1 0.000006653 0.000010830 -0.000000345

79 1 0.000016106 -0.000003400 0.000001196

80 1 0.000016106 0.000003400 0.000001196

81 1 0.000006653 -0.000010830 -0.000000345

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

Cartesian Forces: Max 0.000376111 RMS 0.000090218

Leave Link 716 at Sun Jun 30 20:46:13 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.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.000185585 RMS 0.000037629

Search for a local minimum.

Step number 5 out of a maximum of 486

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .37629D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

DE= -1.07D-05 DEPred=-6.84D-06 R= 1.56D+00

TightC=F SS= 1.41D+00 RLast= 5.13D-02 DXNew= 5.0454D-01 1.5386D-01

Trust test= 1.56D+00 RLast= 5.13D-02 DXMaxT set to 3.00D-01

ITU= 1 1 1 1 0

Eigenvalues --- 0.00262 0.01432 0.01484 0.01500 0.01573

Eigenvalues --- 0.01593 0.01627 0.01656 0.01658 0.01694

Eigenvalues --- 0.01698 0.01705 0.01713 0.01715 0.01725

Eigenvalues --- 0.01725 0.01730 0.01731 0.01735 0.01737

Eigenvalues --- 0.01746 0.01751 0.01759 0.01791 0.01827

Eigenvalues --- 0.01828 0.01829 0.01851 0.01854 0.01860

Eigenvalues --- 0.01869 0.01869 0.01936 0.01955 0.01968

Eigenvalues --- 0.01968 0.01972 0.01972 0.01978 0.01992

Eigenvalues --- 0.01992 0.01993 0.01993 0.02009 0.02080

Eigenvalues --- 0.02080 0.02086 0.02086 0.02089 0.02096

Eigenvalues --- 0.02096 0.02098 0.02098 0.02103 0.02103

Eigenvalues --- 0.02105 0.02106 0.02107 0.02124 0.02124

Eigenvalues --- 0.02137 0.02144 0.02144 0.02147 0.02147

Eigenvalues --- 0.02171 0.02173 0.02213 0.02214 0.02221

Eigenvalues --- 0.02225 0.02233 0.02279 0.02285 0.02346

Eigenvalues --- 0.02391 0.03556 0.05482 0.05591 0.08096

Eigenvalues --- 0.14734 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 0.16004 0.16010 0.16092

Eigenvalues --- 0.16146 0.16275 0.17442 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22500 0.22502 0.22504

Eigenvalues --- 0.22532 0.23234 0.23234 0.23234 0.23696

Eigenvalues --- 0.23939 0.23940 0.23940 0.23955 0.24181

Eigenvalues --- 0.24209 0.24349 0.24541 0.24554 0.24557

Eigenvalues --- 0.24557 0.24561 0.24782 0.24893 0.24896

Eigenvalues --- 0.24969 0.24982 0.24986 0.24990 0.24992

Eigenvalues --- 0.24997 0.24997 0.24998 0.24998 0.26193

Eigenvalues --- 0.32867 0.32950 0.33673 0.33741 0.33837

Eigenvalues --- 0.33888 0.35038 0.35064 0.35181 0.35181

Eigenvalues --- 0.35181 0.35187 0.35202 0.35202 0.35202

Eigenvalues --- 0.35211 0.35231 0.35231 0.35231 0.35240

Eigenvalues --- 0.35249 0.35249 0.35249 0.35270 0.35270

Eigenvalues --- 0.35270 0.35273 0.35279 0.35279 0.35279

Eigenvalues --- 0.35281 0.35408 0.35414 0.35910 0.36350

Eigenvalues --- 0.37281 0.37459 0.37573 0.37969 0.39275

Eigenvalues --- 0.39275 0.39612 0.39612 0.39671 0.40188

Eigenvalues --- 0.40188 0.40257 0.40257 0.40906 0.41001

Eigenvalues --- 0.41047 0.41122 0.41604 0.41759 0.41874

Eigenvalues --- 0.42117 0.42215 0.42398 0.42706 0.42806

Eigenvalues --- 0.42911 0.42971 0.45544 0.45678 0.47124

Eigenvalues --- 0.47124 0.47212 0.47384 0.47386 0.47579

Eigenvalues --- 0.47580 0.48128 0.48218 0.48341 0.48464

Eigenvalues --- 0.48465 0.48680 0.48699 0.48707 0.48729

Eigenvalues --- 0.49091 0.49392 0.49898 0.50397 0.50639

Eigenvalues --- 0.50996 0.51539 0.52485 0.59245 0.59850

Eigenvalues --- 0.60911 0.60987

En-DIIS/RFO-DIIS IScMMF= 0 using points: 5 4 3 2

RFO step: Lambda=-1.72847040D-06.

NNeg= 0 NP= 4 Switch= 2.50D-03 Rises=F DC= 3.95D-05 SmlDif= 1.00D-05

RMS Error= 0.1470740358D-03 NUsed= 4 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.60631 -0.35160 -0.45036 0.19565

Iteration 1 RMS(Cart)= 0.02718744 RMS(Int)= 0.00004869

Iteration 2 RMS(Cart)= 0.00021623 RMS(Int)= 0.00000589

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000589

ITry= 1 IFail=0 DXMaxC= 1.58D-01 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.98D-08 for atom 73.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.57977 0.00009 -0.00006 0.00019 0.00014 2.57991

R2 2.74437 -0.00015 -0.00021 -0.00010 -0.00032 2.74405

R3 2.55892 0.00005 -0.00017 0.00017 0.00000 2.55892

R4 2.57977 0.00009 -0.00006 0.00019 0.00014 2.57991

R5 3.95067 -0.00010 0.00081 -0.00023 0.00058 3.95125

R6 2.74437 -0.00015 -0.00021 -0.00010 -0.00032 2.74405

R7 2.55892 0.00005 -0.00017 0.00017 0.00000 2.55892

R8 2.71261 -0.00001 -0.00010 -0.00003 -0.00014 2.71247

R9 2.60026 0.00000 -0.00009 0.00012 0.00003 2.60029

R10 2.60026 0.00000 -0.00009 0.00012 0.00003 2.60029

R11 2.48303 0.00014 -0.00035 0.00018 -0.00017 2.48286

R12 2.59792 0.00004 -0.00005 0.00008 0.00002 2.59794

R13 2.78729 -0.00019 0.00008 -0.00018 -0.00010 2.78720

R14 2.59792 0.00004 -0.00005 0.00008 0.00002 2.59794

R15 3.92377 -0.00004 -0.00026 0.00008 -0.00018 3.92358

R16 2.78729 -0.00019 0.00008 -0.00018 -0.00010 2.78720

R17 2.48303 0.00014 -0.00035 0.00018 -0.00017 2.48286

R18 2.69195 0.00000 -0.00018 0.00001 -0.00016 2.69178

R19 2.58477 0.00000 -0.00010 0.00010 0.00001 2.58478

R20 2.58477 0.00000 -0.00010 0.00010 0.00001 2.58478

R21 2.48303 0.00014 -0.00035 0.00018 -0.00017 2.48286

R22 2.69195 0.00000 -0.00018 0.00001 -0.00016 2.69178

R23 2.78729 -0.00019 0.00008 -0.00018 -0.00010 2.78720

R24 2.58477 0.00000 -0.00010 0.00010 0.00001 2.58478

R25 2.78729 -0.00019 0.00008 -0.00018 -0.00010 2.78720

R26 2.58477 0.00000 -0.00010 0.00010 0.00001 2.58478

R27 2.59792 0.00004 -0.00005 0.00008 0.00002 2.59794

R28 2.48303 0.00014 -0.00035 0.00018 -0.00017 2.48286

R29 2.59792 0.00004 -0.00005 0.00008 0.00002 2.59794

R30 3.92377 -0.00004 -0.00026 0.00008 -0.00018 3.92358

R31 2.55892 0.00005 -0.00017 0.00017 0.00000 2.55892

R32 2.57977 0.00009 -0.00006 0.00019 0.00014 2.57991

R33 2.57977 0.00009 -0.00006 0.00019 0.00014 2.57991

R34 3.95067 -0.00010 0.00081 -0.00023 0.00058 3.95125

R35 2.74437 -0.00015 -0.00021 -0.00010 -0.00032 2.74405

R36 2.71261 -0.00001 -0.00010 -0.00003 -0.00014 2.71247

R37 2.60026 0.00000 -0.00009 0.00012 0.00003 2.60029

R38 2.74437 -0.00015 -0.00021 -0.00010 -0.00032 2.74405

R39 2.60026 0.00000 -0.00009 0.00012 0.00003 2.60029

R40 2.55892 0.00005 -0.00017 0.00017 0.00000 2.55892

R41 2.69223 -0.00005 -0.00019 0.00012 -0.00007 2.69216

R42 2.05023 -0.00002 0.00001 -0.00005 -0.00004 2.05019

R43 2.71726 -0.00008 -0.00003 -0.00006 -0.00009 2.71717

R44 2.67590 -0.00005 -0.00013 0.00009 -0.00004 2.67586

R45 2.69223 -0.00005 -0.00019 0.00012 -0.00007 2.69216

R46 2.67590 -0.00005 -0.00013 0.00009 -0.00004 2.67586

R47 2.05023 -0.00002 0.00001 -0.00005 -0.00004 2.05019

R48 2.67812 -0.00004 -0.00023 0.00012 -0.00010 2.67802

R49 2.05053 -0.00002 0.00002 -0.00005 -0.00003 2.05050

R50 2.72703 -0.00010 0.00001 -0.00010 -0.00009 2.72695

R51 2.68339 -0.00007 -0.00017 0.00007 -0.00010 2.68328

R52 2.67812 -0.00004 -0.00023 0.00012 -0.00010 2.67802

R53 2.68339 -0.00007 -0.00017 0.00007 -0.00010 2.68328

R54 2.05053 -0.00002 0.00002 -0.00005 -0.00003 2.05050

R55 2.69223 -0.00005 -0.00019 0.00012 -0.00007 2.69216

R56 2.05023 -0.00002 0.00001 -0.00005 -0.00004 2.05019

R57 2.71726 -0.00008 -0.00003 -0.00006 -0.00009 2.71717

R58 2.67590 -0.00005 -0.00013 0.00009 -0.00004 2.67586

R59 2.69223 -0.00005 -0.00019 0.00012 -0.00007 2.69216

R60 2.67590 -0.00005 -0.00013 0.00009 -0.00004 2.67586

R61 2.05023 -0.00002 0.00001 -0.00005 -0.00004 2.05019

R62 2.67812 -0.00004 -0.00023 0.00012 -0.00010 2.67802

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R64 2.72703 -0.00010 0.00001 -0.00010 -0.00009 2.72695

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R70 2.05131 -0.00001 0.00000 -0.00003 -0.00003 2.05129

R71 2.67609 -0.00006 0.00001 -0.00008 -0.00007 2.67602

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R75 2.05131 -0.00001 0.00000 -0.00003 -0.00003 2.05129

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R78 2.66791 -0.00005 -0.00001 -0.00006 -0.00007 2.66784

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A11 2.31740 -0.00004 -0.00007 -0.00002 -0.00010 2.31730

A12 2.11339 0.00001 0.00004 -0.00001 0.00002 2.11342

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A22 2.17058 0.00003 0.00038 -0.00002 0.00036 2.17094

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A73 2.09016 0.00001 0.00004 -0.00003 0.00001 2.09017

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D4 0.15396 -0.00005 -0.00825 -0.00497 -0.01322 0.14073

D5 -0.01119 -0.00001 0.00008 -0.00041 -0.00033 -0.01152

D6 3.14126 0.00002 0.00168 0.00168 0.00336 -3.13857

D7 3.10493 0.00000 -0.00033 0.00019 -0.00014 3.10479

D8 -0.02581 0.00003 0.00127 0.00228 0.00355 -0.02226

D9 0.09327 0.00003 0.00495 0.00314 0.00809 0.10136

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D11 -0.01884 -0.00002 0.00014 -0.00069 -0.00055 -0.01939

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D14 -0.15396 0.00005 0.00825 0.00497 0.01322 -0.14073

D15 -2.95985 0.00004 0.00400 0.00301 0.00702 -2.95284

D16 -0.30510 0.00003 0.00572 0.00269 0.00841 -0.29669

D17 -1.63248 0.00003 0.00486 0.00285 0.00771 -1.62476

D18 0.30510 -0.00003 -0.00572 -0.00269 -0.00841 0.29669

D19 2.95985 -0.00004 -0.00400 -0.00301 -0.00702 2.95284

D20 1.63248 -0.00003 -0.00486 -0.00285 -0.00771 1.62476

D21 0.01119 0.00001 -0.00008 0.00041 0.00033 0.01152

D22 -3.14126 -0.00002 -0.00168 -0.00168 -0.00336 3.13857

D23 -3.10493 0.00000 0.00033 -0.00019 0.00014 -3.10479

D24 0.02581 -0.00003 -0.00127 -0.00228 -0.00355 0.02226

D25 -0.09327 -0.00003 -0.00495 -0.00314 -0.00809 -0.10136

D26 3.01779 -0.00002 -0.00545 -0.00242 -0.00786 3.00992

D27 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D28 3.13229 -0.00003 -0.00137 -0.00180 -0.00317 3.12913

D29 -3.13229 0.00003 0.00137 0.00180 0.00317 -3.12913

D30 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D35 3.13503 -0.00005 -0.00197 -0.00291 -0.00487 3.13015

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D55 -3.00714 -0.00005 0.00296 -0.00129 0.00166 -3.00547

D56 3.00714 0.00005 -0.00296 0.00129 -0.00166 3.00547

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D77 3.07097 0.00001 -0.00228 -0.00026 -0.00255 3.06842

D78 -0.02584 0.00002 -0.00031 0.00092 0.00061 -0.02523

D79 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D80 3.13438 0.00000 -0.00019 -0.00039 -0.00058 3.13380

D81 -3.13438 0.00000 0.00019 0.00039 0.00058 -3.13380

D82 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D83 -3.07999 -0.00001 0.00333 0.00082 0.00415 -3.07584

D84 0.02457 -0.00001 0.00170 -0.00016 0.00154 0.02611

D85 0.05330 -0.00001 0.00311 0.00038 0.00348 0.05678

D86 -3.12532 -0.00002 0.00148 -0.00061 0.00087 -3.12445

D87 -0.00776 0.00000 -0.00030 -0.00014 -0.00043 -0.00819

D88 3.13684 0.00000 -0.00027 -0.00013 -0.00041 3.13643

D89 -3.14001 0.00000 -0.00004 0.00037 0.00032 -3.13969

D90 0.00459 0.00000 -0.00002 0.00037 0.00035 0.00493

D91 -0.02457 0.00001 -0.00170 0.00016 -0.00154 -0.02611

D92 3.07999 0.00001 -0.00333 -0.00082 -0.00415 3.07584

D93 3.12532 0.00002 -0.00148 0.00061 -0.00087 3.12445

D94 -0.05330 0.00001 -0.00311 -0.00038 -0.00348 -0.05678

D95 0.00776 0.00000 0.00030 0.00014 0.00043 0.00819

D96 -3.13684 0.00000 0.00027 0.00013 0.00041 -3.13643

D97 3.14001 0.00000 0.00004 -0.00037 -0.00032 3.13969

D98 -0.00459 0.00000 0.00002 -0.00037 -0.00035 -0.00493

D99 0.04123 -0.00002 0.00285 -0.00027 0.00258 0.04381

D100 -2.90354 0.00002 -0.00152 0.00129 -0.00023 -2.90377

D101 -3.06081 -0.00002 0.00460 0.00077 0.00536 -3.05544

D102 0.27761 0.00003 0.00023 0.00233 0.00256 0.28016

D103 -3.07097 -0.00001 0.00228 0.00026 0.00255 -3.06842

D104 0.02584 -0.00002 0.00031 -0.00092 -0.00061 0.02523

D105 3.06081 0.00002 -0.00460 -0.00077 -0.00536 3.05544

D106 -0.04123 0.00002 -0.00285 0.00027 -0.00258 -0.04381

D107 -0.27761 -0.00003 -0.00023 -0.00233 -0.00256 -0.28016

D108 2.90354 -0.00002 0.00152 -0.00129 0.00023 2.90377

D109 -3.00714 -0.00005 0.00296 -0.00129 0.00166 -3.00547

D110 -1.68288 -0.00003 0.00247 -0.00090 0.00157 -1.68131

D111 -0.35862 -0.00001 0.00198 -0.00051 0.00148 -0.35715

D112 0.35862 0.00001 -0.00198 0.00051 -0.00148 0.35715

D113 1.68288 0.00003 -0.00247 0.00090 -0.00157 1.68131

D114 3.00714 0.00005 -0.00296 0.00129 -0.00166 3.00547

D115 -0.09327 -0.00003 -0.00495 -0.00314 -0.00809 -0.10136

D116 3.01779 -0.00002 -0.00545 -0.00242 -0.00786 3.00992

D117 3.09590 -0.00001 -0.00030 -0.00006 -0.00036 3.09554

D118 -0.01884 -0.00002 0.00014 -0.00069 -0.00055 -0.01939

D119 -0.15396 0.00005 0.00825 0.00497 0.01322 -0.14073

D120 3.01449 0.00004 0.00869 0.00434 0.01303 3.02752

D121 0.01884 0.00002 -0.00014 0.00069 0.00055 0.01939

D122 -3.09590 0.00001 0.00030 0.00006 0.00036 -3.09554

D123 -3.01449 -0.00004 -0.00869 -0.00434 -0.01303 -3.02752

D124 0.15396 -0.00005 -0.00825 -0.00497 -0.01322 0.14073

D125 1.63248 -0.00003 -0.00486 -0.00285 -0.00771 1.62476

D126 2.95985 -0.00004 -0.00400 -0.00301 -0.00702 2.95284

D127 0.30510 -0.00003 -0.00572 -0.00269 -0.00841 0.29669

D128 -1.63248 0.00003 0.00486 0.00285 0.00771 -1.62476

D129 -0.30510 0.00003 0.00572 0.00269 0.00841 -0.29669

D130 -2.95985 0.00004 0.00400 0.00301 0.00702 -2.95284

D131 -3.10493 0.00000 0.00033 -0.00019 0.00014 -3.10479

D132 0.02581 -0.00003 -0.00127 -0.00228 -0.00355 0.02226

D133 0.01119 0.00001 -0.00008 0.00041 0.00033 0.01152

D134 -3.14126 -0.00002 -0.00168 -0.00168 -0.00336 3.13857

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.13229 -0.00003 -0.00137 -0.00180 -0.00317 3.12913

D137 -3.13229 0.00003 0.00137 0.00180 0.00317 -3.12913

D138 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D139 -3.13503 0.00005 0.00197 0.00291 0.00487 -3.13015

D140 0.00609 0.00004 0.00133 0.00210 0.00342 0.00952

D141 -0.00561 0.00001 0.00017 0.00056 0.00073 -0.00488

D142 3.13552 0.00000 -0.00047 -0.00025 -0.00072 3.13480

D143 -0.01119 -0.00001 0.00008 -0.00041 -0.00033 -0.01152

D144 3.10493 0.00000 -0.00033 0.00019 -0.00014 3.10479

D145 3.14126 0.00002 0.00168 0.00168 0.00336 -3.13857

D146 -0.02581 0.00003 0.00127 0.00228 0.00355 -0.02226

D147 0.00561 -0.00001 -0.00017 -0.00056 -0.00073 0.00488

D148 -3.13552 0.00000 0.00047 0.00025 0.00072 -3.13480

D149 3.13503 -0.00005 -0.00197 -0.00291 -0.00487 3.13015

D150 -0.00609 -0.00004 -0.00133 -0.00210 -0.00342 -0.00952

D151 0.09327 0.00003 0.00495 0.00314 0.00809 0.10136

D152 -3.01779 0.00002 0.00545 0.00242 0.00786 -3.00992

D153 0.00762 0.00000 0.00029 0.00013 0.00042 0.00805

D154 -3.13399 0.00000 0.00032 0.00001 0.00033 -3.13365

D155 -3.13692 0.00000 0.00027 0.00013 0.00040 -3.13652

D156 0.00465 0.00000 0.00030 0.00001 0.00031 0.00496

D157 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D158 3.14158 0.00000 0.00003 -0.00012 -0.00009 3.14149

D159 -3.14158 0.00000 -0.00003 0.00012 0.00009 -3.14149

D160 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D161 3.14146 0.00000 -0.00002 0.00009 0.00007 3.14153

D162 -0.00036 0.00000 -0.00002 0.00008 0.00006 -0.00030

D163 -0.00015 0.00000 0.00001 -0.00003 -0.00002 -0.00017

D164 3.14122 0.00000 0.00000 -0.00004 -0.00003 3.14119

D165 -0.00762 0.00000 -0.00029 -0.00013 -0.00042 -0.00805

D166 3.13692 0.00000 -0.00027 -0.00013 -0.00040 3.13652

D167 3.13399 0.00000 -0.00032 -0.00001 -0.00033 3.13365

D168 -0.00465 0.00000 -0.00030 -0.00001 -0.00031 -0.00496

D169 0.00015 0.00000 -0.00001 0.00003 0.00002 0.00017

D170 -3.14122 0.00000 0.00000 0.00004 0.00003 -3.14119

D171 -3.14146 0.00000 0.00002 -0.00009 -0.00007 -3.14153

D172 0.00036 0.00000 0.00002 -0.00008 -0.00006 0.00030

D173 -0.00554 0.00001 0.00017 0.00055 0.00072 -0.00482

D174 3.13757 0.00002 0.00062 0.00096 0.00159 3.13916

D175 3.13559 0.00000 -0.00046 -0.00024 -0.00070 3.13489

D176 -0.00448 0.00001 -0.00001 0.00017 0.00016 -0.00432

D177 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D178 -3.14012 0.00000 0.00044 0.00040 0.00084 -3.13928

D179 3.14012 0.00000 -0.00044 -0.00040 -0.00084 3.13928

D180 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D181 3.14070 -0.00001 -0.00034 -0.00047 -0.00081 3.13989

D182 -0.00173 0.00000 -0.00040 -0.00042 -0.00082 -0.00256

D183 0.00061 0.00000 0.00011 -0.00006 0.00005 0.00065

D184 3.14136 0.00000 0.00004 -0.00001 0.00003 3.14139

D185 0.00554 -0.00001 -0.00017 -0.00055 -0.00072 0.00482

D186 -3.13559 0.00000 0.00046 0.00024 0.00070 -3.13489

D187 -3.13757 -0.00002 -0.00062 -0.00096 -0.00159 -3.13916

D188 0.00448 -0.00001 0.00001 -0.00017 -0.00016 0.00432

D189 -0.00061 0.00000 -0.00011 0.00006 -0.00005 -0.00065

D190 -3.14136 0.00000 -0.00004 0.00001 -0.00003 -3.14139

D191 -3.14070 0.00001 0.00034 0.00047 0.00081 -3.13989

D192 0.00173 0.00000 0.00040 0.00042 0.00082 0.00256

D193 -0.00762 0.00000 -0.00029 -0.00013 -0.00042 -0.00805

D194 3.13399 0.00000 -0.00032 -0.00001 -0.00033 3.13365

D195 3.13692 0.00000 -0.00027 -0.00013 -0.00040 3.13652

D196 -0.00465 0.00000 -0.00030 -0.00001 -0.00031 -0.00496

D197 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D198 -3.14158 0.00000 -0.00003 0.00012 0.00009 -3.14149

D199 3.14158 0.00000 0.00003 -0.00012 -0.00009 3.14149

D200 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D201 -3.14146 0.00000 0.00002 -0.00009 -0.00007 -3.14153

D202 0.00036 0.00000 0.00002 -0.00008 -0.00006 0.00030

D203 0.00015 0.00000 -0.00001 0.00003 0.00002 0.00017

D204 -3.14122 0.00000 0.00000 0.00004 0.00003 -3.14119

D205 0.00762 0.00000 0.00029 0.00013 0.00042 0.00805

D206 -3.13692 0.00000 0.00027 0.00013 0.00040 -3.13652

D207 -3.13399 0.00000 0.00032 0.00001 0.00033 -3.13365

D208 0.00465 0.00000 0.00030 0.00001 0.00031 0.00496

D209 -0.00015 0.00000 0.00001 -0.00003 -0.00002 -0.00017

D210 3.14122 0.00000 0.00000 -0.00004 -0.00003 3.14119

D211 3.14146 0.00000 -0.00002 0.00009 0.00007 3.14153

D212 -0.00036 0.00000 -0.00002 0.00008 0.00006 -0.00030

D213 -0.00554 0.00001 0.00017 0.00055 0.00072 -0.00482

D214 3.13757 0.00002 0.00062 0.00096 0.00159 3.13916

D215 3.13559 0.00000 -0.00046 -0.00024 -0.00070 3.13489

D216 -0.00448 0.00001 -0.00001 0.00017 0.00016 -0.00432

D217 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D218 -3.14012 0.00000 0.00044 0.00040 0.00084 -3.13928

D219 3.14012 0.00000 -0.00044 -0.00040 -0.00084 3.13928

D220 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D221 3.14070 -0.00001 -0.00034 -0.00047 -0.00081 3.13989

D222 -0.00173 0.00000 -0.00040 -0.00042 -0.00082 -0.00256

D223 0.00061 0.00000 0.00011 -0.00006 0.00005 0.00065

D224 3.14136 0.00000 0.00004 -0.00001 0.00003 3.14139

D225 0.00554 -0.00001 -0.00017 -0.00055 -0.00072 0.00482

D226 -3.13559 0.00000 0.00046 0.00024 0.00070 -3.13489

D227 -3.13757 -0.00002 -0.00062 -0.00096 -0.00159 -3.13916

D228 0.00448 -0.00001 0.00001 -0.00017 -0.00016 0.00432

D229 -0.00061 0.00000 -0.00011 0.00006 -0.00005 -0.00065

D230 -3.14136 0.00000 -0.00004 0.00001 -0.00003 -3.14139

D231 -3.14070 0.00001 0.00034 0.00047 0.00081 -3.13989

D232 0.00173 0.00000 0.00040 0.00042 0.00082 0.00256

D233 0.00062 0.00000 0.00011 -0.00006 0.00005 0.00066

D234 -3.14138 0.00000 0.00013 0.00005 0.00018 -3.14120

D235 3.14135 0.00000 0.00004 -0.00001 0.00003 3.14138

D236 -0.00065 0.00000 0.00006 0.00010 0.00016 -0.00048

D237 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D238 3.14119 0.00000 0.00002 0.00011 0.00013 3.14132

D239 -3.14119 0.00000 -0.00002 -0.00011 -0.00013 -3.14132

D240 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D241 -0.00062 0.00000 -0.00011 0.00006 -0.00005 -0.00066

D242 -3.14135 0.00000 -0.00004 0.00001 -0.00003 -3.14138

D243 3.14138 0.00000 -0.00013 -0.00005 -0.00018 3.14120

D244 0.00065 0.00000 -0.00006 -0.00010 -0.00016 0.00048

D245 -0.00015 0.00000 0.00001 -0.00003 -0.00002 -0.00017

D246 -3.14112 0.00000 0.00001 -0.00002 -0.00001 -3.14113

D247 3.14121 0.00000 0.00000 -0.00004 -0.00003 3.14118

D248 0.00024 0.00000 0.00001 -0.00003 -0.00002 0.00022

D249 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D250 -3.14097 0.00000 0.00000 0.00001 0.00001 -3.14096

D251 3.14097 0.00000 0.00000 -0.00001 -0.00001 3.14096

D252 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D253 0.00015 0.00000 -0.00001 0.00003 0.00002 0.00017

D254 -3.14121 0.00000 0.00000 0.00004 0.00003 -3.14118

D255 3.14112 0.00000 -0.00001 0.00002 0.00001 3.14113

D256 -0.00024 0.00000 -0.00001 0.00003 0.00002 -0.00022

D257 0.00062 0.00000 0.00011 -0.00006 0.00005 0.00066

D258 -3.14138 0.00000 0.00013 0.00005 0.00018 -3.14120

D259 3.14135 0.00000 0.00004 -0.00001 0.00003 3.14138

D260 -0.00065 0.00000 0.00006 0.00010 0.00016 -0.00048

D261 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D262 3.14119 0.00000 0.00002 0.00011 0.00013 3.14132

D263 -3.14119 0.00000 -0.00002 -0.00011 -0.00013 -3.14132

D264 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D265 -0.00062 0.00000 -0.00011 0.00006 -0.00005 -0.00066

D266 -3.14135 0.00000 -0.00004 0.00001 -0.00003 -3.14138

D267 3.14138 0.00000 -0.00013 -0.00005 -0.00018 3.14120

D268 0.00065 0.00000 -0.00006 -0.00010 -0.00016 0.00048

D269 0.00015 0.00000 -0.00001 0.00003 0.00002 0.00017

D270 3.14112 0.00000 -0.00001 0.00002 0.00001 3.14113

D271 -3.14121 0.00000 0.00000 0.00004 0.00003 -3.14118

D272 -0.00024 0.00000 -0.00001 0.00003 0.00002 -0.00022

D273 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D274 3.14097 0.00000 0.00000 -0.00001 -0.00001 3.14096

D275 -3.14097 0.00000 0.00000 0.00001 0.00001 -3.14096

D276 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D277 -0.00015 0.00000 0.00001 -0.00003 -0.00002 -0.00017

D278 3.14121 0.00000 0.00000 -0.00004 -0.00003 3.14118

D279 -3.14112 0.00000 0.00001 -0.00002 -0.00001 -3.14113

D280 0.00024 0.00000 0.00001 -0.00003 -0.00002 0.00022

Item Value Threshold Converged?

Maximum Force 0.000186 0.000450 YES

RMS Force 0.000038 0.000300 YES

Maximum Displacement 0.158287 0.001800 NO

RMS Displacement 0.027205 0.001200 NO

Predicted change in Energy=-5.849112D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Jun 30 20:46:28 2019, MaxMem= 1342177280 cpu: 151.2

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

Stoichiometry C48H24N8Zn(3)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C48H24N4)]

Deg. of freedom 61

Full point group C2V NOp 4

RotChk: IX=0 Diff= 7.93D-15

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 1.121188 2.790571 0.183943

2 7 0 0.000000 2.023697 0.320651

3 6 0 -1.121188 2.790571 0.183943

4 6 0 -0.717689 4.168252 -0.034550

5 6 0 0.717689 4.168252 -0.034550

6 7 0 -2.412479 2.383492 0.206461

7 6 0 -2.794692 1.127615 0.260738

8 7 0 -2.011489 0.000000 0.331946

9 6 0 -2.794692 -1.127615 0.260738

10 6 0 -4.208319 -0.712215 0.193717

11 6 0 -4.208319 0.712215 0.193717

12 7 0 2.412479 2.383492 0.206461

13 6 0 4.208319 0.712215 0.193717

14 6 0 4.208319 -0.712215 0.193717

15 6 0 2.794692 -1.127615 0.260738

16 7 0 2.011489 0.000000 0.331946

17 6 0 2.794692 1.127615 0.260738

18 7 0 2.412479 -2.383492 0.206461

19 7 0 0.000000 -2.023697 0.320651

20 6 0 1.121188 -2.790571 0.183943

21 6 0 0.717689 -4.168252 -0.034550

22 6 0 -0.717689 -4.168252 -0.034550

23 6 0 -1.121188 -2.790571 0.183943

24 7 0 -2.412479 -2.383492 0.206461

25 30 0 0.000000 0.000000 0.846545

26 6 0 5.373234 1.426166 0.129384

27 6 0 6.608555 0.718931 0.071407

28 6 0 6.608555 -0.718931 0.071407

29 6 0 5.373234 -1.426166 0.129384

30 6 0 -1.428236 -5.329676 -0.233618

31 6 0 -0.721519 -6.541382 -0.435172

32 6 0 0.721519 -6.541382 -0.435172

33 6 0 1.428236 -5.329676 -0.233618

34 6 0 -5.373234 1.426166 0.129384

35 6 0 -6.608555 0.718931 0.071407

36 6 0 -6.608555 -0.718931 0.071407

37 6 0 -5.373234 -1.426166 0.129384

38 6 0 1.428236 5.329676 -0.233618

39 6 0 0.721519 6.541382 -0.435172

40 6 0 -0.721519 6.541382 -0.435172

41 6 0 -1.428236 5.329676 -0.233618

42 6 0 1.402290 -7.770112 -0.642484

43 6 0 0.708043 -8.939572 -0.839017

44 6 0 -0.708043 -8.939572 -0.839017

45 6 0 -1.402290 -7.770112 -0.642484

46 6 0 7.847913 -1.401327 0.013108

47 6 0 9.035138 -0.705880 -0.042539

48 6 0 9.035138 0.705880 -0.042539

49 6 0 7.847913 1.401327 0.013108

50 6 0 -1.402290 7.770112 -0.642484

51 6 0 -0.708043 8.939572 -0.839017

52 6 0 0.708043 8.939572 -0.839017

53 6 0 1.402290 7.770112 -0.642484

54 6 0 -7.847913 -1.401327 0.013108

55 6 0 -9.035138 -0.705880 -0.042539

56 6 0 -9.035138 0.705880 -0.042539

57 6 0 -7.847913 1.401327 0.013108

58 1 0 5.373128 2.511069 0.124610

59 1 0 5.373128 -2.511069 0.124610

60 1 0 -2.513290 -5.331914 -0.240395

61 1 0 2.513290 -5.331914 -0.240395

62 1 0 -5.373128 2.511069 0.124610

63 1 0 -5.373128 -2.511069 0.124610

64 1 0 2.513290 5.331914 -0.240395

65 1 0 -2.513290 5.331914 -0.240395

66 1 0 2.487782 -7.768617 -0.642035

67 1 0 1.243430 -9.869916 -0.995627

68 1 0 -1.243430 -9.869916 -0.995627

69 1 0 -2.487782 -7.768617 -0.642035

70 1 0 7.846186 -2.486606 0.012803

71 1 0 9.976735 -1.242393 -0.087267

72 1 0 9.976735 1.242393 -0.087267

73 1 0 7.846186 2.486606 0.012803

74 1 0 -2.487782 7.768617 -0.642035

75 1 0 -1.243430 9.869916 -0.995627

76 1 0 1.243430 9.869916 -0.995627

77 1 0 2.487782 7.768617 -0.642035

78 1 0 -7.846186 -2.486606 0.012803

79 1 0 -9.976735 -1.242393 -0.087267

80 1 0 -9.976735 1.242393 -0.087267

81 1 0 -7.846186 2.486606 0.012803

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

Rotational constants (GHZ): 0.0387016 0.0379892 0.0193668

Leave Link 202 at Sun Jun 30 20:46:28 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 307 symmetry adapted cartesian basis functions of A1 symmetry.

There are 278 symmetry adapted cartesian basis functions of A2 symmetry.

There are 289 symmetry adapted cartesian basis functions of B1 symmetry.

There are 289 symmetry adapted cartesian basis functions of B2 symmetry.

There are 289 symmetry adapted basis functions of A1 symmetry.

There are 265 symmetry adapted basis functions of A2 symmetry.

There are 275 symmetry adapted basis functions of B1 symmetry.

There are 275 symmetry adapted basis functions of B2 symmetry.

1104 basis functions, 1951 primitive gaussians, 1163 cartesian basis functions

191 alpha electrons 189 beta electrons

nuclear repulsion energy 6889.3192755826 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= 81 NActive= 81 NUniq= 22 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= -0.2361092784 Hartrees.

Nuclear repulsion after empirical dispersion term = 6889.0831663042 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= 81.

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

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GePol: Number of generator spheres = 81

GePol: Total number of spheres = 81

GePol: Number of exposed spheres = 81 (100.00%)

GePol: Number of points = 6422

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.96D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 386

GePol: Fraction of low-weight points (<1% of avg) = 6.01%

GePol: Cavity surface area = 670.443 Ang\*\*2

GePol: Cavity volume = 694.274 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0170187762 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 6889.0661475280 Hartrees.

Leave Link 301 at Sun Jun 30 20:46:29 2019, MaxMem= 1342177280 cpu: 1.7

(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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36719 LenP2D= 95208.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1104 RedAO= T EigKep= 2.89D-05 NBF= 289 265 275 275

NBsUse= 1104 1.00D-06 EigRej= -1.00D+00 NBFU= 289 265 275 275

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= 1060 1060 1060 1060 1060 MxSgAt= 81 MxSgA2= 81.

Leave Link 302 at Sun Jun 30 20:46:57 2019, MaxMem= 1342177280 cpu: 282.4

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Jun 30 20:46:57 2019, MaxMem= 1342177280 cpu: 4.5

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

Initial guess from the checkpoint file: "ZnNPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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The electronic state of the initial guess is 3-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -2348.36346701668

Leave Link 401 at Sun Jun 30 20:47:27 2019, MaxMem= 1342177280 cpu: 293.2

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4103221 IEndB= 4103221 NGot= 1342177280 MDV= 1339444432

LenX= 1339444432 LenY= 1338090700

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= 420000000 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= 123726252.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.10D-15 for 6418.

Iteration 1 A\*A^-1 deviation from orthogonality is 7.76D-15 for 6408 1184.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.22D-15 for 6418.

Iteration 1 A^-1\*A deviation from orthogonality is 8.58D-10 for 1535 1446.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.77D-15 for 30.

Iteration 2 A\*A^-1 deviation from orthogonality is 6.10D-15 for 3961 602.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 823.

Iteration 2 A^-1\*A deviation from orthogonality is 3.77D-16 for 3613 1019.

E= -2348.12917173102

DIIS: error= 1.24D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2348.12917173102 IErMin= 1 ErrMin= 1.24D-03

ErrMax= 1.24D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.02D-03 BMatP= 3.02D-03

IDIUse=3 WtCom= 9.88D-01 WtEn= 1.24D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.378 Goal= None Shift= 0.000

Gap= 0.459 Goal= None Shift= 0.000

GapD= 0.378 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

RMSDP=3.27D-05 MaxDP=1.32D-03 OVMax= 7.73D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.27D-05 CP: 1.00D+00

E= -2348.13070631679 Delta-E= -0.001534585765 Rises=F Damp=F

DIIS: error= 1.69D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2348.13070631679 IErMin= 2 ErrMin= 1.69D-04

ErrMax= 1.69D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.16D-05 BMatP= 3.02D-03

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.69D-03

Coeff-Com: -0.751D-01 0.108D+01

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

Coeff: -0.750D-01 0.107D+01

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=5.03D-06 MaxDP=2.16D-04 DE=-1.53D-03 OVMax= 1.21D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 3.85D-06 CP: 1.00D+00 1.10D+00

E= -2348.13072868750 Delta-E= -0.000022370716 Rises=F Damp=F

DIIS: error= 2.88D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2348.13072868750 IErMin= 3 ErrMin= 2.88D-05

ErrMax= 2.88D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.55D-06 BMatP= 3.16D-05

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

Coeff-Com: -0.181D-01 0.211D+00 0.807D+00

Coeff: -0.181D-01 0.211D+00 0.807D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.36D-06 MaxDP=1.03D-04 DE=-2.24D-05 OVMax= 3.07D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.33D-06 CP: 1.00D+00 1.11D+00 9.52D-01

E= -2348.13072889250 Delta-E= -0.000000205002 Rises=F Damp=F

DIIS: error= 3.68D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2348.13072889250 IErMin= 3 ErrMin= 2.88D-05

ErrMax= 3.68D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.28D-06 BMatP= 2.55D-06

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

Coeff-Com: -0.419D-02 0.296D-01 0.486D+00 0.488D+00

Coeff: -0.419D-02 0.296D-01 0.486D+00 0.488D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=7.44D-07 MaxDP=8.06D-05 DE=-2.05D-07 OVMax= 2.02D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.38D-07 CP: 1.00D+00 1.11D+00 1.01D+00 5.79D-01

E= -2348.13072938794 Delta-E= -0.000000495438 Rises=F Damp=F

DIIS: error= 1.05D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2348.13072938794 IErMin= 5 ErrMin= 1.05D-05

ErrMax= 1.05D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.70D-07 BMatP= 2.28D-06

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

Coeff-Com: 0.110D-02-0.252D-01 0.103D+00 0.249D+00 0.672D+00

Coeff: 0.110D-02-0.252D-01 0.103D+00 0.249D+00 0.672D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.84D-07 MaxDP=2.31D-05 DE=-4.95D-07 OVMax= 5.04D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.08D-07 CP: 1.00D+00 1.11D+00 1.02D+00 6.30D-01 7.24D-01

E= -2348.13072942234 Delta-E= -0.000000034403 Rises=F Damp=F

DIIS: error= 2.54D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2348.13072942234 IErMin= 6 ErrMin= 2.54D-06

ErrMax= 2.54D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.79D-08 BMatP= 1.70D-07

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

Coeff-Com: 0.803D-03-0.162D-01 0.450D-01 0.133D+00 0.405D+00 0.432D+00

Coeff: 0.803D-03-0.162D-01 0.450D-01 0.133D+00 0.405D+00 0.432D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=6.90D-08 MaxDP=4.68D-06 DE=-3.44D-08 OVMax= 1.68D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 4.37D-08 CP: 1.00D+00 1.11D+00 1.02D+00 6.42D-01 7.29D-01

CP: 5.31D-01

E= -2348.13072942674 Delta-E= -0.000000004398 Rises=F Damp=F

DIIS: error= 6.05D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2348.13072942674 IErMin= 7 ErrMin= 6.05D-07

ErrMax= 6.05D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.82D-10 BMatP= 1.79D-08

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

Coeff-Com: 0.171D-03-0.284D-02 0.202D-02 0.165D-01 0.661D-01 0.196D+00

Coeff-Com: 0.722D+00

Coeff: 0.171D-03-0.284D-02 0.202D-02 0.165D-01 0.661D-01 0.196D+00

Coeff: 0.722D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.91D-08 MaxDP=1.07D-06 DE=-4.40D-09 OVMax= 5.89D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.47D-08 CP: 1.00D+00 1.11D+00 1.02D+00 6.43D-01 7.29D-01

CP: 6.37D-01 9.36D-01

E= -2348.13072942721 Delta-E= -0.000000000469 Rises=F Damp=F

DIIS: error= 2.44D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2348.13072942721 IErMin= 8 ErrMin= 2.44D-07

ErrMax= 2.44D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.65D-10 BMatP= 9.82D-10

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

Coeff-Com: -0.188D-04 0.748D-03-0.540D-02-0.101D-01-0.207D-01 0.506D-01

Coeff-Com: 0.417D+00 0.568D+00

Coeff: -0.188D-04 0.748D-03-0.540D-02-0.101D-01-0.207D-01 0.506D-01

Coeff: 0.417D+00 0.568D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=9.27D-09 MaxDP=6.17D-07 DE=-4.69D-10 OVMax= 3.81D-06

Error on total polarization charges = 0.08833

SCF Done: E(UB3LYP) = -2348.13072943 A.U. after 8 cycles

NFock= 8 Conv=0.93D-08 -V/T= 1.9830

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

<L.S>= 0.000000000000E+00

KE= 2.388746955779D+03 PE=-1.932155301845D+04 EE= 7.695609185719D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -10.68

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0219, after 2.0003

Leave Link 502 at Sun Jun 30 20:54:14 2019, MaxMem= 1342177280 cpu: 4324.0

(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.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36719 LenP2D= 95208.

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 = 195

Leave Link 701 at Sun Jun 30 20:54:49 2019, MaxMem= 1342177280 cpu: 340.5

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sun Jun 30 20:54:49 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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 Sun Jun 30 20:55:34 2019, MaxMem= 1342177280 cpu: 491.6

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-1.31450406D-13 1.02673425D-12 8.85684682D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000007481 0.000107895 -0.000076369

2 7 0.000000000 -0.000165466 0.000184456

3 6 0.000007481 0.000107895 -0.000076369

4 6 0.000019409 -0.000057421 0.000100902

5 6 -0.000019409 -0.000057421 0.000100902

6 7 -0.000048867 0.000184216 0.000004681

7 6 -0.000196702 -0.000190460 0.000048526

8 7 0.000150941 0.000000000 -0.000387409

9 6 -0.000196702 0.000190460 0.000048526

10 6 0.000128603 -0.000061200 0.000084315

11 6 0.000128603 0.000061200 0.000084315

12 7 0.000048867 0.000184216 0.000004681

13 6 -0.000128603 0.000061200 0.000084315

14 6 -0.000128603 -0.000061200 0.000084315

15 6 0.000196702 0.000190460 0.000048526

16 7 -0.000150941 0.000000000 -0.000387409

17 6 0.000196702 -0.000190460 0.000048526

18 7 0.000048867 -0.000184216 0.000004681

19 7 0.000000000 0.000165466 0.000184456

20 6 -0.000007481 -0.000107895 -0.000076369

21 6 -0.000019409 0.000057421 0.000100902

22 6 0.000019409 0.000057421 0.000100902

23 6 0.000007481 -0.000107895 -0.000076369

24 7 -0.000048867 -0.000184216 0.000004681

25 30 0.000000000 0.000000000 0.000052338

26 6 0.000020138 0.000063078 -0.000028002

27 6 -0.000006672 -0.000086891 0.000000082

28 6 -0.000006672 0.000086891 0.000000082

29 6 0.000020138 -0.000063078 -0.000028002

30 6 -0.000082445 0.000022638 -0.000088218

31 6 0.000111121 -0.000012179 0.000001252

32 6 -0.000111121 -0.000012179 0.000001252

33 6 0.000082445 0.000022638 -0.000088218

34 6 -0.000020138 0.000063078 -0.000028002

35 6 0.000006672 -0.000086891 0.000000082

36 6 0.000006672 0.000086891 0.000000082

37 6 -0.000020138 -0.000063078 -0.000028002

38 6 0.000082445 -0.000022638 -0.000088218

39 6 -0.000111121 0.000012179 0.000001252

40 6 0.000111121 0.000012179 0.000001252

41 6 -0.000082445 -0.000022638 -0.000088218

42 6 0.000054559 0.000039711 0.000025076

43 6 -0.000067707 -0.000011557 -0.000015488

44 6 0.000067707 -0.000011557 -0.000015488

45 6 -0.000054559 0.000039711 0.000025076

46 6 -0.000027508 -0.000036935 0.000000147

47 6 0.000007066 0.000043871 -0.000001843

48 6 0.000007066 -0.000043871 -0.000001843

49 6 -0.000027508 0.000036935 0.000000147

50 6 -0.000054559 -0.000039711 0.000025076

51 6 0.000067707 0.000011557 -0.000015488

52 6 -0.000067707 0.000011557 -0.000015488

53 6 0.000054559 -0.000039711 0.000025076

54 6 0.000027508 -0.000036935 0.000000147

55 6 -0.000007066 0.000043871 -0.000001843

56 6 -0.000007066 -0.000043871 -0.000001843

57 6 0.000027508 0.000036935 0.000000147

58 1 0.000011852 -0.000008153 0.000005894

59 1 0.000011852 0.000008153 0.000005894

60 1 0.000008172 -0.000028263 0.000026611

61 1 -0.000008172 -0.000028263 0.000026611

62 1 -0.000011852 -0.000008153 0.000005894

63 1 -0.000011852 0.000008153 0.000005894

64 1 -0.000008172 0.000028263 0.000026611

65 1 0.000008172 0.000028263 0.000026611

66 1 -0.000004001 0.000002971 -0.000000914

67 1 0.000011870 0.000009105 0.000000799

68 1 -0.000011870 0.000009105 0.000000799

69 1 0.000004001 0.000002971 -0.000000914

70 1 -0.000003816 0.000002289 0.000000217

71 1 -0.000008135 -0.000007746 0.000000723

72 1 -0.000008135 0.000007746 0.000000723

73 1 -0.000003816 -0.000002289 0.000000217

74 1 0.000004001 -0.000002971 -0.000000914

75 1 -0.000011870 -0.000009105 0.000000799

76 1 0.000011870 -0.000009105 0.000000799

77 1 -0.000004001 -0.000002971 -0.000000914

78 1 0.000003816 0.000002289 0.000000217

79 1 0.000008135 -0.000007746 0.000000723

80 1 0.000008135 0.000007746 0.000000723

81 1 0.000003816 -0.000002289 0.000000217

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

Cartesian Forces: Max 0.000387409 RMS 0.000075585

Leave Link 716 at Sun Jun 30 20:55:35 2019, MaxMem= 1342177280 cpu: 5.9

(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 0.000146564 RMS 0.000029676

Search for a local minimum.

Step number 6 out of a maximum of 486

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .29676D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

6

DE= -7.37D-06 DEPred=-5.85D-06 R= 1.26D+00

TightC=F SS= 1.41D+00 RLast= 5.73D-02 DXNew= 5.0454D-01 1.7186D-01

Trust test= 1.26D+00 RLast= 5.73D-02 DXMaxT set to 3.00D-01

ITU= 1 1 1 1 1 0

Eigenvalues --- 0.00249 0.01431 0.01482 0.01499 0.01572

Eigenvalues --- 0.01590 0.01627 0.01640 0.01656 0.01694

Eigenvalues --- 0.01698 0.01704 0.01706 0.01713 0.01714

Eigenvalues --- 0.01725 0.01730 0.01730 0.01735 0.01737

Eigenvalues --- 0.01744 0.01751 0.01758 0.01791 0.01827

Eigenvalues --- 0.01827 0.01830 0.01851 0.01854 0.01860

Eigenvalues --- 0.01869 0.01870 0.01937 0.01965 0.01968

Eigenvalues --- 0.01968 0.01972 0.01978 0.01992 0.01992

Eigenvalues --- 0.01993 0.01993 0.01996 0.02013 0.02080

Eigenvalues --- 0.02083 0.02086 0.02086 0.02089 0.02096

Eigenvalues --- 0.02096 0.02098 0.02100 0.02103 0.02103

Eigenvalues --- 0.02105 0.02106 0.02116 0.02124 0.02124

Eigenvalues --- 0.02137 0.02144 0.02144 0.02147 0.02148

Eigenvalues --- 0.02171 0.02173 0.02213 0.02214 0.02225

Eigenvalues --- 0.02225 0.02249 0.02280 0.02286 0.02346

Eigenvalues --- 0.02467 0.03538 0.05455 0.05592 0.08065

Eigenvalues --- 0.14716 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 0.16001 0.16021 0.16047

Eigenvalues --- 0.16145 0.16274 0.17077 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22499 0.22502 0.22504

Eigenvalues --- 0.22537 0.23234 0.23235 0.23236 0.23717

Eigenvalues --- 0.23898 0.23939 0.23939 0.23940 0.23956

Eigenvalues --- 0.24257 0.24348 0.24550 0.24554 0.24557

Eigenvalues --- 0.24557 0.24573 0.24790 0.24890 0.24893

Eigenvalues --- 0.24962 0.24980 0.24984 0.24988 0.24990

Eigenvalues --- 0.24996 0.24996 0.24997 0.24997 0.25800

Eigenvalues --- 0.32865 0.32948 0.33673 0.33728 0.33836

Eigenvalues --- 0.33858 0.35039 0.35067 0.35181 0.35181

Eigenvalues --- 0.35181 0.35187 0.35202 0.35202 0.35202

Eigenvalues --- 0.35211 0.35231 0.35231 0.35231 0.35240

Eigenvalues --- 0.35249 0.35249 0.35249 0.35269 0.35270

Eigenvalues --- 0.35270 0.35270 0.35277 0.35279 0.35279

Eigenvalues --- 0.35279 0.35414 0.35426 0.35797 0.36350

Eigenvalues --- 0.36829 0.37459 0.37562 0.37969 0.38395

Eigenvalues --- 0.39275 0.39276 0.39612 0.39612 0.40188

Eigenvalues --- 0.40188 0.40256 0.40257 0.40906 0.41001

Eigenvalues --- 0.41003 0.41126 0.41604 0.41765 0.41874

Eigenvalues --- 0.42132 0.42215 0.42374 0.42730 0.42806

Eigenvalues --- 0.42906 0.42972 0.44372 0.45696 0.47124

Eigenvalues --- 0.47124 0.47215 0.47384 0.47386 0.47579

Eigenvalues --- 0.47580 0.48124 0.48218 0.48346 0.48424

Eigenvalues --- 0.48462 0.48465 0.48680 0.48707 0.48716

Eigenvalues --- 0.48729 0.49091 0.49414 0.49898 0.50392

Eigenvalues --- 0.51016 0.51285 0.52484 0.58681 0.59243

Eigenvalues --- 0.59863 0.60916

En-DIIS/RFO-DIIS IScMMF= 0 using points: 6 5 4 3 2

RFO step: Lambda=-1.23064900D-06.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 3.95D-05 SmlDif= 1.00D-05

RMS Error= 0.1023158129D-03 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.94510 -1.24670 -0.39264 0.88773 -0.19349

Iteration 1 RMS(Cart)= 0.01203936 RMS(Int)= 0.00000975

Iteration 2 RMS(Cart)= 0.00002859 RMS(Int)= 0.00000679

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000679

ITry= 1 IFail=0 DXMaxC= 6.45D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.38D-08 for atom 73.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.57991 0.00009 0.00030 0.00001 0.00030 2.58020

R2 2.74405 -0.00009 -0.00037 0.00003 -0.00033 2.74371

R3 2.55892 0.00003 0.00024 -0.00006 0.00018 2.55910

R4 2.57991 0.00009 0.00030 0.00001 0.00030 2.58020

R5 3.95125 -0.00006 -0.00117 0.00019 -0.00099 3.95027

R6 2.74405 -0.00009 -0.00037 0.00003 -0.00033 2.74371

R7 2.55892 0.00003 0.00024 -0.00006 0.00018 2.55910

R8 2.71247 0.00001 -0.00015 0.00018 0.00004 2.71251

R9 2.60029 0.00001 0.00009 -0.00001 0.00008 2.60037

R10 2.60029 0.00001 0.00009 -0.00001 0.00008 2.60037

R11 2.48286 0.00014 0.00042 -0.00008 0.00034 2.48320

R12 2.59794 0.00004 0.00010 0.00002 0.00011 2.59805

R13 2.78720 -0.00015 -0.00064 0.00006 -0.00057 2.78662

R14 2.59794 0.00004 0.00010 0.00002 0.00011 2.59805

R15 3.92358 0.00001 -0.00032 0.00017 -0.00015 3.92343

R16 2.78720 -0.00015 -0.00064 0.00006 -0.00057 2.78662

R17 2.48286 0.00014 0.00042 -0.00008 0.00034 2.48320

R18 2.69178 0.00004 -0.00007 0.00022 0.00016 2.69194

R19 2.58478 0.00001 0.00008 -0.00002 0.00006 2.58484

R20 2.58478 0.00001 0.00008 -0.00002 0.00006 2.58484

R21 2.48286 0.00014 0.00042 -0.00008 0.00034 2.48320

R22 2.69178 0.00004 -0.00007 0.00022 0.00016 2.69194

R23 2.78720 -0.00015 -0.00064 0.00006 -0.00057 2.78662

R24 2.58478 0.00001 0.00008 -0.00002 0.00006 2.58484

R25 2.78720 -0.00015 -0.00064 0.00006 -0.00057 2.78662

R26 2.58478 0.00001 0.00008 -0.00002 0.00006 2.58484

R27 2.59794 0.00004 0.00010 0.00002 0.00011 2.59805

R28 2.48286 0.00014 0.00042 -0.00008 0.00034 2.48320

R29 2.59794 0.00004 0.00010 0.00002 0.00011 2.59805

R30 3.92358 0.00001 -0.00032 0.00017 -0.00015 3.92343

R31 2.55892 0.00003 0.00024 -0.00006 0.00018 2.55910

R32 2.57991 0.00009 0.00030 0.00001 0.00030 2.58020

R33 2.57991 0.00009 0.00030 0.00001 0.00030 2.58020

R34 3.95125 -0.00006 -0.00117 0.00019 -0.00099 3.95027

R35 2.74405 -0.00009 -0.00037 0.00003 -0.00033 2.74371

R36 2.71247 0.00001 -0.00015 0.00018 0.00004 2.71251

R37 2.60029 0.00001 0.00009 -0.00001 0.00008 2.60037

R38 2.74405 -0.00009 -0.00037 0.00003 -0.00033 2.74371

R39 2.60029 0.00001 0.00009 -0.00001 0.00008 2.60037

R40 2.55892 0.00003 0.00024 -0.00006 0.00018 2.55910

R41 2.69216 -0.00002 0.00001 -0.00004 -0.00003 2.69212

R42 2.05019 -0.00001 -0.00015 0.00011 -0.00004 2.05015

R43 2.71717 -0.00005 -0.00034 0.00018 -0.00016 2.71700

R44 2.67586 -0.00002 -0.00003 0.00000 -0.00003 2.67584

R45 2.69216 -0.00002 0.00001 -0.00004 -0.00003 2.69212

R46 2.67586 -0.00002 -0.00003 0.00000 -0.00003 2.67584

R47 2.05019 -0.00001 -0.00015 0.00011 -0.00004 2.05015

R48 2.67802 -0.00001 0.00007 -0.00007 0.00000 2.67802

R49 2.05050 -0.00001 -0.00015 0.00012 -0.00004 2.05046

R50 2.72695 -0.00006 -0.00042 0.00020 -0.00022 2.72673

R51 2.68328 -0.00003 -0.00006 0.00001 -0.00005 2.68323

R52 2.67802 -0.00001 0.00007 -0.00007 0.00000 2.67802

R53 2.68328 -0.00003 -0.00006 0.00001 -0.00005 2.68323

R54 2.05050 -0.00001 -0.00015 0.00012 -0.00004 2.05046

R55 2.69216 -0.00002 0.00001 -0.00004 -0.00003 2.69212

R56 2.05019 -0.00001 -0.00015 0.00011 -0.00004 2.05015

R57 2.71717 -0.00005 -0.00034 0.00018 -0.00016 2.71700

R58 2.67586 -0.00002 -0.00003 0.00000 -0.00003 2.67584

R59 2.69216 -0.00002 0.00001 -0.00004 -0.00003 2.69212

R60 2.67586 -0.00002 -0.00003 0.00000 -0.00003 2.67584

R61 2.05019 -0.00001 -0.00015 0.00011 -0.00004 2.05015

R62 2.67802 -0.00001 0.00007 -0.00007 0.00000 2.67802

R63 2.05050 -0.00001 -0.00015 0.00012 -0.00004 2.05046

R64 2.72695 -0.00006 -0.00042 0.00020 -0.00022 2.72673

R65 2.68328 -0.00003 -0.00006 0.00001 -0.00005 2.68323

R66 2.67802 -0.00001 0.00007 -0.00007 0.00000 2.67802

R67 2.68328 -0.00003 -0.00006 0.00001 -0.00005 2.68323

R68 2.05050 -0.00001 -0.00015 0.00012 -0.00004 2.05046

R69 2.59673 0.00002 0.00000 0.00007 0.00007 2.59681

R70 2.05129 0.00000 -0.00010 0.00009 -0.00002 2.05127

R71 2.67602 -0.00003 -0.00034 0.00027 -0.00007 2.67595

R72 2.04990 0.00000 -0.00004 0.00004 0.00000 2.04990

R73 2.59673 0.00002 0.00000 0.00007 0.00007 2.59681

R74 2.04990 0.00000 -0.00004 0.00004 0.00000 2.04990

R75 2.05129 0.00000 -0.00010 0.00009 -0.00002 2.05127

R76 2.60223 0.00001 -0.00004 0.00008 0.00004 2.60227

R77 2.05088 0.00000 -0.00009 0.00009 -0.00001 2.05087

R78 2.66784 -0.00002 -0.00030 0.00026 -0.00004 2.66780

R79 2.04968 0.00000 -0.00005 0.00004 -0.00001 2.04967

R80 2.60223 0.00001 -0.00004 0.00008 0.00004 2.60227

R81 2.04968 0.00000 -0.00005 0.00004 -0.00001 2.04967

R82 2.05088 0.00000 -0.00009 0.00009 -0.00001 2.05087

R83 2.59673 0.00002 0.00000 0.00007 0.00007 2.59681

R84 2.05129 0.00000 -0.00010 0.00009 -0.00002 2.05127

R85 2.67602 -0.00003 -0.00034 0.00027 -0.00007 2.67595

R86 2.04990 0.00000 -0.00004 0.00004 0.00000 2.04990

R87 2.59673 0.00002 0.00000 0.00007 0.00007 2.59681

R88 2.04990 0.00000 -0.00004 0.00004 0.00000 2.04990

R89 2.05129 0.00000 -0.00010 0.00009 -0.00002 2.05127

R90 2.60223 0.00001 -0.00004 0.00008 0.00004 2.60227

R91 2.05088 0.00000 -0.00009 0.00009 -0.00001 2.05087

R92 2.66784 -0.00002 -0.00030 0.00026 -0.00004 2.66780

R93 2.04968 0.00000 -0.00005 0.00004 -0.00001 2.04967

R94 2.60223 0.00001 -0.00004 0.00008 0.00004 2.60227

R95 2.04968 0.00000 -0.00005 0.00004 -0.00001 2.04967

R96 2.05088 0.00000 -0.00009 0.00009 -0.00001 2.05087

A1 1.89631 0.00001 0.00013 -0.00008 0.00002 1.89634

A2 2.23015 0.00002 0.00002 0.00005 0.00009 2.23024

A3 2.15640 -0.00002 -0.00015 0.00004 -0.00010 2.15630

A4 1.92718 -0.00005 -0.00036 0.00016 -0.00018 1.92701

A5 2.17590 0.00003 0.00020 0.00002 0.00028 2.17618

A6 2.17590 0.00003 0.00020 0.00002 0.00028 2.17618

A7 1.89631 0.00001 0.00013 -0.00008 0.00002 1.89634

A8 2.23015 0.00002 0.00002 0.00005 0.00009 2.23024

A9 2.15640 -0.00002 -0.00015 0.00004 -0.00010 2.15630

A10 1.85238 0.00002 0.00006 0.00001 0.00007 1.85245

A11 2.31730 -0.00003 -0.00011 -0.00005 -0.00017 2.31713

A12 2.11342 0.00001 0.00003 0.00004 0.00006 2.11348

A13 1.85238 0.00002 0.00006 0.00001 0.00007 1.85245

A14 2.31730 -0.00003 -0.00011 -0.00005 -0.00017 2.31713

A15 2.11342 0.00001 0.00003 0.00004 0.00006 2.11348

A16 2.17177 -0.00008 -0.00041 -0.00002 -0.00042 2.17135

A17 2.24008 0.00001 -0.00017 0.00001 -0.00016 2.23993

A18 2.14856 -0.00002 -0.00010 0.00007 -0.00001 2.14854

A19 1.89375 0.00001 0.00026 -0.00007 0.00019 1.89394

A20 1.92359 -0.00004 -0.00046 0.00015 -0.00029 1.92330

A21 2.17094 0.00001 -0.00015 -0.00026 -0.00040 2.17054

A22 2.17094 0.00001 -0.00015 -0.00026 -0.00040 2.17054

A23 1.89375 0.00001 0.00026 -0.00007 0.00019 1.89394

A24 2.24008 0.00001 -0.00017 0.00001 -0.00016 2.23993

A25 2.14856 -0.00002 -0.00010 0.00007 -0.00001 2.14854

A26 1.85630 0.00001 -0.00002 0.00000 -0.00002 1.85629

A27 2.30690 -0.00001 -0.00002 -0.00002 -0.00004 2.30685

A28 2.11995 0.00000 0.00003 0.00002 0.00005 2.12000

A29 1.85630 0.00001 -0.00002 0.00000 -0.00002 1.85629

A30 2.30690 -0.00001 -0.00002 -0.00002 -0.00004 2.30685

A31 2.11995 0.00000 0.00003 0.00002 0.00005 2.12000

A32 2.17177 -0.00008 -0.00041 -0.00002 -0.00042 2.17135

A33 1.85630 0.00001 -0.00002 0.00000 -0.00002 1.85629

A34 2.11995 0.00000 0.00003 0.00002 0.00005 2.12000

A35 2.30690 -0.00001 -0.00002 -0.00002 -0.00004 2.30685

A36 1.85630 0.00001 -0.00002 0.00000 -0.00002 1.85629

A37 2.11995 0.00000 0.00003 0.00002 0.00005 2.12000

A38 2.30690 -0.00001 -0.00002 -0.00002 -0.00004 2.30685

A39 1.89375 0.00001 0.00026 -0.00007 0.00019 1.89394

A40 2.14856 -0.00002 -0.00010 0.00007 -0.00001 2.14854

A41 2.24008 0.00001 -0.00017 0.00001 -0.00016 2.23993

A42 1.92359 -0.00004 -0.00046 0.00015 -0.00029 1.92330

A43 2.17094 0.00001 -0.00015 -0.00026 -0.00040 2.17054

A44 2.17094 0.00001 -0.00015 -0.00026 -0.00040 2.17054

A45 2.14856 -0.00002 -0.00010 0.00007 -0.00001 2.14854

A46 2.24008 0.00001 -0.00017 0.00001 -0.00016 2.23993

A47 1.89375 0.00001 0.00026 -0.00007 0.00019 1.89394

A48 2.17177 -0.00008 -0.00041 -0.00002 -0.00042 2.17135

A49 1.92718 -0.00005 -0.00036 0.00016 -0.00018 1.92701

A50 2.17590 0.00003 0.00020 0.00002 0.00028 2.17618

A51 2.17590 0.00003 0.00020 0.00002 0.00028 2.17618

A52 2.23015 0.00002 0.00002 0.00005 0.00009 2.23024

A53 2.15640 -0.00002 -0.00015 0.00004 -0.00010 2.15630

A54 1.89631 0.00001 0.00013 -0.00008 0.00002 1.89634

A55 1.85238 0.00002 0.00006 0.00001 0.00007 1.85245

A56 2.31730 -0.00003 -0.00011 -0.00005 -0.00017 2.31713

A57 2.11342 0.00001 0.00003 0.00004 0.00006 2.11348

A58 1.85238 0.00002 0.00006 0.00001 0.00007 1.85245

A59 2.11342 0.00001 0.00003 0.00004 0.00006 2.11348

A60 2.31730 -0.00003 -0.00011 -0.00005 -0.00017 2.31713

A61 1.89631 0.00001 0.00013 -0.00008 0.00002 1.89634

A62 2.23015 0.00002 0.00002 0.00005 0.00009 2.23024

A63 2.15640 -0.00002 -0.00015 0.00004 -0.00010 2.15630

A64 2.17177 -0.00008 -0.00041 -0.00002 -0.00042 2.17135

A65 1.50842 0.00000 0.00006 0.00001 0.00007 1.50849

A66 1.50842 0.00000 0.00006 0.00001 0.00007 1.50849

A67 2.63310 0.00005 0.00151 0.00050 0.00202 2.63512

A68 2.64068 -0.00002 -0.00100 -0.00041 -0.00141 2.63927

A69 1.50842 0.00000 0.00006 0.00001 0.00007 1.50849

A70 1.50842 0.00000 0.00006 0.00001 0.00007 1.50849

A71 2.07292 -0.00003 -0.00014 -0.00005 -0.00019 2.07273

A72 2.12009 0.00003 0.00018 0.00001 0.00019 2.12029

A73 2.09017 0.00000 -0.00004 0.00004 0.00000 2.09017

A74 2.09028 0.00003 0.00010 0.00003 0.00014 2.09042

A75 2.11926 -0.00004 -0.00010 -0.00010 -0.00020 2.11906

A76 2.07364 0.00001 0.00000 0.00006 0.00007 2.07370

A77 2.09028 0.00003 0.00010 0.00003 0.00014 2.09042

A78 2.07364 0.00001 0.00000 0.00006 0.00007 2.07370

A79 2.11926 -0.00004 -0.00010 -0.00010 -0.00020 2.11906

A80 2.07292 -0.00003 -0.00014 -0.00005 -0.00019 2.07273

A81 2.12009 0.00003 0.00018 0.00001 0.00019 2.12029

A82 2.09017 0.00000 -0.00004 0.00004 0.00000 2.09017

A83 2.07687 -0.00004 -0.00011 -0.00009 -0.00020 2.07667

A84 2.11649 0.00004 0.00024 0.00009 0.00033 2.11682

A85 2.08981 -0.00001 -0.00013 0.00000 -0.00013 2.08969

A86 2.09288 0.00003 0.00009 0.00005 0.00014 2.09302

A87 2.11949 -0.00005 -0.00012 -0.00012 -0.00024 2.11925

A88 2.07081 0.00002 0.00003 0.00007 0.00010 2.07091

A89 2.09288 0.00003 0.00009 0.00005 0.00014 2.09302

A90 2.07081 0.00002 0.00003 0.00007 0.00010 2.07091

A91 2.11949 -0.00005 -0.00012 -0.00012 -0.00024 2.11925

A92 2.07687 -0.00004 -0.00011 -0.00009 -0.00020 2.07667

A93 2.11649 0.00004 0.00024 0.00009 0.00033 2.11682

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A95 2.07292 -0.00003 -0.00014 -0.00005 -0.00019 2.07273

A96 2.12009 0.00003 0.00018 0.00001 0.00019 2.12029

A97 2.09017 0.00000 -0.00004 0.00004 0.00000 2.09017

A98 2.09028 0.00003 0.00010 0.00003 0.00014 2.09042

A99 2.11926 -0.00004 -0.00010 -0.00010 -0.00020 2.11906

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A101 2.09028 0.00003 0.00010 0.00003 0.00014 2.09042

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A120 2.06938 0.00001 0.00001 0.00003 0.00004 2.06943

A121 2.10187 0.00001 0.00001 0.00009 0.00010 2.10197

A122 2.10044 0.00000 0.00000 0.00005 0.00004 2.10048

A123 2.09578 -0.00002 -0.00007 -0.00010 -0.00016 2.09561

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D1 0.01939 0.00000 -0.00016 -0.00018 -0.00034 0.01905

D2 -3.02752 -0.00002 -0.00257 -0.00231 -0.00488 -3.03240

D3 -3.09554 0.00001 -0.00015 -0.00042 -0.00057 -3.09610

D4 0.14073 -0.00002 -0.00256 -0.00255 -0.00510 0.13563

D5 -0.01152 0.00000 0.00009 0.00011 0.00020 -0.01132

D6 -3.13857 0.00002 0.00239 0.00047 0.00286 -3.13571

D7 3.10479 -0.00001 0.00008 0.00034 0.00042 3.10521

D8 -0.02226 0.00002 0.00237 0.00070 0.00307 -0.01919

D9 0.10136 0.00001 0.00179 0.00190 0.00369 0.10505

D10 -3.00992 0.00001 0.00180 0.00163 0.00343 -3.00649

D11 -0.01939 0.00000 0.00016 0.00018 0.00034 -0.01905

D12 3.09554 -0.00001 0.00015 0.00042 0.00057 3.09610

D13 3.02752 0.00002 0.00257 0.00231 0.00488 3.03240

D14 -0.14073 0.00002 0.00256 0.00255 0.00510 -0.13563

D15 -2.95284 0.00003 0.00189 0.00143 0.00332 -2.94952

D16 -0.29669 0.00000 0.00083 0.00100 0.00183 -0.29486

D17 -1.62476 0.00001 0.00136 0.00121 0.00257 -1.62219

D18 0.29669 0.00000 -0.00083 -0.00100 -0.00183 0.29486

D19 2.95284 -0.00003 -0.00189 -0.00143 -0.00332 2.94952

D20 1.62476 -0.00001 -0.00136 -0.00121 -0.00257 1.62219

D21 0.01152 0.00000 -0.00009 -0.00011 -0.00020 0.01132

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D23 -3.10479 0.00001 -0.00008 -0.00034 -0.00042 -3.10521

D24 0.02226 -0.00002 -0.00237 -0.00070 -0.00307 0.01919

D25 -0.10136 -0.00001 -0.00179 -0.00190 -0.00369 -0.10505

D26 3.00992 -0.00001 -0.00180 -0.00163 -0.00343 3.00649

D27 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D28 3.12913 -0.00002 -0.00197 -0.00031 -0.00228 3.12685

D29 -3.12913 0.00002 0.00197 0.00031 0.00228 -3.12685

D30 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D31 -3.13015 0.00002 0.00280 -0.00012 0.00268 -3.12747

D32 0.00952 0.00003 0.00254 0.00071 0.00325 0.01276

D33 -0.00488 0.00000 0.00023 -0.00052 -0.00030 -0.00517

D34 3.13480 0.00001 -0.00003 0.00030 0.00027 3.13506

D35 3.13015 -0.00002 -0.00280 0.00012 -0.00268 3.12747

D36 -0.00952 -0.00003 -0.00254 -0.00071 -0.00325 -0.01276

D37 0.00488 0.00000 -0.00023 0.00052 0.00030 0.00517

D38 -3.13480 -0.00001 0.00003 -0.00030 -0.00027 -3.13506

D39 0.02523 -0.00002 -0.00111 -0.00055 -0.00165 0.02358

D40 -3.06842 -0.00005 -0.00124 -0.00088 -0.00212 -3.07054

D41 -3.05544 -0.00004 -0.00122 -0.00022 -0.00143 -3.05688

D42 0.28016 0.00003 0.00261 0.00185 0.00446 0.28463

D43 0.04381 -0.00003 -0.00111 0.00008 -0.00102 0.04278

D44 -2.90377 0.00005 0.00272 0.00215 0.00487 -2.89890

D45 3.07584 0.00003 0.00075 0.00023 0.00098 3.07682

D46 -0.05678 0.00003 0.00131 0.00040 0.00170 -0.05508

D47 -0.02611 0.00001 0.00065 -0.00005 0.00060 -0.02551

D48 3.12445 0.00001 0.00120 0.00012 0.00132 3.12578

D49 -0.04381 0.00003 0.00111 -0.00008 0.00102 -0.04278

D50 3.05544 0.00004 0.00122 0.00022 0.00143 3.05688

D51 2.90377 -0.00005 -0.00272 -0.00215 -0.00487 2.89890

D52 -0.28016 -0.00003 -0.00261 -0.00185 -0.00446 -0.28463

D53 -0.35715 -0.00002 -0.00143 -0.00090 -0.00233 -0.35948

D54 -1.68131 -0.00005 -0.00220 -0.00115 -0.00335 -1.68467

D55 -3.00547 -0.00007 -0.00296 -0.00141 -0.00438 -3.00985

D56 3.00547 0.00007 0.00296 0.00141 0.00438 3.00985

D57 1.68131 0.00005 0.00220 0.00115 0.00335 1.68467

D58 0.35715 0.00002 0.00143 0.00090 0.00233 0.35948

D59 0.02611 -0.00001 -0.00065 0.00005 -0.00060 0.02551

D60 -3.12445 -0.00001 -0.00120 -0.00012 -0.00132 -3.12578

D61 -3.07584 -0.00003 -0.00075 -0.00023 -0.00098 -3.07682

D62 0.05678 -0.00003 -0.00131 -0.00040 -0.00170 0.05508

D63 -0.02523 0.00002 0.00111 0.00055 0.00165 -0.02358

D64 3.06842 0.00005 0.00124 0.00088 0.00212 3.07054

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13380 0.00000 -0.00048 -0.00015 -0.00063 3.13317

D67 -3.13380 0.00000 0.00048 0.00015 0.00063 -3.13317

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 -3.13969 0.00000 0.00063 0.00020 0.00082 -3.13887

D70 0.00493 0.00000 0.00053 0.00019 0.00072 0.00565

D71 -0.00819 0.00000 0.00001 0.00001 0.00001 -0.00818

D72 3.13643 0.00000 -0.00009 0.00000 -0.00009 3.13635

D73 3.13969 0.00000 -0.00063 -0.00020 -0.00082 3.13887

D74 -0.00493 0.00000 -0.00053 -0.00019 -0.00072 -0.00565

D75 0.00819 0.00000 -0.00001 -0.00001 -0.00001 0.00818

D76 -3.13643 0.00000 0.00009 0.00000 0.00009 -3.13635

D77 3.06842 0.00005 0.00124 0.00088 0.00212 3.07054

D78 -0.02523 0.00002 0.00111 0.00055 0.00165 -0.02358

D79 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D80 3.13380 0.00000 -0.00048 -0.00015 -0.00063 3.13317

D81 -3.13380 0.00000 0.00048 0.00015 0.00063 -3.13317

D82 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D83 -3.07584 -0.00003 -0.00075 -0.00023 -0.00098 -3.07682

D84 0.02611 -0.00001 -0.00065 0.00005 -0.00060 0.02551

D85 0.05678 -0.00003 -0.00131 -0.00040 -0.00170 0.05508

D86 -3.12445 -0.00001 -0.00120 -0.00012 -0.00132 -3.12578

D87 -0.00819 0.00000 0.00001 0.00001 0.00001 -0.00818

D88 3.13643 0.00000 -0.00009 0.00000 -0.00009 3.13635

D89 -3.13969 0.00000 0.00063 0.00020 0.00082 -3.13887

D90 0.00493 0.00000 0.00053 0.00019 0.00072 0.00565

D91 -0.02611 0.00001 0.00065 -0.00005 0.00060 -0.02551

D92 3.07584 0.00003 0.00075 0.00023 0.00098 3.07682

D93 3.12445 0.00001 0.00120 0.00012 0.00132 3.12578

D94 -0.05678 0.00003 0.00131 0.00040 0.00170 -0.05508

D95 0.00819 0.00000 -0.00001 -0.00001 -0.00001 0.00818

D96 -3.13643 0.00000 0.00009 0.00000 0.00009 -3.13635

D97 3.13969 0.00000 -0.00063 -0.00020 -0.00082 3.13887

D98 -0.00493 0.00000 -0.00053 -0.00019 -0.00072 -0.00565

D99 0.04381 -0.00003 -0.00111 0.00008 -0.00102 0.04278

D100 -2.90377 0.00005 0.00272 0.00215 0.00487 -2.89890

D101 -3.05544 -0.00004 -0.00122 -0.00022 -0.00143 -3.05688

D102 0.28016 0.00003 0.00261 0.00185 0.00446 0.28463

D103 -3.06842 -0.00005 -0.00124 -0.00088 -0.00212 -3.07054

D104 0.02523 -0.00002 -0.00111 -0.00055 -0.00165 0.02358

D105 3.05544 0.00004 0.00122 0.00022 0.00143 3.05688

D106 -0.04381 0.00003 0.00111 -0.00008 0.00102 -0.04278

D107 -0.28016 -0.00003 -0.00261 -0.00185 -0.00446 -0.28463

D108 2.90377 -0.00005 -0.00272 -0.00215 -0.00487 2.89890

D109 -3.00547 -0.00007 -0.00296 -0.00141 -0.00438 -3.00985

D110 -1.68131 -0.00005 -0.00220 -0.00115 -0.00335 -1.68467

D111 -0.35715 -0.00002 -0.00143 -0.00090 -0.00233 -0.35948

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D113 1.68131 0.00005 0.00220 0.00115 0.00335 1.68467

D114 3.00547 0.00007 0.00296 0.00141 0.00438 3.00985

D115 -0.10136 -0.00001 -0.00179 -0.00190 -0.00369 -0.10505

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D120 3.02752 0.00002 0.00257 0.00231 0.00488 3.03240

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D122 -3.09554 0.00001 -0.00015 -0.00042 -0.00057 -3.09610

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D124 0.14073 -0.00002 -0.00256 -0.00255 -0.00510 0.13563

D125 1.62476 -0.00001 -0.00136 -0.00121 -0.00257 1.62219

D126 2.95284 -0.00003 -0.00189 -0.00143 -0.00332 2.94952

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D128 -1.62476 0.00001 0.00136 0.00121 0.00257 -1.62219

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D130 -2.95284 0.00003 0.00189 0.00143 0.00332 -2.94952

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D144 3.10479 -0.00001 0.00008 0.00034 0.00042 3.10521

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D146 -0.02226 0.00002 0.00237 0.00070 0.00307 -0.01919

D147 0.00488 0.00000 -0.00023 0.00052 0.00030 0.00517

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D200 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D201 -3.14153 0.00000 -0.00005 -0.00008 -0.00013 3.14152

D202 0.00030 0.00000 -0.00006 -0.00005 -0.00011 0.00019

D203 0.00017 0.00000 0.00003 -0.00003 0.00000 0.00017

D204 -3.14119 0.00000 0.00002 0.00000 0.00002 -3.14116

D205 0.00805 0.00000 -0.00001 -0.00001 -0.00001 0.00803

D206 -3.13652 0.00000 0.00009 0.00000 0.00009 -3.13644

D207 -3.13365 0.00000 -0.00009 -0.00006 -0.00015 -3.13380

D208 0.00496 0.00000 0.00000 -0.00005 -0.00005 0.00491

D209 -0.00017 0.00000 -0.00003 0.00003 0.00000 -0.00017

D210 3.14119 0.00000 -0.00002 0.00000 -0.00002 3.14116

D211 3.14153 0.00000 0.00005 0.00008 0.00013 -3.14152

D212 -0.00030 0.00000 0.00006 0.00005 0.00011 -0.00019

D213 -0.00482 0.00000 0.00022 -0.00052 -0.00029 -0.00511

D214 3.13916 0.00000 0.00067 -0.00036 0.00030 3.13946

D215 3.13489 0.00001 -0.00003 0.00029 0.00026 3.13515

D216 -0.00432 0.00001 0.00041 0.00045 0.00086 -0.00347

D217 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D218 -3.13928 0.00000 0.00043 0.00015 0.00058 -3.13870

D219 3.13928 0.00000 -0.00043 -0.00015 -0.00058 3.13870

D220 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D221 3.13989 -0.00001 -0.00064 -0.00059 -0.00123 3.13866

D222 -0.00256 0.00000 -0.00044 -0.00005 -0.00049 -0.00305

D223 0.00065 -0.00001 -0.00020 -0.00044 -0.00064 0.00001

D224 3.14139 0.00000 0.00000 0.00010 0.00010 3.14149

D225 0.00482 0.00000 -0.00022 0.00052 0.00029 0.00511

D226 -3.13489 -0.00001 0.00003 -0.00029 -0.00026 -3.13515

D227 -3.13916 0.00000 -0.00067 0.00036 -0.00030 -3.13946

D228 0.00432 -0.00001 -0.00041 -0.00045 -0.00086 0.00347

D229 -0.00065 0.00001 0.00020 0.00044 0.00064 -0.00001

D230 -3.14139 0.00000 0.00000 -0.00010 -0.00010 -3.14149

D231 -3.13989 0.00001 0.00064 0.00059 0.00123 -3.13866

D232 0.00256 0.00000 0.00044 0.00005 0.00049 0.00305

D233 0.00066 -0.00001 -0.00020 -0.00045 -0.00065 0.00001

D234 -3.14120 -0.00001 -0.00007 -0.00038 -0.00045 3.14153

D235 3.14138 0.00000 0.00000 0.00010 0.00010 3.14148

D236 -0.00048 0.00000 0.00013 0.00017 0.00030 -0.00019

D237 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D238 3.14132 0.00000 0.00013 0.00006 0.00020 3.14152

D239 -3.14132 0.00000 -0.00013 -0.00006 -0.00020 -3.14152

D240 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D241 -0.00066 0.00001 0.00020 0.00045 0.00065 -0.00001

D242 -3.14138 0.00000 0.00000 -0.00010 -0.00010 -3.14148

D243 3.14120 0.00001 0.00007 0.00038 0.00045 -3.14153

D244 0.00048 0.00000 -0.00013 -0.00017 -0.00030 0.00019

D245 -0.00017 0.00000 -0.00003 0.00004 0.00000 -0.00017

D246 -3.14113 0.00000 -0.00004 0.00003 -0.00001 -3.14114

D247 3.14118 0.00000 -0.00002 0.00000 -0.00002 3.14116

D248 0.00022 0.00000 -0.00002 -0.00001 -0.00003 0.00019

D249 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D250 -3.14096 0.00000 0.00000 -0.00001 -0.00001 -3.14097

D251 3.14096 0.00000 0.00000 0.00001 0.00001 3.14097

D252 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D253 0.00017 0.00000 0.00003 -0.00004 0.00000 0.00017

D254 -3.14118 0.00000 0.00002 0.00000 0.00002 -3.14116

D255 3.14113 0.00000 0.00004 -0.00003 0.00001 3.14114

D256 -0.00022 0.00000 0.00002 0.00001 0.00003 -0.00019

D257 0.00066 -0.00001 -0.00020 -0.00045 -0.00065 0.00001

D258 -3.14120 -0.00001 -0.00007 -0.00038 -0.00045 3.14153

D259 3.14138 0.00000 0.00000 0.00010 0.00010 3.14148

D260 -0.00048 0.00000 0.00013 0.00017 0.00030 -0.00019

D261 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D262 3.14132 0.00000 0.00013 0.00006 0.00020 3.14152

D263 -3.14132 0.00000 -0.00013 -0.00006 -0.00020 -3.14152

D264 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D265 -0.00066 0.00001 0.00020 0.00045 0.00065 -0.00001

D266 -3.14138 0.00000 0.00000 -0.00010 -0.00010 -3.14148

D267 3.14120 0.00001 0.00007 0.00038 0.00045 -3.14153

D268 0.00048 0.00000 -0.00013 -0.00017 -0.00030 0.00019

D269 0.00017 0.00000 0.00003 -0.00004 0.00000 0.00017

D270 3.14113 0.00000 0.00004 -0.00003 0.00001 3.14114

D271 -3.14118 0.00000 0.00002 0.00000 0.00002 -3.14116

D272 -0.00022 0.00000 0.00002 0.00001 0.00003 -0.00019

D273 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D274 3.14096 0.00000 0.00000 0.00001 0.00001 3.14097

D275 -3.14096 0.00000 0.00000 -0.00001 -0.00001 -3.14097

D276 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D277 -0.00017 0.00000 -0.00003 0.00004 0.00000 -0.00017

D278 3.14118 0.00000 -0.00002 0.00000 -0.00002 3.14116

D279 -3.14113 0.00000 -0.00004 0.00003 -0.00001 -3.14114

D280 0.00022 0.00000 -0.00002 -0.00001 -0.00003 0.00019

Item Value Threshold Converged?

Maximum Force 0.000147 0.000450 YES

RMS Force 0.000030 0.000300 YES

Maximum Displacement 0.064489 0.001800 NO

RMS Displacement 0.012039 0.001200 NO

Predicted change in Energy=-6.621958D-07

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Jun 30 20:55:44 2019, MaxMem= 1342177280 cpu: 92.3

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

Stoichiometry C48H24N8Zn(3)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C48H24N4)]

Deg. of freedom 61

Full point group C2V NOp 4

RotChk: IX=0 Diff= 2.60D-14

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 1.121247 2.790405 0.185378

2 7 0 0.000000 2.023722 0.324213

3 6 0 -1.121247 2.790405 0.185378

4 6 0 -0.717700 4.167214 -0.037309

5 6 0 0.717700 4.167214 -0.037309

6 7 0 -2.412715 2.383667 0.209572

7 6 0 -2.794741 1.127549 0.263985

8 7 0 -2.011048 0.000000 0.331938

9 6 0 -2.794741 -1.127549 0.263985

10 6 0 -4.208288 -0.712256 0.201450

11 6 0 -4.208288 0.712256 0.201450

12 7 0 2.412715 2.383667 0.209572

13 6 0 4.208288 0.712256 0.201450

14 6 0 4.208288 -0.712256 0.201450

15 6 0 2.794741 -1.127549 0.263985

16 7 0 2.011048 0.000000 0.331938

17 6 0 2.794741 1.127549 0.263985

18 7 0 2.412715 -2.383667 0.209572

19 7 0 0.000000 -2.023722 0.324213

20 6 0 1.121247 -2.790405 0.185378

21 6 0 0.717700 -4.167214 -0.037309

22 6 0 -0.717700 -4.167214 -0.037309

23 6 0 -1.121247 -2.790405 0.185378

24 7 0 -2.412715 -2.383667 0.209572

25 30 0 0.000000 0.000000 0.847932

26 6 0 5.373354 1.426284 0.140075

27 6 0 6.608706 0.718888 0.085223

28 6 0 6.608706 -0.718888 0.085223

29 6 0 5.373354 -1.426284 0.140075

30 6 0 -1.428345 -5.327547 -0.242583

31 6 0 -0.721461 -6.538123 -0.450236

32 6 0 0.721461 -6.538123 -0.450236

33 6 0 1.428345 -5.327547 -0.242583

34 6 0 -5.373354 1.426284 0.140075

35 6 0 -6.608706 0.718888 0.085223

36 6 0 -6.608706 -0.718888 0.085223

37 6 0 -5.373354 -1.426284 0.140075

38 6 0 1.428345 5.327547 -0.242583

39 6 0 0.721461 6.538123 -0.450236

40 6 0 -0.721461 6.538123 -0.450236

41 6 0 -1.428345 5.327547 -0.242583

42 6 0 1.402342 -7.765576 -0.664444

43 6 0 0.708025 -8.933786 -0.868298

44 6 0 -0.708025 -8.933786 -0.868298

45 6 0 -1.402342 -7.765576 -0.664444

46 6 0 7.848143 -1.401359 0.029895

47 6 0 9.035496 -0.705870 -0.022909

48 6 0 9.035496 0.705870 -0.022909

49 6 0 7.848143 1.401359 0.029895

50 6 0 -1.402342 7.765576 -0.664444

51 6 0 -0.708025 8.933786 -0.868298

52 6 0 0.708025 8.933786 -0.868298

53 6 0 1.402342 7.765576 -0.664444

54 6 0 -7.848143 -1.401359 0.029895

55 6 0 -9.035496 -0.705870 -0.022909

56 6 0 -9.035496 0.705870 -0.022909

57 6 0 -7.848143 1.401359 0.029895

58 1 0 5.373409 2.511166 0.135211

59 1 0 5.373409 -2.511166 0.135211

60 1 0 -2.513380 -5.330072 -0.249178

61 1 0 2.513380 -5.330072 -0.249178

62 1 0 -5.373409 2.511166 0.135211

63 1 0 -5.373409 -2.511166 0.135211

64 1 0 2.513380 5.330072 -0.249178

65 1 0 -2.513380 5.330072 -0.249178

66 1 0 2.487825 -7.764008 -0.664066

67 1 0 1.243528 -9.863100 -1.030539

68 1 0 -1.243528 -9.863100 -1.030539

69 1 0 -2.487825 -7.764008 -0.664066

70 1 0 7.846364 -2.486633 0.029566

71 1 0 9.977150 -1.242461 -0.065372

72 1 0 9.977150 1.242461 -0.065372

73 1 0 7.846364 2.486633 0.029566

74 1 0 -2.487825 7.764008 -0.664066

75 1 0 -1.243528 9.863100 -1.030539

76 1 0 1.243528 9.863100 -1.030539

77 1 0 2.487825 7.764008 -0.664066

78 1 0 -7.846364 -2.486633 0.029566

79 1 0 -9.977150 -1.242461 -0.065372

80 1 0 -9.977150 1.242461 -0.065372

81 1 0 -7.846364 2.486633 0.029566

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

Rotational constants (GHZ): 0.0387223 0.0379705 0.0193757

Leave Link 202 at Sun Jun 30 20:55:44 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 307 symmetry adapted cartesian basis functions of A1 symmetry.

There are 278 symmetry adapted cartesian basis functions of A2 symmetry.

There are 289 symmetry adapted cartesian basis functions of B1 symmetry.

There are 289 symmetry adapted cartesian basis functions of B2 symmetry.

There are 289 symmetry adapted basis functions of A1 symmetry.

There are 265 symmetry adapted basis functions of A2 symmetry.

There are 275 symmetry adapted basis functions of B1 symmetry.

There are 275 symmetry adapted basis functions of B2 symmetry.

1104 basis functions, 1951 primitive gaussians, 1163 cartesian basis functions

191 alpha electrons 189 beta electrons

nuclear repulsion energy 6889.6750275643 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= 81 NActive= 81 NUniq= 22 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= -0.2361178583 Hartrees.

Nuclear repulsion after empirical dispersion term = 6889.4389097060 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= 81.

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 = 81

GePol: Total number of spheres = 81

GePol: Number of exposed spheres = 81 (100.00%)

GePol: Number of points = 6430

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.18D-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) = 6.07%

GePol: Cavity surface area = 670.606 Ang\*\*2

GePol: Cavity volume = 694.433 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0170113837 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 6889.4218983223 Hartrees.

Leave Link 301 at Sun Jun 30 20:55:45 2019, MaxMem= 1342177280 cpu: 1.7

(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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36719 LenP2D= 95212.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1104 RedAO= T EigKep= 2.89D-05 NBF= 289 265 275 275

NBsUse= 1104 1.00D-06 EigRej= -1.00D+00 NBFU= 289 265 275 275

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= 1060 1060 1060 1060 1060 MxSgAt= 81 MxSgA2= 81.

Leave Link 302 at Sun Jun 30 20:56:00 2019, MaxMem= 1342177280 cpu: 158.2

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Jun 30 20:56:01 2019, MaxMem= 1342177280 cpu: 3.9

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

Initial guess from the checkpoint file: "ZnNPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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

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The electronic state of the initial guess is 3-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -2348.36339937327

Leave Link 401 at Sun Jun 30 20:56:33 2019, MaxMem= 1342177280 cpu: 321.1

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4103221 IEndB= 4103221 NGot= 1342177280 MDV= 1339444432

LenX= 1339444432 LenY= 1338090700

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= 420000000 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= 124034700.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.66D-15 for 6416.

Iteration 1 A\*A^-1 deviation from orthogonality is 1.11D-14 for 6416 1184.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.88D-15 for 6416.

Iteration 1 A^-1\*A deviation from orthogonality is 5.64D-09 for 3236 3232.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.89D-15 for 234.

Iteration 2 A\*A^-1 deviation from orthogonality is 4.54D-15 for 5173 178.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.33D-15 for 55.

Iteration 2 A^-1\*A deviation from orthogonality is 4.95D-16 for 2242 212.

E= -2348.13047560961

DIIS: error= 4.53D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2348.13047560961 IErMin= 1 ErrMin= 4.53D-04

ErrMax= 4.53D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.04D-04 BMatP= 5.04D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.53D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.379 Goal= None Shift= 0.000

Gap= 0.459 Goal= None Shift= 0.000

RMSDP=1.60D-05 MaxDP=5.25D-04 OVMax= 2.93D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.60D-05 CP: 1.00D+00

E= -2348.13073222711 Delta-E= -0.000256617503 Rises=F Damp=F

DIIS: error= 6.38D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2348.13073222711 IErMin= 2 ErrMin= 6.38D-05

ErrMax= 6.38D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.63D-06 BMatP= 5.04D-04

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

Coeff-Com: -0.736D-01 0.107D+01

Coeff: -0.736D-01 0.107D+01

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.18D-06 MaxDP=7.78D-05 DE=-2.57D-04 OVMax= 4.73D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.84D-06 CP: 1.00D+00 1.07D+00

E= -2348.13073588168 Delta-E= -0.000003654572 Rises=F Damp=F

DIIS: error= 2.32D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2348.13073588168 IErMin= 3 ErrMin= 2.32D-05

ErrMax= 2.32D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.45D-06 BMatP= 5.63D-06

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

Coeff-Com: -0.305D-01 0.391D+00 0.640D+00

Coeff: -0.305D-01 0.391D+00 0.640D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.07D-06 MaxDP=6.75D-05 DE=-3.65D-06 OVMax= 1.79D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 9.68D-07 CP: 1.00D+00 1.08D+00 7.78D-01

E= -2348.13073601645 Delta-E= -0.000000134762 Rises=F Damp=F

DIIS: error= 1.86D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2348.13073601645 IErMin= 4 ErrMin= 1.86D-05

ErrMax= 1.86D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.18D-07 BMatP= 1.45D-06

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

Coeff-Com: -0.609D-02 0.538D-01 0.437D+00 0.516D+00

Coeff: -0.609D-02 0.538D-01 0.437D+00 0.516D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=5.33D-07 MaxDP=3.16D-05 DE=-1.35D-07 OVMax= 1.18D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.24D-07 CP: 1.00D+00 1.08D+00 9.20D-01 5.92D-01

E= -2348.13073620422 Delta-E= -0.000000187771 Rises=F Damp=F

DIIS: error= 3.54D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2348.13073620422 IErMin= 5 ErrMin= 3.54D-06

ErrMax= 3.54D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.52D-08 BMatP= 9.18D-07

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

Coeff-Com: 0.343D-03-0.179D-01 0.128D+00 0.232D+00 0.658D+00

Coeff: 0.343D-03-0.179D-01 0.128D+00 0.232D+00 0.658D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.17D-07 MaxDP=1.22D-05 DE=-1.88D-07 OVMax= 3.28D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.44D-08 CP: 1.00D+00 1.08D+00 9.33D-01 6.22D-01 7.40D-01

E= -2348.13073620984 Delta-E= -0.000000005619 Rises=F Damp=F

DIIS: error= 2.45D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2348.13073620984 IErMin= 6 ErrMin= 2.45D-06

ErrMax= 2.45D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.31D-08 BMatP= 3.52D-08

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

Coeff-Com: 0.910D-03-0.182D-01 0.332D-01 0.913D-01 0.436D+00 0.457D+00

Coeff: 0.910D-03-0.182D-01 0.332D-01 0.913D-01 0.436D+00 0.457D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=5.28D-08 MaxDP=5.44D-06 DE=-5.62D-09 OVMax= 1.58D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.76D-08 CP: 1.00D+00 1.08D+00 9.34D-01 6.36D-01 8.03D-01

CP: 5.72D-01

E= -2348.13073621256 Delta-E= -0.000000002725 Rises=F Damp=F

DIIS: error= 4.45D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2348.13073621256 IErMin= 7 ErrMin= 4.45D-07

ErrMax= 4.45D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.28D-10 BMatP= 1.31D-08

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

Coeff-Com: 0.293D-03-0.509D-02 0.318D-02 0.168D-01 0.112D+00 0.160D+00

Coeff-Com: 0.713D+00

Coeff: 0.293D-03-0.509D-02 0.318D-02 0.168D-01 0.112D+00 0.160D+00

Coeff: 0.713D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.18D-08 MaxDP=7.23D-07 DE=-2.72D-09 OVMax= 6.18D-06

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.06D-08 CP: 1.00D+00 1.08D+00 9.35D-01 6.38D-01 8.11D-01

CP: 6.13D-01 1.07D+00

E= -2348.13073621282 Delta-E= -0.000000000258 Rises=F Damp=F

DIIS: error= 3.71D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2348.13073621282 IErMin= 8 ErrMin= 3.71D-07

ErrMax= 3.71D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.33D-10 BMatP= 2.28D-10

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

Coeff-Com: -0.353D-04 0.127D-02-0.641D-02-0.120D-01-0.366D-01-0.984D-02

Coeff-Com: 0.469D+00 0.595D+00

Coeff: -0.353D-04 0.127D-02-0.641D-02-0.120D-01-0.366D-01-0.984D-02

Coeff: 0.469D+00 0.595D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=6.94D-09 MaxDP=5.66D-07 DE=-2.58D-10 OVMax= 3.82D-06

Error on total polarization charges = 0.08830

SCF Done: E(UB3LYP) = -2348.13073621 A.U. after 8 cycles

NFock= 8 Conv=0.69D-08 -V/T= 1.9830

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

<L.S>= 0.000000000000E+00

KE= 2.388747093416D+03 PE=-1.932226897255D+04 EE= 7.695969244598D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -10.67

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0219, after 2.0003

Leave Link 502 at Sun Jun 30 21:05:54 2019, MaxMem= 1342177280 cpu: 6093.7

(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.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36719 LenP2D= 95212.

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 = 193

Leave Link 701 at Sun Jun 30 21:06:29 2019, MaxMem= 1342177280 cpu: 350.7

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sun Jun 30 21:06:30 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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 Sun Jun 30 21:07:13 2019, MaxMem= 1342177280 cpu: 439.1

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-2.30926389D-14 1.43529633D-12 8.78664080D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000000603 -0.000007708 -0.000035583

2 7 0.000000000 0.000007716 0.000088025

3 6 0.000000603 -0.000007708 -0.000035583

4 6 -0.000002233 0.000004119 0.000004374

5 6 0.000002233 0.000004119 0.000004374

6 7 0.000017833 0.000002440 -0.000010816

7 6 -0.000016733 -0.000020794 0.000076048

8 7 0.000012754 0.000000000 -0.000281982

9 6 -0.000016733 0.000020794 0.000076048

10 6 0.000014920 -0.000024150 0.000034944

11 6 0.000014920 0.000024150 0.000034944

12 7 -0.000017833 0.000002440 -0.000010816

13 6 -0.000014920 0.000024150 0.000034944

14 6 -0.000014920 -0.000024150 0.000034944

15 6 0.000016733 0.000020794 0.000076048

16 7 -0.000012754 0.000000000 -0.000281982

17 6 0.000016733 -0.000020794 0.000076048

18 7 -0.000017833 -0.000002440 -0.000010816

19 7 0.000000000 -0.000007716 0.000088025

20 6 -0.000000603 0.000007708 -0.000035583

21 6 0.000002233 -0.000004119 0.000004374

22 6 -0.000002233 -0.000004119 0.000004374

23 6 0.000000603 0.000007708 -0.000035583

24 7 0.000017833 -0.000002440 -0.000010816

25 30 0.000000000 0.000000000 0.000128368

26 6 -0.000003842 -0.000009418 -0.000009496

27 6 0.000005563 -0.000004819 0.000001420

28 6 0.000005563 0.000004819 0.000001420

29 6 -0.000003842 0.000009418 -0.000009496

30 6 0.000007761 0.000008748 0.000018187

31 6 0.000004434 -0.000002032 -0.000001627

32 6 -0.000004434 -0.000002032 -0.000001627

33 6 -0.000007761 0.000008748 0.000018187

34 6 0.000003842 -0.000009418 -0.000009496

35 6 -0.000005563 -0.000004819 0.000001420

36 6 -0.000005563 0.000004819 0.000001420

37 6 0.000003842 0.000009418 -0.000009496

38 6 -0.000007761 -0.000008748 0.000018187

39 6 -0.000004434 0.000002032 -0.000001627

40 6 0.000004434 0.000002032 -0.000001627

41 6 0.000007761 -0.000008748 0.000018187

42 6 -0.000005654 -0.000000913 -0.000024846

43 6 -0.000003498 -0.000002499 0.000010045

44 6 0.000003498 -0.000002499 0.000010045

45 6 0.000005654 -0.000000913 -0.000024846

46 6 -0.000000711 0.000003837 -0.000003532

47 6 0.000002123 0.000004658 -0.000000629

48 6 0.000002123 -0.000004658 -0.000000629

49 6 -0.000000711 -0.000003837 -0.000003532

50 6 0.000005654 0.000000913 -0.000024846

51 6 0.000003498 0.000002499 0.000010045

52 6 -0.000003498 0.000002499 0.000010045

53 6 -0.000005654 0.000000913 -0.000024846

54 6 0.000000711 0.000003837 -0.000003532

55 6 -0.000002123 0.000004658 -0.000000629

56 6 -0.000002123 -0.000004658 -0.000000629

57 6 0.000000711 -0.000003837 -0.000003532

58 1 -0.000001014 -0.000000820 0.000002519

59 1 -0.000001014 0.000000820 0.000002519

60 1 0.000001864 0.000001730 -0.000001992

61 1 -0.000001864 0.000001730 -0.000001992

62 1 0.000001014 -0.000000820 0.000002519

63 1 0.000001014 0.000000820 0.000002519

64 1 -0.000001864 -0.000001730 -0.000001992

65 1 0.000001864 -0.000001730 -0.000001992

66 1 -0.000002719 -0.000001861 0.000004705

67 1 -0.000001878 -0.000000527 0.000000424

68 1 0.000001878 -0.000000527 0.000000424

69 1 0.000002719 -0.000001861 0.000004705

70 1 0.000001734 0.000002742 0.000000509

71 1 -0.000000143 0.000001106 0.000000233

72 1 -0.000000143 -0.000001106 0.000000233

73 1 0.000001734 -0.000002742 0.000000509

74 1 0.000002719 0.000001861 0.000004705

75 1 0.000001878 0.000000527 0.000000424

76 1 -0.000001878 0.000000527 0.000000424

77 1 -0.000002719 0.000001861 0.000004705

78 1 -0.000001734 0.000002742 0.000000509

79 1 0.000000143 0.000001106 0.000000233

80 1 0.000000143 -0.000001106 0.000000233

81 1 -0.000001734 -0.000002742 0.000000509

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

Cartesian Forces: Max 0.000281982 RMS 0.000031382

Leave Link 716 at Sun Jun 30 21:07:13 2019, MaxMem= 1342177280 cpu: 4.0

(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 0.000035698 RMS 0.000008481

Search for a local minimum.

Step number 7 out of a maximum of 486

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .84808D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

6 7

DE= -6.79D-06 DEPred=-6.62D-07 R= 1.02D+01

TightC=F SS= 1.41D+00 RLast= 3.12D-02 DXNew= 5.0454D-01 9.3567D-02

Trust test= 1.02D+01 RLast= 3.12D-02 DXMaxT set to 3.00D-01

ITU= 1 1 1 1 1 1 0

Eigenvalues --- 0.00258 0.00880 0.01431 0.01483 0.01499

Eigenvalues --- 0.01572 0.01589 0.01627 0.01656 0.01672

Eigenvalues --- 0.01694 0.01698 0.01705 0.01713 0.01714

Eigenvalues --- 0.01725 0.01730 0.01730 0.01735 0.01737

Eigenvalues --- 0.01744 0.01752 0.01758 0.01791 0.01806

Eigenvalues --- 0.01827 0.01827 0.01830 0.01851 0.01854

Eigenvalues --- 0.01870 0.01870 0.01892 0.01937 0.01968

Eigenvalues --- 0.01968 0.01971 0.01972 0.01978 0.01992

Eigenvalues --- 0.01992 0.01993 0.01993 0.02021 0.02080

Eigenvalues --- 0.02086 0.02086 0.02087 0.02089 0.02096

Eigenvalues --- 0.02096 0.02098 0.02100 0.02103 0.02103

Eigenvalues --- 0.02105 0.02106 0.02124 0.02124 0.02137

Eigenvalues --- 0.02144 0.02144 0.02147 0.02148 0.02169

Eigenvalues --- 0.02173 0.02189 0.02214 0.02214 0.02225

Eigenvalues --- 0.02225 0.02252 0.02280 0.02286 0.02327

Eigenvalues --- 0.02346 0.02989 0.05474 0.05565 0.08105

Eigenvalues --- 0.14652 0.15998 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 0.16001 0.16007 0.16077

Eigenvalues --- 0.16151 0.16260 0.17279 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22499 0.22503 0.22504

Eigenvalues --- 0.22536 0.23232 0.23234 0.23234 0.23681

Eigenvalues --- 0.23939 0.23939 0.23940 0.23954 0.24176

Eigenvalues --- 0.24271 0.24330 0.24550 0.24553 0.24557

Eigenvalues --- 0.24557 0.24575 0.24779 0.24891 0.24894

Eigenvalues --- 0.24962 0.24981 0.24983 0.24985 0.24989

Eigenvalues --- 0.24996 0.24996 0.24997 0.24997 0.26292

Eigenvalues --- 0.32865 0.32947 0.33671 0.33749 0.33835

Eigenvalues --- 0.33864 0.35040 0.35068 0.35181 0.35181

Eigenvalues --- 0.35181 0.35187 0.35202 0.35202 0.35202

Eigenvalues --- 0.35212 0.35231 0.35231 0.35231 0.35238

Eigenvalues --- 0.35249 0.35249 0.35249 0.35261 0.35270

Eigenvalues --- 0.35270 0.35270 0.35275 0.35279 0.35279

Eigenvalues --- 0.35279 0.35414 0.35433 0.35609 0.36349

Eigenvalues --- 0.36740 0.37459 0.37569 0.37969 0.38703

Eigenvalues --- 0.39276 0.39276 0.39612 0.39612 0.40188

Eigenvalues --- 0.40188 0.40257 0.40257 0.40906 0.41001

Eigenvalues --- 0.41019 0.41140 0.41603 0.41771 0.41873

Eigenvalues --- 0.42150 0.42215 0.42374 0.42806 0.42808

Eigenvalues --- 0.42903 0.42970 0.45169 0.45691 0.47124

Eigenvalues --- 0.47124 0.47219 0.47384 0.47386 0.47579

Eigenvalues --- 0.47580 0.48123 0.48218 0.48351 0.48459

Eigenvalues --- 0.48465 0.48680 0.48707 0.48722 0.48729

Eigenvalues --- 0.49091 0.49178 0.49530 0.49898 0.50378

Eigenvalues --- 0.51023 0.51339 0.52482 0.58665 0.59240

Eigenvalues --- 0.59868 0.60916

En-DIIS/RFO-DIIS IScMMF= 0 using points: 7 6 5 4 3

RFO step: Lambda=-3.48397728D-07.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 2.00D-05 SmlDif= 1.00D-05

RMS Error= 0.8689276400D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.60929 -0.43149 -0.52301 0.43215 -0.08694

Iteration 1 RMS(Cart)= 0.00923804 RMS(Int)= 0.00000352

Iteration 2 RMS(Cart)= 0.00001441 RMS(Int)= 0.00000159

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000159

ITry= 1 IFail=0 DXMaxC= 4.39D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 5.01D-08 for atom 69.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58020 -0.00001 0.00019 -0.00011 0.00008 2.58028

R2 2.74371 0.00000 -0.00016 0.00003 -0.00013 2.74358

R3 2.55910 -0.00001 0.00013 -0.00009 0.00004 2.55915

R4 2.58020 -0.00001 0.00019 -0.00011 0.00008 2.58028

R5 3.95027 -0.00001 -0.00063 0.00005 -0.00058 3.94969

R6 2.74371 0.00000 -0.00016 0.00003 -0.00013 2.74358

R7 2.55910 -0.00001 0.00013 -0.00009 0.00004 2.55915

R8 2.71251 -0.00001 0.00007 -0.00006 0.00000 2.71252

R9 2.60037 -0.00001 0.00006 -0.00005 0.00001 2.60038

R10 2.60037 -0.00001 0.00006 -0.00005 0.00001 2.60038

R11 2.48320 0.00000 0.00024 -0.00011 0.00013 2.48333

R12 2.59805 -0.00001 0.00008 -0.00009 0.00000 2.59805

R13 2.78662 -0.00001 -0.00034 0.00007 -0.00027 2.78636

R14 2.59805 -0.00001 0.00008 -0.00009 0.00000 2.59805

R15 3.92343 0.00001 0.00003 -0.00006 -0.00002 3.92341

R16 2.78662 -0.00001 -0.00034 0.00007 -0.00027 2.78636

R17 2.48320 0.00000 0.00024 -0.00011 0.00013 2.48333

R18 2.69194 0.00001 0.00015 -0.00006 0.00009 2.69202

R19 2.58484 0.00000 0.00006 -0.00003 0.00002 2.58486

R20 2.58484 0.00000 0.00006 -0.00003 0.00002 2.58486

R21 2.48320 0.00000 0.00024 -0.00011 0.00013 2.48333

R22 2.69194 0.00001 0.00015 -0.00006 0.00009 2.69202

R23 2.78662 -0.00001 -0.00034 0.00007 -0.00027 2.78636

R24 2.58484 0.00000 0.00006 -0.00003 0.00002 2.58486

R25 2.78662 -0.00001 -0.00034 0.00007 -0.00027 2.78636

R26 2.58484 0.00000 0.00006 -0.00003 0.00002 2.58486

R27 2.59805 -0.00001 0.00008 -0.00009 0.00000 2.59805

R28 2.48320 0.00000 0.00024 -0.00011 0.00013 2.48333

R29 2.59805 -0.00001 0.00008 -0.00009 0.00000 2.59805

R30 3.92343 0.00001 0.00003 -0.00006 -0.00002 3.92341

R31 2.55910 -0.00001 0.00013 -0.00009 0.00004 2.55915

R32 2.58020 -0.00001 0.00019 -0.00011 0.00008 2.58028

R33 2.58020 -0.00001 0.00019 -0.00011 0.00008 2.58028

R34 3.95027 -0.00001 -0.00063 0.00005 -0.00058 3.94969

R35 2.74371 0.00000 -0.00016 0.00003 -0.00013 2.74358

R36 2.71251 -0.00001 0.00007 -0.00006 0.00000 2.71252

R37 2.60037 -0.00001 0.00006 -0.00005 0.00001 2.60038

R38 2.74371 0.00000 -0.00016 0.00003 -0.00013 2.74358

R39 2.60037 -0.00001 0.00006 -0.00005 0.00001 2.60038

R40 2.55910 -0.00001 0.00013 -0.00009 0.00004 2.55915

R41 2.69212 0.00001 0.00002 -0.00001 0.00001 2.69213

R42 2.05015 0.00000 -0.00001 0.00000 -0.00001 2.05014

R43 2.71700 -0.00001 -0.00006 -0.00004 -0.00010 2.71690

R44 2.67584 0.00000 0.00002 -0.00002 0.00000 2.67583

R45 2.69212 0.00001 0.00002 -0.00001 0.00001 2.69213

R46 2.67584 0.00000 0.00002 -0.00002 0.00000 2.67583

R47 2.05015 0.00000 -0.00001 0.00000 -0.00001 2.05014

R48 2.67802 0.00001 0.00003 -0.00001 0.00002 2.67804

R49 2.05046 0.00000 -0.00001 -0.00001 -0.00002 2.05044

R50 2.72673 -0.00001 -0.00009 -0.00002 -0.00011 2.72662

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R52 2.67802 0.00001 0.00003 -0.00001 0.00002 2.67804

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R55 2.69212 0.00001 0.00002 -0.00001 0.00001 2.69213

R56 2.05015 0.00000 -0.00001 0.00000 -0.00001 2.05014

R57 2.71700 -0.00001 -0.00006 -0.00004 -0.00010 2.71690

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R63 2.05046 0.00000 -0.00001 -0.00001 -0.00002 2.05044

R64 2.72673 -0.00001 -0.00009 -0.00002 -0.00011 2.72662

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R66 2.67802 0.00001 0.00003 -0.00001 0.00002 2.67804

R67 2.68323 0.00000 0.00000 0.00000 0.00000 2.68323

R68 2.05046 0.00000 -0.00001 -0.00001 -0.00002 2.05044

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R70 2.05127 0.00000 0.00000 -0.00002 -0.00002 2.05125

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R72 2.04990 0.00000 0.00001 -0.00001 0.00000 2.04991

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R78 2.66780 -0.00001 0.00002 -0.00006 -0.00004 2.66776

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R96 2.05087 0.00000 0.00001 -0.00002 -0.00001 2.05086

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A3 2.15630 0.00000 -0.00002 0.00004 0.00002 2.15632

A4 1.92701 -0.00001 -0.00009 0.00003 -0.00006 1.92694

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A6 2.17618 0.00000 0.00014 0.00004 0.00018 2.17636

A7 1.89634 0.00000 0.00000 0.00001 0.00001 1.89635

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A9 2.15630 0.00000 -0.00002 0.00004 0.00002 2.15632

A10 1.85245 0.00000 0.00004 -0.00002 0.00002 1.85247

A11 2.31713 0.00000 -0.00010 0.00005 -0.00005 2.31709

A12 2.11348 0.00000 0.00004 -0.00003 0.00001 2.11349

A13 1.85245 0.00000 0.00004 -0.00002 0.00002 1.85247

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A15 2.11348 0.00000 0.00004 -0.00003 0.00001 2.11349

A16 2.17135 0.00001 -0.00023 0.00004 -0.00019 2.17116

A17 2.23993 0.00000 -0.00012 -0.00006 -0.00018 2.23974

A18 2.14854 0.00000 0.00000 0.00007 0.00006 2.14861

A19 1.89394 0.00000 0.00013 -0.00002 0.00012 1.89405

A20 1.92330 0.00001 -0.00017 0.00005 -0.00013 1.92317

A21 2.17054 -0.00001 -0.00031 -0.00020 -0.00053 2.17001

A22 2.17054 -0.00001 -0.00031 -0.00020 -0.00053 2.17001

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A29 1.85629 0.00000 -0.00001 -0.00001 -0.00002 1.85626

A30 2.30685 0.00001 -0.00001 0.00004 0.00003 2.30688

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A32 2.17135 0.00001 -0.00023 0.00004 -0.00019 2.17116

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A53 2.15630 0.00000 -0.00002 0.00004 0.00002 2.15632

A54 1.89634 0.00000 0.00000 0.00001 0.00001 1.89635

A55 1.85245 0.00000 0.00004 -0.00002 0.00002 1.85247

A56 2.31713 0.00000 -0.00010 0.00005 -0.00005 2.31709

A57 2.11348 0.00000 0.00004 -0.00003 0.00001 2.11349

A58 1.85245 0.00000 0.00004 -0.00002 0.00002 1.85247

A59 2.11348 0.00000 0.00004 -0.00003 0.00001 2.11349

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A68 2.63927 -0.00002 -0.00113 -0.00031 -0.00144 2.63782

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A71 2.07273 0.00001 -0.00010 0.00007 -0.00003 2.07270

A72 2.12029 0.00000 0.00010 -0.00006 0.00004 2.12033

A73 2.09017 0.00000 0.00000 -0.00001 -0.00001 2.09015

A74 2.09042 0.00000 0.00008 -0.00004 0.00004 2.09046

A75 2.11906 0.00000 -0.00012 0.00007 -0.00005 2.11901

A76 2.07370 0.00000 0.00004 -0.00003 0.00001 2.07372

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A83 2.07667 0.00000 -0.00011 0.00007 -0.00004 2.07663

A84 2.11682 0.00000 0.00020 -0.00010 0.00010 2.11692

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A131 2.10924 0.00000 -0.00006 0.00005 -0.00001 2.10923

A132 2.07208 0.00000 0.00002 -0.00001 0.00001 2.07209

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A141 2.07208 0.00000 0.00002 -0.00001 0.00001 2.07209

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A144 2.06943 0.00000 0.00004 -0.00003 0.00000 2.06943

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A146 2.10048 0.00000 0.00003 -0.00003 0.00000 2.10048

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A148 2.08709 0.00000 0.00009 -0.00005 0.00004 2.08712

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A150 2.08709 0.00000 0.00009 -0.00005 0.00004 2.08712

A151 2.09561 0.00000 -0.00012 0.00008 -0.00004 2.09558

A152 2.11179 0.00001 -0.00009 0.00008 -0.00002 2.11177

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A154 2.10197 0.00000 0.00006 -0.00004 0.00002 2.10198

A155 2.10924 0.00000 -0.00006 0.00005 -0.00001 2.10923

A156 2.07208 0.00000 0.00002 -0.00001 0.00001 2.07209

A157 2.10186 0.00000 0.00004 -0.00004 0.00000 2.10186

A158 2.10024 0.00000 0.00002 -0.00002 0.00000 2.10024

A159 2.09464 0.00000 -0.00008 0.00006 -0.00002 2.09461

A160 2.08831 0.00000 0.00006 -0.00003 0.00003 2.08833

A161 2.10024 0.00000 0.00002 -0.00002 0.00000 2.10024

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A163 2.09464 0.00000 -0.00008 0.00006 -0.00002 2.09461

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D3 -3.09610 0.00000 -0.00034 -0.00050 -0.00084 -3.09694

D4 0.13563 -0.00001 -0.00273 -0.00165 -0.00438 0.13126

D5 -0.01132 -0.00001 -0.00020 0.00018 -0.00002 -0.01133

D6 -3.13571 0.00000 0.00137 -0.00012 0.00125 -3.13446

D7 3.10521 0.00000 0.00044 0.00036 0.00081 3.10601

D8 -0.01919 0.00000 0.00201 0.00006 0.00208 -0.01711

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D11 -0.01905 -0.00001 -0.00033 0.00030 -0.00003 -0.01908

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D13 3.03240 0.00000 0.00205 0.00146 0.00351 3.03591

D14 -0.13563 0.00001 0.00273 0.00165 0.00438 -0.13126

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D16 -0.29486 0.00000 0.00076 0.00050 0.00127 -0.29360

D17 -1.62219 0.00001 0.00135 0.00066 0.00201 -1.62018

D18 0.29486 0.00000 -0.00076 -0.00050 -0.00127 0.29360

D19 2.94952 -0.00002 -0.00195 -0.00081 -0.00276 2.94676

D20 1.62219 -0.00001 -0.00135 -0.00066 -0.00201 1.62018

D21 0.01132 0.00001 0.00020 -0.00018 0.00002 0.01133

D22 3.13571 0.00000 -0.00137 0.00012 -0.00125 3.13446

D23 -3.10521 0.00000 -0.00044 -0.00036 -0.00081 -3.10601

D24 0.01919 0.00000 -0.00201 -0.00006 -0.00208 0.01711

D25 -0.10505 -0.00001 -0.00202 -0.00115 -0.00317 -0.10821

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D27 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D28 3.12685 0.00000 -0.00135 0.00026 -0.00109 3.12576

D29 -3.12685 0.00000 0.00135 -0.00026 0.00109 -3.12576

D30 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D31 -3.12747 0.00001 0.00174 -0.00015 0.00160 -3.12588

D32 0.01276 0.00000 0.00193 -0.00045 0.00148 0.01424

D33 -0.00517 0.00000 -0.00002 0.00019 0.00017 -0.00500

D34 3.13506 0.00000 0.00017 -0.00012 0.00005 3.13511

D35 3.12747 -0.00001 -0.00174 0.00015 -0.00160 3.12588

D36 -0.01276 0.00000 -0.00193 0.00045 -0.00148 -0.01424

D37 0.00517 0.00000 0.00002 -0.00019 -0.00017 0.00500

D38 -3.13506 0.00000 -0.00017 0.00012 -0.00005 -3.13511

D39 0.02358 -0.00002 -0.00119 -0.00082 -0.00201 0.02157

D40 -3.07054 -0.00002 -0.00129 -0.00065 -0.00194 -3.07249

D41 -3.05688 -0.00002 -0.00129 0.00003 -0.00126 -3.05814

D42 0.28463 0.00003 0.00301 0.00189 0.00490 0.28953

D43 0.04278 -0.00002 -0.00120 -0.00011 -0.00132 0.04147

D44 -2.89890 0.00004 0.00309 0.00175 0.00484 -2.89406

D45 3.07682 0.00001 0.00079 -0.00007 0.00072 3.07755

D46 -0.05508 0.00001 0.00123 0.00008 0.00131 -0.05377

D47 -0.02551 0.00001 0.00071 0.00007 0.00078 -0.02472

D48 3.12578 0.00001 0.00115 0.00022 0.00137 3.12715

D49 -0.04278 0.00002 0.00120 0.00011 0.00132 -0.04147

D50 3.05688 0.00002 0.00129 -0.00003 0.00126 3.05814

D51 2.89890 -0.00004 -0.00309 -0.00175 -0.00484 2.89406

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D53 -0.35948 -0.00002 -0.00173 -0.00102 -0.00275 -0.36223

D54 -1.68467 -0.00003 -0.00244 -0.00105 -0.00349 -1.68815

D55 -3.00985 -0.00003 -0.00315 -0.00107 -0.00422 -3.01407

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D59 0.02551 -0.00001 -0.00071 -0.00007 -0.00078 0.02472

D60 -3.12578 -0.00001 -0.00115 -0.00022 -0.00137 -3.12715

D61 -3.07682 -0.00001 -0.00079 0.00007 -0.00072 -3.07755

D62 0.05508 -0.00001 -0.00123 -0.00008 -0.00131 0.05377

D63 -0.02358 0.00002 0.00119 0.00082 0.00201 -0.02157

D64 3.07054 0.00002 0.00129 0.00065 0.00194 3.07249

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13317 0.00000 -0.00038 -0.00013 -0.00051 3.13266

D67 -3.13317 0.00000 0.00038 0.00013 0.00051 -3.13266

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 -3.13887 0.00000 0.00047 0.00031 0.00078 -3.13808

D70 0.00565 0.00000 0.00047 0.00009 0.00056 0.00621

D71 -0.00818 0.00000 -0.00002 0.00015 0.00012 -0.00805

D72 3.13635 0.00000 -0.00003 -0.00007 -0.00010 3.13625

D73 3.13887 0.00000 -0.00047 -0.00031 -0.00078 3.13808

D74 -0.00565 0.00000 -0.00047 -0.00009 -0.00056 -0.00621

D75 0.00818 0.00000 0.00002 -0.00015 -0.00012 0.00805

D76 -3.13635 0.00000 0.00003 0.00007 0.00010 -3.13625

D77 3.07054 0.00002 0.00129 0.00065 0.00194 3.07249

D78 -0.02358 0.00002 0.00119 0.00082 0.00201 -0.02157

D79 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D80 3.13317 0.00000 -0.00038 -0.00013 -0.00051 3.13266

D81 -3.13317 0.00000 0.00038 0.00013 0.00051 -3.13266

D82 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D83 -3.07682 -0.00001 -0.00079 0.00007 -0.00072 -3.07755

D84 0.02551 -0.00001 -0.00071 -0.00007 -0.00078 0.02472

D85 0.05508 -0.00001 -0.00123 -0.00008 -0.00131 0.05377

D86 -3.12578 -0.00001 -0.00115 -0.00022 -0.00137 -3.12715

D87 -0.00818 0.00000 -0.00002 0.00015 0.00012 -0.00805

D88 3.13635 0.00000 -0.00003 -0.00007 -0.00010 3.13625

D89 -3.13887 0.00000 0.00047 0.00031 0.00078 -3.13808

D90 0.00565 0.00000 0.00047 0.00009 0.00056 0.00621

D91 -0.02551 0.00001 0.00071 0.00007 0.00078 -0.02472

D92 3.07682 0.00001 0.00079 -0.00007 0.00072 3.07755

D93 3.12578 0.00001 0.00115 0.00022 0.00137 3.12715

D94 -0.05508 0.00001 0.00123 0.00008 0.00131 -0.05377

D95 0.00818 0.00000 0.00002 -0.00015 -0.00012 0.00805

D96 -3.13635 0.00000 0.00003 0.00007 0.00010 -3.13625

D97 3.13887 0.00000 -0.00047 -0.00031 -0.00078 3.13808

D98 -0.00565 0.00000 -0.00047 -0.00009 -0.00056 -0.00621

D99 0.04278 -0.00002 -0.00120 -0.00011 -0.00132 0.04147

D100 -2.89890 0.00004 0.00309 0.00175 0.00484 -2.89406

D101 -3.05688 -0.00002 -0.00129 0.00003 -0.00126 -3.05814

D102 0.28463 0.00003 0.00301 0.00189 0.00490 0.28953

D103 -3.07054 -0.00002 -0.00129 -0.00065 -0.00194 -3.07249

D104 0.02358 -0.00002 -0.00119 -0.00082 -0.00201 0.02157

D105 3.05688 0.00002 0.00129 -0.00003 0.00126 3.05814

D106 -0.04278 0.00002 0.00120 0.00011 0.00132 -0.04147

D107 -0.28463 -0.00003 -0.00301 -0.00189 -0.00490 -0.28953

D108 2.89890 -0.00004 -0.00309 -0.00175 -0.00484 2.89406

D109 -3.00985 -0.00003 -0.00315 -0.00107 -0.00422 -3.01407

D110 -1.68467 -0.00003 -0.00244 -0.00105 -0.00349 -1.68815

D111 -0.35948 -0.00002 -0.00173 -0.00102 -0.00275 -0.36223

D112 0.35948 0.00002 0.00173 0.00102 0.00275 0.36223

D113 1.68467 0.00003 0.00244 0.00105 0.00349 1.68815

D114 3.00985 0.00003 0.00315 0.00107 0.00422 3.01407

D115 -0.10505 -0.00001 -0.00202 -0.00115 -0.00317 -0.10821

D116 3.00649 0.00000 -0.00125 -0.00093 -0.00218 3.00431

D117 3.09610 0.00000 0.00034 0.00050 0.00084 3.09694

D118 -0.01905 -0.00001 -0.00033 0.00030 -0.00003 -0.01908

D119 -0.13563 0.00001 0.00273 0.00165 0.00438 -0.13126

D120 3.03240 0.00000 0.00205 0.00146 0.00351 3.03591

D121 0.01905 0.00001 0.00033 -0.00030 0.00003 0.01908

D122 -3.09610 0.00000 -0.00034 -0.00050 -0.00084 -3.09694

D123 -3.03240 0.00000 -0.00205 -0.00146 -0.00351 -3.03591

D124 0.13563 -0.00001 -0.00273 -0.00165 -0.00438 0.13126

D125 1.62219 -0.00001 -0.00135 -0.00066 -0.00201 1.62018

D126 2.94952 -0.00002 -0.00195 -0.00081 -0.00276 2.94676

D127 0.29486 0.00000 -0.00076 -0.00050 -0.00127 0.29360

D128 -1.62219 0.00001 0.00135 0.00066 0.00201 -1.62018

D129 -0.29486 0.00000 0.00076 0.00050 0.00127 -0.29360

D130 -2.94952 0.00002 0.00195 0.00081 0.00276 -2.94676

D131 -3.10521 0.00000 -0.00044 -0.00036 -0.00081 -3.10601

D132 0.01919 0.00000 -0.00201 -0.00006 -0.00208 0.01711

D133 0.01132 0.00001 0.00020 -0.00018 0.00002 0.01133

D134 3.13571 0.00000 -0.00137 0.00012 -0.00125 3.13446

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.12685 0.00000 -0.00135 0.00026 -0.00109 3.12576

D137 -3.12685 0.00000 0.00135 -0.00026 0.00109 -3.12576

D138 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D139 -3.12747 0.00001 0.00174 -0.00015 0.00160 -3.12588

D140 0.01276 0.00000 0.00193 -0.00045 0.00148 0.01424

D141 -0.00517 0.00000 -0.00002 0.00019 0.00017 -0.00500

D142 3.13506 0.00000 0.00017 -0.00012 0.00005 3.13511

D143 -0.01132 -0.00001 -0.00020 0.00018 -0.00002 -0.01133

D144 3.10521 0.00000 0.00044 0.00036 0.00081 3.10601

D145 -3.13571 0.00000 0.00137 -0.00012 0.00125 -3.13446

D146 -0.01919 0.00000 0.00201 0.00006 0.00208 -0.01711

D147 0.00517 0.00000 0.00002 -0.00019 -0.00017 0.00500

D148 -3.13506 0.00000 -0.00017 0.00012 -0.00005 -3.13511

D149 3.12747 -0.00001 -0.00174 0.00015 -0.00160 3.12588

D150 -0.01276 0.00000 -0.00193 0.00045 -0.00148 -0.01424

D151 0.10505 0.00001 0.00202 0.00115 0.00317 0.10821

D152 -3.00649 0.00000 0.00125 0.00093 0.00218 -3.00431

D153 0.00803 0.00000 0.00002 -0.00015 -0.00012 0.00791

D154 -3.13380 0.00000 -0.00011 -0.00019 -0.00029 -3.13410

D155 -3.13644 0.00000 0.00003 0.00007 0.00010 -3.13634

D156 0.00491 0.00000 -0.00010 0.00003 -0.00007 0.00484

D157 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D158 3.14136 0.00000 -0.00013 -0.00004 -0.00017 3.14119

D159 -3.14136 0.00000 0.00013 0.00004 0.00017 -3.14119

D160 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D161 -3.14152 0.00000 0.00013 0.00001 0.00014 -3.14138

D162 -0.00019 0.00000 0.00010 0.00006 0.00016 -0.00003

D163 -0.00017 0.00000 0.00000 -0.00003 -0.00003 -0.00020

D164 3.14116 0.00000 -0.00003 0.00002 -0.00001 3.14115

D165 -0.00803 0.00000 -0.00002 0.00015 0.00012 -0.00791

D166 3.13644 0.00000 -0.00003 -0.00007 -0.00010 3.13634

D167 3.13380 0.00000 0.00011 0.00019 0.00029 3.13410

D168 -0.00491 0.00000 0.00010 -0.00003 0.00007 -0.00484

D169 0.00017 0.00000 0.00000 0.00003 0.00003 0.00020

D170 -3.14116 0.00000 0.00003 -0.00002 0.00001 -3.14115

D171 3.14152 0.00000 -0.00013 -0.00001 -0.00014 3.14138

D172 0.00019 0.00000 -0.00010 -0.00006 -0.00016 0.00003

D173 -0.00511 0.00000 -0.00002 0.00019 0.00017 -0.00494

D174 3.13946 0.00000 0.00031 0.00007 0.00038 3.13984

D175 3.13515 0.00000 0.00016 -0.00011 0.00005 3.13520

D176 -0.00347 0.00000 0.00049 -0.00023 0.00027 -0.00320

D177 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D178 -3.13870 0.00000 0.00032 -0.00011 0.00021 -3.13849

D179 3.13870 0.00000 -0.00032 0.00011 -0.00021 3.13849

D180 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D181 3.13866 0.00001 -0.00070 0.00065 -0.00005 3.13861

D182 -0.00305 0.00000 -0.00028 -0.00004 -0.00032 -0.00337

D183 0.00001 0.00001 -0.00038 0.00054 0.00016 0.00017

D184 3.14149 0.00000 0.00005 -0.00015 -0.00010 3.14138

D185 0.00511 0.00000 0.00002 -0.00019 -0.00017 0.00494

D186 -3.13515 0.00000 -0.00016 0.00011 -0.00005 -3.13520

D187 -3.13946 0.00000 -0.00031 -0.00007 -0.00038 -3.13984

D188 0.00347 0.00000 -0.00049 0.00023 -0.00027 0.00320

D189 -0.00001 -0.00001 0.00038 -0.00054 -0.00016 -0.00017

D190 -3.14149 0.00000 -0.00005 0.00015 0.00010 -3.14138

D191 -3.13866 -0.00001 0.00070 -0.00065 0.00005 -3.13861

D192 0.00305 0.00000 0.00028 0.00004 0.00032 0.00337

D193 -0.00803 0.00000 -0.00002 0.00015 0.00012 -0.00791

D194 3.13380 0.00000 0.00011 0.00019 0.00029 3.13410

D195 3.13644 0.00000 -0.00003 -0.00007 -0.00010 3.13634

D196 -0.00491 0.00000 0.00010 -0.00003 0.00007 -0.00484

D197 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D198 -3.14136 0.00000 0.00013 0.00004 0.00017 -3.14119

D199 3.14136 0.00000 -0.00013 -0.00004 -0.00017 3.14119

D200 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D201 3.14152 0.00000 -0.00013 -0.00001 -0.00014 3.14138

D202 0.00019 0.00000 -0.00010 -0.00006 -0.00016 0.00003

D203 0.00017 0.00000 0.00000 0.00003 0.00003 0.00020

D204 -3.14116 0.00000 0.00003 -0.00002 0.00001 -3.14115

D205 0.00803 0.00000 0.00002 -0.00015 -0.00012 0.00791

D206 -3.13644 0.00000 0.00003 0.00007 0.00010 -3.13634

D207 -3.13380 0.00000 -0.00011 -0.00019 -0.00029 -3.13410

D208 0.00491 0.00000 -0.00010 0.00003 -0.00007 0.00484

D209 -0.00017 0.00000 0.00000 -0.00003 -0.00003 -0.00020

D210 3.14116 0.00000 -0.00003 0.00002 -0.00001 3.14115

D211 -3.14152 0.00000 0.00013 0.00001 0.00014 -3.14138

D212 -0.00019 0.00000 0.00010 0.00006 0.00016 -0.00003

D213 -0.00511 0.00000 -0.00002 0.00019 0.00017 -0.00494

D214 3.13946 0.00000 0.00031 0.00007 0.00038 3.13984

D215 3.13515 0.00000 0.00016 -0.00011 0.00005 3.13520

D216 -0.00347 0.00000 0.00049 -0.00023 0.00027 -0.00320

D217 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D218 -3.13870 0.00000 0.00032 -0.00011 0.00021 -3.13849

D219 3.13870 0.00000 -0.00032 0.00011 -0.00021 3.13849

D220 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D221 3.13866 0.00001 -0.00070 0.00065 -0.00005 3.13861

D222 -0.00305 0.00000 -0.00028 -0.00004 -0.00032 -0.00337

D223 0.00001 0.00001 -0.00038 0.00054 0.00016 0.00017

D224 3.14149 0.00000 0.00005 -0.00015 -0.00010 3.14138

D225 0.00511 0.00000 0.00002 -0.00019 -0.00017 0.00494

D226 -3.13515 0.00000 -0.00016 0.00011 -0.00005 -3.13520

D227 -3.13946 0.00000 -0.00031 -0.00007 -0.00038 -3.13984

D228 0.00347 0.00000 -0.00049 0.00023 -0.00027 0.00320

D229 -0.00001 -0.00001 0.00038 -0.00054 -0.00016 -0.00017

D230 -3.14149 0.00000 -0.00005 0.00015 0.00010 -3.14138

D231 -3.13866 -0.00001 0.00070 -0.00065 0.00005 -3.13861

D232 0.00305 0.00000 0.00028 0.00004 0.00032 0.00337

D233 0.00001 0.00001 -0.00038 0.00055 0.00017 0.00018

D234 3.14153 0.00001 -0.00026 0.00042 0.00016 -3.14149

D235 3.14148 0.00000 0.00005 -0.00016 -0.00011 3.14138

D236 -0.00019 0.00000 0.00018 -0.00028 -0.00011 -0.00029

D237 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D238 3.14152 0.00000 0.00012 -0.00013 0.00000 3.14151

D239 -3.14152 0.00000 -0.00012 0.00013 0.00000 -3.14151

D240 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D241 -0.00001 -0.00001 0.00038 -0.00055 -0.00017 -0.00018

D242 -3.14148 0.00000 -0.00005 0.00016 0.00011 -3.14138

D243 -3.14153 -0.00001 0.00026 -0.00042 -0.00016 3.14149

D244 0.00019 0.00000 -0.00018 0.00028 0.00011 0.00029

D245 -0.00017 0.00000 0.00000 -0.00003 -0.00003 -0.00020

D246 -3.14114 0.00000 0.00000 -0.00003 -0.00003 -3.14117

D247 3.14116 0.00000 -0.00003 0.00002 -0.00001 3.14114

D248 0.00019 0.00000 -0.00003 0.00002 -0.00001 0.00017

D249 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D250 -3.14097 0.00000 0.00000 0.00000 0.00000 -3.14097

D251 3.14097 0.00000 0.00000 0.00000 0.00000 3.14097

D252 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D253 0.00017 0.00000 0.00000 0.00003 0.00003 0.00020

D254 -3.14116 0.00000 0.00003 -0.00002 0.00001 -3.14114

D255 3.14114 0.00000 0.00000 0.00003 0.00003 3.14117

D256 -0.00019 0.00000 0.00003 -0.00002 0.00001 -0.00017

D257 0.00001 0.00001 -0.00038 0.00055 0.00017 0.00018

D258 3.14153 0.00001 -0.00026 0.00042 0.00016 -3.14149

D259 3.14148 0.00000 0.00005 -0.00016 -0.00011 3.14138

D260 -0.00019 0.00000 0.00018 -0.00028 -0.00011 -0.00029

D261 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D262 3.14152 0.00000 0.00012 -0.00013 0.00000 3.14151

D263 -3.14152 0.00000 -0.00012 0.00013 0.00000 -3.14151

D264 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D265 -0.00001 -0.00001 0.00038 -0.00055 -0.00017 -0.00018

D266 -3.14148 0.00000 -0.00005 0.00016 0.00011 -3.14138

D267 -3.14153 -0.00001 0.00026 -0.00042 -0.00016 3.14149

D268 0.00019 0.00000 -0.00018 0.00028 0.00011 0.00029

D269 0.00017 0.00000 0.00000 0.00003 0.00003 0.00020

D270 3.14114 0.00000 0.00000 0.00003 0.00003 3.14117

D271 -3.14116 0.00000 0.00003 -0.00002 0.00001 -3.14114

D272 -0.00019 0.00000 0.00003 -0.00002 0.00001 -0.00017

D273 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D274 3.14097 0.00000 0.00000 0.00000 0.00000 3.14097

D275 -3.14097 0.00000 0.00000 0.00000 0.00000 -3.14097

D276 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D277 -0.00017 0.00000 0.00000 -0.00003 -0.00003 -0.00020

D278 3.14116 0.00000 -0.00003 0.00002 -0.00001 3.14114

D279 -3.14114 0.00000 0.00000 -0.00003 -0.00003 -3.14117

D280 0.00019 0.00000 -0.00003 0.00002 -0.00001 0.00017

Item Value Threshold Converged?

Maximum Force 0.000036 0.000450 YES

RMS Force 0.000008 0.000300 YES

Maximum Displacement 0.043918 0.001800 NO

RMS Displacement 0.009240 0.001200 NO

Predicted change in Energy=-2.000443D-06

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Jun 30 21:07:30 2019, MaxMem= 1342177280 cpu: 165.4

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

Stoichiometry C48H24N8Zn(3)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C48H24N4)]

Deg. of freedom 61

Full point group C2V NOp 4

RotChk: IX=0 Diff= 1.88D-14

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 1.121258 2.790235 0.184689

2 7 0 0.000000 2.023799 0.325221

3 6 0 -1.121258 2.790235 0.184689

4 6 0 -0.717701 4.166482 -0.040975

5 6 0 0.717701 4.166482 -0.040975

6 7 0 -2.412779 2.383698 0.210661

7 6 0 -2.794718 1.127499 0.265459

8 7 0 -2.010663 0.000000 0.329977

9 6 0 -2.794718 -1.127499 0.265459

10 6 0 -4.208325 -0.712278 0.207290

11 6 0 -4.208325 0.712278 0.207290

12 7 0 2.412779 2.383698 0.210661

13 6 0 4.208325 0.712278 0.207290

14 6 0 4.208325 -0.712278 0.207290

15 6 0 2.794718 -1.127499 0.265459

16 7 0 2.010663 0.000000 0.329977

17 6 0 2.794718 1.127499 0.265459

18 7 0 2.412779 -2.383698 0.210661

19 7 0 0.000000 -2.023799 0.325221

20 6 0 1.121258 -2.790235 0.184689

21 6 0 0.717701 -4.166482 -0.040975

22 6 0 -0.717701 -4.166482 -0.040975

23 6 0 -1.121258 -2.790235 0.184689

24 7 0 -2.412779 -2.383698 0.210661

25 30 0 0.000000 0.000000 0.847420

26 6 0 5.373561 1.426303 0.148915

27 6 0 6.609022 0.718862 0.097092

28 6 0 6.609022 -0.718862 0.097092

29 6 0 5.373561 -1.426303 0.148915

30 6 0 -1.428361 -5.326137 -0.250034

31 6 0 -0.721432 -6.535980 -0.461839

32 6 0 0.721432 -6.535980 -0.461839

33 6 0 1.428361 -5.326137 -0.250034

34 6 0 -5.373561 1.426303 0.148915

35 6 0 -6.609022 0.718862 0.097092

36 6 0 -6.609022 -0.718862 0.097092

37 6 0 -5.373561 -1.426303 0.148915

38 6 0 1.428361 5.326137 -0.250034

39 6 0 0.721432 6.535980 -0.461839

40 6 0 -0.721432 6.535980 -0.461839

41 6 0 -1.428361 5.326137 -0.250034

42 6 0 1.402333 -7.762632 -0.680515

43 6 0 0.708009 -8.930136 -0.888439

44 6 0 -0.708009 -8.930136 -0.888439

45 6 0 -1.402333 -7.762632 -0.680515

46 6 0 7.848572 -1.401348 0.044594

47 6 0 9.036054 -0.705858 -0.005467

48 6 0 9.036054 0.705858 -0.005467

49 6 0 7.848572 1.401348 0.044594

50 6 0 -1.402333 7.762632 -0.680515

51 6 0 -0.708009 8.930136 -0.888439

52 6 0 0.708009 8.930136 -0.888439

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55 6 0 -9.036054 -0.705858 -0.005467

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57 6 0 -7.848572 1.401348 0.044594

58 1 0 5.373676 2.511178 0.143956

59 1 0 5.373676 -2.511178 0.143956

60 1 0 -2.513386 -5.328741 -0.256608

61 1 0 2.513386 -5.328741 -0.256608

62 1 0 -5.373676 2.511178 0.143956

63 1 0 -5.373676 -2.511178 0.143956

64 1 0 2.513386 5.328741 -0.256608

65 1 0 -2.513386 5.328741 -0.256608

66 1 0 2.487808 -7.761067 -0.680032

67 1 0 1.243546 -9.858861 -1.053912

68 1 0 -1.243546 -9.858861 -1.053912

69 1 0 -2.487808 -7.761067 -0.680032

70 1 0 7.846789 -2.486615 0.044250

71 1 0 9.977787 -1.242475 -0.045752

72 1 0 9.977787 1.242475 -0.045752

73 1 0 7.846789 2.486615 0.044250

74 1 0 -2.487808 7.761067 -0.680032

75 1 0 -1.243546 9.858861 -1.053912

76 1 0 1.243546 9.858861 -1.053912

77 1 0 2.487808 7.761067 -0.680032

78 1 0 -7.846789 -2.486615 0.044250

79 1 0 -9.977787 -1.242475 -0.045752

80 1 0 -9.977787 1.242475 -0.045752

81 1 0 -7.846789 2.486615 0.044250

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

Rotational constants (GHZ): 0.0387348 0.0379554 0.0193810

Leave Link 202 at Sun Jun 30 21:07:30 2019, MaxMem= 1342177280 cpu: 0.7

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

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 307 symmetry adapted cartesian basis functions of A1 symmetry.

There are 278 symmetry adapted cartesian basis functions of A2 symmetry.

There are 289 symmetry adapted cartesian basis functions of B1 symmetry.

There are 289 symmetry adapted cartesian basis functions of B2 symmetry.

There are 289 symmetry adapted basis functions of A1 symmetry.

There are 265 symmetry adapted basis functions of A2 symmetry.

There are 275 symmetry adapted basis functions of B1 symmetry.

There are 275 symmetry adapted basis functions of B2 symmetry.

1104 basis functions, 1951 primitive gaussians, 1163 cartesian basis functions

191 alpha electrons 189 beta electrons

nuclear repulsion energy 6889.8532173806 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= 81 NActive= 81 NUniq= 22 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= -0.2361221601 Hartrees.

Nuclear repulsion after empirical dispersion term = 6889.6170952205 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= 81.

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 = 81

GePol: Total number of spheres = 81

GePol: Number of exposed spheres = 81 (100.00%)

GePol: Number of points = 6438

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.21D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 418

GePol: Fraction of low-weight points (<1% of avg) = 6.49%

GePol: Cavity surface area = 670.736 Ang\*\*2

GePol: Cavity volume = 694.550 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0170087965 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 6889.6000864240 Hartrees.

Leave Link 301 at Sun Jun 30 21:07:31 2019, MaxMem= 1342177280 cpu: 6.3

(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.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36727 LenP2D= 95228.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1104 RedAO= T EigKep= 2.89D-05 NBF= 289 265 275 275

NBsUse= 1104 1.00D-06 EigRej= -1.00D+00 NBFU= 289 265 275 275

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= 1060 1060 1060 1060 1060 MxSgAt= 81 MxSgA2= 81.

Leave Link 302 at Sun Jun 30 21:07:48 2019, MaxMem= 1342177280 cpu: 188.6

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Jun 30 21:07:49 2019, MaxMem= 1342177280 cpu: 2.5

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

Initial guess from the checkpoint file: "ZnNPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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The electronic state of the initial guess is 3-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

Generating alternative initial guess.

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -2348.36337356425

Leave Link 401 at Sun Jun 30 21:08:19 2019, MaxMem= 1342177280 cpu: 305.9

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4103221 IEndB= 4103221 NGot= 1342177280 MDV= 1339444432

LenX= 1339444432 LenY= 1338090700

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= 420000000 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= 124343532.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.15D-14 for 2140.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.83D-15 for 1337 485.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.33D-15 for 1019.

Iteration 1 A^-1\*A deviation from orthogonality is 4.60D-09 for 1524 1449.

Iteration 2 A\*A^-1 deviation from unit magnitude is 1.53D-14 for 1590.

Iteration 2 A\*A^-1 deviation from orthogonality is 1.22D-14 for 1338 486.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.55D-15 for 2128.

Iteration 2 A^-1\*A deviation from orthogonality is 6.42D-16 for 6427 6401.

E= -2348.13059867095

DIIS: error= 3.38D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2348.13059867095 IErMin= 1 ErrMin= 3.38D-04

ErrMax= 3.38D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.72D-04 BMatP= 2.72D-04

IDIUse=3 WtCom= 9.97D-01 WtEn= 3.38D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.379 Goal= None Shift= 0.000

Gap= 0.459 Goal= None Shift= 0.000

RMSDP=1.19D-05 MaxDP=3.31D-04 OVMax= 1.78D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.19D-05 CP: 1.00D+00

E= -2348.13073650619 Delta-E= -0.000137835235 Rises=F Damp=F

DIIS: error= 4.89D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2348.13073650619 IErMin= 2 ErrMin= 4.89D-05

ErrMax= 4.89D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.03D-06 BMatP= 2.72D-04

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

Coeff-Com: -0.747D-01 0.107D+01

Coeff: -0.747D-01 0.107D+01

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.61D-06 MaxDP=5.75D-05 DE=-1.38D-04 OVMax= 4.36D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 1.35D-06 CP: 1.00D+00 1.07D+00

E= -2348.13073851707 Delta-E= -0.000002010880 Rises=F Damp=F

DIIS: error= 1.19D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2348.13073851707 IErMin= 3 ErrMin= 1.19D-05

ErrMax= 1.19D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.70D-07 BMatP= 3.03D-06

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

Coeff-Com: -0.244D-01 0.305D+00 0.720D+00

Coeff: -0.244D-01 0.305D+00 0.720D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=6.81D-07 MaxDP=4.10D-05 DE=-2.01D-06 OVMax= 1.19D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.41D-07 CP: 1.00D+00 1.08D+00 8.66D-01

E= -2348.13073854448 Delta-E= -0.000000027414 Rises=F Damp=F

DIIS: error= 1.21D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2348.13073854448 IErMin= 3 ErrMin= 1.19D-05

ErrMax= 1.21D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.17D-07 BMatP= 4.70D-07

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

Coeff-Com: -0.554D-02 0.494D-01 0.480D+00 0.476D+00

Coeff: -0.554D-02 0.494D-01 0.480D+00 0.476D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=3.76D-07 MaxDP=2.28D-05 DE=-2.74D-08 OVMax= 7.93D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 1.72D-07 CP: 1.00D+00 1.08D+00 9.77D-01 5.46D-01

E= -2348.13073862920 Delta-E= -0.000000084714 Rises=F Damp=F

DIIS: error= 2.21D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2348.13073862920 IErMin= 5 ErrMin= 2.21D-06

ErrMax= 2.21D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.61D-08 BMatP= 4.17D-07

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

Coeff-Com: 0.748D-03-0.216D-01 0.114D+00 0.210D+00 0.697D+00

Coeff: 0.748D-03-0.216D-01 0.114D+00 0.210D+00 0.697D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=7.83D-08 MaxDP=7.43D-06 DE=-8.47D-08 OVMax= 2.78D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.11D-08 CP: 1.00D+00 1.08D+00 9.93D-01 5.91D-01 8.06D-01

E= -2348.13073863215 Delta-E= -0.000000002949 Rises=F Damp=F

DIIS: error= 1.57D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2348.13073863215 IErMin= 6 ErrMin= 1.57D-06

ErrMax= 1.57D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.24D-09 BMatP= 1.61D-08

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

Coeff-Com: 0.931D-03-0.183D-01 0.335D-01 0.955D-01 0.453D+00 0.435D+00

Coeff: 0.931D-03-0.183D-01 0.335D-01 0.955D-01 0.453D+00 0.435D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=3.43D-08 MaxDP=3.61D-06 DE=-2.95D-09 OVMax= 9.81D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 2.15D-08 CP: 1.00D+00 1.08D+00 9.95D-01 6.05D-01 8.41D-01

CP: 6.06D-01

E= -2348.13073863301 Delta-E= -0.000000000860 Rises=F Damp=F

DIIS: error= 2.32D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2348.13073863301 IErMin= 7 ErrMin= 2.32D-07

ErrMax= 2.32D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.02D-10 BMatP= 5.24D-09

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

Coeff-Com: 0.174D-03-0.252D-02-0.359D-02 0.317D-02 0.507D-01 0.117D+00

Coeff-Com: 0.835D+00

Coeff: 0.174D-03-0.252D-02-0.359D-02 0.317D-02 0.507D-01 0.117D+00

Coeff: 0.835D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=9.81D-09 MaxDP=4.27D-07 DE=-8.60D-10 OVMax= 6.46D-06

Error on total polarization charges = 0.08828

SCF Done: E(UB3LYP) = -2348.13073863 A.U. after 7 cycles

NFock= 7 Conv=0.98D-08 -V/T= 1.9830

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

<L.S>= 0.000000000000E+00

KE= 2.388748031760D+03 PE=-1.932262684518D+04 EE= 7.696147988359D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -10.67

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0219, after 2.0003

Leave Link 502 at Sun Jun 30 21:13:13 2019, MaxMem= 1342177280 cpu: 3230.7

(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.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36727 LenP2D= 95228.

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 = 193

Leave Link 701 at Sun Jun 30 21:13:48 2019, MaxMem= 1342177280 cpu: 341.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sun Jun 30 21:13:48 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=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 Sun Jun 30 21:14:38 2019, MaxMem= 1342177280 cpu: 494.7

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-2.16715534D-13 7.95807864D-13 8.77789862D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000015423 -0.000041698 0.000026056

2 7 0.000000000 0.000074216 -0.000014658

3 6 -0.000015423 -0.000041698 0.000026056

4 6 -0.000008725 0.000023340 -0.000044702

5 6 0.000008725 0.000023340 -0.000044702

6 7 0.000027464 -0.000063039 -0.000017350

7 6 0.000052673 0.000059766 0.000038160

8 7 -0.000047709 0.000000000 -0.000120985

9 6 0.000052673 -0.000059766 0.000038160

10 6 -0.000033818 0.000002758 0.000012435

11 6 -0.000033818 -0.000002758 0.000012435

12 7 -0.000027464 -0.000063039 -0.000017350

13 6 0.000033818 -0.000002758 0.000012435

14 6 0.000033818 0.000002758 0.000012435

15 6 -0.000052673 -0.000059766 0.000038160

16 7 0.000047709 0.000000000 -0.000120985

17 6 -0.000052673 0.000059766 0.000038160

18 7 -0.000027464 0.000063039 -0.000017350

19 7 0.000000000 -0.000074216 -0.000014658

20 6 0.000015423 0.000041698 0.000026056

21 6 0.000008725 -0.000023340 -0.000044702

22 6 -0.000008725 -0.000023340 -0.000044702

23 6 -0.000015423 0.000041698 0.000026056

24 7 0.000027464 0.000063039 -0.000017350

25 30 0.000000000 0.000000000 0.000138661

26 6 -0.000007538 -0.000022971 -0.000001983

27 6 0.000005887 0.000031830 0.000001101

28 6 0.000005887 -0.000031830 0.000001101

29 6 -0.000007538 0.000022971 -0.000001983

30 6 0.000030461 -0.000005136 0.000029476

31 6 -0.000039602 0.000001644 -0.000004388

32 6 0.000039602 0.000001644 -0.000004388

33 6 -0.000030461 -0.000005136 0.000029476

34 6 0.000007538 -0.000022971 -0.000001983

35 6 -0.000005887 0.000031830 0.000001101

36 6 -0.000005887 -0.000031830 0.000001101

37 6 0.000007538 0.000022971 -0.000001983

38 6 -0.000030461 0.000005136 0.000029476

39 6 0.000039602 -0.000001644 -0.000004388

40 6 -0.000039602 -0.000001644 -0.000004388

41 6 0.000030461 0.000005136 0.000029476

42 6 -0.000019162 -0.000015685 0.000004500

43 6 0.000026952 0.000006568 0.000003598

44 6 -0.000026952 0.000006568 0.000003598

45 6 0.000019162 -0.000015685 0.000004500

46 6 0.000007209 0.000011926 -0.000000960

47 6 -0.000003279 -0.000016675 -0.000000436

48 6 -0.000003279 0.000016675 -0.000000436

49 6 0.000007209 -0.000011926 -0.000000960

50 6 0.000019162 0.000015685 0.000004500

51 6 -0.000026952 -0.000006568 0.000003598

52 6 0.000026952 -0.000006568 0.000003598

53 6 -0.000019162 0.000015685 0.000004500

54 6 -0.000007209 0.000011926 -0.000000960

55 6 0.000003279 -0.000016675 -0.000000436

56 6 0.000003279 0.000016675 -0.000000436

57 6 -0.000007209 -0.000011926 -0.000000960

58 1 -0.000004893 0.000003239 0.000000959

59 1 -0.000004893 -0.000003239 0.000000959

60 1 -0.000003202 0.000010525 -0.000009143

61 1 0.000003202 0.000010525 -0.000009143

62 1 0.000004893 0.000003239 0.000000959

63 1 0.000004893 -0.000003239 0.000000959

64 1 0.000003202 -0.000010525 -0.000009143

65 1 -0.000003202 -0.000010525 -0.000009143

66 1 0.000002191 -0.000000917 -0.000003220

67 1 -0.000003832 -0.000001927 -0.000000931

68 1 0.000003832 -0.000001927 -0.000000931

69 1 -0.000002191 -0.000000917 -0.000003220

70 1 0.000002847 -0.000001132 0.000000181

71 1 0.000001620 0.000001841 -0.000000197

72 1 0.000001620 -0.000001841 -0.000000197

73 1 0.000002847 0.000001132 0.000000181

74 1 -0.000002191 0.000000917 -0.000003220

75 1 0.000003832 0.000001927 -0.000000931

76 1 -0.000003832 0.000001927 -0.000000931

77 1 0.000002191 0.000000917 -0.000003220

78 1 -0.000002847 -0.000001132 0.000000181

79 1 -0.000001620 0.000001841 -0.000000197

80 1 -0.000001620 -0.000001841 -0.000000197

81 1 -0.000002847 0.000001132 0.000000181

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

Cartesian Forces: Max 0.000138661 RMS 0.000026536

Leave Link 716 at Sun Jun 30 21:14:38 2019, MaxMem= 1342177280 cpu: 4.8

(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 0.000047695 RMS 0.000010215

Search for a local minimum.

Step number 8 out of a maximum of 486

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .10215D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

6 7 8

DE= -2.42D-06 DEPred=-2.00D-06 R= 1.21D+00

TightC=F SS= 1.41D+00 RLast= 2.66D-02 DXNew= 5.0454D-01 7.9863D-02

Trust test= 1.21D+00 RLast= 2.66D-02 DXMaxT set to 3.00D-01

ITU= 1 1 1 1 1 1 1 0

Eigenvalues --- 0.00272 0.00624 0.01432 0.01485 0.01500

Eigenvalues --- 0.01572 0.01589 0.01627 0.01656 0.01670

Eigenvalues --- 0.01694 0.01698 0.01705 0.01713 0.01714

Eigenvalues --- 0.01725 0.01730 0.01730 0.01736 0.01737

Eigenvalues --- 0.01745 0.01753 0.01759 0.01787 0.01791

Eigenvalues --- 0.01827 0.01828 0.01830 0.01851 0.01854

Eigenvalues --- 0.01870 0.01871 0.01891 0.01937 0.01968

Eigenvalues --- 0.01968 0.01972 0.01972 0.01978 0.01992

Eigenvalues --- 0.01992 0.01993 0.01993 0.02024 0.02080

Eigenvalues --- 0.02086 0.02086 0.02089 0.02091 0.02095

Eigenvalues --- 0.02095 0.02098 0.02103 0.02103 0.02104

Eigenvalues --- 0.02105 0.02106 0.02124 0.02124 0.02137

Eigenvalues --- 0.02144 0.02144 0.02147 0.02148 0.02164

Eigenvalues --- 0.02173 0.02178 0.02213 0.02214 0.02225

Eigenvalues --- 0.02227 0.02243 0.02281 0.02286 0.02346

Eigenvalues --- 0.02380 0.03132 0.05493 0.05546 0.08163

Eigenvalues --- 0.14679 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 0.16005 0.16011 0.16095

Eigenvalues --- 0.16156 0.16249 0.17495 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22499 0.22503 0.22504

Eigenvalues --- 0.22537 0.23233 0.23234 0.23234 0.23642

Eigenvalues --- 0.23939 0.23939 0.23940 0.23953 0.24215

Eigenvalues --- 0.24280 0.24311 0.24550 0.24553 0.24557

Eigenvalues --- 0.24557 0.24573 0.24769 0.24891 0.24895

Eigenvalues --- 0.24961 0.24982 0.24983 0.24984 0.24989

Eigenvalues --- 0.24996 0.24996 0.24997 0.24997 0.26437

Eigenvalues --- 0.32865 0.32947 0.33671 0.33751 0.33834

Eigenvalues --- 0.33877 0.35041 0.35068 0.35181 0.35181

Eigenvalues --- 0.35181 0.35188 0.35202 0.35202 0.35202

Eigenvalues --- 0.35212 0.35231 0.35231 0.35231 0.35240

Eigenvalues --- 0.35249 0.35249 0.35249 0.35270 0.35270

Eigenvalues --- 0.35270 0.35273 0.35279 0.35279 0.35279

Eigenvalues --- 0.35280 0.35414 0.35446 0.35814 0.36349

Eigenvalues --- 0.37054 0.37458 0.37573 0.37969 0.39276

Eigenvalues --- 0.39276 0.39288 0.39612 0.39612 0.40188

Eigenvalues --- 0.40188 0.40257 0.40257 0.40906 0.41001

Eigenvalues --- 0.41044 0.41144 0.41603 0.41776 0.41873

Eigenvalues --- 0.42156 0.42215 0.42410 0.42806 0.42835

Eigenvalues --- 0.42902 0.42970 0.45519 0.45684 0.47124

Eigenvalues --- 0.47124 0.47241 0.47384 0.47386 0.47579

Eigenvalues --- 0.47580 0.48122 0.48218 0.48355 0.48456

Eigenvalues --- 0.48465 0.48680 0.48707 0.48729 0.48735

Eigenvalues --- 0.49091 0.49376 0.49898 0.50362 0.50402

Eigenvalues --- 0.51028 0.51300 0.52479 0.59238 0.59871

Eigenvalues --- 0.59957 0.60917

En-DIIS/RFO-DIIS IScMMF= 0 using points: 8 7 6 5 4

RFO step: Lambda=-1.38484984D-07.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 1.07D-05 SmlDif= 1.00D-05

RMS Error= 0.3755309022D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.78396 -1.11923 0.08130 0.41830 -0.16432

Iteration 1 RMS(Cart)= 0.00249031 RMS(Int)= 0.00000072

Iteration 2 RMS(Cart)= 0.00000281 RMS(Int)= 0.00000048

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000048

ITry= 1 IFail=0 DXMaxC= 1.38D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.39D-08 for atom 62.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58028 -0.00003 -0.00008 0.00001 -0.00007 2.58021

R2 2.74358 0.00003 0.00006 0.00002 0.00008 2.74366

R3 2.55915 -0.00002 -0.00005 0.00001 -0.00004 2.55911

R4 2.58028 -0.00003 -0.00008 0.00001 -0.00007 2.58021

R5 3.94969 0.00003 -0.00009 0.00023 0.00014 3.94983

R6 2.74358 0.00003 0.00006 0.00002 0.00008 2.74366

R7 2.55915 -0.00002 -0.00005 0.00001 -0.00004 2.55911

R8 2.71252 0.00000 0.00000 0.00003 0.00003 2.71254

R9 2.60038 -0.00001 -0.00003 0.00000 -0.00003 2.60035

R10 2.60038 -0.00001 -0.00003 0.00000 -0.00003 2.60035

R11 2.48333 -0.00005 -0.00003 -0.00003 -0.00006 2.48327

R12 2.59805 -0.00002 -0.00005 0.00001 -0.00005 2.59800

R13 2.78636 0.00004 0.00004 0.00002 0.00006 2.78642

R14 2.59805 -0.00002 -0.00005 0.00001 -0.00005 2.59800

R15 3.92341 0.00002 0.00004 0.00015 0.00018 3.92359

R16 2.78636 0.00004 0.00004 0.00002 0.00006 2.78642

R17 2.48333 -0.00005 -0.00003 -0.00003 -0.00006 2.48327

R18 2.69202 0.00000 0.00002 0.00000 0.00002 2.69205

R19 2.58486 0.00000 -0.00001 0.00000 -0.00001 2.58485

R20 2.58486 0.00000 -0.00001 0.00000 -0.00001 2.58485

R21 2.48333 -0.00005 -0.00003 -0.00003 -0.00006 2.48327

R22 2.69202 0.00000 0.00002 0.00000 0.00002 2.69205

R23 2.78636 0.00004 0.00004 0.00002 0.00006 2.78642

R24 2.58486 0.00000 -0.00001 0.00000 -0.00001 2.58485

R25 2.78636 0.00004 0.00004 0.00002 0.00006 2.78642

R26 2.58486 0.00000 -0.00001 0.00000 -0.00001 2.58485

R27 2.59805 -0.00002 -0.00005 0.00001 -0.00005 2.59800

R28 2.48333 -0.00005 -0.00003 -0.00003 -0.00006 2.48327

R29 2.59805 -0.00002 -0.00005 0.00001 -0.00005 2.59800

R30 3.92341 0.00002 0.00004 0.00015 0.00018 3.92359

R31 2.55915 -0.00002 -0.00005 0.00001 -0.00004 2.55911

R32 2.58028 -0.00003 -0.00008 0.00001 -0.00007 2.58021

R33 2.58028 -0.00003 -0.00008 0.00001 -0.00007 2.58021

R34 3.94969 0.00003 -0.00009 0.00023 0.00014 3.94983

R35 2.74358 0.00003 0.00006 0.00002 0.00008 2.74366

R36 2.71252 0.00000 0.00000 0.00003 0.00003 2.71254

R37 2.60038 -0.00001 -0.00003 0.00000 -0.00003 2.60035

R38 2.74358 0.00003 0.00006 0.00002 0.00008 2.74366

R39 2.60038 -0.00001 -0.00003 0.00000 -0.00003 2.60035

R40 2.55915 -0.00002 -0.00005 0.00001 -0.00004 2.55911

R41 2.69213 0.00001 0.00002 -0.00001 0.00001 2.69214

R42 2.05014 0.00000 0.00001 0.00000 0.00001 2.05015

R43 2.71690 0.00002 0.00000 0.00005 0.00005 2.71696

R44 2.67583 0.00001 0.00001 -0.00001 0.00000 2.67583

R45 2.69213 0.00001 0.00002 -0.00001 0.00001 2.69214

R46 2.67583 0.00001 0.00001 -0.00001 0.00000 2.67583

R47 2.05014 0.00000 0.00001 0.00000 0.00001 2.05015

R48 2.67804 0.00000 0.00002 -0.00002 0.00000 2.67804

R49 2.05044 0.00000 0.00001 0.00000 0.00001 2.05046

R50 2.72662 0.00002 0.00001 0.00005 0.00006 2.72668

R51 2.68323 0.00001 0.00003 -0.00003 0.00000 2.68323

R52 2.67804 0.00000 0.00002 -0.00002 0.00000 2.67804

R53 2.68323 0.00001 0.00003 -0.00003 0.00000 2.68323

R54 2.05044 0.00000 0.00001 0.00000 0.00001 2.05046

R55 2.69213 0.00001 0.00002 -0.00001 0.00001 2.69214

R56 2.05014 0.00000 0.00001 0.00000 0.00001 2.05015

R57 2.71690 0.00002 0.00000 0.00005 0.00005 2.71696

R58 2.67583 0.00001 0.00001 -0.00001 0.00000 2.67583

R59 2.69213 0.00001 0.00002 -0.00001 0.00001 2.69214

R60 2.67583 0.00001 0.00001 -0.00001 0.00000 2.67583

R61 2.05014 0.00000 0.00001 0.00000 0.00001 2.05015

R62 2.67804 0.00000 0.00002 -0.00002 0.00000 2.67804

R63 2.05044 0.00000 0.00001 0.00000 0.00001 2.05046

R64 2.72662 0.00002 0.00001 0.00005 0.00006 2.72668

R65 2.68323 0.00001 0.00003 -0.00003 0.00000 2.68323

R66 2.67804 0.00000 0.00002 -0.00002 0.00000 2.67804

R67 2.68323 0.00001 0.00003 -0.00003 0.00000 2.68323

R68 2.05044 0.00000 0.00001 0.00000 0.00001 2.05046

R69 2.59683 -0.00001 -0.00001 -0.00002 -0.00002 2.59681

R70 2.05125 0.00000 0.00000 0.00001 0.00001 2.05126

R71 2.67589 0.00001 -0.00001 0.00004 0.00003 2.67592

R72 2.04991 0.00000 0.00000 0.00000 0.00000 2.04990

R73 2.59683 -0.00001 -0.00001 -0.00002 -0.00002 2.59681

R74 2.04991 0.00000 0.00000 0.00000 0.00000 2.04990

R75 2.05125 0.00000 0.00000 0.00001 0.00001 2.05126

R76 2.60229 0.00000 0.00000 -0.00001 -0.00001 2.60228

R77 2.05086 0.00000 0.00000 0.00001 0.00000 2.05086

R78 2.66776 0.00001 -0.00001 0.00003 0.00002 2.66778

R79 2.04967 0.00000 0.00000 0.00000 0.00000 2.04967

R80 2.60229 0.00000 0.00000 -0.00001 -0.00001 2.60228

R81 2.04967 0.00000 0.00000 0.00000 0.00000 2.04967

R82 2.05086 0.00000 0.00000 0.00001 0.00000 2.05086

R83 2.59683 -0.00001 -0.00001 -0.00002 -0.00002 2.59681

R84 2.05125 0.00000 0.00000 0.00001 0.00001 2.05126

R85 2.67589 0.00001 -0.00001 0.00004 0.00003 2.67592

R86 2.04991 0.00000 0.00000 0.00000 0.00000 2.04990

R87 2.59683 -0.00001 -0.00001 -0.00002 -0.00002 2.59681

R88 2.04991 0.00000 0.00000 0.00000 0.00000 2.04990

R89 2.05125 0.00000 0.00000 0.00001 0.00001 2.05126

R90 2.60229 0.00000 0.00000 -0.00001 -0.00001 2.60228

R91 2.05086 0.00000 0.00000 0.00001 0.00000 2.05086

R92 2.66776 0.00001 -0.00001 0.00003 0.00002 2.66778

R93 2.04967 0.00000 0.00000 0.00000 0.00000 2.04967

R94 2.60229 0.00000 0.00000 -0.00001 -0.00001 2.60228

R95 2.04967 0.00000 0.00000 0.00000 0.00000 2.04967

R96 2.05086 0.00000 0.00000 0.00001 0.00000 2.05086

A1 1.89635 0.00000 -0.00001 -0.00004 -0.00005 1.89630

A2 2.23023 -0.00001 -0.00007 0.00002 -0.00005 2.23018

A3 2.15632 0.00001 0.00008 0.00003 0.00011 2.15643

A4 1.92694 0.00002 0.00005 0.00005 0.00011 1.92705

A5 2.17636 -0.00001 -0.00004 0.00000 -0.00004 2.17632

A6 2.17636 -0.00001 -0.00004 0.00000 -0.00004 2.17632

A7 1.89635 0.00000 -0.00001 -0.00004 -0.00005 1.89630

A8 2.23023 -0.00001 -0.00007 0.00002 -0.00005 2.23018

A9 2.15632 0.00001 0.00008 0.00003 0.00011 2.15643

A10 1.85247 -0.00001 -0.00002 0.00001 0.00000 1.85246

A11 2.31709 0.00001 0.00004 -0.00001 0.00003 2.31712

A12 2.11349 0.00000 -0.00002 0.00000 -0.00002 2.11347

A13 1.85247 -0.00001 -0.00002 0.00001 0.00000 1.85246

A14 2.31709 0.00001 0.00004 -0.00001 0.00003 2.31712

A15 2.11349 0.00000 -0.00002 0.00000 -0.00002 2.11347

A16 2.17116 0.00003 0.00004 0.00002 0.00006 2.17122

A17 2.23974 0.00000 -0.00006 -0.00001 -0.00007 2.23967

A18 2.14861 0.00001 0.00007 0.00003 0.00009 2.14870

A19 1.89405 -0.00001 0.00000 -0.00002 -0.00002 1.89403

A20 1.92317 0.00003 0.00005 0.00003 0.00008 1.92325

A21 2.17001 -0.00001 -0.00028 -0.00006 -0.00034 2.16966

A22 2.17001 -0.00001 -0.00028 -0.00006 -0.00034 2.16966

A23 1.89405 -0.00001 0.00000 -0.00002 -0.00002 1.89403

A24 2.23974 0.00000 -0.00006 -0.00001 -0.00007 2.23967

A25 2.14861 0.00001 0.00007 0.00003 0.00009 2.14870

A26 1.85626 0.00000 -0.00001 0.00001 0.00000 1.85626

A27 2.30688 0.00000 0.00004 -0.00002 0.00002 2.30690

A28 2.12000 0.00000 -0.00003 0.00001 -0.00002 2.11998

A29 1.85626 0.00000 -0.00001 0.00001 0.00000 1.85626

A30 2.30688 0.00000 0.00004 -0.00002 0.00002 2.30690

A31 2.12000 0.00000 -0.00003 0.00001 -0.00002 2.11998

A32 2.17116 0.00003 0.00004 0.00002 0.00006 2.17122

A33 1.85626 0.00000 -0.00001 0.00001 0.00000 1.85626

A34 2.12000 0.00000 -0.00003 0.00001 -0.00002 2.11998

A35 2.30688 0.00000 0.00004 -0.00002 0.00002 2.30690

A36 1.85626 0.00000 -0.00001 0.00001 0.00000 1.85626

A37 2.12000 0.00000 -0.00003 0.00001 -0.00002 2.11998

A38 2.30688 0.00000 0.00004 -0.00002 0.00002 2.30690

A39 1.89405 -0.00001 0.00000 -0.00002 -0.00002 1.89403

A40 2.14861 0.00001 0.00007 0.00003 0.00009 2.14870

A41 2.23974 0.00000 -0.00006 -0.00001 -0.00007 2.23967

A42 1.92317 0.00003 0.00005 0.00003 0.00008 1.92325

A43 2.17001 -0.00001 -0.00028 -0.00006 -0.00034 2.16966

A44 2.17001 -0.00001 -0.00028 -0.00006 -0.00034 2.16966

A45 2.14861 0.00001 0.00007 0.00003 0.00009 2.14870

A46 2.23974 0.00000 -0.00006 -0.00001 -0.00007 2.23967

A47 1.89405 -0.00001 0.00000 -0.00002 -0.00002 1.89403

A48 2.17116 0.00003 0.00004 0.00002 0.00006 2.17122

A49 1.92694 0.00002 0.00005 0.00005 0.00011 1.92705

A50 2.17636 -0.00001 -0.00004 0.00000 -0.00004 2.17632

A51 2.17636 -0.00001 -0.00004 0.00000 -0.00004 2.17632

A52 2.23023 -0.00001 -0.00007 0.00002 -0.00005 2.23018

A53 2.15632 0.00001 0.00008 0.00003 0.00011 2.15643

A54 1.89635 0.00000 -0.00001 -0.00004 -0.00005 1.89630

A55 1.85247 -0.00001 -0.00002 0.00001 0.00000 1.85246

A56 2.31709 0.00001 0.00004 -0.00001 0.00003 2.31712

A57 2.11349 0.00000 -0.00002 0.00000 -0.00002 2.11347

A58 1.85247 -0.00001 -0.00002 0.00001 0.00000 1.85246

A59 2.11349 0.00000 -0.00002 0.00000 -0.00002 2.11347

A60 2.31709 0.00001 0.00004 -0.00001 0.00003 2.31712

A61 1.89635 0.00000 -0.00001 -0.00004 -0.00005 1.89630

A62 2.23023 -0.00001 -0.00007 0.00002 -0.00005 2.23018

A63 2.15632 0.00001 0.00008 0.00003 0.00011 2.15643

A64 2.17116 0.00003 0.00004 0.00002 0.00006 2.17122

A65 1.50849 0.00000 -0.00004 -0.00004 -0.00009 1.50840

A66 1.50849 0.00000 -0.00004 -0.00004 -0.00009 1.50840

A67 2.63655 -0.00001 0.00028 -0.00020 0.00008 2.63663

A68 2.63782 -0.00001 -0.00065 -0.00015 -0.00079 2.63703

A69 1.50849 0.00000 -0.00004 -0.00004 -0.00009 1.50840

A70 1.50849 0.00000 -0.00004 -0.00004 -0.00009 1.50840

A71 2.07270 0.00001 0.00006 -0.00002 0.00004 2.07275

A72 2.12033 -0.00001 -0.00006 0.00000 -0.00005 2.12027

A73 2.09015 0.00000 -0.00001 0.00002 0.00001 2.09016

A74 2.09046 -0.00001 -0.00003 0.00000 -0.00003 2.09043

A75 2.11901 0.00001 0.00005 -0.00001 0.00004 2.11905

A76 2.07372 0.00000 -0.00002 0.00001 -0.00001 2.07371

A77 2.09046 -0.00001 -0.00003 0.00000 -0.00003 2.09043

A78 2.07372 0.00000 -0.00002 0.00001 -0.00001 2.07371

A79 2.11901 0.00001 0.00005 -0.00001 0.00004 2.11905

A80 2.07270 0.00001 0.00006 -0.00002 0.00004 2.07275

A81 2.12033 -0.00001 -0.00006 0.00000 -0.00005 2.12027

A82 2.09015 0.00000 -0.00001 0.00002 0.00001 2.09016

A83 2.07663 0.00001 0.00005 -0.00001 0.00005 2.07668

A84 2.11692 -0.00002 -0.00006 -0.00002 -0.00008 2.11684

A85 2.08963 0.00000 0.00001 0.00002 0.00003 2.08967

A86 2.09305 -0.00001 -0.00003 0.00000 -0.00003 2.09302

A87 2.11920 0.00002 0.00006 -0.00002 0.00004 2.11925

A88 2.07093 -0.00001 -0.00003 0.00001 -0.00001 2.07091

A89 2.09305 -0.00001 -0.00003 0.00000 -0.00003 2.09302

A90 2.07093 -0.00001 -0.00003 0.00001 -0.00001 2.07091

A91 2.11920 0.00002 0.00006 -0.00002 0.00004 2.11925

A92 2.07663 0.00001 0.00005 -0.00001 0.00005 2.07668

A93 2.11692 -0.00002 -0.00006 -0.00002 -0.00008 2.11684

A94 2.08963 0.00000 0.00001 0.00002 0.00003 2.08967

A95 2.07270 0.00001 0.00006 -0.00002 0.00004 2.07275

A96 2.12033 -0.00001 -0.00006 0.00000 -0.00005 2.12027

A97 2.09015 0.00000 -0.00001 0.00002 0.00001 2.09016

A98 2.09046 -0.00001 -0.00003 0.00000 -0.00003 2.09043

A99 2.11901 0.00001 0.00005 -0.00001 0.00004 2.11905

A100 2.07372 0.00000 -0.00002 0.00001 -0.00001 2.07371

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A105 2.12033 -0.00001 -0.00006 0.00000 -0.00005 2.12027

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A107 2.07663 0.00001 0.00005 -0.00001 0.00005 2.07668

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A116 2.07663 0.00001 0.00005 -0.00001 0.00005 2.07668

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A121 2.10198 0.00000 -0.00003 0.00002 -0.00002 2.10196

A122 2.10048 0.00000 -0.00002 0.00001 0.00000 2.10048

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A124 2.08712 0.00000 -0.00003 0.00000 -0.00002 2.08710

A125 2.10048 0.00000 -0.00002 0.00001 0.00000 2.10048

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A127 2.09558 0.00000 0.00004 -0.00002 0.00003 2.09560

A128 2.11177 0.00001 0.00005 -0.00003 0.00002 2.11179

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A132 2.07209 0.00000 0.00000 0.00002 0.00002 2.07211

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A134 2.10024 0.00000 -0.00001 0.00001 0.00000 2.10024

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D1 0.01908 0.00000 -0.00016 0.00022 0.00006 0.01914

D2 -3.03591 0.00000 0.00021 -0.00038 -0.00017 -3.03608

D3 -3.09694 0.00000 -0.00050 -0.00011 -0.00062 -3.09756

D4 0.13126 0.00000 -0.00013 -0.00072 -0.00085 0.13041

D5 -0.01133 0.00000 0.00010 -0.00013 -0.00003 -0.01137

D6 -3.13446 -0.00001 -0.00037 -0.00041 -0.00078 -3.13524

D7 3.10601 0.00000 0.00042 0.00018 0.00060 3.10661

D8 -0.01711 -0.00001 -0.00005 -0.00010 -0.00015 -0.01726

D9 0.10821 0.00000 0.00025 0.00043 0.00069 0.10890

D10 -3.00431 0.00000 -0.00013 0.00006 -0.00007 -3.00438

D11 -0.01908 0.00000 0.00016 -0.00022 -0.00006 -0.01914

D12 3.09694 0.00000 0.00050 0.00011 0.00062 3.09756

D13 3.03591 0.00000 -0.00021 0.00038 0.00017 3.03608

D14 -0.13126 0.00000 0.00013 0.00072 0.00085 -0.13041

D15 -2.94676 0.00001 0.00011 0.00041 0.00052 -2.94624

D16 -0.29360 -0.00001 -0.00053 0.00028 -0.00025 -0.29385

D17 -1.62018 0.00000 -0.00021 0.00035 0.00014 -1.62004

D18 0.29360 0.00001 0.00053 -0.00028 0.00025 0.29385

D19 2.94676 -0.00001 -0.00011 -0.00041 -0.00052 2.94624

D20 1.62018 0.00000 0.00021 -0.00035 -0.00014 1.62004

D21 0.01133 0.00000 -0.00010 0.00013 0.00003 0.01137

D22 3.13446 0.00001 0.00037 0.00041 0.00078 3.13524

D23 -3.10601 0.00000 -0.00042 -0.00018 -0.00060 -3.10661

D24 0.01711 0.00001 0.00005 0.00010 0.00015 0.01726

D25 -0.10821 0.00000 -0.00025 -0.00043 -0.00069 -0.10890

D26 3.00431 0.00000 0.00013 -0.00006 0.00007 3.00438

D27 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D28 3.12576 0.00001 0.00040 0.00024 0.00064 3.12640

D29 -3.12576 -0.00001 -0.00040 -0.00024 -0.00064 -3.12640

D30 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D31 -3.12588 -0.00001 -0.00047 -0.00045 -0.00091 -3.12679

D32 0.01424 -0.00001 -0.00049 -0.00029 -0.00078 0.01346

D33 -0.00500 0.00000 0.00006 -0.00013 -0.00007 -0.00508

D34 3.13511 0.00000 0.00004 0.00003 0.00006 3.13518

D35 3.12588 0.00001 0.00047 0.00045 0.00091 3.12679

D36 -0.01424 0.00001 0.00049 0.00029 0.00078 -0.01346

D37 0.00500 0.00000 -0.00006 0.00013 0.00007 0.00508

D38 -3.13511 0.00000 -0.00004 -0.00003 -0.00006 -3.13518

D39 0.02157 -0.00001 -0.00080 -0.00039 -0.00119 0.02038

D40 -3.07249 -0.00001 -0.00105 -0.00014 -0.00119 -3.07367

D41 -3.05814 0.00000 -0.00089 0.00028 -0.00061 -3.05874

D42 0.28953 0.00002 0.00174 0.00077 0.00252 0.29204

D43 0.04147 0.00000 -0.00067 0.00006 -0.00060 0.04086

D44 -2.89406 0.00002 0.00196 0.00056 0.00252 -2.89154

D45 3.07755 0.00000 0.00060 -0.00024 0.00036 3.07790

D46 -0.05377 0.00000 0.00070 -0.00014 0.00056 -0.05321

D47 -0.02472 0.00000 0.00040 -0.00004 0.00036 -0.02436

D48 3.12715 0.00000 0.00050 0.00006 0.00056 3.12771

D49 -0.04147 0.00000 0.00067 -0.00006 0.00060 -0.04086

D50 3.05814 0.00000 0.00089 -0.00028 0.00061 3.05874

D51 2.89406 -0.00002 -0.00196 -0.00056 -0.00252 2.89154

D52 -0.28953 -0.00002 -0.00174 -0.00077 -0.00252 -0.29204

D53 -0.36223 -0.00002 -0.00132 -0.00037 -0.00169 -0.36392

D54 -1.68815 -0.00001 -0.00148 -0.00027 -0.00175 -1.68990

D55 -3.01407 0.00000 -0.00163 -0.00018 -0.00182 -3.01589

D56 3.01407 0.00000 0.00163 0.00018 0.00182 3.01589

D57 1.68815 0.00001 0.00148 0.00027 0.00175 1.68990

D58 0.36223 0.00002 0.00132 0.00037 0.00169 0.36392

D59 0.02472 0.00000 -0.00040 0.00004 -0.00036 0.02436

D60 -3.12715 0.00000 -0.00050 -0.00006 -0.00056 -3.12771

D61 -3.07755 0.00000 -0.00060 0.00024 -0.00036 -3.07790

D62 0.05377 0.00000 -0.00070 0.00014 -0.00056 0.05321

D63 -0.02157 0.00001 0.00080 0.00039 0.00119 -0.02038

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D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13266 0.00000 -0.00009 -0.00009 -0.00017 3.13249

D67 -3.13266 0.00000 0.00009 0.00009 0.00017 -3.13249

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 -3.13808 0.00000 0.00028 -0.00001 0.00027 -3.13782

D70 0.00621 0.00000 0.00011 0.00009 0.00020 0.00641

D71 -0.00805 0.00000 0.00016 -0.00012 0.00004 -0.00801

D72 3.13625 0.00000 -0.00001 -0.00002 -0.00002 3.13622

D73 3.13808 0.00000 -0.00028 0.00001 -0.00027 3.13782

D74 -0.00621 0.00000 -0.00011 -0.00009 -0.00020 -0.00641

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D76 -3.13625 0.00000 0.00001 0.00002 0.00002 -3.13622

D77 3.07249 0.00001 0.00105 0.00014 0.00119 3.07367

D78 -0.02157 0.00001 0.00080 0.00039 0.00119 -0.02038

D79 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D80 3.13266 0.00000 -0.00009 -0.00009 -0.00017 3.13249

D81 -3.13266 0.00000 0.00009 0.00009 0.00017 -3.13249

D82 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D83 -3.07755 0.00000 -0.00060 0.00024 -0.00036 -3.07790

D84 0.02472 0.00000 -0.00040 0.00004 -0.00036 0.02436

D85 0.05377 0.00000 -0.00070 0.00014 -0.00056 0.05321

D86 -3.12715 0.00000 -0.00050 -0.00006 -0.00056 -3.12771

D87 -0.00805 0.00000 0.00016 -0.00012 0.00004 -0.00801

D88 3.13625 0.00000 -0.00001 -0.00002 -0.00002 3.13622

D89 -3.13808 0.00000 0.00028 -0.00001 0.00027 -3.13782

D90 0.00621 0.00000 0.00011 0.00009 0.00020 0.00641

D91 -0.02472 0.00000 0.00040 -0.00004 0.00036 -0.02436

D92 3.07755 0.00000 0.00060 -0.00024 0.00036 3.07790

D93 3.12715 0.00000 0.00050 0.00006 0.00056 3.12771

D94 -0.05377 0.00000 0.00070 -0.00014 0.00056 -0.05321

D95 0.00805 0.00000 -0.00016 0.00012 -0.00004 0.00801

D96 -3.13625 0.00000 0.00001 0.00002 0.00002 -3.13622

D97 3.13808 0.00000 -0.00028 0.00001 -0.00027 3.13782

D98 -0.00621 0.00000 -0.00011 -0.00009 -0.00020 -0.00641

D99 0.04147 0.00000 -0.00067 0.00006 -0.00060 0.04086

D100 -2.89406 0.00002 0.00196 0.00056 0.00252 -2.89154

D101 -3.05814 0.00000 -0.00089 0.00028 -0.00061 -3.05874

D102 0.28953 0.00002 0.00174 0.00077 0.00252 0.29204

D103 -3.07249 -0.00001 -0.00105 -0.00014 -0.00119 -3.07367

D104 0.02157 -0.00001 -0.00080 -0.00039 -0.00119 0.02038

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D106 -0.04147 0.00000 0.00067 -0.00006 0.00060 -0.04086

D107 -0.28953 -0.00002 -0.00174 -0.00077 -0.00252 -0.29204

D108 2.89406 -0.00002 -0.00196 -0.00056 -0.00252 2.89154

D109 -3.01407 0.00000 -0.00163 -0.00018 -0.00182 -3.01589

D110 -1.68815 -0.00001 -0.00148 -0.00027 -0.00175 -1.68990

D111 -0.36223 -0.00002 -0.00132 -0.00037 -0.00169 -0.36392

D112 0.36223 0.00002 0.00132 0.00037 0.00169 0.36392

D113 1.68815 0.00001 0.00148 0.00027 0.00175 1.68990

D114 3.01407 0.00000 0.00163 0.00018 0.00182 3.01589

D115 -0.10821 0.00000 -0.00025 -0.00043 -0.00069 -0.10890

D116 3.00431 0.00000 0.00013 -0.00006 0.00007 3.00438

D117 3.09694 0.00000 0.00050 0.00011 0.00062 3.09756

D118 -0.01908 0.00000 0.00016 -0.00022 -0.00006 -0.01914

D119 -0.13126 0.00000 0.00013 0.00072 0.00085 -0.13041

D120 3.03591 0.00000 -0.00021 0.00038 0.00017 3.03608

D121 0.01908 0.00000 -0.00016 0.00022 0.00006 0.01914

D122 -3.09694 0.00000 -0.00050 -0.00011 -0.00062 -3.09756

D123 -3.03591 0.00000 0.00021 -0.00038 -0.00017 -3.03608

D124 0.13126 0.00000 -0.00013 -0.00072 -0.00085 0.13041

D125 1.62018 0.00000 0.00021 -0.00035 -0.00014 1.62004

D126 2.94676 -0.00001 -0.00011 -0.00041 -0.00052 2.94624

D127 0.29360 0.00001 0.00053 -0.00028 0.00025 0.29385

D128 -1.62018 0.00000 -0.00021 0.00035 0.00014 -1.62004

D129 -0.29360 -0.00001 -0.00053 0.00028 -0.00025 -0.29385

D130 -2.94676 0.00001 0.00011 0.00041 0.00052 -2.94624

D131 -3.10601 0.00000 -0.00042 -0.00018 -0.00060 -3.10661

D132 0.01711 0.00001 0.00005 0.00010 0.00015 0.01726

D133 0.01133 0.00000 -0.00010 0.00013 0.00003 0.01137

D134 3.13446 0.00001 0.00037 0.00041 0.00078 3.13524

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D137 -3.12576 -0.00001 -0.00040 -0.00024 -0.00064 -3.12640

D138 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D139 -3.12588 -0.00001 -0.00047 -0.00045 -0.00091 -3.12679

D140 0.01424 -0.00001 -0.00049 -0.00029 -0.00078 0.01346

D141 -0.00500 0.00000 0.00006 -0.00013 -0.00007 -0.00508

D142 3.13511 0.00000 0.00004 0.00003 0.00006 3.13518

D143 -0.01133 0.00000 0.00010 -0.00013 -0.00003 -0.01137

D144 3.10601 0.00000 0.00042 0.00018 0.00060 3.10661

D145 -3.13446 -0.00001 -0.00037 -0.00041 -0.00078 -3.13524

D146 -0.01711 -0.00001 -0.00005 -0.00010 -0.00015 -0.01726

D147 0.00500 0.00000 -0.00006 0.00013 0.00007 0.00508

D148 -3.13511 0.00000 -0.00004 -0.00003 -0.00006 -3.13518

D149 3.12588 0.00001 0.00047 0.00045 0.00091 3.12679

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D157 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D159 -3.14119 0.00000 0.00005 0.00006 0.00011 -3.14108

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D164 3.14115 0.00000 0.00001 -0.00002 -0.00001 3.14114

D165 -0.00791 0.00000 0.00016 -0.00012 0.00004 -0.00787

D166 3.13634 0.00000 -0.00001 -0.00002 -0.00002 3.13631

D167 3.13410 0.00000 0.00021 -0.00006 0.00015 3.13425

D168 -0.00484 0.00000 0.00005 0.00004 0.00009 -0.00475

D169 0.00020 0.00000 0.00002 -0.00004 -0.00002 0.00017

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D171 3.14138 0.00000 -0.00003 -0.00010 -0.00013 3.14125

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D179 3.13849 0.00000 0.00014 0.00011 0.00025 3.13874

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D187 -3.13984 0.00000 0.00009 0.00024 0.00033 -3.13951

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D216 -0.00320 0.00000 -0.00011 -0.00008 -0.00020 -0.00340

D217 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D218 -3.13849 0.00000 -0.00014 -0.00011 -0.00025 -3.13874

D219 3.13849 0.00000 0.00014 0.00011 0.00025 3.13874

D220 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D221 3.13861 0.00000 0.00049 -0.00027 0.00022 3.13883

D222 -0.00337 0.00000 0.00003 0.00029 0.00032 -0.00305

D223 0.00017 0.00000 0.00034 -0.00038 -0.00004 0.00013

D224 3.14138 0.00000 -0.00011 0.00018 0.00006 3.14144

D225 0.00494 0.00000 -0.00006 0.00013 0.00007 0.00502

D226 -3.13520 0.00000 -0.00004 -0.00003 -0.00006 -3.13526

D227 -3.13984 0.00000 0.00009 0.00024 0.00033 -3.13951

D228 0.00320 0.00000 0.00011 0.00008 0.00020 0.00340

D229 -0.00017 0.00000 -0.00034 0.00038 0.00004 -0.00013

D230 -3.14138 0.00000 0.00011 -0.00018 -0.00006 -3.14144

D231 -3.13861 0.00000 -0.00049 0.00027 -0.00022 -3.13883

D232 0.00337 0.00000 -0.00003 -0.00029 -0.00032 0.00305

D233 0.00018 0.00000 0.00035 -0.00039 -0.00004 0.00014

D234 -3.14149 0.00000 0.00026 -0.00034 -0.00008 -3.14157

D235 3.14138 0.00000 -0.00012 0.00018 0.00006 3.14144

D236 -0.00029 0.00000 -0.00021 0.00023 0.00002 -0.00027

D237 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D238 3.14151 0.00000 -0.00009 0.00005 -0.00004 3.14148

D239 -3.14151 0.00000 0.00009 -0.00005 0.00004 -3.14148

D240 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D241 -0.00018 0.00000 -0.00035 0.00039 0.00004 -0.00014

D242 -3.14138 0.00000 0.00012 -0.00018 -0.00006 -3.14144

D243 3.14149 0.00000 -0.00026 0.00034 0.00008 3.14157

D244 0.00029 0.00000 0.00021 -0.00023 -0.00002 0.00027

D245 -0.00020 0.00000 -0.00002 0.00004 0.00002 -0.00018

D246 -3.14117 0.00000 -0.00002 0.00004 0.00002 -3.14115

D247 3.14114 0.00000 0.00001 -0.00002 -0.00001 3.14113

D248 0.00017 0.00000 0.00001 -0.00002 -0.00001 0.00016

D249 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D250 -3.14097 0.00000 0.00000 0.00000 0.00000 -3.14098

D251 3.14097 0.00000 0.00000 0.00000 0.00000 3.14098

D252 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D253 0.00020 0.00000 0.00002 -0.00004 -0.00002 0.00018

D254 -3.14114 0.00000 -0.00001 0.00002 0.00001 -3.14113

D255 3.14117 0.00000 0.00002 -0.00004 -0.00002 3.14115

D256 -0.00017 0.00000 -0.00001 0.00002 0.00001 -0.00016

D257 0.00018 0.00000 0.00035 -0.00039 -0.00004 0.00014

D258 -3.14149 0.00000 0.00026 -0.00034 -0.00008 -3.14157

D259 3.14138 0.00000 -0.00012 0.00018 0.00006 3.14144

D260 -0.00029 0.00000 -0.00021 0.00023 0.00002 -0.00027

D261 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D262 3.14151 0.00000 -0.00009 0.00005 -0.00004 3.14148

D263 -3.14151 0.00000 0.00009 -0.00005 0.00004 -3.14148

D264 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D265 -0.00018 0.00000 -0.00035 0.00039 0.00004 -0.00014

D266 -3.14138 0.00000 0.00012 -0.00018 -0.00006 -3.14144

D267 3.14149 0.00000 -0.00026 0.00034 0.00008 3.14157

D268 0.00029 0.00000 0.00021 -0.00023 -0.00002 0.00027

D269 0.00020 0.00000 0.00002 -0.00004 -0.00002 0.00018

D270 3.14117 0.00000 0.00002 -0.00004 -0.00002 3.14115

D271 -3.14114 0.00000 -0.00001 0.00002 0.00001 -3.14113

D272 -0.00017 0.00000 -0.00001 0.00002 0.00001 -0.00016

D273 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D274 3.14097 0.00000 0.00000 0.00000 0.00000 3.14098

D275 -3.14097 0.00000 0.00000 0.00000 0.00000 -3.14098

D276 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D277 -0.00020 0.00000 -0.00002 0.00004 0.00002 -0.00018

D278 3.14114 0.00000 0.00001 -0.00002 -0.00001 3.14113

D279 -3.14117 0.00000 -0.00002 0.00004 0.00002 -3.14115

D280 0.00017 0.00000 0.00001 -0.00002 -0.00001 0.00016

Item Value Threshold Converged?

Maximum Force 0.000048 0.000450 YES

RMS Force 0.000010 0.000300 YES

Maximum Displacement 0.013819 0.001800 NO

RMS Displacement 0.002491 0.001200 NO

Predicted change in Energy=-2.579389D-07

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Jun 30 21:14:55 2019, MaxMem= 1342177280 cpu: 166.0

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

Stoichiometry C48H24N8Zn(3)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C48H24N4)]

Deg. of freedom 61

Full point group C2V NOp 4

RotChk: IX=0 Diff= 5.81D-15

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 1.121270 2.790226 0.181888

2 7 0 0.000000 2.023891 0.322518

3 6 0 -1.121270 2.790226 0.181888

4 6 0 -0.717708 4.166495 -0.043908

5 6 0 0.717708 4.166495 -0.043908

6 7 0 -2.412746 2.383662 0.208594

7 6 0 -2.794688 1.127508 0.263602

8 7 0 -2.010551 0.000000 0.326388

9 6 0 -2.794688 -1.127508 0.263602

10 6 0 -4.208422 -0.712285 0.207703

11 6 0 -4.208422 0.712285 0.207703

12 7 0 2.412746 2.383662 0.208594

13 6 0 4.208422 0.712285 0.207703

14 6 0 4.208422 -0.712285 0.207703

15 6 0 2.794688 -1.127508 0.263602

16 7 0 2.010551 0.000000 0.326388

17 6 0 2.794688 1.127508 0.263602

18 7 0 2.412746 -2.383662 0.208594

19 7 0 0.000000 -2.023891 0.322518

20 6 0 1.121270 -2.790226 0.181888

21 6 0 0.717708 -4.166495 -0.043908

22 6 0 -0.717708 -4.166495 -0.043908

23 6 0 -1.121270 -2.790226 0.181888

24 7 0 -2.412746 -2.383662 0.208594

25 30 0 0.000000 0.000000 0.844654

26 6 0 5.373745 1.426286 0.150998

27 6 0 6.609301 0.718876 0.100889

28 6 0 6.609301 -0.718876 0.100889

29 6 0 5.373745 -1.426286 0.150998

30 6 0 -1.428341 -5.326265 -0.252326

31 6 0 -0.721448 -6.536261 -0.463376

32 6 0 0.721448 -6.536261 -0.463376

33 6 0 1.428341 -5.326265 -0.252326

34 6 0 -5.373745 1.426286 0.150998

35 6 0 -6.609301 0.718876 0.100889

36 6 0 -6.609301 -0.718876 0.100889

37 6 0 -5.373745 -1.426286 0.150998

38 6 0 1.428341 5.326265 -0.252326

39 6 0 0.721448 6.536261 -0.463376

40 6 0 -0.721448 6.536261 -0.463376

41 6 0 -1.428341 5.326265 -0.252326

42 6 0 1.402331 -7.763115 -0.680976

43 6 0 0.708017 -8.930785 -0.887917

44 6 0 -0.708017 -8.930785 -0.887917

45 6 0 -1.402331 -7.763115 -0.680976

46 6 0 7.848924 -1.401349 0.049980

47 6 0 9.036463 -0.705864 0.001415

48 6 0 9.036463 0.705864 0.001415

49 6 0 7.848924 1.401349 0.049980

50 6 0 -1.402331 7.763115 -0.680976

51 6 0 -0.708017 8.930785 -0.887917

52 6 0 0.708017 8.930785 -0.887917

53 6 0 1.402331 7.763115 -0.680976

54 6 0 -7.848924 -1.401349 0.049980

55 6 0 -9.036463 -0.705864 0.001415

56 6 0 -9.036463 0.705864 0.001415

57 6 0 -7.848924 1.401349 0.049980

58 1 0 5.373826 2.511167 0.146018

59 1 0 5.373826 -2.511167 0.146018

60 1 0 -2.513372 -5.328815 -0.258829

61 1 0 2.513372 -5.328815 -0.258829

62 1 0 -5.373826 2.511167 0.146018

63 1 0 -5.373826 -2.511167 0.146018

64 1 0 2.513372 5.328815 -0.258829

65 1 0 -2.513372 5.328815 -0.258829

66 1 0 2.487810 -7.761553 -0.680555

67 1 0 1.243532 -9.859653 -1.052648

68 1 0 -1.243532 -9.859653 -1.052648

69 1 0 -2.487810 -7.761553 -0.680555

70 1 0 7.847171 -2.486618 0.049623

71 1 0 9.978249 -1.242473 -0.037682

72 1 0 9.978249 1.242473 -0.037682

73 1 0 7.847171 2.486618 0.049623

74 1 0 -2.487810 7.761553 -0.680555

75 1 0 -1.243532 9.859653 -1.052648

76 1 0 1.243532 9.859653 -1.052648

77 1 0 2.487810 7.761553 -0.680555

78 1 0 -7.847171 -2.486618 0.049623

79 1 0 -9.978249 -1.242473 -0.037682

80 1 0 -9.978249 1.242473 -0.037682

81 1 0 -7.847171 2.486618 0.049623

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

Rotational constants (GHZ): 0.0387320 0.0379537 0.0193793

Leave Link 202 at Sun Jun 30 21:14:55 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 307 symmetry adapted cartesian basis functions of A1 symmetry.

There are 278 symmetry adapted cartesian basis functions of A2 symmetry.

There are 289 symmetry adapted cartesian basis functions of B1 symmetry.

There are 289 symmetry adapted cartesian basis functions of B2 symmetry.

There are 289 symmetry adapted basis functions of A1 symmetry.

There are 265 symmetry adapted basis functions of A2 symmetry.

There are 275 symmetry adapted basis functions of B1 symmetry.

There are 275 symmetry adapted basis functions of B2 symmetry.

1104 basis functions, 1951 primitive gaussians, 1163 cartesian basis functions

191 alpha electrons 189 beta electrons

nuclear repulsion energy 6889.7517718007 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= 81 NActive= 81 NUniq= 22 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= -0.2361216656 Hartrees.

Nuclear repulsion after empirical dispersion term = 6889.5156501352 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= 81.

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 = 81

GePol: Total number of spheres = 81

GePol: Number of exposed spheres = 81 (100.00%)

GePol: Number of points = 6430

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.48D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 410

GePol: Fraction of low-weight points (<1% of avg) = 6.38%

GePol: Cavity surface area = 670.749 Ang\*\*2

GePol: Cavity volume = 694.564 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0170090706 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 6889.4986410645 Hartrees.

Leave Link 301 at Sun Jun 30 21:14:55 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.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36719 LenP2D= 95220.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1104 RedAO= T EigKep= 2.89D-05 NBF= 289 265 275 275

NBsUse= 1104 1.00D-06 EigRej= -1.00D+00 NBFU= 289 265 275 275

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= 1060 1060 1060 1060 1060 MxSgAt= 81 MxSgA2= 81.

Leave Link 302 at Sun Jun 30 21:15:24 2019, MaxMem= 1342177280 cpu: 282.3

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Jun 30 21:15:24 2019, MaxMem= 1342177280 cpu: 4.3

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

Initial guess from the checkpoint file: "ZnNPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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

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The electronic state of the initial guess is 3-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

Leave Link 401 at Sun Jun 30 21:15:45 2019, MaxMem= 1342177280 cpu: 220.9

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4103221 IEndB= 4103221 NGot= 1342177280 MDV= 1339444432

LenX= 1339444432 LenY= 1338090700

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= 420000000 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= 124034700.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.55D-15 for 6408.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.34D-15 for 5167 193.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.77D-15 for 6408.

Iteration 1 A^-1\*A deviation from orthogonality is 8.69D-09 for 5290 5270.

Iteration 2 A\*A^-1 deviation from unit magnitude is 4.00D-15 for 432.

Iteration 2 A\*A^-1 deviation from orthogonality is 4.73D-15 for 3064 747.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 2406.

Iteration 2 A^-1\*A deviation from orthogonality is 3.46D-16 for 6288 1751.

E= -2348.13071867411

DIIS: error= 1.30D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2348.13071867411 IErMin= 1 ErrMin= 1.30D-04

ErrMax= 1.30D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.03D-05 BMatP= 4.03D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.30D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.379 Goal= None Shift= 0.000

Gap= 0.459 Goal= None Shift= 0.000

RMSDP=5.00D-06 MaxDP=1.72D-04 OVMax= 6.80D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 5.00D-06 CP: 1.00D+00

E= -2348.13073898422 Delta-E= -0.000020310110 Rises=F Damp=F

DIIS: error= 1.85D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2348.13073898422 IErMin= 2 ErrMin= 1.85D-05

ErrMax= 1.85D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.78D-07 BMatP= 4.03D-05

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

Coeff-Com: -0.745D-01 0.107D+01

Coeff: -0.745D-01 0.107D+01

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=6.40D-07 MaxDP=2.80D-05 DE=-2.03D-05 OVMax= 1.80D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 5.46D-07 CP: 1.00D+00 1.07D+00

E= -2348.13073927871 Delta-E= -0.000000294493 Rises=F Damp=F

DIIS: error= 9.46D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2348.13073927871 IErMin= 3 ErrMin= 9.46D-06

ErrMax= 9.46D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.86D-08 BMatP= 4.78D-07

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

Coeff-Com: -0.261D-01 0.331D+00 0.695D+00

Coeff: -0.261D-01 0.331D+00 0.695D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.23D-07 MaxDP=1.52D-05 DE=-2.94D-07 OVMax= 4.33D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.14D-07 CP: 1.00D+00 1.07D+00 9.12D-01

E= -2348.13073928376 Delta-E= -0.000000005053 Rises=F Damp=F

DIIS: error= 5.83D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2348.13073928376 IErMin= 4 ErrMin= 5.83D-06

ErrMax= 5.83D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.18D-08 BMatP= 8.86D-08

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

Coeff-Com: -0.654D-02 0.650D-01 0.467D+00 0.474D+00

Coeff: -0.654D-02 0.650D-01 0.467D+00 0.474D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.23D-07 MaxDP=9.62D-06 DE=-5.05D-09 OVMax= 2.69D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 7.30D-08 CP: 1.00D+00 1.07D+00 9.82D-01 5.85D-01

E= -2348.13073929856 Delta-E= -0.000000014796 Rises=F Damp=F

DIIS: error= 1.43D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2348.13073929856 IErMin= 5 ErrMin= 1.43D-06

ErrMax= 1.43D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.10D-09 BMatP= 7.18D-08

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

Coeff-Com: 0.362D-03-0.170D-01 0.123D+00 0.221D+00 0.673D+00

Coeff: 0.362D-03-0.170D-01 0.123D+00 0.221D+00 0.673D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=3.50D-08 MaxDP=2.06D-06 DE=-1.48D-08 OVMax= 1.16D-05

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.37D-08 CP: 1.00D+00 1.07D+00 9.98D-01 6.67D-01 7.75D-01

E= -2348.13073929906 Delta-E= -0.000000000498 Rises=F Damp=F

DIIS: error= 1.34D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2348.13073929906 IErMin= 6 ErrMin= 1.34D-06

ErrMax= 1.34D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.64D-10 BMatP= 3.10D-09

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

Coeff-Com: 0.907D-03-0.178D-01 0.251D-01 0.835D-01 0.412D+00 0.496D+00

Coeff: 0.907D-03-0.178D-01 0.251D-01 0.835D-01 0.412D+00 0.496D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.36D-08 MaxDP=5.59D-07 DE=-4.98D-10 OVMax= 3.77D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 8.98D-09 CP: 1.00D+00 1.07D+00 1.00D+00 6.62D-01 8.32D-01

CP: 6.38D-01

E= -2348.13073929912 Delta-E= -0.000000000062 Rises=F Damp=F

DIIS: error= 8.63D-08 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2348.13073929912 IErMin= 7 ErrMin= 8.63D-08

ErrMax= 8.63D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.88D-11 BMatP= 7.64D-10

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

Coeff-Com: 0.346D-03-0.597D-02 0.103D-02 0.176D-01 0.120D+00 0.207D+00

Coeff-Com: 0.659D+00

Coeff: 0.346D-03-0.597D-02 0.103D-02 0.176D-01 0.120D+00 0.207D+00

Coeff: 0.659D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=4.26D-09 MaxDP=1.96D-07 DE=-6.18D-11 OVMax= 1.99D-06

Error on total polarization charges = 0.08828

SCF Done: E(UB3LYP) = -2348.13073930 A.U. after 7 cycles

NFock= 7 Conv=0.43D-08 -V/T= 1.9830

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

<L.S>= 0.000000000000E+00

KE= 2.388748100429D+03 PE=-1.932242216688D+04 EE= 7.696044686089D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -10.67

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0219, after 2.0003

Leave Link 502 at Sun Jun 30 21:24:16 2019, MaxMem= 1342177280 cpu: 5448.5

(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.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36719 LenP2D= 95220.

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 = 192

Leave Link 701 at Sun Jun 30 21:24:51 2019, MaxMem= 1342177280 cpu: 341.5

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sun Jun 30 21:24:51 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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 Sun Jun 30 21:25:40 2019, MaxMem= 1342177280 cpu: 489.3

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 3.10862447D-13-1.16173737D-12 8.83872530D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 0.000001198 -0.000009254 0.000022549

2 7 0.000000000 0.000015872 -0.000020423

3 6 -0.000001198 -0.000009254 0.000022549

4 6 0.000001048 0.000002346 -0.000030893

5 6 -0.000001048 0.000002346 -0.000030893

6 7 0.000007137 -0.000024106 -0.000007348

7 6 0.000017899 0.000023831 0.000007819

8 7 -0.000009136 0.000000000 -0.000024741

9 6 0.000017899 -0.000023831 0.000007819

10 6 -0.000009880 0.000010125 0.000000958

11 6 -0.000009880 -0.000010125 0.000000958

12 7 -0.000007137 -0.000024106 -0.000007348

13 6 0.000009880 -0.000010125 0.000000958

14 6 0.000009880 0.000010125 0.000000958

15 6 -0.000017899 -0.000023831 0.000007819

16 7 0.000009136 0.000000000 -0.000024741

17 6 -0.000017899 0.000023831 0.000007819

18 7 -0.000007137 0.000024106 -0.000007348

19 7 0.000000000 -0.000015872 -0.000020423

20 6 0.000001198 0.000009254 0.000022549

21 6 -0.000001048 -0.000002346 -0.000030893

22 6 0.000001048 -0.000002346 -0.000030893

23 6 -0.000001198 0.000009254 0.000022549

24 7 0.000007137 0.000024106 -0.000007348

25 30 0.000000000 0.000000000 0.000058279

26 6 -0.000000380 -0.000004789 0.000004630

27 6 0.000000026 0.000009376 -0.000001158

28 6 0.000000026 -0.000009376 -0.000001158

29 6 -0.000000380 0.000004789 0.000004630

30 6 0.000009431 -0.000005280 0.000021124

31 6 -0.000011965 0.000000703 0.000003416

32 6 0.000011965 0.000000703 0.000003416

33 6 -0.000009431 -0.000005280 0.000021124

34 6 0.000000380 -0.000004789 0.000004630

35 6 -0.000000026 0.000009376 -0.000001158

36 6 -0.000000026 -0.000009376 -0.000001158

37 6 0.000000380 0.000004789 0.000004630

38 6 -0.000009431 0.000005280 0.000021124

39 6 0.000011965 -0.000000703 0.000003416

40 6 -0.000011965 -0.000000703 0.000003416

41 6 0.000009431 0.000005280 0.000021124

42 6 -0.000005844 -0.000002624 -0.000009138

43 6 0.000005559 0.000000263 0.000001382

44 6 -0.000005559 0.000000263 0.000001382

45 6 0.000005844 -0.000002624 -0.000009138

46 6 0.000002415 0.000003972 -0.000001734

47 6 0.000000236 -0.000003644 0.000000395

48 6 0.000000236 0.000003644 0.000000395

49 6 0.000002415 -0.000003972 -0.000001734

50 6 0.000005844 0.000002624 -0.000009138

51 6 -0.000005559 -0.000000263 0.000001382

52 6 0.000005559 -0.000000263 0.000001382

53 6 -0.000005844 0.000002624 -0.000009138

54 6 -0.000002415 0.000003972 -0.000001734

55 6 -0.000000236 -0.000003644 0.000000395

56 6 -0.000000236 0.000003644 0.000000395

57 6 -0.000002415 -0.000003972 -0.000001734

58 1 -0.000001587 0.000000646 -0.000000847

59 1 -0.000001587 -0.000000646 -0.000000847

60 1 -0.000000844 0.000003237 -0.000005919

61 1 0.000000844 0.000003237 -0.000005919

62 1 0.000001587 0.000000646 -0.000000847

63 1 0.000001587 -0.000000646 -0.000000847

64 1 0.000000844 -0.000003237 -0.000005919

65 1 -0.000000844 -0.000003237 -0.000005919

66 1 0.000000212 -0.000000545 0.000001009

67 1 -0.000001342 -0.000001951 0.000001267

68 1 0.000001342 -0.000001951 0.000001267

69 1 -0.000000212 -0.000000545 0.000001009

70 1 0.000000791 -0.000000101 0.000000466

71 1 0.000001107 0.000000623 0.000000035

72 1 0.000001107 -0.000000623 0.000000035

73 1 0.000000791 0.000000101 0.000000466

74 1 -0.000000212 0.000000545 0.000001009

75 1 0.000001342 0.000001951 0.000001267

76 1 -0.000001342 0.000001951 0.000001267

77 1 0.000000212 0.000000545 0.000001009

78 1 -0.000000791 -0.000000101 0.000000466

79 1 -0.000001107 0.000000623 0.000000035

80 1 -0.000001107 -0.000000623 0.000000035

81 1 -0.000000791 0.000000101 0.000000466

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

Cartesian Forces: Max 0.000058279 RMS 0.000009965

Leave Link 716 at Sun Jun 30 21:25:41 2019, MaxMem= 1342177280 cpu: 4.5

(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 0.000018485 RMS 0.000003835

Search for a local minimum.

Step number 9 out of a maximum of 486

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .38355D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

6 7 8 9

DE= -6.66D-07 DEPred=-2.58D-07 R= 2.58D+00

Trust test= 2.58D+00 RLast= 1.13D-02 DXMaxT set to 3.00D-01

ITU= 0 1 1 1 1 1 1 1 0

Eigenvalues --- 0.00234 0.00633 0.01432 0.01486 0.01500

Eigenvalues --- 0.01541 0.01572 0.01588 0.01627 0.01656

Eigenvalues --- 0.01675 0.01694 0.01698 0.01705 0.01713

Eigenvalues --- 0.01714 0.01725 0.01730 0.01730 0.01736

Eigenvalues --- 0.01737 0.01751 0.01753 0.01758 0.01791

Eigenvalues --- 0.01827 0.01828 0.01830 0.01851 0.01854

Eigenvalues --- 0.01870 0.01871 0.01906 0.01936 0.01968

Eigenvalues --- 0.01968 0.01972 0.01975 0.01978 0.01992

Eigenvalues --- 0.01992 0.01993 0.01993 0.02020 0.02080

Eigenvalues --- 0.02084 0.02086 0.02087 0.02089 0.02095

Eigenvalues --- 0.02096 0.02096 0.02098 0.02103 0.02103

Eigenvalues --- 0.02105 0.02106 0.02124 0.02124 0.02137

Eigenvalues --- 0.02144 0.02144 0.02144 0.02147 0.02148

Eigenvalues --- 0.02171 0.02173 0.02213 0.02214 0.02225

Eigenvalues --- 0.02230 0.02241 0.02281 0.02286 0.02346

Eigenvalues --- 0.02409 0.03111 0.05504 0.05546 0.07907

Eigenvalues --- 0.14665 0.15971 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 0.16008 0.16037

Eigenvalues --- 0.16159 0.16246 0.16966 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22499 0.22503 0.22504

Eigenvalues --- 0.22542 0.23234 0.23234 0.23234 0.23620

Eigenvalues --- 0.23939 0.23939 0.23939 0.23952 0.23953

Eigenvalues --- 0.24279 0.24301 0.24550 0.24553 0.24557

Eigenvalues --- 0.24557 0.24570 0.24759 0.24892 0.24897

Eigenvalues --- 0.24962 0.24982 0.24984 0.24985 0.24989

Eigenvalues --- 0.24996 0.24996 0.24997 0.24997 0.25914

Eigenvalues --- 0.32865 0.32946 0.33670 0.33735 0.33834

Eigenvalues --- 0.33853 0.35041 0.35068 0.35181 0.35181

Eigenvalues --- 0.35181 0.35187 0.35202 0.35202 0.35202

Eigenvalues --- 0.35210 0.35231 0.35231 0.35231 0.35231

Eigenvalues --- 0.35244 0.35249 0.35249 0.35249 0.35270

Eigenvalues --- 0.35270 0.35270 0.35275 0.35279 0.35279

Eigenvalues --- 0.35279 0.35414 0.35448 0.35530 0.36349

Eigenvalues --- 0.36542 0.37458 0.37552 0.37969 0.38237

Eigenvalues --- 0.39276 0.39276 0.39612 0.39612 0.40188

Eigenvalues --- 0.40188 0.40257 0.40257 0.40906 0.41001

Eigenvalues --- 0.41003 0.41146 0.41603 0.41778 0.41873

Eigenvalues --- 0.42158 0.42215 0.42380 0.42806 0.42855

Eigenvalues --- 0.42901 0.42970 0.44425 0.45680 0.47124

Eigenvalues --- 0.47124 0.47239 0.47384 0.47386 0.47579

Eigenvalues --- 0.47580 0.47979 0.48122 0.48218 0.48360

Eigenvalues --- 0.48455 0.48465 0.48680 0.48707 0.48729

Eigenvalues --- 0.48739 0.49092 0.49409 0.49898 0.50353

Eigenvalues --- 0.51028 0.51279 0.52478 0.58195 0.59237

Eigenvalues --- 0.59872 0.60917

En-DIIS/RFO-DIIS IScMMF= 0 using points: 9 8 7 6 5

RFO step: Lambda=-2.82494127D-08.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 7.37D-06 SmlDif= 1.00D-05

RMS Error= 0.2027745755D-04 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.35836 -0.24645 -0.19973 0.16724 -0.07942

Iteration 1 RMS(Cart)= 0.00376033 RMS(Int)= 0.00000087

Iteration 2 RMS(Cart)= 0.00000237 RMS(Int)= 0.00000072

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000072

ITry= 1 IFail=0 DXMaxC= 1.80D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.94D-08 for atom 78.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58021 -0.00001 -0.00003 0.00001 -0.00002 2.58019

R2 2.74366 0.00001 0.00002 0.00001 0.00003 2.74369

R3 2.55911 -0.00001 -0.00002 0.00000 -0.00003 2.55908

R4 2.58021 -0.00001 -0.00003 0.00001 -0.00002 2.58019

R5 3.94983 0.00001 0.00012 0.00008 0.00020 3.95002

R6 2.74366 0.00001 0.00002 0.00001 0.00003 2.74369

R7 2.55911 -0.00001 -0.00002 0.00000 -0.00003 2.55908

R8 2.71254 0.00000 0.00000 -0.00001 -0.00001 2.71253

R9 2.60035 0.00000 -0.00001 0.00001 0.00000 2.60035

R10 2.60035 0.00000 -0.00001 0.00001 0.00000 2.60035

R11 2.48327 -0.00002 -0.00005 -0.00001 -0.00006 2.48320

R12 2.59800 0.00000 -0.00003 0.00000 -0.00002 2.59798

R13 2.78642 0.00001 0.00004 0.00000 0.00004 2.78646

R14 2.59800 0.00000 -0.00003 0.00000 -0.00002 2.59798

R15 3.92359 0.00000 0.00006 0.00001 0.00007 3.92366

R16 2.78642 0.00001 0.00004 0.00000 0.00004 2.78646

R17 2.48327 -0.00002 -0.00005 -0.00001 -0.00006 2.48320

R18 2.69205 -0.00001 -0.00001 -0.00001 -0.00002 2.69203

R19 2.58485 0.00000 -0.00001 0.00001 0.00000 2.58485

R20 2.58485 0.00000 -0.00001 0.00001 0.00000 2.58485

R21 2.48327 -0.00002 -0.00005 -0.00001 -0.00006 2.48320

R22 2.69205 -0.00001 -0.00001 -0.00001 -0.00002 2.69203

R23 2.78642 0.00001 0.00004 0.00000 0.00004 2.78646

R24 2.58485 0.00000 -0.00001 0.00001 0.00000 2.58485

R25 2.78642 0.00001 0.00004 0.00000 0.00004 2.78646

R26 2.58485 0.00000 -0.00001 0.00001 0.00000 2.58485

R27 2.59800 0.00000 -0.00003 0.00000 -0.00002 2.59798

R28 2.48327 -0.00002 -0.00005 -0.00001 -0.00006 2.48320

R29 2.59800 0.00000 -0.00003 0.00000 -0.00002 2.59798

R30 3.92359 0.00000 0.00006 0.00001 0.00007 3.92366

R31 2.55911 -0.00001 -0.00002 0.00000 -0.00003 2.55908

R32 2.58021 -0.00001 -0.00003 0.00001 -0.00002 2.58019

R33 2.58021 -0.00001 -0.00003 0.00001 -0.00002 2.58019

R34 3.94983 0.00001 0.00012 0.00008 0.00020 3.95002

R35 2.74366 0.00001 0.00002 0.00001 0.00003 2.74369

R36 2.71254 0.00000 0.00000 -0.00001 -0.00001 2.71253

R37 2.60035 0.00000 -0.00001 0.00001 0.00000 2.60035

R38 2.74366 0.00001 0.00002 0.00001 0.00003 2.74369

R39 2.60035 0.00000 -0.00001 0.00001 0.00000 2.60035

R40 2.55911 -0.00001 -0.00002 0.00000 -0.00003 2.55908

R41 2.69214 0.00000 0.00000 0.00000 0.00000 2.69214

R42 2.05015 0.00000 0.00000 0.00000 0.00001 2.05015

R43 2.71696 0.00001 0.00001 0.00001 0.00003 2.71698

R44 2.67583 0.00000 0.00000 0.00001 0.00000 2.67584

R45 2.69214 0.00000 0.00000 0.00000 0.00000 2.69214

R46 2.67583 0.00000 0.00000 0.00001 0.00000 2.67584

R47 2.05015 0.00000 0.00000 0.00000 0.00001 2.05015

R48 2.67804 0.00000 -0.00001 0.00000 -0.00001 2.67803

R49 2.05046 0.00000 0.00000 0.00000 0.00001 2.05046

R50 2.72668 0.00001 0.00002 0.00001 0.00003 2.72671

R51 2.68323 0.00000 0.00000 0.00001 0.00000 2.68323

R52 2.67804 0.00000 -0.00001 0.00000 -0.00001 2.67803

R53 2.68323 0.00000 0.00000 0.00001 0.00000 2.68323

R54 2.05046 0.00000 0.00000 0.00000 0.00001 2.05046

R55 2.69214 0.00000 0.00000 0.00000 0.00000 2.69214

R56 2.05015 0.00000 0.00000 0.00000 0.00001 2.05015

R57 2.71696 0.00001 0.00001 0.00001 0.00003 2.71698

R58 2.67583 0.00000 0.00000 0.00001 0.00000 2.67584

R59 2.69214 0.00000 0.00000 0.00000 0.00000 2.69214

R60 2.67583 0.00000 0.00000 0.00001 0.00000 2.67584

R61 2.05015 0.00000 0.00000 0.00000 0.00001 2.05015

R62 2.67804 0.00000 -0.00001 0.00000 -0.00001 2.67803

R63 2.05046 0.00000 0.00000 0.00000 0.00001 2.05046

R64 2.72668 0.00001 0.00002 0.00001 0.00003 2.72671

R65 2.68323 0.00000 0.00000 0.00001 0.00000 2.68323

R66 2.67804 0.00000 -0.00001 0.00000 -0.00001 2.67803

R67 2.68323 0.00000 0.00000 0.00001 0.00000 2.68323

R68 2.05046 0.00000 0.00000 0.00000 0.00001 2.05046

R69 2.59681 0.00000 -0.00001 0.00001 -0.00001 2.59680

R70 2.05126 0.00000 0.00000 0.00000 0.00000 2.05126

R71 2.67592 0.00000 0.00001 0.00001 0.00001 2.67593

R72 2.04990 0.00000 0.00000 0.00000 0.00000 2.04990

R73 2.59681 0.00000 -0.00001 0.00001 -0.00001 2.59680

R74 2.04990 0.00000 0.00000 0.00000 0.00000 2.04990

R75 2.05126 0.00000 0.00000 0.00000 0.00000 2.05126

R76 2.60228 0.00000 -0.00001 0.00001 0.00000 2.60227

R77 2.05086 0.00000 0.00000 0.00000 0.00000 2.05087

R78 2.66778 0.00000 0.00000 0.00001 0.00001 2.66779

R79 2.04967 0.00000 0.00000 0.00000 0.00000 2.04967

R80 2.60228 0.00000 -0.00001 0.00001 0.00000 2.60227

R81 2.04967 0.00000 0.00000 0.00000 0.00000 2.04967

R82 2.05086 0.00000 0.00000 0.00000 0.00000 2.05087

R83 2.59681 0.00000 -0.00001 0.00001 -0.00001 2.59680

R84 2.05126 0.00000 0.00000 0.00000 0.00000 2.05126

R85 2.67592 0.00000 0.00001 0.00001 0.00001 2.67593

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A3 2.15643 0.00000 0.00003 -0.00001 0.00002 2.15645

A4 1.92705 0.00000 0.00003 -0.00001 0.00001 1.92706

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A11 2.31712 0.00000 0.00001 0.00000 0.00002 2.31714

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A18 2.14870 0.00000 0.00004 0.00001 0.00005 2.14875

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A20 1.92325 0.00001 0.00002 -0.00001 0.00002 1.92327

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D2 -3.03608 0.00000 -0.00106 -0.00048 -0.00155 -3.03763

D3 -3.09756 0.00000 -0.00024 -0.00006 -0.00030 -3.09786

D4 0.13041 0.00000 -0.00140 -0.00015 -0.00155 0.12886

D5 -0.01137 0.00000 -0.00006 0.00023 0.00018 -0.01119

D6 -3.13524 0.00000 -0.00012 0.00008 -0.00004 -3.13528

D7 3.10661 0.00000 0.00026 -0.00008 0.00018 3.10679

D8 -0.01726 -0.00001 0.00019 -0.00023 -0.00004 -0.01730

D9 0.10890 0.00000 0.00092 0.00011 0.00103 0.10993

D10 -3.00438 0.00001 0.00054 0.00048 0.00102 -3.00336

D11 -0.01914 0.00000 -0.00010 0.00039 0.00029 -0.01884

D12 3.09756 0.00000 0.00024 0.00006 0.00030 3.09786

D13 3.03608 0.00000 0.00106 0.00048 0.00155 3.03763

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D17 -1.62004 0.00000 0.00066 0.00005 0.00071 -1.61933

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D29 -3.12640 0.00000 -0.00006 -0.00013 -0.00019 -3.12658

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D31 -3.12679 0.00000 0.00000 -0.00007 -0.00007 -3.12686

D32 0.01346 -0.00001 -0.00013 -0.00019 -0.00032 0.01314

D33 -0.00508 0.00000 0.00008 0.00010 0.00017 -0.00490

D34 3.13518 0.00000 -0.00005 -0.00003 -0.00008 3.13510

D35 3.12679 0.00000 0.00000 0.00007 0.00007 3.12686

D36 -0.01346 0.00001 0.00013 0.00019 0.00032 -0.01314

D37 0.00508 0.00000 -0.00008 -0.00010 -0.00017 0.00490

D38 -3.13518 0.00000 0.00005 0.00003 0.00008 -3.13510

D39 0.02038 0.00000 -0.00055 -0.00013 -0.00069 0.01970

D40 -3.07367 0.00000 -0.00025 -0.00015 -0.00040 -3.07407

D41 -3.05874 0.00001 0.00019 0.00015 0.00035 -3.05839

D42 0.29204 0.00001 0.00126 0.00028 0.00154 0.29359

D43 0.04086 0.00000 -0.00007 0.00017 0.00010 0.04096

D44 -2.89154 0.00001 0.00100 0.00029 0.00129 -2.89025

D45 3.07790 0.00000 -0.00021 -0.00009 -0.00029 3.07761

D46 -0.05321 0.00000 -0.00008 -0.00006 -0.00014 -0.05335

D47 -0.02436 0.00000 0.00004 -0.00010 -0.00006 -0.02442

D48 3.12771 0.00000 0.00017 -0.00007 0.00010 3.12781

D49 -0.04086 0.00000 0.00007 -0.00017 -0.00010 -0.04096

D50 3.05874 -0.00001 -0.00019 -0.00015 -0.00035 3.05839

D51 2.89154 -0.00001 -0.00100 -0.00029 -0.00129 2.89025

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D53 -0.36392 -0.00001 -0.00059 -0.00017 -0.00076 -0.36468

D54 -1.68990 0.00000 -0.00060 -0.00007 -0.00067 -1.69058

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D56 3.01589 -0.00001 0.00061 -0.00002 0.00059 3.01648

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D58 0.36392 0.00001 0.00059 0.00017 0.00076 0.36468

D59 0.02436 0.00000 -0.00004 0.00010 0.00006 0.02442

D60 -3.12771 0.00000 -0.00017 0.00007 -0.00010 -3.12781

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D62 0.05321 0.00000 0.00008 0.00006 0.00014 0.05335

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D67 -3.13249 0.00000 0.00011 0.00003 0.00014 -3.13235

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 -3.13782 0.00000 0.00014 0.00010 0.00023 -3.13758

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D77 3.07367 0.00000 0.00025 0.00015 0.00040 3.07407

D78 -0.02038 0.00000 0.00055 0.00013 0.00069 -0.01970

D79 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D80 3.13249 0.00000 -0.00011 -0.00003 -0.00014 3.13235

D81 -3.13249 0.00000 0.00011 0.00003 0.00014 -3.13235

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D83 -3.07790 0.00000 0.00021 0.00009 0.00029 -3.07761

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D85 0.05321 0.00000 0.00008 0.00006 0.00014 0.05335

D86 -3.12771 0.00000 -0.00017 0.00007 -0.00010 -3.12781

D87 -0.00801 0.00000 -0.00001 0.00006 0.00006 -0.00795

D88 3.13622 0.00000 -0.00004 -0.00003 -0.00007 3.13615

D89 -3.13782 0.00000 0.00014 0.00010 0.00023 -3.13758

D90 0.00641 0.00000 0.00010 0.00001 0.00011 0.00652

D91 -0.02436 0.00000 0.00004 -0.00010 -0.00006 -0.02442

D92 3.07790 0.00000 -0.00021 -0.00009 -0.00029 3.07761

D93 3.12771 0.00000 0.00017 -0.00007 0.00010 3.12781

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D96 -3.13622 0.00000 0.00004 0.00003 0.00007 -3.13615

D97 3.13782 0.00000 -0.00014 -0.00010 -0.00023 3.13758

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D101 -3.05874 0.00001 0.00019 0.00015 0.00035 -3.05839

D102 0.29204 0.00001 0.00126 0.00028 0.00154 0.29359

D103 -3.07367 0.00000 -0.00025 -0.00015 -0.00040 -3.07407

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D107 -0.29204 -0.00001 -0.00126 -0.00028 -0.00154 -0.29359

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D111 -0.36392 -0.00001 -0.00059 -0.00017 -0.00076 -0.36468

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D113 1.68990 0.00000 0.00060 0.00007 0.00067 1.69058

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D115 -0.10890 0.00000 -0.00092 -0.00011 -0.00103 -0.10993

D116 3.00438 -0.00001 -0.00054 -0.00048 -0.00102 3.00336

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D120 3.03608 0.00000 0.00106 0.00048 0.00155 3.03763

D121 0.01914 0.00000 0.00010 -0.00039 -0.00029 0.01884

D122 -3.09756 0.00000 -0.00024 -0.00006 -0.00030 -3.09786

D123 -3.03608 0.00000 -0.00106 -0.00048 -0.00155 -3.03763

D124 0.13041 0.00000 -0.00140 -0.00015 -0.00155 0.12886

D125 1.62004 0.00000 -0.00066 -0.00005 -0.00071 1.61933

D126 2.94624 0.00000 -0.00076 -0.00008 -0.00085 2.94539

D127 0.29385 0.00000 -0.00056 -0.00002 -0.00058 0.29327

D128 -1.62004 0.00000 0.00066 0.00005 0.00071 -1.61933

D129 -0.29385 0.00000 0.00056 0.00002 0.00058 -0.29327

D130 -2.94624 0.00000 0.00076 0.00008 0.00085 -2.94539

D131 -3.10661 0.00000 -0.00026 0.00008 -0.00018 -3.10679

D132 0.01726 0.00001 -0.00019 0.00023 0.00004 0.01730

D133 0.01137 0.00000 0.00006 -0.00023 -0.00018 0.01119

D134 3.13524 0.00000 0.00012 -0.00008 0.00004 3.13528

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.12640 0.00000 0.00006 0.00013 0.00019 3.12658

D137 -3.12640 0.00000 -0.00006 -0.00013 -0.00019 -3.12658

D138 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D139 -3.12679 0.00000 0.00000 -0.00007 -0.00007 -3.12686

D140 0.01346 -0.00001 -0.00013 -0.00019 -0.00032 0.01314

D141 -0.00508 0.00000 0.00008 0.00010 0.00017 -0.00490

D142 3.13518 0.00000 -0.00005 -0.00003 -0.00008 3.13510

D143 -0.01137 0.00000 -0.00006 0.00023 0.00018 -0.01119

D144 3.10661 0.00000 0.00026 -0.00008 0.00018 3.10679

D145 -3.13524 0.00000 -0.00012 0.00008 -0.00004 -3.13528

D146 -0.01726 -0.00001 0.00019 -0.00023 -0.00004 -0.01730

D147 0.00508 0.00000 -0.00008 -0.00010 -0.00017 0.00490

D148 -3.13518 0.00000 0.00005 0.00003 0.00008 -3.13510

D149 3.12679 0.00000 0.00000 0.00007 0.00007 3.12686

D150 -0.01346 0.00001 0.00013 0.00019 0.00032 -0.01314

D151 0.10890 0.00000 0.00092 0.00011 0.00103 0.10993

D152 -3.00438 0.00001 0.00054 0.00048 0.00102 -3.00336

D153 0.00787 0.00000 0.00001 -0.00006 -0.00006 0.00781

D154 -3.13425 0.00000 -0.00005 -0.00005 -0.00010 -3.13435

D155 -3.13631 0.00000 0.00004 0.00003 0.00007 -3.13624

D156 0.00475 0.00000 -0.00001 0.00004 0.00003 0.00478

D157 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D158 3.14108 0.00000 -0.00005 0.00001 -0.00004 3.14104

D159 -3.14108 0.00000 0.00005 -0.00001 0.00004 -3.14104

D160 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D161 -3.14125 0.00000 0.00006 -0.00003 0.00003 -3.14122

D162 0.00007 0.00000 0.00005 0.00000 0.00005 0.00012

D163 -0.00017 0.00000 0.00000 -0.00002 -0.00001 -0.00019

D164 3.14114 0.00000 -0.00001 0.00002 0.00001 3.14115

D165 -0.00787 0.00000 -0.00001 0.00006 0.00006 -0.00781

D166 3.13631 0.00000 -0.00004 -0.00003 -0.00007 3.13624

D167 3.13425 0.00000 0.00005 0.00005 0.00010 3.13435

D168 -0.00475 0.00000 0.00001 -0.00004 -0.00003 -0.00478

D169 0.00017 0.00000 0.00000 0.00002 0.00001 0.00019

D170 -3.14114 0.00000 0.00001 -0.00002 -0.00001 -3.14115

D171 3.14125 0.00000 -0.00006 0.00003 -0.00003 3.14122

D172 -0.00007 0.00000 -0.00005 0.00000 -0.00005 -0.00012

D173 -0.00502 0.00000 0.00008 0.00010 0.00017 -0.00484

D174 3.13951 0.00000 0.00002 0.00018 0.00021 3.13972

D175 3.13526 0.00000 -0.00005 -0.00002 -0.00008 3.13518

D176 -0.00340 0.00000 -0.00010 0.00006 -0.00004 -0.00344

D177 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D178 -3.13874 0.00000 -0.00005 0.00008 0.00003 -3.13871

D179 3.13874 0.00000 0.00005 -0.00008 -0.00003 3.13871

D180 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D181 3.13883 0.00000 0.00012 -0.00005 0.00007 3.13890

D182 -0.00305 0.00000 0.00006 -0.00010 -0.00004 -0.00308

D183 0.00013 0.00000 0.00006 0.00004 0.00010 0.00024

D184 3.14144 0.00000 0.00001 -0.00001 0.00000 3.14144

D185 0.00502 0.00000 -0.00008 -0.00010 -0.00017 0.00484

D186 -3.13526 0.00000 0.00005 0.00002 0.00008 -3.13518

D187 -3.13951 0.00000 -0.00002 -0.00018 -0.00021 -3.13972

D188 0.00340 0.00000 0.00010 -0.00006 0.00004 0.00344

D189 -0.00013 0.00000 -0.00006 -0.00004 -0.00010 -0.00024

D190 -3.14144 0.00000 -0.00001 0.00001 0.00000 -3.14144

D191 -3.13883 0.00000 -0.00012 0.00005 -0.00007 -3.13890

D192 0.00305 0.00000 -0.00006 0.00010 0.00004 0.00308

D193 -0.00787 0.00000 -0.00001 0.00006 0.00006 -0.00781

D194 3.13425 0.00000 0.00005 0.00005 0.00010 3.13435

D195 3.13631 0.00000 -0.00004 -0.00003 -0.00007 3.13624

D196 -0.00475 0.00000 0.00001 -0.00004 -0.00003 -0.00478

D197 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D198 -3.14108 0.00000 0.00005 -0.00001 0.00004 -3.14104

D199 3.14108 0.00000 -0.00005 0.00001 -0.00004 3.14104

D200 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D201 3.14125 0.00000 -0.00006 0.00003 -0.00003 3.14122

D202 -0.00007 0.00000 -0.00005 0.00000 -0.00005 -0.00012

D203 0.00017 0.00000 0.00000 0.00002 0.00001 0.00019

D204 -3.14114 0.00000 0.00001 -0.00002 -0.00001 -3.14115

D205 0.00787 0.00000 0.00001 -0.00006 -0.00006 0.00781

D206 -3.13631 0.00000 0.00004 0.00003 0.00007 -3.13624

D207 -3.13425 0.00000 -0.00005 -0.00005 -0.00010 -3.13435

D208 0.00475 0.00000 -0.00001 0.00004 0.00003 0.00478

D209 -0.00017 0.00000 0.00000 -0.00002 -0.00001 -0.00019

D210 3.14114 0.00000 -0.00001 0.00002 0.00001 3.14115

D211 -3.14125 0.00000 0.00006 -0.00003 0.00003 -3.14122

D212 0.00007 0.00000 0.00005 0.00000 0.00005 0.00012

D213 -0.00502 0.00000 0.00008 0.00010 0.00017 -0.00484

D214 3.13951 0.00000 0.00002 0.00018 0.00021 3.13972

D215 3.13526 0.00000 -0.00005 -0.00002 -0.00008 3.13518

D216 -0.00340 0.00000 -0.00010 0.00006 -0.00004 -0.00344

D217 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D218 -3.13874 0.00000 -0.00005 0.00008 0.00003 -3.13871

D219 3.13874 0.00000 0.00005 -0.00008 -0.00003 3.13871

D220 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D221 3.13883 0.00000 0.00012 -0.00005 0.00007 3.13890

D222 -0.00305 0.00000 0.00006 -0.00010 -0.00004 -0.00308

D223 0.00013 0.00000 0.00006 0.00004 0.00010 0.00024

D224 3.14144 0.00000 0.00001 -0.00001 0.00000 3.14144

D225 0.00502 0.00000 -0.00008 -0.00010 -0.00017 0.00484

D226 -3.13526 0.00000 0.00005 0.00002 0.00008 -3.13518

D227 -3.13951 0.00000 -0.00002 -0.00018 -0.00021 -3.13972

D228 0.00340 0.00000 0.00010 -0.00006 0.00004 0.00344

D229 -0.00013 0.00000 -0.00006 -0.00004 -0.00010 -0.00024

D230 -3.14144 0.00000 -0.00001 0.00001 0.00000 -3.14144

D231 -3.13883 0.00000 -0.00012 0.00005 -0.00007 -3.13890

D232 0.00305 0.00000 -0.00006 0.00010 0.00004 0.00308

D233 0.00014 0.00000 0.00006 0.00004 0.00010 0.00024

D234 -3.14157 0.00000 0.00004 0.00008 0.00013 -3.14145

D235 3.14144 0.00000 0.00000 -0.00001 -0.00001 3.14144

D236 -0.00027 0.00000 -0.00002 0.00003 0.00002 -0.00025

D237 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D238 3.14148 0.00000 -0.00002 0.00004 0.00002 3.14150

D239 -3.14148 0.00000 0.00002 -0.00004 -0.00002 -3.14150

D240 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D241 -0.00014 0.00000 -0.00006 -0.00004 -0.00010 -0.00024

D242 -3.14144 0.00000 0.00000 0.00001 0.00001 -3.14144

D243 3.14157 0.00000 -0.00004 -0.00008 -0.00013 3.14145

D244 0.00027 0.00000 0.00002 -0.00003 -0.00002 0.00025

D245 -0.00018 0.00000 0.00000 -0.00002 -0.00001 -0.00019

D246 -3.14115 0.00000 0.00000 -0.00002 -0.00002 -3.14117

D247 3.14113 0.00000 -0.00001 0.00002 0.00001 3.14115

D248 0.00016 0.00000 0.00000 0.00001 0.00001 0.00017

D249 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D250 -3.14098 0.00000 0.00000 0.00000 0.00000 -3.14098

D251 3.14098 0.00000 0.00000 0.00000 0.00000 3.14098

D252 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D253 0.00018 0.00000 0.00000 0.00002 0.00001 0.00019

D254 -3.14113 0.00000 0.00001 -0.00002 -0.00001 -3.14115

D255 3.14115 0.00000 0.00000 0.00002 0.00002 3.14117

D256 -0.00016 0.00000 0.00000 -0.00001 -0.00001 -0.00017

D257 0.00014 0.00000 0.00006 0.00004 0.00010 0.00024

D258 -3.14157 0.00000 0.00004 0.00008 0.00013 -3.14145

D259 3.14144 0.00000 0.00000 -0.00001 -0.00001 3.14144

D260 -0.00027 0.00000 -0.00002 0.00003 0.00002 -0.00025

D261 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D262 3.14148 0.00000 -0.00002 0.00004 0.00002 3.14150

D263 -3.14148 0.00000 0.00002 -0.00004 -0.00002 -3.14150

D264 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D265 -0.00014 0.00000 -0.00006 -0.00004 -0.00010 -0.00024

D266 -3.14144 0.00000 0.00000 0.00001 0.00001 -3.14144

D267 3.14157 0.00000 -0.00004 -0.00008 -0.00013 3.14145

D268 0.00027 0.00000 0.00002 -0.00003 -0.00002 0.00025

D269 0.00018 0.00000 0.00000 0.00002 0.00001 0.00019

D270 3.14115 0.00000 0.00000 0.00002 0.00002 3.14117

D271 -3.14113 0.00000 0.00001 -0.00002 -0.00001 -3.14115

D272 -0.00016 0.00000 0.00000 -0.00001 -0.00001 -0.00017

D273 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D274 3.14098 0.00000 0.00000 0.00000 0.00000 3.14098

D275 -3.14098 0.00000 0.00000 0.00000 0.00000 -3.14098

D276 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D277 -0.00018 0.00000 0.00000 -0.00002 -0.00001 -0.00019

D278 3.14113 0.00000 -0.00001 0.00002 0.00001 3.14115

D279 -3.14115 0.00000 0.00000 -0.00002 -0.00002 -3.14117

D280 0.00016 0.00000 0.00000 0.00001 0.00001 0.00017

Item Value Threshold Converged?

Maximum Force 0.000018 0.000450 YES

RMS Force 0.000004 0.000300 YES

Maximum Displacement 0.017978 0.001800 NO

RMS Displacement 0.003761 0.001200 NO

Predicted change in Energy=-1.093616D-07

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Jun 30 21:25:57 2019, MaxMem= 1342177280 cpu: 165.1

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

Stoichiometry C48H24N8Zn(3)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C48H24N4)]

Deg. of freedom 61

Full point group C2V NOp 4

RotChk: IX=0 Diff= 6.79D-15

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 1.121266 2.790101 0.181795

2 7 0 0.000000 2.023940 0.323286

3 6 0 -1.121266 2.790101 0.181795

4 6 0 -0.717705 4.166064 -0.045955

5 6 0 0.717705 4.166064 -0.045955

6 7 0 -2.412727 2.383588 0.209280

7 6 0 -2.794689 1.127506 0.264967

8 7 0 -2.010515 0.000000 0.327083

9 6 0 -2.794689 -1.127506 0.264967

10 6 0 -4.208496 -0.712281 0.210406

11 6 0 -4.208496 0.712281 0.210406

12 7 0 2.412727 2.383588 0.209280

13 6 0 4.208496 0.712281 0.210406

14 6 0 4.208496 -0.712281 0.210406

15 6 0 2.794689 -1.127506 0.264967

16 7 0 2.010515 0.000000 0.327083

17 6 0 2.794689 1.127506 0.264967

18 7 0 2.412727 -2.383588 0.209280

19 7 0 0.000000 -2.023940 0.323286

20 6 0 1.121266 -2.790101 0.181795

21 6 0 0.717705 -4.166064 -0.045955

22 6 0 -0.717705 -4.166064 -0.045955

23 6 0 -1.121266 -2.790101 0.181795

24 7 0 -2.412727 -2.383588 0.209280

25 30 0 0.000000 0.000000 0.845647

26 6 0 5.373866 1.426279 0.154645

27 6 0 6.609470 0.718882 0.105467

28 6 0 6.609470 -0.718882 0.105467

29 6 0 5.373866 -1.426279 0.154645

30 6 0 -1.428325 -5.325582 -0.255804

31 6 0 -0.721455 -6.535289 -0.468560

32 6 0 0.721455 -6.535289 -0.468560

33 6 0 1.428325 -5.325582 -0.255804

34 6 0 -5.373866 1.426279 0.154645

35 6 0 -6.609470 0.718882 0.105467

36 6 0 -6.609470 -0.718882 0.105467

37 6 0 -5.373866 -1.426279 0.154645

38 6 0 1.428325 5.325582 -0.255804

39 6 0 0.721455 6.535289 -0.468560

40 6 0 -0.721455 6.535289 -0.468560

41 6 0 -1.428325 5.325582 -0.255804

42 6 0 1.402326 -7.761835 -0.687930

43 6 0 0.708020 -8.929227 -0.896436

44 6 0 -0.708020 -8.929227 -0.896436

45 6 0 -1.402326 -7.761835 -0.687930

46 6 0 7.849135 -1.401347 0.055441

47 6 0 9.036710 -0.705866 0.007740

48 6 0 9.036710 0.705866 0.007740

49 6 0 7.849135 1.401347 0.055441

50 6 0 -1.402326 7.761835 -0.687930

51 6 0 -0.708020 8.929227 -0.896436

52 6 0 0.708020 8.929227 -0.896436

53 6 0 1.402326 7.761835 -0.687930

54 6 0 -7.849135 -1.401347 0.055441

55 6 0 -9.036710 -0.705866 0.007740

56 6 0 -9.036710 0.705866 0.007740

57 6 0 -7.849135 1.401347 0.055441

58 1 0 5.373926 2.511161 0.149601

59 1 0 5.373926 -2.511161 0.149601

60 1 0 -2.513360 -5.328083 -0.262376

61 1 0 2.513360 -5.328083 -0.262376

62 1 0 -5.373926 2.511161 0.149601

63 1 0 -5.373926 -2.511161 0.149601

64 1 0 2.513360 5.328083 -0.262376

65 1 0 -2.513360 5.328083 -0.262376

66 1 0 2.487807 -7.760275 -0.687504

67 1 0 1.243523 -9.857885 -1.062395

68 1 0 -1.243523 -9.857885 -1.062395

69 1 0 -2.487807 -7.760275 -0.687504

70 1 0 7.847397 -2.486617 0.055092

71 1 0 9.978528 -1.242471 -0.030671

72 1 0 9.978528 1.242471 -0.030671

73 1 0 7.847397 2.486617 0.055092

74 1 0 -2.487807 7.760275 -0.687504

75 1 0 -1.243523 9.857885 -1.062395

76 1 0 1.243523 9.857885 -1.062395

77 1 0 2.487807 7.760275 -0.687504

78 1 0 -7.847397 -2.486617 0.055092

79 1 0 -9.978528 -1.242471 -0.030671

80 1 0 -9.978528 1.242471 -0.030671

81 1 0 -7.847397 2.486617 0.055092

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

Rotational constants (GHZ): 0.0387371 0.0379462 0.0193816

Leave Link 202 at Sun Jun 30 21:25:58 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 307 symmetry adapted cartesian basis functions of A1 symmetry.

There are 278 symmetry adapted cartesian basis functions of A2 symmetry.

There are 289 symmetry adapted cartesian basis functions of B1 symmetry.

There are 289 symmetry adapted cartesian basis functions of B2 symmetry.

There are 289 symmetry adapted basis functions of A1 symmetry.

There are 265 symmetry adapted basis functions of A2 symmetry.

There are 275 symmetry adapted basis functions of B1 symmetry.

There are 275 symmetry adapted basis functions of B2 symmetry.

1104 basis functions, 1951 primitive gaussians, 1163 cartesian basis functions

191 alpha electrons 189 beta electrons

nuclear repulsion energy 6889.7875009412 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= 81 NActive= 81 NUniq= 22 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= -0.2361215374 Hartrees.

Nuclear repulsion after empirical dispersion term = 6889.5513794038 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= 81.

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 = 81

GePol: Total number of spheres = 81

GePol: Number of exposed spheres = 81 (100.00%)

GePol: Number of points = 6432

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.99D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 396

GePol: Fraction of low-weight points (<1% of avg) = 6.16%

GePol: Cavity surface area = 670.784 Ang\*\*2

GePol: Cavity volume = 694.599 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0170124300 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 6889.5343669738 Hartrees.

Leave Link 301 at Sun Jun 30 21:25:58 2019, MaxMem= 1342177280 cpu: 0.8

(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

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36719 LenP2D= 95220.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1104 RedAO= T EigKep= 2.89D-05 NBF= 289 265 275 275

NBsUse= 1104 1.00D-06 EigRej= -1.00D+00 NBFU= 289 265 275 275

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= 1060 1060 1060 1060 1060 MxSgAt= 81 MxSgA2= 81.

Leave Link 302 at Sun Jun 30 21:26:26 2019, MaxMem= 1342177280 cpu: 309.9

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Jun 30 21:26:27 2019, MaxMem= 1342177280 cpu: 4.3

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

Initial guess from the checkpoint file: "ZnNPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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

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

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The electronic state of the initial guess is 3-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

Leave Link 401 at Sun Jun 30 21:26:47 2019, MaxMem= 1342177280 cpu: 204.3

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4103221 IEndB= 4103221 NGot= 1342177280 MDV= 1339444432

LenX= 1339444432 LenY= 1338090700

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= 420000000 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= 124111872.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.33D-15 for 6412.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.54D-15 for 4942 4876.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.77D-15 for 6412.

Iteration 1 A^-1\*A deviation from orthogonality is 6.85D-09 for 2934 2923.

Iteration 2 A\*A^-1 deviation from unit magnitude is 3.77D-15 for 333.

Iteration 2 A\*A^-1 deviation from orthogonality is 5.33D-15 for 1627 1252.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 4.

Iteration 2 A^-1\*A deviation from orthogonality is 5.45D-16 for 6315 1163.

E= -2348.13071898170

DIIS: error= 1.36D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2348.13071898170 IErMin= 1 ErrMin= 1.36D-04

ErrMax= 1.36D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.99D-05 BMatP= 3.99D-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= 0.379 Goal= None Shift= 0.000

Gap= 0.459 Goal= None Shift= 0.000

RMSDP=4.50D-06 MaxDP=1.50D-04 OVMax= 7.12D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.50D-06 CP: 1.00D+00

E= -2348.13073907787 Delta-E= -0.000020096169 Rises=F Damp=F

DIIS: error= 1.94D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2348.13073907787 IErMin= 2 ErrMin= 1.94D-05

ErrMax= 1.94D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.24D-07 BMatP= 3.99D-05

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

Coeff-Com: -0.737D-01 0.107D+01

Coeff: -0.737D-01 0.107D+01

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=5.99D-07 MaxDP=2.18D-05 DE=-2.01D-05 OVMax= 1.28D-04

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.94D-07 CP: 1.00D+00 1.08D+00

E= -2348.13073936463 Delta-E= -0.000000286755 Rises=F Damp=F

DIIS: error= 7.59D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2348.13073936463 IErMin= 3 ErrMin= 7.59D-06

ErrMax= 7.59D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.74D-08 BMatP= 4.24D-07

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

Coeff-Com: -0.259D-01 0.330D+00 0.696D+00

Coeff: -0.259D-01 0.330D+00 0.696D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.14D-07 MaxDP=2.17D-05 DE=-2.87D-07 OVMax= 5.50D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.07D-07 CP: 1.00D+00 1.08D+00 9.07D-01

E= -2348.13073936782 Delta-E= -0.000000003196 Rises=F Damp=F

DIIS: error= 6.71D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2348.13073936782 IErMin= 4 ErrMin= 6.71D-06

ErrMax= 6.71D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.90D-08 BMatP= 7.74D-08

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

Coeff-Com: -0.495D-02 0.389D-01 0.480D+00 0.486D+00

Coeff: -0.495D-02 0.389D-01 0.480D+00 0.486D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.12D-07 MaxDP=1.32D-05 DE=-3.20D-09 OVMax= 3.08D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 5.94D-08 CP: 1.00D+00 1.08D+00 9.94D-01 5.97D-01

E= -2348.13073938308 Delta-E= -0.000000015258 Rises=F Damp=F

DIIS: error= 1.38D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2348.13073938308 IErMin= 5 ErrMin= 1.38D-06

ErrMax= 1.38D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.11D-09 BMatP= 6.90D-08

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

Coeff-Com: 0.764D-03-0.228D-01 0.128D+00 0.207D+00 0.687D+00

Coeff: 0.764D-03-0.228D-01 0.128D+00 0.207D+00 0.687D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.88D-08 MaxDP=1.78D-06 DE=-1.53D-08 OVMax= 7.15D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 2.12D-08 CP: 1.00D+00 1.08D+00 1.01D+00 6.38D-01 7.48D-01

E= -2348.13073938329 Delta-E= -0.000000000207 Rises=F Damp=F

DIIS: error= 1.16D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2348.13073938329 IErMin= 6 ErrMin= 1.16D-06

ErrMax= 1.16D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.61D-10 BMatP= 2.11D-09

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

Coeff-Com: 0.833D-03-0.166D-01 0.363D-01 0.820D-01 0.402D+00 0.495D+00

Coeff: 0.833D-03-0.166D-01 0.363D-01 0.820D-01 0.402D+00 0.495D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.22D-08 MaxDP=5.85D-07 DE=-2.07D-10 OVMax= 2.56D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 7.60D-09 CP: 1.00D+00 1.08D+00 1.01D+00 6.42D-01 8.06D-01

CP: 5.91D-01

E= -2348.13073938344 Delta-E= -0.000000000153 Rises=F Damp=F

DIIS: error= 5.13D-08 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2348.13073938344 IErMin= 7 ErrMin= 5.13D-08

ErrMax= 5.13D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.46D-11 BMatP= 4.61D-10

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

Coeff-Com: 0.192D-03-0.302D-02-0.842D-03 0.573D-02 0.638D-01 0.160D+00

Coeff-Com: 0.774D+00

Coeff: 0.192D-03-0.302D-02-0.842D-03 0.573D-02 0.638D-01 0.160D+00

Coeff: 0.774D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=3.86D-09 MaxDP=1.69D-07 DE=-1.53D-10 OVMax= 1.70D-06

Error on total polarization charges = 0.08827

SCF Done: E(UB3LYP) = -2348.13073938 A.U. after 7 cycles

NFock= 7 Conv=0.39D-08 -V/T= 1.9830

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

<L.S>= 0.000000000000E+00

KE= 2.388748342829D+03 PE=-1.932249370745D+04 EE= 7.696080258259D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -10.68

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0219, after 2.0003

Leave Link 502 at Sun Jun 30 21:36:03 2019, MaxMem= 1342177280 cpu: 5990.5

(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.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36719 LenP2D= 95220.

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 = 192

Leave Link 701 at Sun Jun 30 21:36:41 2019, MaxMem= 1342177280 cpu: 373.3

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sun Jun 30 21:36:41 2019, MaxMem= 1342177280 cpu: 0.1

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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 Sun Jun 30 21:37:28 2019, MaxMem= 1342177280 cpu: 491.0

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole = 4.88498131D-13 1.26121336D-12 8.84339442D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000003350 0.000001475 -0.000008283

2 7 0.000000000 0.000000348 0.000002764

3 6 0.000003350 0.000001475 -0.000008283

4 6 0.000003457 -0.000002433 -0.000001007

5 6 -0.000003457 -0.000002433 -0.000001007

6 7 -0.000002596 -0.000001310 0.000000031

7 6 -0.000003481 0.000000988 0.000001178

8 7 0.000006715 0.000000000 0.000000309

9 6 -0.000003481 -0.000000988 0.000001178

10 6 0.000001136 0.000003712 -0.000001289

11 6 0.000001136 -0.000003712 -0.000001289

12 7 0.000002596 -0.000001310 0.000000031

13 6 -0.000001136 -0.000003712 -0.000001289

14 6 -0.000001136 0.000003712 -0.000001289

15 6 0.000003481 -0.000000988 0.000001178

16 7 -0.000006715 0.000000000 0.000000309

17 6 0.000003481 0.000000988 0.000001178

18 7 0.000002596 0.000001310 0.000000031

19 7 0.000000000 -0.000000348 0.000002764

20 6 -0.000003350 -0.000001475 -0.000008283

21 6 -0.000003457 0.000002433 -0.000001007

22 6 0.000003457 0.000002433 -0.000001007

23 6 0.000003350 -0.000001475 -0.000008283

24 7 -0.000002596 0.000001310 0.000000031

25 30 0.000000000 0.000000000 0.000021448

26 6 0.000000993 0.000002079 -0.000001097

27 6 -0.000000994 -0.000000892 0.000000618

28 6 -0.000000994 0.000000892 0.000000618

29 6 0.000000993 -0.000002079 -0.000001097

30 6 -0.000002504 -0.000000165 -0.000000648

31 6 0.000002152 0.000000696 0.000000103

32 6 -0.000002152 0.000000696 0.000000103

33 6 0.000002504 -0.000000165 -0.000000648

34 6 -0.000000993 0.000002079 -0.000001097

35 6 0.000000994 -0.000000892 0.000000618

36 6 0.000000994 0.000000892 0.000000618

37 6 -0.000000993 -0.000002079 -0.000001097

38 6 0.000002504 0.000000165 -0.000000648

39 6 -0.000002152 -0.000000696 0.000000103

40 6 0.000002152 -0.000000696 0.000000103

41 6 -0.000002504 0.000000165 -0.000000648

42 6 0.000001805 -0.000001160 0.000003583

43 6 -0.000001753 -0.000000608 -0.000000561

44 6 0.000001753 -0.000000608 -0.000000561

45 6 -0.000001805 -0.000001160 0.000003583

46 6 0.000000919 -0.000000078 0.000000538

47 6 0.000000248 0.000000763 -0.000000158

48 6 0.000000248 -0.000000763 -0.000000158

49 6 0.000000919 0.000000078 0.000000538

50 6 -0.000001805 0.000001160 0.000003583

51 6 0.000001753 0.000000608 -0.000000561

52 6 -0.000001753 0.000000608 -0.000000561

53 6 0.000001805 0.000001160 0.000003583

54 6 -0.000000919 -0.000000078 0.000000538

55 6 -0.000000248 0.000000763 -0.000000158

56 6 -0.000000248 -0.000000763 -0.000000158

57 6 -0.000000919 0.000000078 0.000000538

58 1 -0.000000039 -0.000000525 -0.000000008

59 1 -0.000000039 0.000000525 -0.000000008

60 1 0.000000403 -0.000000962 0.000001277

61 1 -0.000000403 -0.000000962 0.000001277

62 1 0.000000039 -0.000000525 -0.000000008

63 1 0.000000039 0.000000525 -0.000000008

64 1 -0.000000403 0.000000962 0.000001277

65 1 0.000000403 0.000000962 0.000001277

66 1 -0.000000389 0.000000019 -0.000000525

67 1 0.000000248 0.000000194 -0.000000489

68 1 -0.000000248 0.000000194 -0.000000489

69 1 0.000000389 0.000000019 -0.000000525

70 1 -0.000000058 0.000000260 -0.000000096

71 1 0.000000033 -0.000000057 -0.000000066

72 1 0.000000033 0.000000057 -0.000000066

73 1 -0.000000058 -0.000000260 -0.000000096

74 1 0.000000389 -0.000000019 -0.000000525

75 1 -0.000000248 -0.000000194 -0.000000489

76 1 0.000000248 -0.000000194 -0.000000489

77 1 -0.000000389 -0.000000019 -0.000000525

78 1 0.000000058 0.000000260 -0.000000096

79 1 -0.000000033 -0.000000057 -0.000000066

80 1 -0.000000033 0.000000057 -0.000000066

81 1 0.000000058 -0.000000260 -0.000000096

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

Cartesian Forces: Max 0.000021448 RMS 0.000002329

Leave Link 716 at Sun Jun 30 21:37:29 2019, MaxMem= 1342177280 cpu: 3.7

(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 0.000005270 RMS 0.000001249

Search for a local minimum.

Step number 10 out of a maximum of 486

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .12485D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

6 7 8 9 10

DE= -8.43D-08 DEPred=-1.09D-07 R= 7.71D-01

Trust test= 7.71D-01 RLast= 7.87D-03 DXMaxT set to 3.00D-01

ITU= 0 0 1 1 1 1 1 1 1 0

Eigenvalues --- 0.00286 0.00549 0.01288 0.01432 0.01486

Eigenvalues --- 0.01500 0.01572 0.01588 0.01628 0.01656

Eigenvalues --- 0.01672 0.01694 0.01698 0.01706 0.01713

Eigenvalues --- 0.01714 0.01725 0.01730 0.01730 0.01736

Eigenvalues --- 0.01738 0.01749 0.01754 0.01758 0.01791

Eigenvalues --- 0.01827 0.01828 0.01830 0.01851 0.01854

Eigenvalues --- 0.01870 0.01871 0.01913 0.01936 0.01968

Eigenvalues --- 0.01968 0.01972 0.01977 0.01978 0.01992

Eigenvalues --- 0.01992 0.01993 0.01993 0.02010 0.02080

Eigenvalues --- 0.02085 0.02086 0.02089 0.02090 0.02096

Eigenvalues --- 0.02096 0.02097 0.02098 0.02103 0.02103

Eigenvalues --- 0.02105 0.02106 0.02124 0.02124 0.02137

Eigenvalues --- 0.02144 0.02144 0.02147 0.02148 0.02169

Eigenvalues --- 0.02173 0.02197 0.02213 0.02214 0.02225

Eigenvalues --- 0.02228 0.02281 0.02286 0.02346 0.02360

Eigenvalues --- 0.02438 0.02953 0.05507 0.05549 0.07576

Eigenvalues --- 0.14639 0.15974 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 0.16001 0.16008 0.16040

Eigenvalues --- 0.16161 0.16245 0.16997 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22499 0.22504 0.22504

Eigenvalues --- 0.22541 0.23231 0.23234 0.23234 0.23612

Eigenvalues --- 0.23939 0.23939 0.23939 0.23952 0.23987

Eigenvalues --- 0.24282 0.24296 0.24550 0.24553 0.24557

Eigenvalues --- 0.24557 0.24570 0.24765 0.24891 0.24897

Eigenvalues --- 0.24961 0.24982 0.24984 0.24985 0.24989

Eigenvalues --- 0.24996 0.24996 0.24997 0.24997 0.25916

Eigenvalues --- 0.32864 0.32946 0.33670 0.33738 0.33834

Eigenvalues --- 0.33859 0.35041 0.35069 0.35089 0.35181

Eigenvalues --- 0.35181 0.35181 0.35188 0.35202 0.35202

Eigenvalues --- 0.35202 0.35212 0.35231 0.35231 0.35231

Eigenvalues --- 0.35242 0.35249 0.35249 0.35249 0.35270

Eigenvalues --- 0.35270 0.35270 0.35274 0.35279 0.35279

Eigenvalues --- 0.35279 0.35345 0.35414 0.35470 0.36350

Eigenvalues --- 0.36427 0.37458 0.37569 0.37969 0.38163

Eigenvalues --- 0.39275 0.39276 0.39612 0.39612 0.40188

Eigenvalues --- 0.40188 0.40257 0.40257 0.40906 0.41001

Eigenvalues --- 0.41013 0.41149 0.41603 0.41779 0.41873

Eigenvalues --- 0.42163 0.42215 0.42381 0.42806 0.42892

Eigenvalues --- 0.42901 0.42970 0.44425 0.45679 0.47124

Eigenvalues --- 0.47124 0.47249 0.47384 0.47386 0.47579

Eigenvalues --- 0.47580 0.47901 0.48121 0.48218 0.48361

Eigenvalues --- 0.48454 0.48465 0.48680 0.48707 0.48729

Eigenvalues --- 0.48754 0.49092 0.49418 0.49898 0.50349

Eigenvalues --- 0.51030 0.51284 0.52477 0.57879 0.59236

Eigenvalues --- 0.59873 0.60917

En-DIIS/RFO-DIIS IScMMF= 0 using points: 10 9 8 7 6

RFO step: Lambda= 0.00000000D+00.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 6.79D-06 SmlDif= 1.00D-05

RMS Error= 0.9658897525D-05 NUsed= 5 EDIIS=F

DidBck=T Rises=F RFO-DIIS coefs: 0.71721 0.43525 -0.18340 -0.00145 0.03240

Iteration 1 RMS(Cart)= 0.00161303 RMS(Int)= 0.00000020

Iteration 2 RMS(Cart)= 0.00000063 RMS(Int)= 0.00000014

ITry= 1 IFail=0 DXMaxC= 9.06D-03 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.99D-08 for atom 69.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58019 0.00000 -0.00002 0.00001 -0.00001 2.58018

R2 2.74369 0.00000 0.00002 -0.00001 0.00001 2.74370

R3 2.55908 0.00000 -0.00001 0.00001 0.00000 2.55908

R4 2.58019 0.00000 -0.00002 0.00001 -0.00001 2.58018

R5 3.95002 0.00000 0.00002 0.00000 0.00002 3.95004

R6 2.74369 0.00000 0.00002 -0.00001 0.00001 2.74370

R7 2.55908 0.00000 -0.00001 0.00001 0.00000 2.55908

R8 2.71253 0.00000 0.00001 -0.00001 0.00000 2.71253

R9 2.60035 0.00000 -0.00001 0.00001 0.00000 2.60035

R10 2.60035 0.00000 -0.00001 0.00001 0.00000 2.60035

R11 2.48320 0.00000 -0.00001 0.00001 0.00000 2.48320

R12 2.59798 0.00000 0.00000 0.00001 0.00000 2.59799

R13 2.78646 0.00000 0.00003 -0.00001 0.00001 2.78647

R14 2.59798 0.00000 0.00000 0.00001 0.00000 2.59799

R15 3.92366 0.00000 0.00001 0.00000 0.00001 3.92368

R16 2.78646 0.00000 0.00003 -0.00001 0.00001 2.78647

R17 2.48320 0.00000 -0.00001 0.00001 0.00000 2.48320

R18 2.69203 0.00000 0.00000 -0.00001 -0.00001 2.69202

R19 2.58485 0.00000 0.00000 0.00001 0.00000 2.58485

R20 2.58485 0.00000 0.00000 0.00001 0.00000 2.58485

R21 2.48320 0.00000 -0.00001 0.00001 0.00000 2.48320

R22 2.69203 0.00000 0.00000 -0.00001 -0.00001 2.69202

R23 2.78646 0.00000 0.00003 -0.00001 0.00001 2.78647

R24 2.58485 0.00000 0.00000 0.00001 0.00000 2.58485

R25 2.78646 0.00000 0.00003 -0.00001 0.00001 2.78647

R26 2.58485 0.00000 0.00000 0.00001 0.00000 2.58485

R27 2.59798 0.00000 0.00000 0.00001 0.00000 2.59799

R28 2.48320 0.00000 -0.00001 0.00001 0.00000 2.48320

R29 2.59798 0.00000 0.00000 0.00001 0.00000 2.59799

R30 3.92366 0.00000 0.00001 0.00000 0.00001 3.92368

R31 2.55908 0.00000 -0.00001 0.00001 0.00000 2.55908

R32 2.58019 0.00000 -0.00002 0.00001 -0.00001 2.58018

R33 2.58019 0.00000 -0.00002 0.00001 -0.00001 2.58018

R34 3.95002 0.00000 0.00002 0.00000 0.00002 3.95004

R35 2.74369 0.00000 0.00002 -0.00001 0.00001 2.74370

R36 2.71253 0.00000 0.00001 -0.00001 0.00000 2.71253

R37 2.60035 0.00000 -0.00001 0.00001 0.00000 2.60035

R38 2.74369 0.00000 0.00002 -0.00001 0.00001 2.74370

R39 2.60035 0.00000 -0.00001 0.00001 0.00000 2.60035

R40 2.55908 0.00000 -0.00001 0.00001 0.00000 2.55908

R41 2.69214 0.00000 0.00000 0.00000 0.00000 2.69214

R42 2.05015 0.00000 0.00000 0.00000 0.00000 2.05015

R43 2.71698 0.00000 0.00001 -0.00001 0.00000 2.71698

R44 2.67584 0.00000 0.00000 0.00000 0.00000 2.67584

R45 2.69214 0.00000 0.00000 0.00000 0.00000 2.69214

R46 2.67584 0.00000 0.00000 0.00000 0.00000 2.67584

R47 2.05015 0.00000 0.00000 0.00000 0.00000 2.05015

R48 2.67803 0.00000 0.00000 0.00000 0.00000 2.67803

R49 2.05046 0.00000 0.00000 0.00000 0.00000 2.05046

R50 2.72671 0.00000 0.00001 -0.00001 0.00000 2.72671

R51 2.68323 0.00000 0.00000 0.00000 0.00000 2.68323

R52 2.67803 0.00000 0.00000 0.00000 0.00000 2.67803

R53 2.68323 0.00000 0.00000 0.00000 0.00000 2.68323

R54 2.05046 0.00000 0.00000 0.00000 0.00000 2.05046

R55 2.69214 0.00000 0.00000 0.00000 0.00000 2.69214

R56 2.05015 0.00000 0.00000 0.00000 0.00000 2.05015

R57 2.71698 0.00000 0.00001 -0.00001 0.00000 2.71698

R58 2.67584 0.00000 0.00000 0.00000 0.00000 2.67584

R59 2.69214 0.00000 0.00000 0.00000 0.00000 2.69214

R60 2.67584 0.00000 0.00000 0.00000 0.00000 2.67584

R61 2.05015 0.00000 0.00000 0.00000 0.00000 2.05015

R62 2.67803 0.00000 0.00000 0.00000 0.00000 2.67803

R63 2.05046 0.00000 0.00000 0.00000 0.00000 2.05046

R64 2.72671 0.00000 0.00001 -0.00001 0.00000 2.72671

R65 2.68323 0.00000 0.00000 0.00000 0.00000 2.68323

R66 2.67803 0.00000 0.00000 0.00000 0.00000 2.67803

R67 2.68323 0.00000 0.00000 0.00000 0.00000 2.68323

R68 2.05046 0.00000 0.00000 0.00000 0.00000 2.05046

R69 2.59680 0.00000 -0.00001 0.00001 0.00000 2.59680

R70 2.05126 0.00000 0.00000 0.00000 0.00000 2.05126

R71 2.67593 0.00000 0.00001 -0.00001 0.00000 2.67593

R72 2.04990 0.00000 0.00000 0.00000 0.00000 2.04990

R73 2.59680 0.00000 -0.00001 0.00001 0.00000 2.59680

R74 2.04990 0.00000 0.00000 0.00000 0.00000 2.04990

R75 2.05126 0.00000 0.00000 0.00000 0.00000 2.05126

R76 2.60227 0.00000 0.00000 0.00000 0.00000 2.60227

R77 2.05087 0.00000 0.00000 0.00000 0.00000 2.05087

R78 2.66779 0.00000 0.00000 -0.00001 0.00000 2.66778

R79 2.04967 0.00000 0.00000 0.00000 0.00000 2.04967

R80 2.60227 0.00000 0.00000 0.00000 0.00000 2.60227

R81 2.04967 0.00000 0.00000 0.00000 0.00000 2.04967

R82 2.05087 0.00000 0.00000 0.00000 0.00000 2.05087

R83 2.59680 0.00000 -0.00001 0.00001 0.00000 2.59680

R84 2.05126 0.00000 0.00000 0.00000 0.00000 2.05126

R85 2.67593 0.00000 0.00001 -0.00001 0.00000 2.67593

R86 2.04990 0.00000 0.00000 0.00000 0.00000 2.04990

R87 2.59680 0.00000 -0.00001 0.00001 0.00000 2.59680

R88 2.04990 0.00000 0.00000 0.00000 0.00000 2.04990

R89 2.05126 0.00000 0.00000 0.00000 0.00000 2.05126

R90 2.60227 0.00000 0.00000 0.00000 0.00000 2.60227

R91 2.05087 0.00000 0.00000 0.00000 0.00000 2.05087

R92 2.66779 0.00000 0.00000 -0.00001 0.00000 2.66778

R93 2.04967 0.00000 0.00000 0.00000 0.00000 2.04967

R94 2.60227 0.00000 0.00000 0.00000 0.00000 2.60227

R95 2.04967 0.00000 0.00000 0.00000 0.00000 2.04967

R96 2.05087 0.00000 0.00000 0.00000 0.00000 2.05087

A1 1.89630 0.00000 -0.00001 0.00001 0.00000 1.89630

A2 2.23016 0.00000 -0.00001 0.00000 -0.00001 2.23016

A3 2.15645 0.00000 0.00002 -0.00001 0.00001 2.15646

A4 1.92706 0.00000 0.00002 -0.00002 0.00000 1.92707

A5 2.17636 0.00000 -0.00003 0.00001 -0.00002 2.17634

A6 2.17636 0.00000 -0.00003 0.00001 -0.00002 2.17634

A7 1.89630 0.00000 -0.00001 0.00001 0.00000 1.89630

A8 2.23016 0.00000 -0.00001 0.00000 -0.00001 2.23016

A9 2.15645 0.00000 0.00002 -0.00001 0.00001 2.15646

A10 1.85246 0.00000 0.00000 0.00000 0.00000 1.85246

A11 2.31714 0.00000 0.00001 0.00000 0.00001 2.31714

A12 2.11346 0.00000 0.00000 0.00000 0.00000 2.11346

A13 1.85246 0.00000 0.00000 0.00000 0.00000 1.85246

A14 2.31714 0.00000 0.00001 0.00000 0.00001 2.31714

A15 2.11346 0.00000 0.00000 0.00000 0.00000 2.11346

A16 2.17124 0.00000 0.00002 -0.00001 0.00001 2.17125

A17 2.23962 0.00000 0.00001 0.00000 0.00001 2.23963

A18 2.14875 0.00000 0.00000 -0.00001 -0.00001 2.14874

A19 1.89402 0.00000 -0.00001 0.00001 0.00000 1.89402

A20 1.92327 0.00000 0.00002 -0.00002 0.00000 1.92327

A21 2.16954 0.00000 0.00001 0.00001 0.00002 2.16956

A22 2.16954 0.00000 0.00001 0.00001 0.00002 2.16956

A23 1.89402 0.00000 -0.00001 0.00001 0.00000 1.89402

A24 2.23962 0.00000 0.00001 0.00000 0.00001 2.23963

A25 2.14875 0.00000 0.00000 -0.00001 -0.00001 2.14874

A26 1.85626 0.00000 0.00000 0.00000 0.00000 1.85626

A27 2.30691 0.00000 0.00000 0.00000 0.00000 2.30690

A28 2.11998 0.00000 0.00000 0.00000 0.00000 2.11998

A29 1.85626 0.00000 0.00000 0.00000 0.00000 1.85626

A30 2.30691 0.00000 0.00000 0.00000 0.00000 2.30690

A31 2.11998 0.00000 0.00000 0.00000 0.00000 2.11998

A32 2.17124 0.00000 0.00002 -0.00001 0.00001 2.17125

A33 1.85626 0.00000 0.00000 0.00000 0.00000 1.85626

A34 2.11998 0.00000 0.00000 0.00000 0.00000 2.11998

A35 2.30691 0.00000 0.00000 0.00000 0.00000 2.30690

A36 1.85626 0.00000 0.00000 0.00000 0.00000 1.85626

A37 2.11998 0.00000 0.00000 0.00000 0.00000 2.11998

A38 2.30691 0.00000 0.00000 0.00000 0.00000 2.30690

A39 1.89402 0.00000 -0.00001 0.00001 0.00000 1.89402

A40 2.14875 0.00000 0.00000 -0.00001 -0.00001 2.14874

A41 2.23962 0.00000 0.00001 0.00000 0.00001 2.23963

A42 1.92327 0.00000 0.00002 -0.00002 0.00000 1.92327

A43 2.16954 0.00000 0.00001 0.00001 0.00002 2.16956

A44 2.16954 0.00000 0.00001 0.00001 0.00002 2.16956

A45 2.14875 0.00000 0.00000 -0.00001 -0.00001 2.14874

A46 2.23962 0.00000 0.00001 0.00000 0.00001 2.23963

A47 1.89402 0.00000 -0.00001 0.00001 0.00000 1.89402

A48 2.17124 0.00000 0.00002 -0.00001 0.00001 2.17125

A49 1.92706 0.00000 0.00002 -0.00002 0.00000 1.92707

A50 2.17636 0.00000 -0.00003 0.00001 -0.00002 2.17634

A51 2.17636 0.00000 -0.00003 0.00001 -0.00002 2.17634

A52 2.23016 0.00000 -0.00001 0.00000 -0.00001 2.23016

A53 2.15645 0.00000 0.00002 -0.00001 0.00001 2.15646

A54 1.89630 0.00000 -0.00001 0.00001 0.00000 1.89630

A55 1.85246 0.00000 0.00000 0.00000 0.00000 1.85246

A56 2.31714 0.00000 0.00001 0.00000 0.00001 2.31714

A57 2.11346 0.00000 0.00000 0.00000 0.00000 2.11346

A58 1.85246 0.00000 0.00000 0.00000 0.00000 1.85246

A59 2.11346 0.00000 0.00000 0.00000 0.00000 2.11346

A60 2.31714 0.00000 0.00001 0.00000 0.00001 2.31714

A61 1.89630 0.00000 -0.00001 0.00001 0.00000 1.89630

A62 2.23016 0.00000 -0.00001 0.00000 -0.00001 2.23016

A63 2.15645 0.00000 0.00002 -0.00001 0.00001 2.15646

A64 2.17124 0.00000 0.00002 -0.00001 0.00001 2.17125

A65 1.50834 0.00000 0.00000 -0.00002 -0.00002 1.50833

A66 1.50834 0.00000 0.00000 -0.00002 -0.00002 1.50833

A67 2.63643 0.00000 -0.00004 -0.00007 -0.00011 2.63632

A68 2.63674 0.00000 0.00005 -0.00006 -0.00001 2.63673

A69 1.50834 0.00000 0.00000 -0.00002 -0.00002 1.50833

A70 1.50834 0.00000 0.00000 -0.00002 -0.00002 1.50833

A71 2.07276 0.00000 0.00001 -0.00001 0.00000 2.07277

A72 2.12025 0.00000 -0.00001 0.00001 0.00000 2.12025

A73 2.09017 0.00000 0.00000 0.00000 0.00000 2.09017

A74 2.09042 0.00000 -0.00001 0.00000 0.00000 2.09041

A75 2.11907 0.00000 0.00001 0.00000 0.00000 2.11907

A76 2.07370 0.00000 0.00000 0.00000 0.00000 2.07370

A77 2.09042 0.00000 -0.00001 0.00000 0.00000 2.09041

A78 2.07370 0.00000 0.00000 0.00000 0.00000 2.07370

A79 2.11907 0.00000 0.00001 0.00000 0.00000 2.11907

A80 2.07276 0.00000 0.00001 -0.00001 0.00000 2.07277

A81 2.12025 0.00000 -0.00001 0.00001 0.00000 2.12025

A82 2.09017 0.00000 0.00000 0.00000 0.00000 2.09017

A83 2.07671 0.00000 0.00001 -0.00001 0.00000 2.07671

A84 2.11680 0.00000 -0.00002 0.00001 0.00000 2.11680

A85 2.08968 0.00000 0.00001 -0.00001 0.00000 2.08968

A86 2.09301 0.00000 -0.00001 0.00000 0.00000 2.09300

A87 2.11927 0.00000 0.00001 0.00000 0.00000 2.11928

A88 2.07090 0.00000 0.00000 0.00000 0.00000 2.07090

A89 2.09301 0.00000 -0.00001 0.00000 0.00000 2.09300

A90 2.07090 0.00000 0.00000 0.00000 0.00000 2.07090

A91 2.11927 0.00000 0.00001 0.00000 0.00000 2.11928

A92 2.07671 0.00000 0.00001 -0.00001 0.00000 2.07671

A93 2.11680 0.00000 -0.00002 0.00001 0.00000 2.11680

A94 2.08968 0.00000 0.00001 -0.00001 0.00000 2.08968

A95 2.07276 0.00000 0.00001 -0.00001 0.00000 2.07277

A96 2.12025 0.00000 -0.00001 0.00001 0.00000 2.12025

A97 2.09017 0.00000 0.00000 0.00000 0.00000 2.09017

A98 2.09042 0.00000 -0.00001 0.00000 0.00000 2.09041

A99 2.11907 0.00000 0.00001 0.00000 0.00000 2.11907

A100 2.07370 0.00000 0.00000 0.00000 0.00000 2.07370

A101 2.09042 0.00000 -0.00001 0.00000 0.00000 2.09041

A102 2.07370 0.00000 0.00000 0.00000 0.00000 2.07370

A103 2.11907 0.00000 0.00001 0.00000 0.00000 2.11907

A104 2.07276 0.00000 0.00001 -0.00001 0.00000 2.07277

A105 2.12025 0.00000 -0.00001 0.00001 0.00000 2.12025

A106 2.09017 0.00000 0.00000 0.00000 0.00000 2.09017

A107 2.07671 0.00000 0.00001 -0.00001 0.00000 2.07671

A108 2.11680 0.00000 -0.00002 0.00001 0.00000 2.11680

A109 2.08968 0.00000 0.00001 -0.00001 0.00000 2.08968

A110 2.09301 0.00000 -0.00001 0.00000 0.00000 2.09300

A111 2.11927 0.00000 0.00001 0.00000 0.00000 2.11928

A112 2.07090 0.00000 0.00000 0.00000 0.00000 2.07090

A113 2.09301 0.00000 -0.00001 0.00000 0.00000 2.09300

A114 2.07090 0.00000 0.00000 0.00000 0.00000 2.07090

A115 2.11927 0.00000 0.00001 0.00000 0.00000 2.11928

A116 2.07671 0.00000 0.00001 -0.00001 0.00000 2.07671

A117 2.11680 0.00000 -0.00002 0.00001 0.00000 2.11680

A118 2.08968 0.00000 0.00001 -0.00001 0.00000 2.08968

A119 2.11181 0.00000 0.00000 0.00000 0.00000 2.11181

A120 2.06942 0.00000 0.00000 0.00000 0.00000 2.06942

A121 2.10196 0.00000 0.00000 0.00000 0.00000 2.10195

A122 2.10047 0.00000 0.00000 0.00000 0.00000 2.10047

A123 2.09562 0.00000 0.00001 0.00000 0.00000 2.09563

A124 2.08709 0.00000 0.00000 0.00000 0.00000 2.08709

A125 2.10047 0.00000 0.00000 0.00000 0.00000 2.10047

A126 2.08709 0.00000 0.00000 0.00000 0.00000 2.08709

A127 2.09562 0.00000 0.00001 0.00000 0.00000 2.09563

A128 2.11181 0.00000 0.00000 0.00000 0.00000 2.11181

A129 2.06942 0.00000 0.00000 0.00000 0.00000 2.06942

A130 2.10196 0.00000 0.00000 0.00000 0.00000 2.10195

A131 2.10925 0.00000 0.00000 0.00000 0.00000 2.10926

A132 2.07211 0.00000 0.00000 0.00000 0.00000 2.07211

A133 2.10182 0.00000 0.00000 0.00000 0.00000 2.10182

A134 2.10023 0.00000 0.00000 0.00000 0.00000 2.10023

A135 2.09463 0.00000 0.00000 0.00000 0.00000 2.09463

A136 2.08832 0.00000 0.00000 0.00000 0.00000 2.08832

A137 2.10023 0.00000 0.00000 0.00000 0.00000 2.10023

A138 2.08832 0.00000 0.00000 0.00000 0.00000 2.08832

A139 2.09463 0.00000 0.00000 0.00000 0.00000 2.09463

A140 2.10925 0.00000 0.00000 0.00000 0.00000 2.10926

A141 2.07211 0.00000 0.00000 0.00000 0.00000 2.07211

A142 2.10182 0.00000 0.00000 0.00000 0.00000 2.10182

A143 2.11181 0.00000 0.00000 0.00000 0.00000 2.11181

A144 2.06942 0.00000 0.00000 0.00000 0.00000 2.06942

A145 2.10196 0.00000 0.00000 0.00000 0.00000 2.10195

A146 2.10047 0.00000 0.00000 0.00000 0.00000 2.10047

A147 2.09562 0.00000 0.00001 0.00000 0.00000 2.09563

A148 2.08709 0.00000 0.00000 0.00000 0.00000 2.08709

A149 2.10047 0.00000 0.00000 0.00000 0.00000 2.10047

A150 2.08709 0.00000 0.00000 0.00000 0.00000 2.08709

A151 2.09562 0.00000 0.00001 0.00000 0.00000 2.09563

A152 2.11181 0.00000 0.00000 0.00000 0.00000 2.11181

A153 2.06942 0.00000 0.00000 0.00000 0.00000 2.06942

A154 2.10196 0.00000 0.00000 0.00000 0.00000 2.10195

A155 2.10925 0.00000 0.00000 0.00000 0.00000 2.10926

A156 2.07211 0.00000 0.00000 0.00000 0.00000 2.07211

A157 2.10182 0.00000 0.00000 0.00000 0.00000 2.10182

A158 2.10023 0.00000 0.00000 0.00000 0.00000 2.10023

A159 2.09463 0.00000 0.00000 0.00000 0.00000 2.09463

A160 2.08832 0.00000 0.00000 0.00000 0.00000 2.08832

A161 2.10023 0.00000 0.00000 0.00000 0.00000 2.10023

A162 2.08832 0.00000 0.00000 0.00000 0.00000 2.08832

A163 2.09463 0.00000 0.00000 0.00000 0.00000 2.09463

A164 2.10925 0.00000 0.00000 0.00000 0.00000 2.10926

A165 2.07211 0.00000 0.00000 0.00000 0.00000 2.07211

A166 2.10182 0.00000 0.00000 0.00000 0.00000 2.10182

D1 0.01884 0.00000 0.00010 0.00004 0.00015 0.01899

D2 -3.03763 0.00001 0.00068 0.00004 0.00071 -3.03691

D3 -3.09786 0.00000 0.00004 0.00001 0.00004 -3.09782

D4 0.12886 0.00000 0.00061 0.00000 0.00061 0.12947

D5 -0.01119 0.00000 -0.00006 -0.00003 -0.00009 -0.01128

D6 -3.13528 0.00000 -0.00024 -0.00011 -0.00035 -3.13563

D7 3.10679 0.00000 0.00000 0.00001 0.00001 3.10680

D8 -0.01730 0.00000 -0.00018 -0.00007 -0.00025 -0.01754

D9 0.10993 0.00000 -0.00040 0.00003 -0.00038 0.10955

D10 -3.00336 0.00000 -0.00048 -0.00002 -0.00049 -3.00386

D11 -0.01884 0.00000 -0.00010 -0.00004 -0.00015 -0.01899

D12 3.09786 0.00000 -0.00004 -0.00001 -0.00004 3.09782

D13 3.03763 -0.00001 -0.00068 -0.00004 -0.00071 3.03691

D14 -0.12886 0.00000 -0.00061 0.00000 -0.00061 -0.12947

D15 -2.94539 0.00000 -0.00035 0.00003 -0.00032 -2.94571

D16 -0.29327 0.00000 -0.00030 -0.00002 -0.00033 -0.29360

D17 -1.61933 0.00000 -0.00033 0.00000 -0.00032 -1.61965

D18 0.29327 0.00000 0.00030 0.00002 0.00033 0.29360

D19 2.94539 0.00000 0.00035 -0.00003 0.00032 2.94571

D20 1.61933 0.00000 0.00033 0.00000 0.00032 1.61965

D21 0.01119 0.00000 0.00006 0.00003 0.00009 0.01128

D22 3.13528 0.00000 0.00024 0.00011 0.00035 3.13563

D23 -3.10679 0.00000 0.00000 -0.00001 -0.00001 -3.10680

D24 0.01730 0.00000 0.00018 0.00007 0.00025 0.01754

D25 -0.10993 0.00000 0.00040 -0.00003 0.00038 -0.10955

D26 3.00336 0.00000 0.00048 0.00002 0.00049 3.00386

D27 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D28 3.12658 0.00000 0.00015 0.00007 0.00022 3.12681

D29 -3.12658 0.00000 -0.00015 -0.00007 -0.00022 -3.12681

D30 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D31 -3.12686 0.00000 -0.00026 -0.00007 -0.00032 -3.12718

D32 0.01314 0.00000 -0.00018 -0.00005 -0.00023 0.01292

D33 -0.00490 0.00000 -0.00006 0.00003 -0.00003 -0.00493

D34 3.13510 0.00000 0.00002 0.00004 0.00006 3.13516

D35 3.12686 0.00000 0.00026 0.00007 0.00032 3.12718

D36 -0.01314 0.00000 0.00018 0.00005 0.00023 -0.01292

D37 0.00490 0.00000 0.00006 -0.00003 0.00003 0.00493

D38 -3.13510 0.00000 -0.00002 -0.00004 -0.00006 -3.13516

D39 0.01970 0.00000 0.00013 0.00001 0.00014 0.01983

D40 -3.07407 0.00000 0.00006 0.00001 0.00007 -3.07400

D41 -3.05839 0.00000 -0.00010 0.00002 -0.00008 -3.05848

D42 0.29359 0.00000 -0.00035 0.00003 -0.00031 0.29327

D43 0.04096 0.00000 -0.00005 0.00002 -0.00003 0.04093

D44 -2.89025 0.00000 -0.00029 0.00003 -0.00026 -2.89051

D45 3.07761 0.00000 0.00008 -0.00002 0.00007 3.07768

D46 -0.05335 0.00000 0.00003 -0.00001 0.00002 -0.05333

D47 -0.02442 0.00000 0.00003 -0.00001 0.00002 -0.02440

D48 3.12781 0.00000 -0.00003 -0.00001 -0.00003 3.12777

D49 -0.04096 0.00000 0.00005 -0.00002 0.00003 -0.04093

D50 3.05839 0.00000 0.00010 -0.00002 0.00008 3.05848

D51 2.89025 0.00000 0.00029 -0.00003 0.00026 2.89051

D52 -0.29359 0.00000 0.00035 -0.00003 0.00031 -0.29327

D53 -0.36468 0.00000 0.00012 -0.00004 0.00008 -0.36460

D54 -1.69058 0.00000 0.00014 -0.00001 0.00013 -1.69044

D55 -3.01648 0.00000 0.00016 0.00002 0.00019 -3.01629

D56 3.01648 0.00000 -0.00016 -0.00002 -0.00019 3.01629

D57 1.69058 0.00000 -0.00014 0.00001 -0.00013 1.69044

D58 0.36468 0.00000 -0.00012 0.00004 -0.00008 0.36460

D59 0.02442 0.00000 -0.00003 0.00001 -0.00002 0.02440

D60 -3.12781 0.00000 0.00003 0.00001 0.00003 -3.12777

D61 -3.07761 0.00000 -0.00008 0.00002 -0.00007 -3.07768

D62 0.05335 0.00000 -0.00003 0.00001 -0.00002 0.05333

D63 -0.01970 0.00000 -0.00013 -0.00001 -0.00014 -0.01983

D64 3.07407 0.00000 -0.00006 -0.00001 -0.00007 3.07400

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13235 0.00000 0.00005 0.00000 0.00004 3.13240

D67 -3.13235 0.00000 -0.00005 0.00000 -0.00004 -3.13240

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 -3.13758 0.00000 -0.00008 0.00001 -0.00006 -3.13765

D70 0.00652 0.00000 -0.00004 0.00000 -0.00004 0.00648

D71 -0.00795 0.00000 -0.00001 0.00001 -0.00001 -0.00796

D72 3.13615 0.00000 0.00002 -0.00001 0.00001 3.13616

D73 3.13758 0.00000 0.00008 -0.00001 0.00006 3.13765

D74 -0.00652 0.00000 0.00004 0.00000 0.00004 -0.00648

D75 0.00795 0.00000 0.00001 -0.00001 0.00001 0.00796

D76 -3.13615 0.00000 -0.00002 0.00001 -0.00001 -3.13616

D77 3.07407 0.00000 -0.00006 -0.00001 -0.00007 3.07400

D78 -0.01970 0.00000 -0.00013 -0.00001 -0.00014 -0.01983

D79 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D80 3.13235 0.00000 0.00005 0.00000 0.00004 3.13240

D81 -3.13235 0.00000 -0.00005 0.00000 -0.00004 -3.13240

D82 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D83 -3.07761 0.00000 -0.00008 0.00002 -0.00007 -3.07768

D84 0.02442 0.00000 -0.00003 0.00001 -0.00002 0.02440

D85 0.05335 0.00000 -0.00003 0.00001 -0.00002 0.05333

D86 -3.12781 0.00000 0.00003 0.00001 0.00003 -3.12777

D87 -0.00795 0.00000 -0.00001 0.00001 -0.00001 -0.00796

D88 3.13615 0.00000 0.00002 -0.00001 0.00001 3.13616

D89 -3.13758 0.00000 -0.00008 0.00001 -0.00006 -3.13765

D90 0.00652 0.00000 -0.00004 0.00000 -0.00004 0.00648

D91 -0.02442 0.00000 0.00003 -0.00001 0.00002 -0.02440

D92 3.07761 0.00000 0.00008 -0.00002 0.00007 3.07768

D93 3.12781 0.00000 -0.00003 -0.00001 -0.00003 3.12777

D94 -0.05335 0.00000 0.00003 -0.00001 0.00002 -0.05333

D95 0.00795 0.00000 0.00001 -0.00001 0.00001 0.00796

D96 -3.13615 0.00000 -0.00002 0.00001 -0.00001 -3.13616

D97 3.13758 0.00000 0.00008 -0.00001 0.00006 3.13765

D98 -0.00652 0.00000 0.00004 0.00000 0.00004 -0.00648

D99 0.04096 0.00000 -0.00005 0.00002 -0.00003 0.04093

D100 -2.89025 0.00000 -0.00029 0.00003 -0.00026 -2.89051

D101 -3.05839 0.00000 -0.00010 0.00002 -0.00008 -3.05848

D102 0.29359 0.00000 -0.00035 0.00003 -0.00031 0.29327

D103 -3.07407 0.00000 0.00006 0.00001 0.00007 -3.07400

D104 0.01970 0.00000 0.00013 0.00001 0.00014 0.01983

D105 3.05839 0.00000 0.00010 -0.00002 0.00008 3.05848

D106 -0.04096 0.00000 0.00005 -0.00002 0.00003 -0.04093

D107 -0.29359 0.00000 0.00035 -0.00003 0.00031 -0.29327

D108 2.89025 0.00000 0.00029 -0.00003 0.00026 2.89051

D109 -3.01648 0.00000 0.00016 0.00002 0.00019 -3.01629

D110 -1.69058 0.00000 0.00014 -0.00001 0.00013 -1.69044

D111 -0.36468 0.00000 0.00012 -0.00004 0.00008 -0.36460

D112 0.36468 0.00000 -0.00012 0.00004 -0.00008 0.36460

D113 1.69058 0.00000 -0.00014 0.00001 -0.00013 1.69044

D114 3.01648 0.00000 -0.00016 -0.00002 -0.00019 3.01629

D115 -0.10993 0.00000 0.00040 -0.00003 0.00038 -0.10955

D116 3.00336 0.00000 0.00048 0.00002 0.00049 3.00386

D117 3.09786 0.00000 -0.00004 -0.00001 -0.00004 3.09782

D118 -0.01884 0.00000 -0.00010 -0.00004 -0.00015 -0.01899

D119 -0.12886 0.00000 -0.00061 0.00000 -0.00061 -0.12947

D120 3.03763 -0.00001 -0.00068 -0.00004 -0.00071 3.03691

D121 0.01884 0.00000 0.00010 0.00004 0.00015 0.01899

D122 -3.09786 0.00000 0.00004 0.00001 0.00004 -3.09782

D123 -3.03763 0.00001 0.00068 0.00004 0.00071 -3.03691

D124 0.12886 0.00000 0.00061 0.00000 0.00061 0.12947

D125 1.61933 0.00000 0.00033 0.00000 0.00032 1.61965

D126 2.94539 0.00000 0.00035 -0.00003 0.00032 2.94571

D127 0.29327 0.00000 0.00030 0.00002 0.00033 0.29360

D128 -1.61933 0.00000 -0.00033 0.00000 -0.00032 -1.61965

D129 -0.29327 0.00000 -0.00030 -0.00002 -0.00033 -0.29360

D130 -2.94539 0.00000 -0.00035 0.00003 -0.00032 -2.94571

D131 -3.10679 0.00000 0.00000 -0.00001 -0.00001 -3.10680

D132 0.01730 0.00000 0.00018 0.00007 0.00025 0.01754

D133 0.01119 0.00000 0.00006 0.00003 0.00009 0.01128

D134 3.13528 0.00000 0.00024 0.00011 0.00035 3.13563

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.12658 0.00000 0.00015 0.00007 0.00022 3.12681

D137 -3.12658 0.00000 -0.00015 -0.00007 -0.00022 -3.12681

D138 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D139 -3.12686 0.00000 -0.00026 -0.00007 -0.00032 -3.12718

D140 0.01314 0.00000 -0.00018 -0.00005 -0.00023 0.01292

D141 -0.00490 0.00000 -0.00006 0.00003 -0.00003 -0.00493

D142 3.13510 0.00000 0.00002 0.00004 0.00006 3.13516

D143 -0.01119 0.00000 -0.00006 -0.00003 -0.00009 -0.01128

D144 3.10679 0.00000 0.00000 0.00001 0.00001 3.10680

D145 -3.13528 0.00000 -0.00024 -0.00011 -0.00035 -3.13563

D146 -0.01730 0.00000 -0.00018 -0.00007 -0.00025 -0.01754

D147 0.00490 0.00000 0.00006 -0.00003 0.00003 0.00493

D148 -3.13510 0.00000 -0.00002 -0.00004 -0.00006 -3.13516

D149 3.12686 0.00000 0.00026 0.00007 0.00032 3.12718

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D151 0.10993 0.00000 -0.00040 0.00003 -0.00038 0.10955

D152 -3.00336 0.00000 -0.00048 -0.00002 -0.00049 -3.00386

D153 0.00781 0.00000 0.00001 -0.00001 0.00001 0.00782

D154 -3.13435 0.00000 0.00002 0.00000 0.00002 -3.13433

D155 -3.13624 0.00000 -0.00002 0.00001 -0.00001 -3.13626

D156 0.00478 0.00000 -0.00002 0.00001 -0.00001 0.00478

D157 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D158 3.14104 0.00000 0.00000 0.00000 0.00001 3.14105

D159 -3.14104 0.00000 0.00000 0.00000 -0.00001 -3.14105

D160 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D161 -3.14122 0.00000 0.00000 -0.00001 0.00000 -3.14122

D162 0.00012 0.00000 -0.00001 0.00000 -0.00001 0.00011

D163 -0.00019 0.00000 0.00001 0.00000 0.00000 -0.00018

D164 3.14115 0.00000 0.00000 0.00000 0.00000 3.14115

D165 -0.00781 0.00000 -0.00001 0.00001 -0.00001 -0.00782

D166 3.13624 0.00000 0.00002 -0.00001 0.00001 3.13626

D167 3.13435 0.00000 -0.00002 0.00000 -0.00002 3.13433

D168 -0.00478 0.00000 0.00002 -0.00001 0.00001 -0.00478

D169 0.00019 0.00000 -0.00001 0.00000 0.00000 0.00018

D170 -3.14115 0.00000 0.00000 0.00000 0.00000 -3.14115

D171 3.14122 0.00000 0.00000 0.00001 0.00000 3.14122

D172 -0.00012 0.00000 0.00001 0.00000 0.00001 -0.00011

D173 -0.00484 0.00000 -0.00006 0.00003 -0.00003 -0.00487

D174 3.13972 0.00000 -0.00013 0.00004 -0.00009 3.13963

D175 3.13518 0.00000 0.00002 0.00004 0.00006 3.13525

D176 -0.00344 0.00000 -0.00005 0.00006 0.00000 -0.00344

D177 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D178 -3.13871 0.00000 -0.00007 0.00001 -0.00006 -3.13877

D179 3.13871 0.00000 0.00007 -0.00001 0.00006 3.13877

D180 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D181 3.13890 0.00000 0.00006 -0.00001 0.00004 3.13894

D182 -0.00308 0.00000 0.00009 -0.00003 0.00006 -0.00303

D183 0.00024 0.00000 -0.00002 0.00000 -0.00002 0.00022

D184 3.14144 0.00000 0.00001 -0.00001 0.00000 3.14144

D185 0.00484 0.00000 0.00006 -0.00003 0.00003 0.00487

D186 -3.13518 0.00000 -0.00002 -0.00004 -0.00006 -3.13525

D187 -3.13972 0.00000 0.00013 -0.00004 0.00009 -3.13963

D188 0.00344 0.00000 0.00005 -0.00006 0.00000 0.00344

D189 -0.00024 0.00000 0.00002 0.00000 0.00002 -0.00022

D190 -3.14144 0.00000 -0.00001 0.00001 0.00000 -3.14144

D191 -3.13890 0.00000 -0.00006 0.00001 -0.00004 -3.13894

D192 0.00308 0.00000 -0.00009 0.00003 -0.00006 0.00303

D193 -0.00781 0.00000 -0.00001 0.00001 -0.00001 -0.00782

D194 3.13435 0.00000 -0.00002 0.00000 -0.00002 3.13433

D195 3.13624 0.00000 0.00002 -0.00001 0.00001 3.13626

D196 -0.00478 0.00000 0.00002 -0.00001 0.00001 -0.00478

D197 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D198 -3.14104 0.00000 0.00000 0.00000 -0.00001 -3.14105

D199 3.14104 0.00000 0.00000 0.00000 0.00001 3.14105

D200 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D201 3.14122 0.00000 0.00000 0.00001 0.00000 3.14122

D202 -0.00012 0.00000 0.00001 0.00000 0.00001 -0.00011

D203 0.00019 0.00000 -0.00001 0.00000 0.00000 0.00018

D204 -3.14115 0.00000 0.00000 0.00000 0.00000 -3.14115

D205 0.00781 0.00000 0.00001 -0.00001 0.00001 0.00782

D206 -3.13624 0.00000 -0.00002 0.00001 -0.00001 -3.13626

D207 -3.13435 0.00000 0.00002 0.00000 0.00002 -3.13433

D208 0.00478 0.00000 -0.00002 0.00001 -0.00001 0.00478

D209 -0.00019 0.00000 0.00001 0.00000 0.00000 -0.00018

D210 3.14115 0.00000 0.00000 0.00000 0.00000 3.14115

D211 -3.14122 0.00000 0.00000 -0.00001 0.00000 -3.14122

D212 0.00012 0.00000 -0.00001 0.00000 -0.00001 0.00011

D213 -0.00484 0.00000 -0.00006 0.00003 -0.00003 -0.00487

D214 3.13972 0.00000 -0.00013 0.00004 -0.00009 3.13963

D215 3.13518 0.00000 0.00002 0.00004 0.00006 3.13525

D216 -0.00344 0.00000 -0.00005 0.00006 0.00000 -0.00344

D217 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D218 -3.13871 0.00000 -0.00007 0.00001 -0.00006 -3.13877

D219 3.13871 0.00000 0.00007 -0.00001 0.00006 3.13877

D220 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D221 3.13890 0.00000 0.00006 -0.00001 0.00004 3.13894

D222 -0.00308 0.00000 0.00009 -0.00003 0.00006 -0.00303

D223 0.00024 0.00000 -0.00002 0.00000 -0.00002 0.00022

D224 3.14144 0.00000 0.00001 -0.00001 0.00000 3.14144

D225 0.00484 0.00000 0.00006 -0.00003 0.00003 0.00487

D226 -3.13518 0.00000 -0.00002 -0.00004 -0.00006 -3.13525

D227 -3.13972 0.00000 0.00013 -0.00004 0.00009 -3.13963

D228 0.00344 0.00000 0.00005 -0.00006 0.00000 0.00344

D229 -0.00024 0.00000 0.00002 0.00000 0.00002 -0.00022

D230 -3.14144 0.00000 -0.00001 0.00001 0.00000 -3.14144

D231 -3.13890 0.00000 -0.00006 0.00001 -0.00004 -3.13894

D232 0.00308 0.00000 -0.00009 0.00003 -0.00006 0.00303

D233 0.00024 0.00000 -0.00002 0.00000 -0.00002 0.00023

D234 -3.14145 0.00000 -0.00004 0.00002 -0.00002 -3.14147

D235 3.14144 0.00000 0.00001 -0.00001 0.00000 3.14143

D236 -0.00025 0.00000 -0.00001 0.00000 -0.00001 -0.00026

D237 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D238 3.14150 0.00000 -0.00002 0.00001 0.00000 3.14149

D239 -3.14150 0.00000 0.00002 -0.00001 0.00000 -3.14149

D240 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D241 -0.00024 0.00000 0.00002 0.00000 0.00002 -0.00023

D242 -3.14144 0.00000 -0.00001 0.00001 0.00000 -3.14143

D243 3.14145 0.00000 0.00004 -0.00002 0.00002 3.14147

D244 0.00025 0.00000 0.00001 0.00000 0.00001 0.00026

D245 -0.00019 0.00000 0.00001 0.00000 0.00000 -0.00019

D246 -3.14117 0.00000 0.00001 0.00000 0.00000 -3.14116

D247 3.14115 0.00000 0.00000 0.00000 0.00000 3.14115

D248 0.00017 0.00000 0.00000 0.00000 0.00000 0.00017

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D250 -3.14098 0.00000 0.00000 0.00000 0.00000 -3.14098

D251 3.14098 0.00000 0.00000 0.00000 0.00000 3.14098

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D253 0.00019 0.00000 -0.00001 0.00000 0.00000 0.00019

D254 -3.14115 0.00000 0.00000 0.00000 0.00000 -3.14115

D255 3.14117 0.00000 -0.00001 0.00000 0.00000 3.14116

D256 -0.00017 0.00000 0.00000 0.00000 0.00000 -0.00017

D257 0.00024 0.00000 -0.00002 0.00000 -0.00002 0.00023

D258 -3.14145 0.00000 -0.00004 0.00002 -0.00002 -3.14147

D259 3.14144 0.00000 0.00001 -0.00001 0.00000 3.14143

D260 -0.00025 0.00000 -0.00001 0.00000 -0.00001 -0.00026

D261 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D262 3.14150 0.00000 -0.00002 0.00001 0.00000 3.14149

D263 -3.14150 0.00000 0.00002 -0.00001 0.00000 -3.14149

D264 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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D266 -3.14144 0.00000 -0.00001 0.00001 0.00000 -3.14143

D267 3.14145 0.00000 0.00004 -0.00002 0.00002 3.14147

D268 0.00025 0.00000 0.00001 0.00000 0.00001 0.00026

D269 0.00019 0.00000 -0.00001 0.00000 0.00000 0.00019

D270 3.14117 0.00000 -0.00001 0.00000 0.00000 3.14116

D271 -3.14115 0.00000 0.00000 0.00000 0.00000 -3.14115

D272 -0.00017 0.00000 0.00000 0.00000 0.00000 -0.00017

D273 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D274 3.14098 0.00000 0.00000 0.00000 0.00000 3.14098

D275 -3.14098 0.00000 0.00000 0.00000 0.00000 -3.14098

D276 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D277 -0.00019 0.00000 0.00001 0.00000 0.00000 -0.00019

D278 3.14115 0.00000 0.00000 0.00000 0.00000 3.14115

D279 -3.14117 0.00000 0.00001 0.00000 0.00000 -3.14116

D280 0.00017 0.00000 0.00000 0.00000 0.00000 0.00017

Item Value Threshold Converged?

Maximum Force 0.000005 0.000450 YES

RMS Force 0.000001 0.000300 YES

Maximum Displacement 0.009055 0.001800 NO

RMS Displacement 0.001613 0.001200 NO

Predicted change in Energy=-2.498760D-08

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sun Jun 30 21:37:30 2019, MaxMem= 1342177280 cpu: 12.0

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

Stoichiometry C48H24N8Zn(3)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C48H24N4)]

Deg. of freedom 61

Full point group C2V NOp 4

RotChk: IX=0 Diff= 7.26D-15

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 1.121263 2.790136 0.181319

2 7 0 0.000000 2.023921 0.322495

3 6 0 -1.121263 2.790136 0.181319

4 6 0 -0.717705 4.166232 -0.045670

5 6 0 0.717705 4.166232 -0.045670

6 7 0 -2.412721 2.383597 0.208594

7 6 0 -2.794679 1.127507 0.264121

8 7 0 -2.010517 0.000000 0.326394

9 6 0 -2.794679 -1.127507 0.264121

10 6 0 -4.208479 -0.712278 0.209240

11 6 0 -4.208479 0.712278 0.209240

12 7 0 2.412721 2.383597 0.208594

13 6 0 4.208479 0.712278 0.209240

14 6 0 4.208479 -0.712278 0.209240

15 6 0 2.794679 -1.127507 0.264121

16 7 0 2.010517 0.000000 0.326394

17 6 0 2.794679 1.127507 0.264121

18 7 0 2.412721 -2.383597 0.208594

19 7 0 0.000000 -2.023921 0.322495

20 6 0 1.121263 -2.790136 0.181319

21 6 0 0.717705 -4.166232 -0.045670

22 6 0 -0.717705 -4.166232 -0.045670

23 6 0 -1.121263 -2.790136 0.181319

24 7 0 -2.412721 -2.383597 0.208594

25 30 0 0.000000 0.000000 0.844972

26 6 0 5.373840 1.426277 0.153267

27 6 0 6.609437 0.718883 0.103873

28 6 0 6.609437 -0.718883 0.103873

29 6 0 5.373840 -1.426277 0.153267

30 6 0 -1.428324 -5.325913 -0.254618

31 6 0 -0.721456 -6.535793 -0.466397

32 6 0 0.721456 -6.535793 -0.466397

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34 6 0 -5.373840 1.426277 0.153267

35 6 0 -6.609437 0.718883 0.103873

36 6 0 -6.609437 -0.718883 0.103873

37 6 0 -5.373840 -1.426277 0.153267

38 6 0 1.428324 5.325913 -0.254618

39 6 0 0.721456 6.535793 -0.466397

40 6 0 -0.721456 6.535793 -0.466397

41 6 0 -1.428324 5.325913 -0.254618

42 6 0 1.402325 -7.762532 -0.684704

43 6 0 0.708020 -8.930102 -0.892216

44 6 0 -0.708020 -8.930102 -0.892216

45 6 0 -1.402325 -7.762532 -0.684704

46 6 0 7.849096 -1.401345 0.053640

47 6 0 9.036663 -0.705865 0.005736

48 6 0 9.036663 0.705865 0.005736

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51 6 0 -0.708020 8.930102 -0.892216

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56 6 0 -9.036663 0.705865 0.005736

57 6 0 -7.849096 1.401345 0.053640

58 1 0 5.373896 2.511159 0.148236

59 1 0 5.373896 -2.511159 0.148236

60 1 0 -2.513359 -5.328428 -0.261130

61 1 0 2.513359 -5.328428 -0.261130

62 1 0 -5.373896 2.511159 0.148236

63 1 0 -5.373896 -2.511159 0.148236

64 1 0 2.513359 5.328428 -0.261130

65 1 0 -2.513359 5.328428 -0.261130

66 1 0 2.487805 -7.760976 -0.684277

67 1 0 1.243521 -9.858901 -1.057387

68 1 0 -1.243521 -9.858901 -1.057387

69 1 0 -2.487805 -7.760976 -0.684277

70 1 0 7.847357 -2.486615 0.053291

71 1 0 9.978475 -1.242469 -0.032837

72 1 0 9.978475 1.242469 -0.032837

73 1 0 7.847357 2.486615 0.053291

74 1 0 -2.487805 7.760976 -0.684277

75 1 0 -1.243521 9.858901 -1.057387

76 1 0 1.243521 9.858901 -1.057387

77 1 0 2.487805 7.760976 -0.684277

78 1 0 -7.847357 -2.486615 0.053291

79 1 0 -9.978475 -1.242469 -0.032837

80 1 0 -9.978475 1.242469 -0.032837

81 1 0 -7.847357 2.486615 0.053291

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

Rotational constants (GHZ): 0.0387342 0.0379494 0.0193803

Leave Link 202 at Sun Jun 30 21:37:30 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 307 symmetry adapted cartesian basis functions of A1 symmetry.

There are 278 symmetry adapted cartesian basis functions of A2 symmetry.

There are 289 symmetry adapted cartesian basis functions of B1 symmetry.

There are 289 symmetry adapted cartesian basis functions of B2 symmetry.

There are 289 symmetry adapted basis functions of A1 symmetry.

There are 265 symmetry adapted basis functions of A2 symmetry.

There are 275 symmetry adapted basis functions of B1 symmetry.

There are 275 symmetry adapted basis functions of B2 symmetry.

1104 basis functions, 1951 primitive gaussians, 1163 cartesian basis functions

191 alpha electrons 189 beta electrons

nuclear repulsion energy 6889.7501375888 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= 81 NActive= 81 NUniq= 22 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= -0.2361210428 Hartrees.

Nuclear repulsion after empirical dispersion term = 6889.5140165460 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= 81.

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 = 81

GePol: Total number of spheres = 81

GePol: Number of exposed spheres = 81 (100.00%)

GePol: Number of points = 6432

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.57D-11

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 396

GePol: Fraction of low-weight points (<1% of avg) = 6.16%

GePol: Cavity surface area = 670.763 Ang\*\*2

GePol: Cavity volume = 694.580 Ang\*\*3

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

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PCM non-electrostatic energy = -0.0170117479 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 6889.4970047981 Hartrees.

Leave Link 301 at Sun Jun 30 21:37:30 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.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36719 LenP2D= 95220.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1104 RedAO= T EigKep= 2.89D-05 NBF= 289 265 275 275

NBsUse= 1104 1.00D-06 EigRej= -1.00D+00 NBFU= 289 265 275 275

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= 1060 1060 1060 1060 1060 MxSgAt= 81 MxSgA2= 81.

Leave Link 302 at Sun Jun 30 21:37:59 2019, MaxMem= 1342177280 cpu: 279.6

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

DipDrv: MaxL=1.

Leave Link 303 at Sun Jun 30 21:37:59 2019, MaxMem= 1342177280 cpu: 6.3

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

Initial guess from the checkpoint file: "ZnNPC3.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess orbital symmetries:

Alpha Orbitals:

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The electronic state of the initial guess is 3-B2.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

Leave Link 401 at Sun Jun 30 21:38:19 2019, MaxMem= 1342177280 cpu: 208.1

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

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4103221 IEndB= 4103221 NGot= 1342177280 MDV= 1339444432

LenX= 1339444432 LenY= 1338090700

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= 420000000 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= 124111872.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.44D-15 for 6397.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.78D-15 for 6417 1184.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.33D-15 for 6397.

Iteration 1 A^-1\*A deviation from orthogonality is 3.42D-09 for 4307 4218.

Iteration 2 A\*A^-1 deviation from unit magnitude is 4.88D-15 for 368.

Iteration 2 A\*A^-1 deviation from orthogonality is 4.56D-15 for 5182 185.

Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 152.

Iteration 2 A^-1\*A deviation from orthogonality is 3.99D-16 for 5452 4533.

E= -2348.13073462693

DIIS: error= 6.81D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2348.13073462693 IErMin= 1 ErrMin= 6.81D-05

ErrMax= 6.81D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.20D-06 BMatP= 9.20D-06

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

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.379 Goal= None Shift= 0.000

Gap= 0.459 Goal= None Shift= 0.000

RMSDP=1.84D-06 MaxDP=7.26D-05 OVMax= 4.29D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.84D-06 CP: 1.00D+00

E= -2348.13073933613 Delta-E= -0.000004709203 Rises=F Damp=F

DIIS: error= 9.49D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2348.13073933613 IErMin= 2 ErrMin= 9.49D-06

ErrMax= 9.49D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.36D-08 BMatP= 9.20D-06

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

Coeff-Com: -0.751D-01 0.108D+01

Coeff: -0.751D-01 0.108D+01

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=2.70D-07 MaxDP=1.17D-05 DE=-4.71D-06 OVMax= 6.72D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.05D-07 CP: 1.00D+00 1.10D+00

E= -2348.13073940598 Delta-E= -0.000000069844 Rises=F Damp=F

DIIS: error= 1.30D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2348.13073940598 IErMin= 3 ErrMin= 1.30D-06

ErrMax= 1.30D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.77D-09 BMatP= 9.36D-08

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

Coeff-Com: -0.157D-01 0.176D+00 0.840D+00

Coeff: -0.157D-01 0.176D+00 0.840D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=7.13D-08 MaxDP=3.01D-06 DE=-6.98D-08 OVMax= 1.15D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 6.94D-08 CP: 1.00D+00 1.10D+00 9.86D-01

E= -2348.13073940624 Delta-E= -0.000000000266 Rises=F Damp=F

DIIS: error= 1.01D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2348.13073940624 IErMin= 4 ErrMin= 1.01D-06

ErrMax= 1.01D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.38D-09 BMatP= 5.77D-09

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

Coeff-Com: -0.316D-02 0.160D-01 0.464D+00 0.523D+00

Coeff: -0.316D-02 0.160D-01 0.464D+00 0.523D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=4.48D-08 MaxDP=2.28D-06 DE=-2.66D-10 OVMax= 1.01D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.53D-08 CP: 1.00D+00 1.10D+00 1.05D+00 5.13D-01

E= -2348.13073940721 Delta-E= -0.000000000970 Rises=F Damp=F

DIIS: error= 4.79D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2348.13073940721 IErMin= 5 ErrMin= 4.79D-07

ErrMax= 4.79D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.71D-10 BMatP= 4.38D-09

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

Coeff-Com: 0.112D-02-0.256D-01 0.112D+00 0.311D+00 0.601D+00

Coeff: 0.112D-02-0.256D-01 0.112D+00 0.311D+00 0.601D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=1.35D-08 MaxDP=1.05D-06 DE=-9.70D-10 OVMax= 3.42D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 6.31D-09 CP: 1.00D+00 1.10D+00 1.05D+00 6.18D-01 6.38D-01

E= -2348.13073940738 Delta-E= -0.000000000166 Rises=F Damp=F

DIIS: error= 1.74D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2348.13073940738 IErMin= 6 ErrMin= 1.74D-07

ErrMax= 1.74D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.31D-11 BMatP= 6.71D-10

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

Coeff-Com: 0.792D-03-0.159D-01 0.484D-01 0.166D+00 0.363D+00 0.438D+00

Coeff: 0.792D-03-0.159D-01 0.484D-01 0.166D+00 0.363D+00 0.438D+00

Gap= 0.042 Goal= None Shift= 0.000

Gap= 0.084 Goal= None Shift= 0.000

RMSDP=3.70D-09 MaxDP=3.09D-07 DE=-1.66D-10 OVMax= 1.35D-06

Error on total polarization charges = 0.08827

SCF Done: E(UB3LYP) = -2348.13073941 A.U. after 6 cycles

NFock= 6 Conv=0.37D-08 -V/T= 1.9830

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0219 S= 1.0073

<L.S>= 0.000000000000E+00

KE= 2.388748248272D+03 PE=-1.932241869603D+04 EE= 7.696042703553D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -10.68

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0219, after 2.0003

Leave Link 502 at Sun Jun 30 21:44:05 2019, MaxMem= 1342177280 cpu: 3809.6

(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.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36719 LenP2D= 95220.

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 = 192

Leave Link 701 at Sun Jun 30 21:44:39 2019, MaxMem= 1342177280 cpu: 363.6

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sun Jun 30 21:44:39 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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 Sun Jun 30 21:45:18 2019, MaxMem= 1342177280 cpu: 442.8

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-8.08242362D-13 1.09068310D-12 8.85704743D-01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 6 -0.000001480 0.000003673 0.000001021

2 7 0.000000000 -0.000003920 -0.000002549

3 6 0.000001480 0.000003673 0.000001021

4 6 0.000000935 -0.000002365 -0.000001548

5 6 -0.000000935 -0.000002365 -0.000001548

6 7 -0.000002257 0.000003361 -0.000000118

7 6 -0.000004512 -0.000001862 -0.000000052

8 7 0.000005474 0.000000000 -0.000000029

9 6 -0.000004512 0.000001862 -0.000000052

10 6 0.000002372 0.000000917 -0.000000344

11 6 0.000002372 -0.000000917 -0.000000344

12 7 0.000002257 0.000003361 -0.000000118

13 6 -0.000002372 -0.000000917 -0.000000344

14 6 -0.000002372 0.000000917 -0.000000344

15 6 0.000004512 0.000001862 -0.000000052

16 7 -0.000005474 0.000000000 -0.000000029

17 6 0.000004512 -0.000001862 -0.000000052

18 7 0.000002257 -0.000003361 -0.000000118

19 7 0.000000000 0.000003920 -0.000002549

20 6 -0.000001480 -0.000003673 0.000001021

21 6 -0.000000935 0.000002365 -0.000001548

22 6 0.000000935 0.000002365 -0.000001548

23 6 0.000001480 -0.000003673 0.000001021

24 7 -0.000002257 -0.000003361 -0.000000118

25 30 0.000000000 0.000000000 0.000007297

26 6 0.000001077 0.000002068 -0.000000437

27 6 -0.000000881 -0.000001672 0.000000167

28 6 -0.000000881 0.000001672 0.000000167

29 6 0.000001077 -0.000002068 -0.000000437

30 6 -0.000002292 0.000000353 0.000000278

31 6 0.000002502 0.000000040 0.000000236

32 6 -0.000002502 0.000000040 0.000000236

33 6 0.000002292 0.000000353 0.000000278

34 6 -0.000001077 0.000002068 -0.000000437

35 6 0.000000881 -0.000001672 0.000000167

36 6 0.000000881 0.000001672 0.000000167

37 6 -0.000001077 -0.000002068 -0.000000437

38 6 0.000002292 -0.000000353 0.000000278

39 6 -0.000002502 -0.000000040 0.000000236

40 6 0.000002502 -0.000000040 0.000000236

41 6 -0.000002292 -0.000000353 0.000000278

42 6 0.000001460 0.000000497 0.000000213

43 6 -0.000001578 -0.000000266 -0.000000016

44 6 0.000001578 -0.000000266 -0.000000016

45 6 -0.000001460 0.000000497 0.000000213

46 6 0.000000167 -0.000000781 0.000000215

47 6 -0.000000013 0.000000585 -0.000000025

48 6 -0.000000013 -0.000000585 -0.000000025

49 6 0.000000167 0.000000781 0.000000215

50 6 -0.000001460 -0.000000497 0.000000213

51 6 0.000001578 0.000000266 -0.000000016

52 6 -0.000001578 0.000000266 -0.000000016

53 6 0.000001460 -0.000000497 0.000000213

54 6 -0.000000167 -0.000000781 0.000000215

55 6 0.000000013 0.000000585 -0.000000025

56 6 0.000000013 -0.000000585 -0.000000025

57 6 -0.000000167 0.000000781 0.000000215

58 1 0.000000192 -0.000000257 -0.000000009

59 1 0.000000192 0.000000257 -0.000000009

60 1 0.000000245 -0.000000706 0.000000047

61 1 -0.000000245 -0.000000706 0.000000047

62 1 -0.000000192 -0.000000257 -0.000000009

63 1 -0.000000192 0.000000257 -0.000000009

64 1 -0.000000245 0.000000706 0.000000047

65 1 0.000000245 0.000000706 0.000000047

66 1 -0.000000106 0.000000029 0.000000082

67 1 0.000000338 0.000000224 -0.000000189

68 1 -0.000000338 0.000000224 -0.000000189

69 1 0.000000106 0.000000029 0.000000082

70 1 -0.000000158 0.000000007 -0.000000048

71 1 -0.000000154 -0.000000228 -0.000000008

72 1 -0.000000154 0.000000228 -0.000000008

73 1 -0.000000158 -0.000000007 -0.000000048

74 1 0.000000106 -0.000000029 0.000000082

75 1 -0.000000338 -0.000000224 -0.000000189

76 1 0.000000338 -0.000000224 -0.000000189

77 1 -0.000000106 -0.000000029 0.000000082

78 1 0.000000158 0.000000007 -0.000000048

79 1 0.000000154 -0.000000228 -0.000000008

80 1 0.000000154 0.000000228 -0.000000008

81 1 0.000000158 -0.000000007 -0.000000048

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

Cartesian Forces: Max 0.000007297 RMS 0.000001516

Leave Link 716 at Sun Jun 30 21:45:18 2019, MaxMem= 1342177280 cpu: 4.3

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

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000002613 RMS 0.000000698

Search for a local minimum.

Step number 11 out of a maximum of 486

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .69821D-06 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 1 2 3 4 5

6 7 8 9 10

11

DE= -2.39D-08 DEPred=-2.50D-08 R= 9.58D-01

Trust test= 9.58D-01 RLast= 3.03D-03 DXMaxT set to 3.00D-01

ITU= 0 0 0 1 1 1 1 1 1 1 0

Eigenvalues --- 0.00297 0.00600 0.01183 0.01432 0.01486

Eigenvalues --- 0.01500 0.01572 0.01588 0.01628 0.01656

Eigenvalues --- 0.01670 0.01694 0.01698 0.01706 0.01713

Eigenvalues --- 0.01714 0.01725 0.01730 0.01730 0.01736

Eigenvalues --- 0.01738 0.01747 0.01754 0.01758 0.01791

Eigenvalues --- 0.01827 0.01828 0.01830 0.01851 0.01854

Eigenvalues --- 0.01870 0.01871 0.01927 0.01936 0.01968

Eigenvalues --- 0.01968 0.01972 0.01978 0.01979 0.01992

Eigenvalues --- 0.01992 0.01993 0.01993 0.02025 0.02080

Eigenvalues --- 0.02086 0.02086 0.02089 0.02093 0.02096

Eigenvalues --- 0.02096 0.02098 0.02103 0.02103 0.02104

Eigenvalues --- 0.02105 0.02106 0.02124 0.02124 0.02137

Eigenvalues --- 0.02144 0.02144 0.02147 0.02148 0.02170

Eigenvalues --- 0.02173 0.02208 0.02214 0.02215 0.02224

Eigenvalues --- 0.02225 0.02281 0.02286 0.02346 0.02444

Eigenvalues --- 0.02609 0.02967 0.05508 0.05551 0.07254

Eigenvalues --- 0.14648 0.15991 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 0.16009 0.16054

Eigenvalues --- 0.16160 0.16246 0.17091 0.22000 0.22000

Eigenvalues --- 0.22000 0.22000 0.22499 0.22503 0.22504

Eigenvalues --- 0.22543 0.23231 0.23234 0.23234 0.23613

Eigenvalues --- 0.23939 0.23939 0.23939 0.23952 0.24068

Eigenvalues --- 0.24280 0.24297 0.24550 0.24553 0.24557

Eigenvalues --- 0.24557 0.24570 0.24767 0.24892 0.24897

Eigenvalues --- 0.24962 0.24982 0.24984 0.24986 0.24989

Eigenvalues --- 0.24996 0.24996 0.24997 0.24997 0.26126

Eigenvalues --- 0.32865 0.32946 0.33670 0.33746 0.33834

Eigenvalues --- 0.33862 0.35041 0.35069 0.35181 0.35181

Eigenvalues --- 0.35181 0.35187 0.35202 0.35202 0.35202

Eigenvalues --- 0.35211 0.35219 0.35231 0.35231 0.35231

Eigenvalues --- 0.35245 0.35249 0.35249 0.35249 0.35270

Eigenvalues --- 0.35270 0.35270 0.35275 0.35279 0.35279

Eigenvalues --- 0.35279 0.35414 0.35421 0.35498 0.36350

Eigenvalues --- 0.36550 0.37458 0.37563 0.37969 0.38372

Eigenvalues --- 0.39275 0.39276 0.39612 0.39612 0.40188

Eigenvalues --- 0.40188 0.40257 0.40257 0.40906 0.41001

Eigenvalues --- 0.41019 0.41152 0.41603 0.41785 0.41874

Eigenvalues --- 0.42164 0.42215 0.42392 0.42806 0.42901

Eigenvalues --- 0.42929 0.42970 0.44720 0.45679 0.47124

Eigenvalues --- 0.47124 0.47263 0.47384 0.47386 0.47579

Eigenvalues --- 0.47580 0.48121 0.48218 0.48305 0.48372

Eigenvalues --- 0.48454 0.48465 0.48680 0.48707 0.48729

Eigenvalues --- 0.48768 0.49092 0.49422 0.49898 0.50350

Eigenvalues --- 0.51029 0.51233 0.52478 0.58084 0.59236

Eigenvalues --- 0.59872 0.60917

En-DIIS/RFO-DIIS IScMMF= 0 using points: 11 10 9 8 7

RFO step: Lambda= 0.00000000D+00.

NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 2.42D-06 SmlDif= 1.00D-05

RMS Error= 0.1781951812D-05 NUsed= 5 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.13769 -0.06432 -0.11819 0.05196 -0.00713

Iteration 1 RMS(Cart)= 0.00009886 RMS(Int)= 0.00000000

Iteration 2 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000000

ITry= 1 IFail=0 DXMaxC= 5.95D-04 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 3.57D-08 for atom 73.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.58018 0.00000 0.00000 0.00000 0.00000 2.58019

R2 2.74370 0.00000 0.00000 -0.00001 -0.00001 2.74369

R3 2.55908 0.00000 0.00000 0.00000 0.00000 2.55909

R4 2.58018 0.00000 0.00000 0.00000 0.00000 2.58019

R5 3.95004 0.00000 0.00001 0.00001 0.00001 3.95006

R6 2.74370 0.00000 0.00000 -0.00001 -0.00001 2.74369

R7 2.55908 0.00000 0.00000 0.00000 0.00000 2.55909

R8 2.71253 0.00000 0.00000 0.00000 0.00000 2.71253

R9 2.60035 0.00000 0.00000 0.00000 0.00000 2.60035

R10 2.60035 0.00000 0.00000 0.00000 0.00000 2.60035

R11 2.48320 0.00000 0.00000 0.00000 0.00000 2.48320

R12 2.59799 0.00000 0.00000 0.00001 0.00001 2.59799

R13 2.78647 0.00000 0.00000 0.00000 -0.00001 2.78646

R14 2.59799 0.00000 0.00000 0.00001 0.00001 2.59799

R15 3.92368 0.00000 0.00000 0.00001 0.00001 3.92368

R16 2.78647 0.00000 0.00000 0.00000 -0.00001 2.78646

R17 2.48320 0.00000 0.00000 0.00000 0.00000 2.48320

R18 2.69202 0.00000 0.00000 0.00000 0.00000 2.69202

R19 2.58485 0.00000 0.00000 0.00000 0.00000 2.58485

R20 2.58485 0.00000 0.00000 0.00000 0.00000 2.58485

R21 2.48320 0.00000 0.00000 0.00000 0.00000 2.48320

R22 2.69202 0.00000 0.00000 0.00000 0.00000 2.69202

R23 2.78647 0.00000 0.00000 0.00000 -0.00001 2.78646

R24 2.58485 0.00000 0.00000 0.00000 0.00000 2.58485

R25 2.78647 0.00000 0.00000 0.00000 -0.00001 2.78646

R26 2.58485 0.00000 0.00000 0.00000 0.00000 2.58485

R27 2.59799 0.00000 0.00000 0.00001 0.00001 2.59799

R28 2.48320 0.00000 0.00000 0.00000 0.00000 2.48320

R29 2.59799 0.00000 0.00000 0.00001 0.00001 2.59799

R30 3.92368 0.00000 0.00000 0.00001 0.00001 3.92368

R31 2.55908 0.00000 0.00000 0.00000 0.00000 2.55909

R32 2.58018 0.00000 0.00000 0.00000 0.00000 2.58019

R33 2.58018 0.00000 0.00000 0.00000 0.00000 2.58019

R34 3.95004 0.00000 0.00001 0.00001 0.00001 3.95006

R35 2.74370 0.00000 0.00000 -0.00001 -0.00001 2.74369

R36 2.71253 0.00000 0.00000 0.00000 0.00000 2.71253

R37 2.60035 0.00000 0.00000 0.00000 0.00000 2.60035

R38 2.74370 0.00000 0.00000 -0.00001 -0.00001 2.74369

R39 2.60035 0.00000 0.00000 0.00000 0.00000 2.60035

R40 2.55908 0.00000 0.00000 0.00000 0.00000 2.55909

R41 2.69214 0.00000 0.00000 0.00000 0.00000 2.69214

R42 2.05015 0.00000 0.00000 0.00000 0.00000 2.05015

R43 2.71698 0.00000 0.00000 0.00000 0.00000 2.71698

R44 2.67584 0.00000 0.00000 0.00000 0.00000 2.67584

R45 2.69214 0.00000 0.00000 0.00000 0.00000 2.69214

R46 2.67584 0.00000 0.00000 0.00000 0.00000 2.67584

R47 2.05015 0.00000 0.00000 0.00000 0.00000 2.05015

R48 2.67803 0.00000 0.00000 0.00000 0.00000 2.67803

R49 2.05046 0.00000 0.00000 0.00000 0.00000 2.05046

R50 2.72671 0.00000 0.00000 0.00000 0.00000 2.72670

R51 2.68323 0.00000 0.00000 0.00000 0.00000 2.68323

R52 2.67803 0.00000 0.00000 0.00000 0.00000 2.67803

R53 2.68323 0.00000 0.00000 0.00000 0.00000 2.68323

R54 2.05046 0.00000 0.00000 0.00000 0.00000 2.05046

R55 2.69214 0.00000 0.00000 0.00000 0.00000 2.69214

R56 2.05015 0.00000 0.00000 0.00000 0.00000 2.05015

R57 2.71698 0.00000 0.00000 0.00000 0.00000 2.71698

R58 2.67584 0.00000 0.00000 0.00000 0.00000 2.67584

R59 2.69214 0.00000 0.00000 0.00000 0.00000 2.69214

R60 2.67584 0.00000 0.00000 0.00000 0.00000 2.67584

R61 2.05015 0.00000 0.00000 0.00000 0.00000 2.05015

R62 2.67803 0.00000 0.00000 0.00000 0.00000 2.67803

R63 2.05046 0.00000 0.00000 0.00000 0.00000 2.05046

R64 2.72671 0.00000 0.00000 0.00000 0.00000 2.72670

R65 2.68323 0.00000 0.00000 0.00000 0.00000 2.68323

R66 2.67803 0.00000 0.00000 0.00000 0.00000 2.67803

R67 2.68323 0.00000 0.00000 0.00000 0.00000 2.68323

R68 2.05046 0.00000 0.00000 0.00000 0.00000 2.05046

R69 2.59680 0.00000 0.00000 0.00000 0.00000 2.59680

R70 2.05126 0.00000 0.00000 0.00000 0.00000 2.05126

R71 2.67593 0.00000 0.00000 0.00000 0.00000 2.67593

R72 2.04990 0.00000 0.00000 0.00000 0.00000 2.04990

R73 2.59680 0.00000 0.00000 0.00000 0.00000 2.59680

R74 2.04990 0.00000 0.00000 0.00000 0.00000 2.04990

R75 2.05126 0.00000 0.00000 0.00000 0.00000 2.05126

R76 2.60227 0.00000 0.00000 0.00000 0.00000 2.60227

R77 2.05087 0.00000 0.00000 0.00000 0.00000 2.05087

R78 2.66778 0.00000 0.00000 0.00000 0.00000 2.66778

R79 2.04967 0.00000 0.00000 0.00000 0.00000 2.04967

R80 2.60227 0.00000 0.00000 0.00000 0.00000 2.60227

R81 2.04967 0.00000 0.00000 0.00000 0.00000 2.04967

R82 2.05087 0.00000 0.00000 0.00000 0.00000 2.05087

R83 2.59680 0.00000 0.00000 0.00000 0.00000 2.59680

R84 2.05126 0.00000 0.00000 0.00000 0.00000 2.05126

R85 2.67593 0.00000 0.00000 0.00000 0.00000 2.67593

R86 2.04990 0.00000 0.00000 0.00000 0.00000 2.04990

R87 2.59680 0.00000 0.00000 0.00000 0.00000 2.59680

R88 2.04990 0.00000 0.00000 0.00000 0.00000 2.04990

R89 2.05126 0.00000 0.00000 0.00000 0.00000 2.05126

R90 2.60227 0.00000 0.00000 0.00000 0.00000 2.60227

R91 2.05087 0.00000 0.00000 0.00000 0.00000 2.05087

R92 2.66778 0.00000 0.00000 0.00000 0.00000 2.66778

R93 2.04967 0.00000 0.00000 0.00000 0.00000 2.04967

R94 2.60227 0.00000 0.00000 0.00000 0.00000 2.60227

R95 2.04967 0.00000 0.00000 0.00000 0.00000 2.04967

R96 2.05087 0.00000 0.00000 0.00000 0.00000 2.05087

A1 1.89630 0.00000 0.00000 0.00000 0.00000 1.89630

A2 2.23016 0.00000 0.00000 0.00000 0.00000 2.23016

A3 2.15646 0.00000 0.00000 0.00000 -0.00001 2.15645

A4 1.92707 0.00000 0.00000 0.00000 -0.00001 1.92706

A5 2.17634 0.00000 0.00000 0.00000 0.00000 2.17634

A6 2.17634 0.00000 0.00000 0.00000 0.00000 2.17634

A7 1.89630 0.00000 0.00000 0.00000 0.00000 1.89630

A8 2.23016 0.00000 0.00000 0.00000 0.00000 2.23016

A9 2.15646 0.00000 0.00000 0.00000 -0.00001 2.15645

A10 1.85246 0.00000 0.00000 0.00000 0.00000 1.85246

A11 2.31714 0.00000 0.00000 0.00000 0.00000 2.31714

A12 2.11346 0.00000 0.00000 0.00000 0.00000 2.11347

A13 1.85246 0.00000 0.00000 0.00000 0.00000 1.85246

A14 2.31714 0.00000 0.00000 0.00000 0.00000 2.31714

A15 2.11346 0.00000 0.00000 0.00000 0.00000 2.11347

A16 2.17125 0.00000 0.00000 -0.00001 -0.00001 2.17124

A17 2.23963 0.00000 0.00000 0.00000 0.00000 2.23963

A18 2.14874 0.00000 0.00000 0.00000 0.00000 2.14874

A19 1.89402 0.00000 0.00000 0.00000 0.00000 1.89403

A20 1.92327 0.00000 0.00000 0.00000 -0.00001 1.92326

A21 2.16956 0.00000 0.00001 0.00000 0.00001 2.16957

A22 2.16956 0.00000 0.00001 0.00000 0.00001 2.16957

A23 1.89402 0.00000 0.00000 0.00000 0.00000 1.89403

A24 2.23963 0.00000 0.00000 0.00000 0.00000 2.23963

A25 2.14874 0.00000 0.00000 0.00000 0.00000 2.14874

A26 1.85626 0.00000 0.00000 0.00000 0.00000 1.85626

A27 2.30690 0.00000 0.00000 0.00000 0.00000 2.30690

A28 2.11998 0.00000 0.00000 0.00000 0.00000 2.11998

A29 1.85626 0.00000 0.00000 0.00000 0.00000 1.85626

A30 2.30690 0.00000 0.00000 0.00000 0.00000 2.30690

A31 2.11998 0.00000 0.00000 0.00000 0.00000 2.11998

A32 2.17125 0.00000 0.00000 -0.00001 -0.00001 2.17124

A33 1.85626 0.00000 0.00000 0.00000 0.00000 1.85626

A34 2.11998 0.00000 0.00000 0.00000 0.00000 2.11998

A35 2.30690 0.00000 0.00000 0.00000 0.00000 2.30690

A36 1.85626 0.00000 0.00000 0.00000 0.00000 1.85626

A37 2.11998 0.00000 0.00000 0.00000 0.00000 2.11998

A38 2.30690 0.00000 0.00000 0.00000 0.00000 2.30690

A39 1.89402 0.00000 0.00000 0.00000 0.00000 1.89403

A40 2.14874 0.00000 0.00000 0.00000 0.00000 2.14874

A41 2.23963 0.00000 0.00000 0.00000 0.00000 2.23963

A42 1.92327 0.00000 0.00000 0.00000 -0.00001 1.92326

A43 2.16956 0.00000 0.00001 0.00000 0.00001 2.16957

A44 2.16956 0.00000 0.00001 0.00000 0.00001 2.16957

A45 2.14874 0.00000 0.00000 0.00000 0.00000 2.14874

A46 2.23963 0.00000 0.00000 0.00000 0.00000 2.23963

A47 1.89402 0.00000 0.00000 0.00000 0.00000 1.89403

A48 2.17125 0.00000 0.00000 -0.00001 -0.00001 2.17124

A49 1.92707 0.00000 0.00000 0.00000 -0.00001 1.92706

A50 2.17634 0.00000 0.00000 0.00000 0.00000 2.17634

A51 2.17634 0.00000 0.00000 0.00000 0.00000 2.17634

A52 2.23016 0.00000 0.00000 0.00000 0.00000 2.23016

A53 2.15646 0.00000 0.00000 0.00000 -0.00001 2.15645

A54 1.89630 0.00000 0.00000 0.00000 0.00000 1.89630

A55 1.85246 0.00000 0.00000 0.00000 0.00000 1.85246

A56 2.31714 0.00000 0.00000 0.00000 0.00000 2.31714

A57 2.11346 0.00000 0.00000 0.00000 0.00000 2.11347

A58 1.85246 0.00000 0.00000 0.00000 0.00000 1.85246

A59 2.11346 0.00000 0.00000 0.00000 0.00000 2.11347

A60 2.31714 0.00000 0.00000 0.00000 0.00000 2.31714

A61 1.89630 0.00000 0.00000 0.00000 0.00000 1.89630

A62 2.23016 0.00000 0.00000 0.00000 0.00000 2.23016

A63 2.15646 0.00000 0.00000 0.00000 -0.00001 2.15645

A64 2.17125 0.00000 0.00000 -0.00001 -0.00001 2.17124

A65 1.50833 0.00000 0.00000 -0.00001 -0.00001 1.50832

A66 1.50833 0.00000 0.00000 -0.00001 -0.00001 1.50832

A67 2.63632 0.00000 -0.00002 -0.00002 -0.00005 2.63628

A68 2.63673 0.00000 0.00000 -0.00002 -0.00002 2.63671

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A70 1.50833 0.00000 0.00000 -0.00001 -0.00001 1.50832

A71 2.07277 0.00000 0.00000 0.00000 0.00000 2.07276

A72 2.12025 0.00000 0.00000 0.00000 0.00000 2.12025

A73 2.09017 0.00000 0.00000 0.00000 0.00000 2.09017

A74 2.09041 0.00000 0.00000 0.00000 0.00000 2.09042

A75 2.11907 0.00000 0.00000 0.00000 0.00000 2.11907

A76 2.07370 0.00000 0.00000 0.00000 0.00000 2.07370

A77 2.09041 0.00000 0.00000 0.00000 0.00000 2.09042

A78 2.07370 0.00000 0.00000 0.00000 0.00000 2.07370

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A80 2.07277 0.00000 0.00000 0.00000 0.00000 2.07276

A81 2.12025 0.00000 0.00000 0.00000 0.00000 2.12025

A82 2.09017 0.00000 0.00000 0.00000 0.00000 2.09017

A83 2.07671 0.00000 0.00000 0.00000 0.00000 2.07670

A84 2.11680 0.00000 0.00000 0.00001 0.00001 2.11681

A85 2.08968 0.00000 0.00000 0.00000 0.00000 2.08967

A86 2.09300 0.00000 0.00000 0.00000 0.00000 2.09301

A87 2.11928 0.00000 0.00000 0.00000 0.00000 2.11927

A88 2.07090 0.00000 0.00000 0.00000 0.00000 2.07090

A89 2.09300 0.00000 0.00000 0.00000 0.00000 2.09301

A90 2.07090 0.00000 0.00000 0.00000 0.00000 2.07090

A91 2.11928 0.00000 0.00000 0.00000 0.00000 2.11927

A92 2.07671 0.00000 0.00000 0.00000 0.00000 2.07670

A93 2.11680 0.00000 0.00000 0.00001 0.00001 2.11681

A94 2.08968 0.00000 0.00000 0.00000 0.00000 2.08967

A95 2.07277 0.00000 0.00000 0.00000 0.00000 2.07276

A96 2.12025 0.00000 0.00000 0.00000 0.00000 2.12025

A97 2.09017 0.00000 0.00000 0.00000 0.00000 2.09017

A98 2.09041 0.00000 0.00000 0.00000 0.00000 2.09042

A99 2.11907 0.00000 0.00000 0.00000 0.00000 2.11907

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A103 2.11907 0.00000 0.00000 0.00000 0.00000 2.11907

A104 2.07277 0.00000 0.00000 0.00000 0.00000 2.07276

A105 2.12025 0.00000 0.00000 0.00000 0.00000 2.12025

A106 2.09017 0.00000 0.00000 0.00000 0.00000 2.09017

A107 2.07671 0.00000 0.00000 0.00000 0.00000 2.07670

A108 2.11680 0.00000 0.00000 0.00001 0.00001 2.11681

A109 2.08968 0.00000 0.00000 0.00000 0.00000 2.08967

A110 2.09300 0.00000 0.00000 0.00000 0.00000 2.09301

A111 2.11928 0.00000 0.00000 0.00000 0.00000 2.11927

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A113 2.09300 0.00000 0.00000 0.00000 0.00000 2.09301

A114 2.07090 0.00000 0.00000 0.00000 0.00000 2.07090

A115 2.11928 0.00000 0.00000 0.00000 0.00000 2.11927

A116 2.07671 0.00000 0.00000 0.00000 0.00000 2.07670

A117 2.11680 0.00000 0.00000 0.00001 0.00001 2.11681

A118 2.08968 0.00000 0.00000 0.00000 0.00000 2.08967

A119 2.11181 0.00000 0.00000 0.00000 0.00000 2.11181

A120 2.06942 0.00000 0.00000 0.00000 0.00000 2.06942

A121 2.10195 0.00000 0.00000 0.00000 0.00000 2.10196

A122 2.10047 0.00000 0.00000 0.00000 0.00000 2.10047

A123 2.09563 0.00000 0.00000 0.00000 0.00000 2.09562

A124 2.08709 0.00000 0.00000 0.00000 0.00000 2.08709

A125 2.10047 0.00000 0.00000 0.00000 0.00000 2.10047

A126 2.08709 0.00000 0.00000 0.00000 0.00000 2.08709

A127 2.09563 0.00000 0.00000 0.00000 0.00000 2.09562

A128 2.11181 0.00000 0.00000 0.00000 0.00000 2.11181

A129 2.06942 0.00000 0.00000 0.00000 0.00000 2.06942

A130 2.10195 0.00000 0.00000 0.00000 0.00000 2.10196

A131 2.10926 0.00000 0.00000 0.00000 0.00000 2.10926

A132 2.07211 0.00000 0.00000 0.00000 0.00000 2.07211

A133 2.10182 0.00000 0.00000 0.00000 0.00000 2.10182

A134 2.10023 0.00000 0.00000 0.00000 0.00000 2.10023

A135 2.09463 0.00000 0.00000 0.00000 0.00000 2.09463

A136 2.08832 0.00000 0.00000 0.00000 0.00000 2.08832

A137 2.10023 0.00000 0.00000 0.00000 0.00000 2.10023

A138 2.08832 0.00000 0.00000 0.00000 0.00000 2.08832

A139 2.09463 0.00000 0.00000 0.00000 0.00000 2.09463

A140 2.10926 0.00000 0.00000 0.00000 0.00000 2.10926

A141 2.07211 0.00000 0.00000 0.00000 0.00000 2.07211

A142 2.10182 0.00000 0.00000 0.00000 0.00000 2.10182

A143 2.11181 0.00000 0.00000 0.00000 0.00000 2.11181

A144 2.06942 0.00000 0.00000 0.00000 0.00000 2.06942

A145 2.10195 0.00000 0.00000 0.00000 0.00000 2.10196

A146 2.10047 0.00000 0.00000 0.00000 0.00000 2.10047

A147 2.09563 0.00000 0.00000 0.00000 0.00000 2.09562

A148 2.08709 0.00000 0.00000 0.00000 0.00000 2.08709

A149 2.10047 0.00000 0.00000 0.00000 0.00000 2.10047

A150 2.08709 0.00000 0.00000 0.00000 0.00000 2.08709

A151 2.09563 0.00000 0.00000 0.00000 0.00000 2.09562

A152 2.11181 0.00000 0.00000 0.00000 0.00000 2.11181

A153 2.06942 0.00000 0.00000 0.00000 0.00000 2.06942

A154 2.10195 0.00000 0.00000 0.00000 0.00000 2.10196

A155 2.10926 0.00000 0.00000 0.00000 0.00000 2.10926

A156 2.07211 0.00000 0.00000 0.00000 0.00000 2.07211

A157 2.10182 0.00000 0.00000 0.00000 0.00000 2.10182

A158 2.10023 0.00000 0.00000 0.00000 0.00000 2.10023

A159 2.09463 0.00000 0.00000 0.00000 0.00000 2.09463

A160 2.08832 0.00000 0.00000 0.00000 0.00000 2.08832

A161 2.10023 0.00000 0.00000 0.00000 0.00000 2.10023

A162 2.08832 0.00000 0.00000 0.00000 0.00000 2.08832

A163 2.09463 0.00000 0.00000 0.00000 0.00000 2.09463

A164 2.10926 0.00000 0.00000 0.00000 0.00000 2.10926

A165 2.07211 0.00000 0.00000 0.00000 0.00000 2.07211

A166 2.10182 0.00000 0.00000 0.00000 0.00000 2.10182

D1 0.01899 0.00000 0.00000 -0.00001 -0.00002 0.01897

D2 -3.03691 0.00000 -0.00003 -0.00001 -0.00004 -3.03696

D3 -3.09782 0.00000 0.00001 0.00000 0.00000 -3.09781

D4 0.12947 0.00000 -0.00002 0.00000 -0.00002 0.12945

D5 -0.01128 0.00000 0.00000 0.00001 0.00001 -0.01127

D6 -3.13563 0.00000 -0.00001 0.00000 -0.00001 -3.13564

D7 3.10680 0.00000 -0.00001 0.00000 -0.00001 3.10679

D8 -0.01754 0.00000 -0.00002 -0.00002 -0.00003 -0.01758

D9 0.10955 0.00000 0.00002 0.00001 0.00002 0.10957

D10 -3.00386 0.00000 0.00003 0.00002 0.00005 -3.00381

D11 -0.01899 0.00000 0.00000 0.00001 0.00002 -0.01897

D12 3.09782 0.00000 -0.00001 0.00000 0.00000 3.09781

D13 3.03691 0.00000 0.00003 0.00001 0.00004 3.03696

D14 -0.12947 0.00000 0.00002 0.00000 0.00002 -0.12945

D15 -2.94571 0.00000 0.00001 0.00001 0.00002 -2.94569

D16 -0.29360 0.00000 0.00002 -0.00001 0.00001 -0.29359

D17 -1.61965 0.00000 0.00002 0.00000 0.00001 -1.61964

D18 0.29360 0.00000 -0.00002 0.00001 -0.00001 0.29359

D19 2.94571 0.00000 -0.00001 -0.00001 -0.00002 2.94569

D20 1.61965 0.00000 -0.00002 0.00000 -0.00001 1.61964

D21 0.01128 0.00000 0.00000 -0.00001 -0.00001 0.01127

D22 3.13563 0.00000 0.00001 0.00000 0.00001 3.13564

D23 -3.10680 0.00000 0.00001 0.00000 0.00001 -3.10679

D24 0.01754 0.00000 0.00002 0.00002 0.00003 0.01758

D25 -0.10955 0.00000 -0.00002 -0.00001 -0.00002 -0.10957

D26 3.00386 0.00000 -0.00003 -0.00002 -0.00005 3.00381

D27 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D28 3.12681 0.00000 0.00001 0.00001 0.00002 3.12683

D29 -3.12681 0.00000 -0.00001 -0.00001 -0.00002 -3.12683

D30 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D31 -3.12718 0.00000 0.00000 -0.00002 -0.00002 -3.12720

D32 0.01292 0.00000 -0.00001 0.00000 -0.00001 0.01290

D33 -0.00493 0.00000 0.00001 -0.00001 0.00001 -0.00493

D34 3.13516 0.00000 0.00000 0.00001 0.00001 3.13517

D35 3.12718 0.00000 0.00000 0.00002 0.00002 3.12720

D36 -0.01292 0.00000 0.00001 0.00000 0.00001 -0.01290

D37 0.00493 0.00000 -0.00001 0.00001 -0.00001 0.00493

D38 -3.13516 0.00000 0.00000 -0.00001 -0.00001 -3.13517

D39 0.01983 0.00000 0.00001 0.00000 0.00000 0.01984

D40 -3.07400 0.00000 0.00002 0.00001 0.00003 -3.07397

D41 -3.05848 0.00000 0.00003 0.00000 0.00004 -3.05844

D42 0.29327 0.00000 -0.00001 0.00002 0.00001 0.29328

D43 0.04093 0.00000 0.00002 -0.00001 0.00001 0.04094

D44 -2.89051 0.00000 -0.00002 0.00001 -0.00001 -2.89052

D45 3.07768 0.00000 -0.00002 -0.00001 -0.00003 3.07765

D46 -0.05333 0.00000 -0.00002 -0.00001 -0.00003 -0.05336

D47 -0.02440 0.00000 -0.00001 0.00001 -0.00001 -0.02441

D48 3.12777 0.00000 -0.00001 0.00001 -0.00001 3.12777

D49 -0.04093 0.00000 -0.00002 0.00001 -0.00001 -0.04094

D50 3.05848 0.00000 -0.00003 0.00000 -0.00004 3.05844

D51 2.89051 0.00000 0.00002 -0.00001 0.00001 2.89052

D52 -0.29327 0.00000 0.00001 -0.00002 -0.00001 -0.29328

D53 -0.36460 0.00000 0.00001 -0.00002 -0.00001 -0.36461

D54 -1.69044 0.00000 0.00002 -0.00001 0.00001 -1.69043

D55 -3.01629 0.00000 0.00003 0.00000 0.00004 -3.01626

D56 3.01629 0.00000 -0.00003 0.00000 -0.00004 3.01626

D57 1.69044 0.00000 -0.00002 0.00001 -0.00001 1.69043

D58 0.36460 0.00000 -0.00001 0.00002 0.00001 0.36461

D59 0.02440 0.00000 0.00001 -0.00001 0.00001 0.02441

D60 -3.12777 0.00000 0.00001 -0.00001 0.00001 -3.12777

D61 -3.07768 0.00000 0.00002 0.00001 0.00003 -3.07765

D62 0.05333 0.00000 0.00002 0.00001 0.00003 0.05336

D63 -0.01983 0.00000 -0.00001 0.00000 0.00000 -0.01984

D64 3.07400 0.00000 -0.00002 -0.00001 -0.00003 3.07397

D65 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D66 3.13240 0.00000 0.00000 0.00000 0.00000 3.13240

D67 -3.13240 0.00000 0.00000 0.00000 0.00000 -3.13240

D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D69 -3.13765 0.00000 0.00000 -0.00001 -0.00001 -3.13766

D70 0.00648 0.00000 0.00000 0.00000 0.00000 0.00648

D71 -0.00796 0.00000 0.00000 -0.00001 -0.00001 -0.00797

D72 3.13616 0.00000 0.00000 0.00000 0.00000 3.13616

D73 3.13765 0.00000 0.00000 0.00001 0.00001 3.13766

D74 -0.00648 0.00000 0.00000 0.00000 0.00000 -0.00648

D75 0.00796 0.00000 0.00000 0.00001 0.00001 0.00797

D76 -3.13616 0.00000 0.00000 0.00000 0.00000 -3.13616

D77 3.07400 0.00000 -0.00002 -0.00001 -0.00003 3.07397

D78 -0.01983 0.00000 -0.00001 0.00000 0.00000 -0.01984

D79 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D80 3.13240 0.00000 0.00000 0.00000 0.00000 3.13240

D81 -3.13240 0.00000 0.00000 0.00000 0.00000 -3.13240

D82 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D83 -3.07768 0.00000 0.00002 0.00001 0.00003 -3.07765

D84 0.02440 0.00000 0.00001 -0.00001 0.00001 0.02441

D85 0.05333 0.00000 0.00002 0.00001 0.00003 0.05336

D86 -3.12777 0.00000 0.00001 -0.00001 0.00001 -3.12777

D87 -0.00796 0.00000 0.00000 -0.00001 -0.00001 -0.00797

D88 3.13616 0.00000 0.00000 0.00000 0.00000 3.13616

D89 -3.13765 0.00000 0.00000 -0.00001 -0.00001 -3.13766

D90 0.00648 0.00000 0.00000 0.00000 0.00000 0.00648

D91 -0.02440 0.00000 -0.00001 0.00001 -0.00001 -0.02441

D92 3.07768 0.00000 -0.00002 -0.00001 -0.00003 3.07765

D93 3.12777 0.00000 -0.00001 0.00001 -0.00001 3.12777

D94 -0.05333 0.00000 -0.00002 -0.00001 -0.00003 -0.05336

D95 0.00796 0.00000 0.00000 0.00001 0.00001 0.00797

D96 -3.13616 0.00000 0.00000 0.00000 0.00000 -3.13616

D97 3.13765 0.00000 0.00000 0.00001 0.00001 3.13766

D98 -0.00648 0.00000 0.00000 0.00000 0.00000 -0.00648

D99 0.04093 0.00000 0.00002 -0.00001 0.00001 0.04094

D100 -2.89051 0.00000 -0.00002 0.00001 -0.00001 -2.89052

D101 -3.05848 0.00000 0.00003 0.00000 0.00004 -3.05844

D102 0.29327 0.00000 -0.00001 0.00002 0.00001 0.29328

D103 -3.07400 0.00000 0.00002 0.00001 0.00003 -3.07397

D104 0.01983 0.00000 0.00001 0.00000 0.00000 0.01984

D105 3.05848 0.00000 -0.00003 0.00000 -0.00004 3.05844

D106 -0.04093 0.00000 -0.00002 0.00001 -0.00001 -0.04094

D107 -0.29327 0.00000 0.00001 -0.00002 -0.00001 -0.29328

D108 2.89051 0.00000 0.00002 -0.00001 0.00001 2.89052

D109 -3.01629 0.00000 0.00003 0.00000 0.00004 -3.01626

D110 -1.69044 0.00000 0.00002 -0.00001 0.00001 -1.69043

D111 -0.36460 0.00000 0.00001 -0.00002 -0.00001 -0.36461

D112 0.36460 0.00000 -0.00001 0.00002 0.00001 0.36461

D113 1.69044 0.00000 -0.00002 0.00001 -0.00001 1.69043

D114 3.01629 0.00000 -0.00003 0.00000 -0.00004 3.01626

D115 -0.10955 0.00000 -0.00002 -0.00001 -0.00002 -0.10957

D116 3.00386 0.00000 -0.00003 -0.00002 -0.00005 3.00381

D117 3.09782 0.00000 -0.00001 0.00000 0.00000 3.09781

D118 -0.01899 0.00000 0.00000 0.00001 0.00002 -0.01897

D119 -0.12947 0.00000 0.00002 0.00000 0.00002 -0.12945

D120 3.03691 0.00000 0.00003 0.00001 0.00004 3.03696

D121 0.01899 0.00000 0.00000 -0.00001 -0.00002 0.01897

D122 -3.09782 0.00000 0.00001 0.00000 0.00000 -3.09781

D123 -3.03691 0.00000 -0.00003 -0.00001 -0.00004 -3.03696

D124 0.12947 0.00000 -0.00002 0.00000 -0.00002 0.12945

D125 1.61965 0.00000 -0.00002 0.00000 -0.00001 1.61964

D126 2.94571 0.00000 -0.00001 -0.00001 -0.00002 2.94569

D127 0.29360 0.00000 -0.00002 0.00001 -0.00001 0.29359

D128 -1.61965 0.00000 0.00002 0.00000 0.00001 -1.61964

D129 -0.29360 0.00000 0.00002 -0.00001 0.00001 -0.29359

D130 -2.94571 0.00000 0.00001 0.00001 0.00002 -2.94569

D131 -3.10680 0.00000 0.00001 0.00000 0.00001 -3.10679

D132 0.01754 0.00000 0.00002 0.00002 0.00003 0.01758

D133 0.01128 0.00000 0.00000 -0.00001 -0.00001 0.01127

D134 3.13563 0.00000 0.00001 0.00000 0.00001 3.13564

D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D136 3.12681 0.00000 0.00001 0.00001 0.00002 3.12683

D137 -3.12681 0.00000 -0.00001 -0.00001 -0.00002 -3.12683

D138 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D139 -3.12718 0.00000 0.00000 -0.00002 -0.00002 -3.12720

D140 0.01292 0.00000 -0.00001 0.00000 -0.00001 0.01290

D141 -0.00493 0.00000 0.00001 -0.00001 0.00001 -0.00493

D142 3.13516 0.00000 0.00000 0.00001 0.00001 3.13517

D143 -0.01128 0.00000 0.00000 0.00001 0.00001 -0.01127

D144 3.10680 0.00000 -0.00001 0.00000 -0.00001 3.10679

D145 -3.13563 0.00000 -0.00001 0.00000 -0.00001 -3.13564

D146 -0.01754 0.00000 -0.00002 -0.00002 -0.00003 -0.01758

D147 0.00493 0.00000 -0.00001 0.00001 -0.00001 0.00493

D148 -3.13516 0.00000 0.00000 -0.00001 -0.00001 -3.13517

D149 3.12718 0.00000 0.00000 0.00002 0.00002 3.12720

D150 -0.01292 0.00000 0.00001 0.00000 0.00001 -0.01290

D151 0.10955 0.00000 0.00002 0.00001 0.00002 0.10957

D152 -3.00386 0.00000 0.00003 0.00002 0.00005 -3.00381

D153 0.00782 0.00000 0.00000 0.00001 0.00001 0.00783

D154 -3.13433 0.00000 0.00000 0.00001 0.00001 -3.13432

D155 -3.13626 0.00000 0.00000 0.00000 0.00000 -3.13626

D156 0.00478 0.00000 0.00000 0.00000 0.00000 0.00478

D157 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D158 3.14105 0.00000 0.00000 0.00000 0.00000 3.14105

D159 -3.14105 0.00000 0.00000 0.00000 0.00000 -3.14105

D160 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D161 -3.14122 0.00000 0.00000 0.00001 0.00000 -3.14122

D162 0.00011 0.00000 0.00000 0.00000 0.00000 0.00011

D163 -0.00018 0.00000 0.00000 0.00000 0.00000 -0.00018

D164 3.14115 0.00000 0.00000 0.00000 0.00000 3.14115

D165 -0.00782 0.00000 0.00000 -0.00001 -0.00001 -0.00783

D166 3.13626 0.00000 0.00000 0.00000 0.00000 3.13626

D167 3.13433 0.00000 0.00000 -0.00001 -0.00001 3.13432

D168 -0.00478 0.00000 0.00000 0.00000 0.00000 -0.00478

D169 0.00018 0.00000 0.00000 0.00000 0.00000 0.00018

D170 -3.14115 0.00000 0.00000 0.00000 0.00000 -3.14115

D171 3.14122 0.00000 0.00000 -0.00001 0.00000 3.14122

D172 -0.00011 0.00000 0.00000 0.00000 0.00000 -0.00011

D173 -0.00487 0.00000 0.00001 -0.00001 0.00001 -0.00487

D174 3.13963 0.00000 0.00002 -0.00001 0.00001 3.13964

D175 3.13525 0.00000 0.00000 0.00001 0.00001 3.13525

D176 -0.00344 0.00000 0.00001 0.00001 0.00001 -0.00343

D177 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D178 -3.13877 0.00000 0.00001 0.00000 0.00000 -3.13876

D179 3.13877 0.00000 -0.00001 0.00000 0.00000 3.13876

D180 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D181 3.13894 0.00000 0.00000 -0.00002 -0.00001 3.13893

D182 -0.00303 0.00000 -0.00001 0.00001 0.00000 -0.00303

D183 0.00022 0.00000 0.00001 -0.00002 -0.00001 0.00021

D184 3.14144 0.00000 0.00000 0.00001 0.00000 3.14144

D185 0.00487 0.00000 -0.00001 0.00001 -0.00001 0.00487

D186 -3.13525 0.00000 0.00000 -0.00001 -0.00001 -3.13525

D187 -3.13963 0.00000 -0.00002 0.00001 -0.00001 -3.13964

D188 0.00344 0.00000 -0.00001 -0.00001 -0.00001 0.00343

D189 -0.00022 0.00000 -0.00001 0.00002 0.00001 -0.00021

D190 -3.14144 0.00000 0.00000 -0.00001 0.00000 -3.14144

D191 -3.13894 0.00000 0.00000 0.00002 0.00001 -3.13893

D192 0.00303 0.00000 0.00001 -0.00001 0.00000 0.00303

D193 -0.00782 0.00000 0.00000 -0.00001 -0.00001 -0.00783

D194 3.13433 0.00000 0.00000 -0.00001 -0.00001 3.13432

D195 3.13626 0.00000 0.00000 0.00000 0.00000 3.13626

D196 -0.00478 0.00000 0.00000 0.00000 0.00000 -0.00478

D197 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D198 -3.14105 0.00000 0.00000 0.00000 0.00000 -3.14105

D199 3.14105 0.00000 0.00000 0.00000 0.00000 3.14105

D200 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D201 3.14122 0.00000 0.00000 -0.00001 0.00000 3.14122

D202 -0.00011 0.00000 0.00000 0.00000 0.00000 -0.00011

D203 0.00018 0.00000 0.00000 0.00000 0.00000 0.00018

D204 -3.14115 0.00000 0.00000 0.00000 0.00000 -3.14115

D205 0.00782 0.00000 0.00000 0.00001 0.00001 0.00783

D206 -3.13626 0.00000 0.00000 0.00000 0.00000 -3.13626

D207 -3.13433 0.00000 0.00000 0.00001 0.00001 -3.13432

D208 0.00478 0.00000 0.00000 0.00000 0.00000 0.00478

D209 -0.00018 0.00000 0.00000 0.00000 0.00000 -0.00018

D210 3.14115 0.00000 0.00000 0.00000 0.00000 3.14115

D211 -3.14122 0.00000 0.00000 0.00001 0.00000 -3.14122

D212 0.00011 0.00000 0.00000 0.00000 0.00000 0.00011

D213 -0.00487 0.00000 0.00001 -0.00001 0.00001 -0.00487

D214 3.13963 0.00000 0.00002 -0.00001 0.00001 3.13964

D215 3.13525 0.00000 0.00000 0.00001 0.00001 3.13525

D216 -0.00344 0.00000 0.00001 0.00001 0.00001 -0.00343

D217 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D218 -3.13877 0.00000 0.00001 0.00000 0.00000 -3.13876

D219 3.13877 0.00000 -0.00001 0.00000 0.00000 3.13876

D220 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D221 3.13894 0.00000 0.00000 -0.00002 -0.00001 3.13893

D222 -0.00303 0.00000 -0.00001 0.00001 0.00000 -0.00303

D223 0.00022 0.00000 0.00001 -0.00002 -0.00001 0.00021

D224 3.14144 0.00000 0.00000 0.00001 0.00000 3.14144

D225 0.00487 0.00000 -0.00001 0.00001 -0.00001 0.00487

D226 -3.13525 0.00000 0.00000 -0.00001 -0.00001 -3.13525

D227 -3.13963 0.00000 -0.00002 0.00001 -0.00001 -3.13964

D228 0.00344 0.00000 -0.00001 -0.00001 -0.00001 0.00343

D229 -0.00022 0.00000 -0.00001 0.00002 0.00001 -0.00021

D230 -3.14144 0.00000 0.00000 -0.00001 0.00000 -3.14144

D231 -3.13894 0.00000 0.00000 0.00002 0.00001 -3.13893

D232 0.00303 0.00000 0.00001 -0.00001 0.00000 0.00303

D233 0.00023 0.00000 0.00001 -0.00002 -0.00001 0.00021

D234 -3.14147 0.00000 0.00001 -0.00003 -0.00001 -3.14148

D235 3.14143 0.00000 0.00000 0.00001 0.00000 3.14144

D236 -0.00026 0.00000 0.00000 0.00000 0.00000 -0.00026

D237 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D238 3.14149 0.00000 0.00000 -0.00001 0.00000 3.14149

D239 -3.14149 0.00000 0.00000 0.00001 0.00000 -3.14149

D240 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D241 -0.00023 0.00000 -0.00001 0.00002 0.00001 -0.00021

D242 -3.14143 0.00000 0.00000 -0.00001 0.00000 -3.14144

D243 3.14147 0.00000 -0.00001 0.00003 0.00001 3.14148

D244 0.00026 0.00000 0.00000 0.00000 0.00000 0.00026

D245 -0.00019 0.00000 0.00000 0.00000 0.00000 -0.00018

D246 -3.14116 0.00000 0.00000 0.00000 0.00000 -3.14116

D247 3.14115 0.00000 0.00000 0.00000 0.00000 3.14114

D248 0.00017 0.00000 0.00000 0.00000 0.00000 0.00017

D249 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D250 -3.14098 0.00000 0.00000 0.00000 0.00000 -3.14098

D251 3.14098 0.00000 0.00000 0.00000 0.00000 3.14098

D252 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D253 0.00019 0.00000 0.00000 0.00000 0.00000 0.00018

D254 -3.14115 0.00000 0.00000 0.00000 0.00000 -3.14114

D255 3.14116 0.00000 0.00000 0.00000 0.00000 3.14116

D256 -0.00017 0.00000 0.00000 0.00000 0.00000 -0.00017

D257 0.00023 0.00000 0.00001 -0.00002 -0.00001 0.00021

D258 -3.14147 0.00000 0.00001 -0.00003 -0.00001 -3.14148

D259 3.14143 0.00000 0.00000 0.00001 0.00000 3.14144

D260 -0.00026 0.00000 0.00000 0.00000 0.00000 -0.00026

D261 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D262 3.14149 0.00000 0.00000 -0.00001 0.00000 3.14149

D263 -3.14149 0.00000 0.00000 0.00001 0.00000 -3.14149

D264 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D265 -0.00023 0.00000 -0.00001 0.00002 0.00001 -0.00021

D266 -3.14143 0.00000 0.00000 -0.00001 0.00000 -3.14144

D267 3.14147 0.00000 -0.00001 0.00003 0.00001 3.14148

D268 0.00026 0.00000 0.00000 0.00000 0.00000 0.00026

D269 0.00019 0.00000 0.00000 0.00000 0.00000 0.00018

D270 3.14116 0.00000 0.00000 0.00000 0.00000 3.14116

D271 -3.14115 0.00000 0.00000 0.00000 0.00000 -3.14114

D272 -0.00017 0.00000 0.00000 0.00000 0.00000 -0.00017

D273 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D274 3.14098 0.00000 0.00000 0.00000 0.00000 3.14098

D275 -3.14098 0.00000 0.00000 0.00000 0.00000 -3.14098

D276 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D277 -0.00019 0.00000 0.00000 0.00000 0.00000 -0.00018

D278 3.14115 0.00000 0.00000 0.00000 0.00000 3.14114

D279 -3.14116 0.00000 0.00000 0.00000 0.00000 -3.14116

D280 0.00017 0.00000 0.00000 0.00000 0.00000 0.00017

Item Value Threshold Converged?

Maximum Force 0.000003 0.000450 YES

RMS Force 0.000001 0.000300 YES

Maximum Displacement 0.000595 0.001800 YES

RMS Displacement 0.000099 0.001200 YES

Predicted change in Energy=-8.383201D-10

Optimization completed.

-- Stationary point found.

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! Optimized Parameters !

! (Angstroms and Degrees) !

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! Name Definition Value Derivative Info. !

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

! R1 R(1,2) 1.3654 -DE/DX = 0.0 !

! R2 R(1,5) 1.4519 -DE/DX = 0.0 !

! R3 R(1,12) 1.3542 -DE/DX = 0.0 !

! R4 R(2,3) 1.3654 -DE/DX = 0.0 !

! R5 R(2,25) 2.0903 -DE/DX = 0.0 !

! R6 R(3,4) 1.4519 -DE/DX = 0.0 !

! R7 R(3,6) 1.3542 -DE/DX = 0.0 !

! R8 R(4,5) 1.4354 -DE/DX = 0.0 !

! R9 R(4,41) 1.376 -DE/DX = 0.0 !

! R10 R(5,38) 1.376 -DE/DX = 0.0 !

! R11 R(6,7) 1.3141 -DE/DX = 0.0 !

! R12 R(7,8) 1.3748 -DE/DX = 0.0 !

! R13 R(7,11) 1.4745 -DE/DX = 0.0 !

! R14 R(8,9) 1.3748 -DE/DX = 0.0 !

! R15 R(8,25) 2.0763 -DE/DX = 0.0 !

! R16 R(9,10) 1.4745 -DE/DX = 0.0 !

! R17 R(9,24) 1.3141 -DE/DX = 0.0 !

! R18 R(10,11) 1.4246 -DE/DX = 0.0 !

! R19 R(10,37) 1.3678 -DE/DX = 0.0 !

! R20 R(11,34) 1.3678 -DE/DX = 0.0 !

! R21 R(12,17) 1.3141 -DE/DX = 0.0 !

! R22 R(13,14) 1.4246 -DE/DX = 0.0 !

! R23 R(13,17) 1.4745 -DE/DX = 0.0 !

! R24 R(13,26) 1.3678 -DE/DX = 0.0 !

! R25 R(14,15) 1.4745 -DE/DX = 0.0 !

! R26 R(14,29) 1.3678 -DE/DX = 0.0 !

! R27 R(15,16) 1.3748 -DE/DX = 0.0 !

! R28 R(15,18) 1.3141 -DE/DX = 0.0 !

! R29 R(16,17) 1.3748 -DE/DX = 0.0 !

! R30 R(16,25) 2.0763 -DE/DX = 0.0 !

! R31 R(18,20) 1.3542 -DE/DX = 0.0 !

! R32 R(19,20) 1.3654 -DE/DX = 0.0 !

! R33 R(19,23) 1.3654 -DE/DX = 0.0 !

! R34 R(19,25) 2.0903 -DE/DX = 0.0 !

! R35 R(20,21) 1.4519 -DE/DX = 0.0 !

! R36 R(21,22) 1.4354 -DE/DX = 0.0 !

! R37 R(21,33) 1.376 -DE/DX = 0.0 !

! R38 R(22,23) 1.4519 -DE/DX = 0.0 !

! R39 R(22,30) 1.376 -DE/DX = 0.0 !

! R40 R(23,24) 1.3542 -DE/DX = 0.0 !

! R41 R(26,27) 1.4246 -DE/DX = 0.0 !

! R42 R(26,58) 1.0849 -DE/DX = 0.0 !

! R43 R(27,28) 1.4378 -DE/DX = 0.0 !

! R44 R(27,49) 1.416 -DE/DX = 0.0 !

! R45 R(28,29) 1.4246 -DE/DX = 0.0 !

! R46 R(28,46) 1.416 -DE/DX = 0.0 !

! R47 R(29,59) 1.0849 -DE/DX = 0.0 !

! R48 R(30,31) 1.4172 -DE/DX = 0.0 !

! R49 R(30,60) 1.0851 -DE/DX = 0.0 !

! R50 R(31,32) 1.4429 -DE/DX = 0.0 !

! R51 R(31,45) 1.4199 -DE/DX = 0.0 !

! R52 R(32,33) 1.4172 -DE/DX = 0.0 !

! R53 R(32,42) 1.4199 -DE/DX = 0.0 !

! R54 R(33,61) 1.0851 -DE/DX = 0.0 !

! R55 R(34,35) 1.4246 -DE/DX = 0.0 !

! R56 R(34,62) 1.0849 -DE/DX = 0.0 !

! R57 R(35,36) 1.4378 -DE/DX = 0.0 !

! R58 R(35,57) 1.416 -DE/DX = 0.0 !

! R59 R(36,37) 1.4246 -DE/DX = 0.0 !

! R60 R(36,54) 1.416 -DE/DX = 0.0 !

! R61 R(37,63) 1.0849 -DE/DX = 0.0 !

! R62 R(38,39) 1.4172 -DE/DX = 0.0 !

! R63 R(38,64) 1.0851 -DE/DX = 0.0 !

! R64 R(39,40) 1.4429 -DE/DX = 0.0 !

! R65 R(39,53) 1.4199 -DE/DX = 0.0 !

! R66 R(40,41) 1.4172 -DE/DX = 0.0 !

! R67 R(40,50) 1.4199 -DE/DX = 0.0 !

! R68 R(41,65) 1.0851 -DE/DX = 0.0 !

! R69 R(42,43) 1.3742 -DE/DX = 0.0 !

! R70 R(42,66) 1.0855 -DE/DX = 0.0 !

! R71 R(43,44) 1.416 -DE/DX = 0.0 !

! R72 R(43,67) 1.0848 -DE/DX = 0.0 !

! R73 R(44,45) 1.3742 -DE/DX = 0.0 !

! R74 R(44,68) 1.0848 -DE/DX = 0.0 !

! R75 R(45,69) 1.0855 -DE/DX = 0.0 !

! R76 R(46,47) 1.3771 -DE/DX = 0.0 !

! R77 R(46,70) 1.0853 -DE/DX = 0.0 !

! R78 R(47,48) 1.4117 -DE/DX = 0.0 !

! R79 R(47,71) 1.0846 -DE/DX = 0.0 !

! R80 R(48,49) 1.3771 -DE/DX = 0.0 !

! R81 R(48,72) 1.0846 -DE/DX = 0.0 !

! R82 R(49,73) 1.0853 -DE/DX = 0.0 !

! R83 R(50,51) 1.3742 -DE/DX = 0.0 !

! R84 R(50,74) 1.0855 -DE/DX = 0.0 !

! R85 R(51,52) 1.416 -DE/DX = 0.0 !

! R86 R(51,75) 1.0848 -DE/DX = 0.0 !

! R87 R(52,53) 1.3742 -DE/DX = 0.0 !

! R88 R(52,76) 1.0848 -DE/DX = 0.0 !

! R89 R(53,77) 1.0855 -DE/DX = 0.0 !

! R90 R(54,55) 1.3771 -DE/DX = 0.0 !

! R91 R(54,78) 1.0853 -DE/DX = 0.0 !

! R92 R(55,56) 1.4117 -DE/DX = 0.0 !

! R93 R(55,79) 1.0846 -DE/DX = 0.0 !

! R94 R(56,57) 1.3771 -DE/DX = 0.0 !

! R95 R(56,80) 1.0846 -DE/DX = 0.0 !

! R96 R(57,81) 1.0853 -DE/DX = 0.0 !

! A1 A(2,1,5) 108.6498 -DE/DX = 0.0 !

! A2 A(2,1,12) 127.7785 -DE/DX = 0.0 !

! A3 A(5,1,12) 123.5559 -DE/DX = 0.0 !

! A4 A(1,2,3) 110.4128 -DE/DX = 0.0 !

! A5 A(1,2,25) 124.695 -DE/DX = 0.0 !

! A6 A(3,2,25) 124.695 -DE/DX = 0.0 !

! A7 A(2,3,4) 108.6498 -DE/DX = 0.0 !

! A8 A(2,3,6) 127.7785 -DE/DX = 0.0 !

! A9 A(4,3,6) 123.5559 -DE/DX = 0.0 !

! A10 A(3,4,5) 106.138 -DE/DX = 0.0 !

! A11 A(3,4,41) 132.7624 -DE/DX = 0.0 !

! A12 A(5,4,41) 121.0926 -DE/DX = 0.0 !

! A13 A(1,5,4) 106.138 -DE/DX = 0.0 !

! A14 A(1,5,38) 132.7624 -DE/DX = 0.0 !

! A15 A(4,5,38) 121.0926 -DE/DX = 0.0 !

! A16 A(3,6,7) 124.4034 -DE/DX = 0.0 !

! A17 A(6,7,8) 128.3213 -DE/DX = 0.0 !

! A18 A(6,7,11) 123.1138 -DE/DX = 0.0 !

! A19 A(8,7,11) 108.5196 -DE/DX = 0.0 !

! A20 A(7,8,9) 110.1952 -DE/DX = 0.0 !

! A21 A(7,8,25) 124.3066 -DE/DX = 0.0 !

! A22 A(9,8,25) 124.3066 -DE/DX = 0.0 !

! A23 A(8,9,10) 108.5196 -DE/DX = 0.0 !

! A24 A(8,9,24) 128.3213 -DE/DX = 0.0 !

! A25 A(10,9,24) 123.1138 -DE/DX = 0.0 !

! A26 A(9,10,11) 106.3557 -DE/DX = 0.0 !

! A27 A(9,10,37) 132.1759 -DE/DX = 0.0 !

! A28 A(11,10,37) 121.4658 -DE/DX = 0.0 !

! A29 A(7,11,10) 106.3557 -DE/DX = 0.0 !

! A30 A(7,11,34) 132.1759 -DE/DX = 0.0 !

! A31 A(10,11,34) 121.4658 -DE/DX = 0.0 !

! A32 A(1,12,17) 124.4034 -DE/DX = 0.0 !

! A33 A(14,13,17) 106.3557 -DE/DX = 0.0 !

! A34 A(14,13,26) 121.4658 -DE/DX = 0.0 !

! A35 A(17,13,26) 132.1759 -DE/DX = 0.0 !

! A36 A(13,14,15) 106.3557 -DE/DX = 0.0 !

! A37 A(13,14,29) 121.4658 -DE/DX = 0.0 !

! A38 A(15,14,29) 132.1759 -DE/DX = 0.0 !

! A39 A(14,15,16) 108.5196 -DE/DX = 0.0 !

! A40 A(14,15,18) 123.1138 -DE/DX = 0.0 !

! A41 A(16,15,18) 128.3213 -DE/DX = 0.0 !

! A42 A(15,16,17) 110.1952 -DE/DX = 0.0 !

! A43 A(15,16,25) 124.3066 -DE/DX = 0.0 !

! A44 A(17,16,25) 124.3066 -DE/DX = 0.0 !

! A45 A(12,17,13) 123.1138 -DE/DX = 0.0 !

! A46 A(12,17,16) 128.3213 -DE/DX = 0.0 !

! A47 A(13,17,16) 108.5196 -DE/DX = 0.0 !

! A48 A(15,18,20) 124.4034 -DE/DX = 0.0 !

! A49 A(20,19,23) 110.4128 -DE/DX = 0.0 !

! A50 A(20,19,25) 124.695 -DE/DX = 0.0 !

! A51 A(23,19,25) 124.695 -DE/DX = 0.0 !

! A52 A(18,20,19) 127.7785 -DE/DX = 0.0 !

! A53 A(18,20,21) 123.5559 -DE/DX = 0.0 !

! A54 A(19,20,21) 108.6498 -DE/DX = 0.0 !

! A55 A(20,21,22) 106.138 -DE/DX = 0.0 !

! A56 A(20,21,33) 132.7624 -DE/DX = 0.0 !

! A57 A(22,21,33) 121.0926 -DE/DX = 0.0 !

! A58 A(21,22,23) 106.138 -DE/DX = 0.0 !

! A59 A(21,22,30) 121.0926 -DE/DX = 0.0 !

! A60 A(23,22,30) 132.7624 -DE/DX = 0.0 !

! A61 A(19,23,22) 108.6498 -DE/DX = 0.0 !

! A62 A(19,23,24) 127.7785 -DE/DX = 0.0 !

! A63 A(22,23,24) 123.5559 -DE/DX = 0.0 !

! A64 A(9,24,23) 124.4034 -DE/DX = 0.0 !

! A65 A(2,25,8) 86.4208 -DE/DX = 0.0 !

! A66 A(2,25,16) 86.4208 -DE/DX = 0.0 !

! A67 A(2,25,19) 151.0502 -DE/DX = 0.0 !

! A68 A(8,25,16) 151.0736 -DE/DX = 0.0 !

! A69 A(8,25,19) 86.4208 -DE/DX = 0.0 !

! A70 A(16,25,19) 86.4208 -DE/DX = 0.0 !

! A71 A(13,26,27) 118.7608 -DE/DX = 0.0 !

! A72 A(13,26,58) 121.4811 -DE/DX = 0.0 !

! A73 A(27,26,58) 119.758 -DE/DX = 0.0 !

! A74 A(26,27,28) 119.7719 -DE/DX = 0.0 !

! A75 A(26,27,49) 121.4141 -DE/DX = 0.0 !

! A76 A(28,27,49) 118.814 -DE/DX = 0.0 !

! A77 A(27,28,29) 119.7719 -DE/DX = 0.0 !

! A78 A(27,28,46) 118.814 -DE/DX = 0.0 !

! A79 A(29,28,46) 121.4141 -DE/DX = 0.0 !

! A80 A(14,29,28) 118.7608 -DE/DX = 0.0 !

! A81 A(14,29,59) 121.4811 -DE/DX = 0.0 !

! A82 A(28,29,59) 119.758 -DE/DX = 0.0 !

! A83 A(22,30,31) 118.9865 -DE/DX = 0.0 !

! A84 A(22,30,60) 121.2837 -DE/DX = 0.0 !

! A85 A(31,30,60) 119.7297 -DE/DX = 0.0 !

! A86 A(30,31,32) 119.9203 -DE/DX = 0.0 !

! A87 A(30,31,45) 121.4256 -DE/DX = 0.0 !

! A88 A(32,31,45) 118.6539 -DE/DX = 0.0 !

! A89 A(31,32,33) 119.9203 -DE/DX = 0.0 !

! A90 A(31,32,42) 118.6539 -DE/DX = 0.0 !

! A91 A(33,32,42) 121.4256 -DE/DX = 0.0 !

! A92 A(21,33,32) 118.9865 -DE/DX = 0.0 !

! A93 A(21,33,61) 121.2837 -DE/DX = 0.0 !

! A94 A(32,33,61) 119.7297 -DE/DX = 0.0 !

! A95 A(11,34,35) 118.7608 -DE/DX = 0.0 !

! A96 A(11,34,62) 121.4811 -DE/DX = 0.0 !

! A97 A(35,34,62) 119.758 -DE/DX = 0.0 !

! A98 A(34,35,36) 119.7719 -DE/DX = 0.0 !

! A99 A(34,35,57) 121.4141 -DE/DX = 0.0 !

! A100 A(36,35,57) 118.814 -DE/DX = 0.0 !

! A101 A(35,36,37) 119.7719 -DE/DX = 0.0 !

! A102 A(35,36,54) 118.814 -DE/DX = 0.0 !

! A103 A(37,36,54) 121.4141 -DE/DX = 0.0 !

! A104 A(10,37,36) 118.7608 -DE/DX = 0.0 !

! A105 A(10,37,63) 121.4811 -DE/DX = 0.0 !

! A106 A(36,37,63) 119.758 -DE/DX = 0.0 !

! A107 A(5,38,39) 118.9865 -DE/DX = 0.0 !

! A108 A(5,38,64) 121.2837 -DE/DX = 0.0 !

! A109 A(39,38,64) 119.7297 -DE/DX = 0.0 !

! A110 A(38,39,40) 119.9203 -DE/DX = 0.0 !

! A111 A(38,39,53) 121.4256 -DE/DX = 0.0 !

! A112 A(40,39,53) 118.6539 -DE/DX = 0.0 !

! A113 A(39,40,41) 119.9203 -DE/DX = 0.0 !

! A114 A(39,40,50) 118.6539 -DE/DX = 0.0 !

! A115 A(41,40,50) 121.4256 -DE/DX = 0.0 !

! A116 A(4,41,40) 118.9865 -DE/DX = 0.0 !

! A117 A(4,41,65) 121.2837 -DE/DX = 0.0 !

! A118 A(40,41,65) 119.7297 -DE/DX = 0.0 !

! A119 A(32,42,43) 120.9978 -DE/DX = 0.0 !

! A120 A(32,42,66) 118.5691 -DE/DX = 0.0 !

! A121 A(43,42,66) 120.4331 -DE/DX = 0.0 !

! A122 A(42,43,44) 120.3483 -DE/DX = 0.0 !

! A123 A(42,43,67) 120.0705 -DE/DX = 0.0 !

! A124 A(44,43,67) 119.5812 -DE/DX = 0.0 !

! A125 A(43,44,45) 120.3483 -DE/DX = 0.0 !

! A126 A(43,44,68) 119.5812 -DE/DX = 0.0 !

! A127 A(45,44,68) 120.0705 -DE/DX = 0.0 !

! A128 A(31,45,44) 120.9978 -DE/DX = 0.0 !

! A129 A(31,45,69) 118.5691 -DE/DX = 0.0 !

! A130 A(44,45,69) 120.4331 -DE/DX = 0.0 !

! A131 A(28,46,47) 120.8516 -DE/DX = 0.0 !

! A132 A(28,46,70) 118.7231 -DE/DX = 0.0 !

! A133 A(47,46,70) 120.4254 -DE/DX = 0.0 !

! A134 A(46,47,48) 120.3344 -DE/DX = 0.0 !

! A135 A(46,47,71) 120.0136 -DE/DX = 0.0 !

! A136 A(48,47,71) 119.652 -DE/DX = 0.0 !

! A137 A(47,48,49) 120.3344 -DE/DX = 0.0 !

! A138 A(47,48,72) 119.652 -DE/DX = 0.0 !

! A139 A(49,48,72) 120.0136 -DE/DX = 0.0 !

! A140 A(27,49,48) 120.8516 -DE/DX = 0.0 !

! A141 A(27,49,73) 118.7231 -DE/DX = 0.0 !

! A142 A(48,49,73) 120.4254 -DE/DX = 0.0 !

! A143 A(40,50,51) 120.9978 -DE/DX = 0.0 !

! A144 A(40,50,74) 118.5691 -DE/DX = 0.0 !

! A145 A(51,50,74) 120.4331 -DE/DX = 0.0 !

! A146 A(50,51,52) 120.3483 -DE/DX = 0.0 !

! A147 A(50,51,75) 120.0705 -DE/DX = 0.0 !

! A148 A(52,51,75) 119.5812 -DE/DX = 0.0 !

! A149 A(51,52,53) 120.3483 -DE/DX = 0.0 !

! A150 A(51,52,76) 119.5812 -DE/DX = 0.0 !

! A151 A(53,52,76) 120.0705 -DE/DX = 0.0 !

! A152 A(39,53,52) 120.9978 -DE/DX = 0.0 !

! A153 A(39,53,77) 118.5691 -DE/DX = 0.0 !

! A154 A(52,53,77) 120.4331 -DE/DX = 0.0 !

! A155 A(36,54,55) 120.8516 -DE/DX = 0.0 !

! A156 A(36,54,78) 118.7231 -DE/DX = 0.0 !

! A157 A(55,54,78) 120.4254 -DE/DX = 0.0 !

! A158 A(54,55,56) 120.3344 -DE/DX = 0.0 !

! A159 A(54,55,79) 120.0136 -DE/DX = 0.0 !

! A160 A(56,55,79) 119.652 -DE/DX = 0.0 !

! A161 A(55,56,57) 120.3344 -DE/DX = 0.0 !

! A162 A(55,56,80) 119.652 -DE/DX = 0.0 !

! A163 A(57,56,80) 120.0136 -DE/DX = 0.0 !

! A164 A(35,57,56) 120.8516 -DE/DX = 0.0 !

! A165 A(35,57,81) 118.7231 -DE/DX = 0.0 !

! A166 A(56,57,81) 120.4254 -DE/DX = 0.0 !

! D1 D(5,1,2,3) 1.0879 -DE/DX = 0.0 !

! D2 D(5,1,2,25) -174.0023 -DE/DX = 0.0 !

! D3 D(12,1,2,3) -177.4917 -DE/DX = 0.0 !

! D4 D(12,1,2,25) 7.418 -DE/DX = 0.0 !

! D5 D(2,1,5,4) -0.6462 -DE/DX = 0.0 !

! D6 D(2,1,5,38) -179.6581 -DE/DX = 0.0 !

! D7 D(12,1,5,4) 178.0067 -DE/DX = 0.0 !

! D8 D(12,1,5,38) -1.0052 -DE/DX = 0.0 !

! D9 D(2,1,12,17) 6.2767 -DE/DX = 0.0 !

! D10 D(5,1,12,17) -172.1083 -DE/DX = 0.0 !

! D11 D(1,2,3,4) -1.0879 -DE/DX = 0.0 !

! D12 D(1,2,3,6) 177.4917 -DE/DX = 0.0 !

! D13 D(25,2,3,4) 174.0023 -DE/DX = 0.0 !

! D14 D(25,2,3,6) -7.418 -DE/DX = 0.0 !

! D15 D(1,2,25,8) -168.7768 -DE/DX = 0.0 !

! D16 D(1,2,25,16) -16.8218 -DE/DX = 0.0 !

! D17 D(1,2,25,19) -92.7993 -DE/DX = 0.0 !

! D18 D(3,2,25,8) 16.8218 -DE/DX = 0.0 !

! D19 D(3,2,25,16) 168.7768 -DE/DX = 0.0 !

! D20 D(3,2,25,19) 92.7993 -DE/DX = 0.0 !

! D21 D(2,3,4,5) 0.6462 -DE/DX = 0.0 !

! D22 D(2,3,4,41) 179.6581 -DE/DX = 0.0 !

! D23 D(6,3,4,5) -178.0067 -DE/DX = 0.0 !

! D24 D(6,3,4,41) 1.0052 -DE/DX = 0.0 !

! D25 D(2,3,6,7) -6.2767 -DE/DX = 0.0 !

! D26 D(4,3,6,7) 172.1083 -DE/DX = 0.0 !

! D27 D(3,4,5,1) 0.0 -DE/DX = 0.0 !

! D28 D(3,4,5,38) 179.1529 -DE/DX = 0.0 !

! D29 D(41,4,5,1) -179.1529 -DE/DX = 0.0 !

! D30 D(41,4,5,38) 0.0 -DE/DX = 0.0 !

! D31 D(3,4,41,40) -179.1742 -DE/DX = 0.0 !

! D32 D(3,4,41,65) 0.74 -DE/DX = 0.0 !

! D33 D(5,4,41,40) -0.2826 -DE/DX = 0.0 !

! D34 D(5,4,41,65) 179.6316 -DE/DX = 0.0 !

! D35 D(1,5,38,39) 179.1742 -DE/DX = 0.0 !

! D36 D(1,5,38,64) -0.74 -DE/DX = 0.0 !

! D37 D(4,5,38,39) 0.2826 -DE/DX = 0.0 !

! D38 D(4,5,38,64) -179.6316 -DE/DX = 0.0 !

! D39 D(3,6,7,8) 1.1363 -DE/DX = 0.0 !

! D40 D(3,6,7,11) -176.1272 -DE/DX = 0.0 !

! D41 D(6,7,8,9) -175.2377 -DE/DX = 0.0 !

! D42 D(6,7,8,25) 16.8032 -DE/DX = 0.0 !

! D43 D(11,7,8,9) 2.3452 -DE/DX = 0.0 !

! D44 D(11,7,8,25) -165.6139 -DE/DX = 0.0 !

! D45 D(6,7,11,10) 176.3379 -DE/DX = 0.0 !

! D46 D(6,7,11,34) -3.0558 -DE/DX = 0.0 !

! D47 D(8,7,11,10) -1.3982 -DE/DX = 0.0 !

! D48 D(8,7,11,34) 179.2081 -DE/DX = 0.0 !

! D49 D(7,8,9,10) -2.3452 -DE/DX = 0.0 !

! D50 D(7,8,9,24) 175.2377 -DE/DX = 0.0 !

! D51 D(25,8,9,10) 165.6139 -DE/DX = 0.0 !

! D52 D(25,8,9,24) -16.8032 -DE/DX = 0.0 !

! D53 D(7,8,25,2) -20.8899 -DE/DX = 0.0 !

! D54 D(7,8,25,16) -96.8553 -DE/DX = 0.0 !

! D55 D(7,8,25,19) -172.8207 -DE/DX = 0.0 !

! D56 D(9,8,25,2) 172.8207 -DE/DX = 0.0 !

! D57 D(9,8,25,16) 96.8553 -DE/DX = 0.0 !

! D58 D(9,8,25,19) 20.8899 -DE/DX = 0.0 !

! D59 D(8,9,10,11) 1.3982 -DE/DX = 0.0 !

! D60 D(8,9,10,37) -179.2081 -DE/DX = 0.0 !

! D61 D(24,9,10,11) -176.3379 -DE/DX = 0.0 !

! D62 D(24,9,10,37) 3.0558 -DE/DX = 0.0 !

! D63 D(8,9,24,23) -1.1363 -DE/DX = 0.0 !

! D64 D(10,9,24,23) 176.1272 -DE/DX = 0.0 !

! D65 D(9,10,11,7) 0.0 -DE/DX = 0.0 !

! D66 D(9,10,11,34) 179.4732 -DE/DX = 0.0 !

! D67 D(37,10,11,7) -179.4732 -DE/DX = 0.0 !

! D68 D(37,10,11,34) 0.0 -DE/DX = 0.0 !

! D69 D(9,10,37,36) -179.7739 -DE/DX = 0.0 !

! D70 D(9,10,37,63) 0.3711 -DE/DX = 0.0 !

! D71 D(11,10,37,36) -0.456 -DE/DX = 0.0 !

! D72 D(11,10,37,63) 179.689 -DE/DX = 0.0 !

! D73 D(7,11,34,35) 179.7739 -DE/DX = 0.0 !

! D74 D(7,11,34,62) -0.3711 -DE/DX = 0.0 !

! D75 D(10,11,34,35) 0.456 -DE/DX = 0.0 !

! D76 D(10,11,34,62) -179.689 -DE/DX = 0.0 !

! D77 D(1,12,17,13) 176.1272 -DE/DX = 0.0 !

! D78 D(1,12,17,16) -1.1363 -DE/DX = 0.0 !

! D79 D(17,13,14,15) 0.0 -DE/DX = 0.0 !

! D80 D(17,13,14,29) 179.4732 -DE/DX = 0.0 !

! D81 D(26,13,14,15) -179.4732 -DE/DX = 0.0 !

! D82 D(26,13,14,29) 0.0 -DE/DX = 0.0 !

! D83 D(14,13,17,12) -176.3379 -DE/DX = 0.0 !

! D84 D(14,13,17,16) 1.3982 -DE/DX = 0.0 !

! D85 D(26,13,17,12) 3.0558 -DE/DX = 0.0 !

! D86 D(26,13,17,16) -179.2081 -DE/DX = 0.0 !

! D87 D(14,13,26,27) -0.456 -DE/DX = 0.0 !

! D88 D(14,13,26,58) 179.689 -DE/DX = 0.0 !

! D89 D(17,13,26,27) -179.7739 -DE/DX = 0.0 !

! D90 D(17,13,26,58) 0.3711 -DE/DX = 0.0 !

! D91 D(13,14,15,16) -1.3982 -DE/DX = 0.0 !

! D92 D(13,14,15,18) 176.3379 -DE/DX = 0.0 !

! D93 D(29,14,15,16) 179.2081 -DE/DX = 0.0 !

! D94 D(29,14,15,18) -3.0558 -DE/DX = 0.0 !

! D95 D(13,14,29,28) 0.456 -DE/DX = 0.0 !

! D96 D(13,14,29,59) -179.689 -DE/DX = 0.0 !

! D97 D(15,14,29,28) 179.7739 -DE/DX = 0.0 !

! D98 D(15,14,29,59) -0.3711 -DE/DX = 0.0 !

! D99 D(14,15,16,17) 2.3452 -DE/DX = 0.0 !

! D100 D(14,15,16,25) -165.6139 -DE/DX = 0.0 !

! D101 D(18,15,16,17) -175.2377 -DE/DX = 0.0 !

! D102 D(18,15,16,25) 16.8032 -DE/DX = 0.0 !

! D103 D(14,15,18,20) -176.1272 -DE/DX = 0.0 !

! D104 D(16,15,18,20) 1.1363 -DE/DX = 0.0 !

! D105 D(15,16,17,12) 175.2377 -DE/DX = 0.0 !

! D106 D(15,16,17,13) -2.3452 -DE/DX = 0.0 !

! D107 D(25,16,17,12) -16.8032 -DE/DX = 0.0 !

! D108 D(25,16,17,13) 165.6139 -DE/DX = 0.0 !

! D109 D(15,16,25,2) -172.8207 -DE/DX = 0.0 !

! D110 D(15,16,25,8) -96.8553 -DE/DX = 0.0 !

! D111 D(15,16,25,19) -20.8899 -DE/DX = 0.0 !

! D112 D(17,16,25,2) 20.8899 -DE/DX = 0.0 !

! D113 D(17,16,25,8) 96.8553 -DE/DX = 0.0 !

! D114 D(17,16,25,19) 172.8207 -DE/DX = 0.0 !

! D115 D(15,18,20,19) -6.2767 -DE/DX = 0.0 !

! D116 D(15,18,20,21) 172.1083 -DE/DX = 0.0 !

! D117 D(23,19,20,18) 177.4917 -DE/DX = 0.0 !

! D118 D(23,19,20,21) -1.0879 -DE/DX = 0.0 !

! D119 D(25,19,20,18) -7.418 -DE/DX = 0.0 !

! D120 D(25,19,20,21) 174.0023 -DE/DX = 0.0 !

! D121 D(20,19,23,22) 1.0879 -DE/DX = 0.0 !

! D122 D(20,19,23,24) -177.4917 -DE/DX = 0.0 !

! D123 D(25,19,23,22) -174.0023 -DE/DX = 0.0 !

! D124 D(25,19,23,24) 7.418 -DE/DX = 0.0 !

! D125 D(20,19,25,2) 92.7993 -DE/DX = 0.0 !

! D126 D(20,19,25,8) 168.7768 -DE/DX = 0.0 !

! D127 D(20,19,25,16) 16.8218 -DE/DX = 0.0 !

! D128 D(23,19,25,2) -92.7993 -DE/DX = 0.0 !

! D129 D(23,19,25,8) -16.8218 -DE/DX = 0.0 !

! D130 D(23,19,25,16) -168.7768 -DE/DX = 0.0 !

! D131 D(18,20,21,22) -178.0067 -DE/DX = 0.0 !

! D132 D(18,20,21,33) 1.0052 -DE/DX = 0.0 !

! D133 D(19,20,21,22) 0.6462 -DE/DX = 0.0 !

! D134 D(19,20,21,33) 179.6581 -DE/DX = 0.0 !

! D135 D(20,21,22,23) 0.0 -DE/DX = 0.0 !

! D136 D(20,21,22,30) 179.1529 -DE/DX = 0.0 !

! D137 D(33,21,22,23) -179.1529 -DE/DX = 0.0 !

! D138 D(33,21,22,30) 0.0 -DE/DX = 0.0 !

! D139 D(20,21,33,32) -179.1742 -DE/DX = 0.0 !

! D140 D(20,21,33,61) 0.74 -DE/DX = 0.0 !

! D141 D(22,21,33,32) -0.2826 -DE/DX = 0.0 !

! D142 D(22,21,33,61) 179.6316 -DE/DX = 0.0 !

! D143 D(21,22,23,19) -0.6462 -DE/DX = 0.0 !

! D144 D(21,22,23,24) 178.0067 -DE/DX = 0.0 !

! D145 D(30,22,23,19) -179.6581 -DE/DX = 0.0 !

! D146 D(30,22,23,24) -1.0052 -DE/DX = 0.0 !

! D147 D(21,22,30,31) 0.2826 -DE/DX = 0.0 !

! D148 D(21,22,30,60) -179.6316 -DE/DX = 0.0 !

! D149 D(23,22,30,31) 179.1742 -DE/DX = 0.0 !

! D150 D(23,22,30,60) -0.74 -DE/DX = 0.0 !

! D151 D(19,23,24,9) 6.2767 -DE/DX = 0.0 !

! D152 D(22,23,24,9) -172.1083 -DE/DX = 0.0 !

! D153 D(13,26,27,28) 0.4481 -DE/DX = 0.0 !

! D154 D(13,26,27,49) -179.5839 -DE/DX = 0.0 !

! D155 D(58,26,27,28) -179.6943 -DE/DX = 0.0 !

! D156 D(58,26,27,49) 0.2736 -DE/DX = 0.0 !

! D157 D(26,27,28,29) 0.0 -DE/DX = 0.0 !

! D158 D(26,27,28,46) 179.9688 -DE/DX = 0.0 !

! D159 D(49,27,28,29) -179.9688 -DE/DX = 0.0 !

! D160 D(49,27,28,46) 0.0 -DE/DX = 0.0 !

! D161 D(26,27,49,48) -179.9788 -DE/DX = 0.0 !

! D162 D(26,27,49,73) 0.0065 -DE/DX = 0.0 !

! D163 D(28,27,49,48) -0.0105 -DE/DX = 0.0 !

! D164 D(28,27,49,73) 179.9748 -DE/DX = 0.0 !

! D165 D(27,28,29,14) -0.4481 -DE/DX = 0.0 !

! D166 D(27,28,29,59) 179.6943 -DE/DX = 0.0 !

! D167 D(46,28,29,14) 179.5839 -DE/DX = 0.0 !

! D168 D(46,28,29,59) -0.2736 -DE/DX = 0.0 !

! D169 D(27,28,46,47) 0.0105 -DE/DX = 0.0 !

! D170 D(27,28,46,70) -179.9748 -DE/DX = 0.0 !

! D171 D(29,28,46,47) 179.9788 -DE/DX = 0.0 !

! D172 D(29,28,46,70) -0.0065 -DE/DX = 0.0 !

! D173 D(22,30,31,32) -0.2792 -DE/DX = 0.0 !

! D174 D(22,30,31,45) 179.8873 -DE/DX = 0.0 !

! D175 D(60,30,31,32) 179.6363 -DE/DX = 0.0 !

! D176 D(60,30,31,45) -0.1971 -DE/DX = 0.0 !

! D177 D(30,31,32,33) 0.0 -DE/DX = 0.0 !

! D178 D(30,31,32,42) -179.838 -DE/DX = 0.0 !

! D179 D(45,31,32,33) 179.838 -DE/DX = 0.0 !

! D180 D(45,31,32,42) 0.0 -DE/DX = 0.0 !

! D181 D(30,31,45,44) 179.8482 -DE/DX = 0.0 !

! D182 D(30,31,45,69) -0.1734 -DE/DX = 0.0 !

! D183 D(32,31,45,44) 0.0127 -DE/DX = 0.0 !

! D184 D(32,31,45,69) 179.9911 -DE/DX = 0.0 !

! D185 D(31,32,33,21) 0.2792 -DE/DX = 0.0 !

! D186 D(31,32,33,61) -179.6363 -DE/DX = 0.0 !

! D187 D(42,32,33,21) -179.8873 -DE/DX = 0.0 !

! D188 D(42,32,33,61) 0.1971 -DE/DX = 0.0 !

! D189 D(31,32,42,43) -0.0127 -DE/DX = 0.0 !

! D190 D(31,32,42,66) -179.9911 -DE/DX = 0.0 !

! D191 D(33,32,42,43) -179.8482 -DE/DX = 0.0 !

! D192 D(33,32,42,66) 0.1734 -DE/DX = 0.0 !

! D193 D(11,34,35,36) -0.4481 -DE/DX = 0.0 !

! D194 D(11,34,35,57) 179.5839 -DE/DX = 0.0 !

! D195 D(62,34,35,36) 179.6943 -DE/DX = 0.0 !

! D196 D(62,34,35,57) -0.2736 -DE/DX = 0.0 !

! D197 D(34,35,36,37) 0.0 -DE/DX = 0.0 !

! D198 D(34,35,36,54) -179.9688 -DE/DX = 0.0 !

! D199 D(57,35,36,37) 179.9688 -DE/DX = 0.0 !

! D200 D(57,35,36,54) 0.0 -DE/DX = 0.0 !

! D201 D(34,35,57,56) 179.9788 -DE/DX = 0.0 !

! D202 D(34,35,57,81) -0.0065 -DE/DX = 0.0 !

! D203 D(36,35,57,56) 0.0105 -DE/DX = 0.0 !

! D204 D(36,35,57,81) -179.9748 -DE/DX = 0.0 !

! D205 D(35,36,37,10) 0.4481 -DE/DX = 0.0 !

! D206 D(35,36,37,63) -179.6943 -DE/DX = 0.0 !

! D207 D(54,36,37,10) -179.5839 -DE/DX = 0.0 !

! D208 D(54,36,37,63) 0.2736 -DE/DX = 0.0 !

! D209 D(35,36,54,55) -0.0105 -DE/DX = 0.0 !

! D210 D(35,36,54,78) 179.9748 -DE/DX = 0.0 !

! D211 D(37,36,54,55) -179.9788 -DE/DX = 0.0 !

! D212 D(37,36,54,78) 0.0065 -DE/DX = 0.0 !

! D213 D(5,38,39,40) -0.2792 -DE/DX = 0.0 !

! D214 D(5,38,39,53) 179.8873 -DE/DX = 0.0 !

! D215 D(64,38,39,40) 179.6363 -DE/DX = 0.0 !

! D216 D(64,38,39,53) -0.1971 -DE/DX = 0.0 !

! D217 D(38,39,40,41) 0.0 -DE/DX = 0.0 !

! D218 D(38,39,40,50) -179.838 -DE/DX = 0.0 !

! D219 D(53,39,40,41) 179.838 -DE/DX = 0.0 !

! D220 D(53,39,40,50) 0.0 -DE/DX = 0.0 !

! D221 D(38,39,53,52) 179.8482 -DE/DX = 0.0 !

! D222 D(38,39,53,77) -0.1734 -DE/DX = 0.0 !

! D223 D(40,39,53,52) 0.0127 -DE/DX = 0.0 !

! D224 D(40,39,53,77) 179.9911 -DE/DX = 0.0 !

! D225 D(39,40,41,4) 0.2792 -DE/DX = 0.0 !

! D226 D(39,40,41,65) -179.6363 -DE/DX = 0.0 !

! D227 D(50,40,41,4) -179.8873 -DE/DX = 0.0 !

! D228 D(50,40,41,65) 0.1971 -DE/DX = 0.0 !

! D229 D(39,40,50,51) -0.0127 -DE/DX = 0.0 !

! D230 D(39,40,50,74) -179.9911 -DE/DX = 0.0 !

! D231 D(41,40,50,51) -179.8482 -DE/DX = 0.0 !

! D232 D(41,40,50,74) 0.1734 -DE/DX = 0.0 !

! D233 D(32,42,43,44) 0.0129 -DE/DX = 0.0 !

! D234 D(32,42,43,67) -179.9928 -DE/DX = 0.0 !

! D235 D(66,42,43,44) 179.991 -DE/DX = 0.0 !

! D236 D(66,42,43,67) -0.0148 -DE/DX = 0.0 !

! D237 D(42,43,44,45) 0.0 -DE/DX = 0.0 !

! D238 D(42,43,44,68) 179.9943 -DE/DX = 0.0 !

! D239 D(67,43,44,45) -179.9943 -DE/DX = 0.0 !

! D240 D(67,43,44,68) 0.0 -DE/DX = 0.0 !

! D241 D(43,44,45,31) -0.0129 -DE/DX = 0.0 !

! D242 D(43,44,45,69) -179.991 -DE/DX = 0.0 !

! D243 D(68,44,45,31) 179.9928 -DE/DX = 0.0 !

! D244 D(68,44,45,69) 0.0148 -DE/DX = 0.0 !

! D245 D(28,46,47,48) -0.0107 -DE/DX = 0.0 !

! D246 D(28,46,47,71) -179.9753 -DE/DX = 0.0 !

! D247 D(70,46,47,48) 179.9744 -DE/DX = 0.0 !

! D248 D(70,46,47,71) 0.0098 -DE/DX = 0.0 !

! D249 D(46,47,48,49) 0.0 -DE/DX = 0.0 !

! D250 D(46,47,48,72) -179.9647 -DE/DX = 0.0 !

! D251 D(71,47,48,49) 179.9647 -DE/DX = 0.0 !

! D252 D(71,47,48,72) 0.0 -DE/DX = 0.0 !

! D253 D(47,48,49,27) 0.0107 -DE/DX = 0.0 !

! D254 D(47,48,49,73) -179.9744 -DE/DX = 0.0 !

! D255 D(72,48,49,27) 179.9753 -DE/DX = 0.0 !

! D256 D(72,48,49,73) -0.0098 -DE/DX = 0.0 !

! D257 D(40,50,51,52) 0.0129 -DE/DX = 0.0 !

! D258 D(40,50,51,75) -179.9928 -DE/DX = 0.0 !

! D259 D(74,50,51,52) 179.991 -DE/DX = 0.0 !

! D260 D(74,50,51,75) -0.0148 -DE/DX = 0.0 !

! D261 D(50,51,52,53) 0.0 -DE/DX = 0.0 !

! D262 D(50,51,52,76) 179.9943 -DE/DX = 0.0 !

! D263 D(75,51,52,53) -179.9943 -DE/DX = 0.0 !

! D264 D(75,51,52,76) 0.0 -DE/DX = 0.0 !

! D265 D(51,52,53,39) -0.0129 -DE/DX = 0.0 !

! D266 D(51,52,53,77) -179.991 -DE/DX = 0.0 !

! D267 D(76,52,53,39) 179.9928 -DE/DX = 0.0 !

! D268 D(76,52,53,77) 0.0148 -DE/DX = 0.0 !

! D269 D(36,54,55,56) 0.0107 -DE/DX = 0.0 !

! D270 D(36,54,55,79) 179.9753 -DE/DX = 0.0 !

! D271 D(78,54,55,56) -179.9744 -DE/DX = 0.0 !

! D272 D(78,54,55,79) -0.0098 -DE/DX = 0.0 !

! D273 D(54,55,56,57) 0.0 -DE/DX = 0.0 !

! D274 D(54,55,56,80) 179.9647 -DE/DX = 0.0 !

! D275 D(79,55,56,57) -179.9647 -DE/DX = 0.0 !

! D276 D(79,55,56,80) 0.0 -DE/DX = 0.0 !

! D277 D(55,56,57,35) -0.0107 -DE/DX = 0.0 !

! D278 D(55,56,57,81) 179.9744 -DE/DX = 0.0 !

! D279 D(80,56,57,35) -179.9753 -DE/DX = 0.0 !

! D280 D(80,56,57,81) 0.0098 -DE/DX = 0.0 !

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

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Largest change from initial coordinates is atom 67 0.110 Angstoms.

Leave Link 103 at Sun Jun 30 21:45:21 2019, MaxMem= 1342177280 cpu: 25.6

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

Stoichiometry C48H24N8Zn(3)

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C48H24N4)]

Deg. of freedom 61

Full point group C2V NOp 4

RotChk: IX=0 Diff= 2.36D-16

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 1.121263 2.790136 0.181319

2 7 0 0.000000 2.023921 0.322495

3 6 0 -1.121263 2.790136 0.181319

4 6 0 -0.717705 4.166232 -0.045670

5 6 0 0.717705 4.166232 -0.045670

6 7 0 -2.412721 2.383597 0.208594

7 6 0 -2.794679 1.127507 0.264121

8 7 0 -2.010517 0.000000 0.326394

9 6 0 -2.794679 -1.127507 0.264121

10 6 0 -4.208479 -0.712278 0.209240

11 6 0 -4.208479 0.712278 0.209240

12 7 0 2.412721 2.383597 0.208594

13 6 0 4.208479 0.712278 0.209240

14 6 0 4.208479 -0.712278 0.209240

15 6 0 2.794679 -1.127507 0.264121

16 7 0 2.010517 0.000000 0.326394

17 6 0 2.794679 1.127507 0.264121

18 7 0 2.412721 -2.383597 0.208594

19 7 0 0.000000 -2.023921 0.322495

20 6 0 1.121263 -2.790136 0.181319

21 6 0 0.717705 -4.166232 -0.045670

22 6 0 -0.717705 -4.166232 -0.045670

23 6 0 -1.121263 -2.790136 0.181319

24 7 0 -2.412721 -2.383597 0.208594

25 30 0 0.000000 0.000000 0.844972

26 6 0 5.373840 1.426277 0.153267

27 6 0 6.609437 0.718883 0.103873

28 6 0 6.609437 -0.718883 0.103873

29 6 0 5.373840 -1.426277 0.153267

30 6 0 -1.428324 -5.325913 -0.254618

31 6 0 -0.721456 -6.535793 -0.466397

32 6 0 0.721456 -6.535793 -0.466397

33 6 0 1.428324 -5.325913 -0.254618

34 6 0 -5.373840 1.426277 0.153267

35 6 0 -6.609437 0.718883 0.103873

36 6 0 -6.609437 -0.718883 0.103873

37 6 0 -5.373840 -1.426277 0.153267

38 6 0 1.428324 5.325913 -0.254618

39 6 0 0.721456 6.535793 -0.466397

40 6 0 -0.721456 6.535793 -0.466397

41 6 0 -1.428324 5.325913 -0.254618

42 6 0 1.402325 -7.762532 -0.684704

43 6 0 0.708020 -8.930102 -0.892216

44 6 0 -0.708020 -8.930102 -0.892216

45 6 0 -1.402325 -7.762532 -0.684704

46 6 0 7.849096 -1.401345 0.053640

47 6 0 9.036663 -0.705865 0.005736

48 6 0 9.036663 0.705865 0.005736

49 6 0 7.849096 1.401345 0.053640

50 6 0 -1.402325 7.762532 -0.684704

51 6 0 -0.708020 8.930102 -0.892216

52 6 0 0.708020 8.930102 -0.892216

53 6 0 1.402325 7.762532 -0.684704

54 6 0 -7.849096 -1.401345 0.053640

55 6 0 -9.036663 -0.705865 0.005736

56 6 0 -9.036663 0.705865 0.005736

57 6 0 -7.849096 1.401345 0.053640

58 1 0 5.373896 2.511159 0.148236

59 1 0 5.373896 -2.511159 0.148236

60 1 0 -2.513359 -5.328428 -0.261130

61 1 0 2.513359 -5.328428 -0.261130

62 1 0 -5.373896 2.511159 0.148236

63 1 0 -5.373896 -2.511159 0.148236

64 1 0 2.513359 5.328428 -0.261130

65 1 0 -2.513359 5.328428 -0.261130

66 1 0 2.487805 -7.760976 -0.684277

67 1 0 1.243521 -9.858901 -1.057387

68 1 0 -1.243521 -9.858901 -1.057387

69 1 0 -2.487805 -7.760976 -0.684277

70 1 0 7.847357 -2.486615 0.053291

71 1 0 9.978475 -1.242469 -0.032837

72 1 0 9.978475 1.242469 -0.032837

73 1 0 7.847357 2.486615 0.053291

74 1 0 -2.487805 7.760976 -0.684277

75 1 0 -1.243521 9.858901 -1.057387

76 1 0 1.243521 9.858901 -1.057387

77 1 0 2.487805 7.760976 -0.684277

78 1 0 -7.847357 -2.486615 0.053291

79 1 0 -9.978475 -1.242469 -0.032837

80 1 0 -9.978475 1.242469 -0.032837

81 1 0 -7.847357 2.486615 0.053291

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

Rotational constants (GHZ): 0.0387342 0.0379494 0.0193803

Leave Link 202 at Sun Jun 30 21:45:22 2019, MaxMem= 1342177280 cpu: 0.7

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

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

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

Population analysis using the SCF density.

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

Orbital symmetries:

Alpha Orbitals:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The electronic state is 3-B2.

Alpha occ. eigenvalues -- -14.31802 -14.31802 -14.30864 -14.30864 -14.30811

Alpha occ. eigenvalues -- -14.30811 -14.30811 -14.30810 -10.25609 -10.25609

Alpha occ. eigenvalues -- -10.25608 -10.25608 -10.24764 -10.24764 -10.24763

Alpha occ. eigenvalues -- -10.24763 -10.19388 -10.19388 -10.19349 -10.19349

Alpha occ. eigenvalues -- -10.19030 -10.19030 -10.18992 -10.18992 -10.18863

Alpha occ. eigenvalues -- -10.18863 -10.18863 -10.18863 -10.18650 -10.18650

Alpha occ. eigenvalues -- -10.18607 -10.18607 -10.18559 -10.18559 -10.18558

Alpha occ. eigenvalues -- -10.18558 -10.18106 -10.18106 -10.18066 -10.18066

Alpha occ. eigenvalues -- -10.17891 -10.17891 -10.17889 -10.17889 -10.17806

Alpha occ. eigenvalues -- -10.17806 -10.17763 -10.17763 -10.17699 -10.17699

Alpha occ. eigenvalues -- -10.17699 -10.17699 -10.17583 -10.17583 -10.17540

Alpha occ. eigenvalues -- -10.17540 -1.00492 -0.99172 -0.99093 -0.96422

Alpha occ. eigenvalues -- -0.94273 -0.90565 -0.89963 -0.88546 -0.88185

Alpha occ. eigenvalues -- -0.88078 -0.87962 -0.86545 -0.83103 -0.83040

Alpha occ. eigenvalues -- -0.82669 -0.82662 -0.79225 -0.78712 -0.78547

Alpha occ. eigenvalues -- -0.78492 -0.75694 -0.75647 -0.75638 -0.75325

Alpha occ. eigenvalues -- -0.75222 -0.73742 -0.73695 -0.73014 -0.70809

Alpha occ. eigenvalues -- -0.69549 -0.68848 -0.66005 -0.65684 -0.65306

Alpha occ. eigenvalues -- -0.65058 -0.63109 -0.62596 -0.61040 -0.60946

Alpha occ. eigenvalues -- -0.60539 -0.60472 -0.60469 -0.60190 -0.60119

Alpha occ. eigenvalues -- -0.59845 -0.58005 -0.56830 -0.56609 -0.56555

Alpha occ. eigenvalues -- -0.55911 -0.54584 -0.54506 -0.54181 -0.53644

Alpha occ. eigenvalues -- -0.53575 -0.53290 -0.51861 -0.51801 -0.51676

Alpha occ. eigenvalues -- -0.51661 -0.51427 -0.51203 -0.50827 -0.50766

Alpha occ. eigenvalues -- -0.49166 -0.46570 -0.45814 -0.45801 -0.45695

Alpha occ. eigenvalues -- -0.45610 -0.45522 -0.45158 -0.45111 -0.45109

Alpha occ. eigenvalues -- -0.44918 -0.44379 -0.44104 -0.43830 -0.43679

Alpha occ. eigenvalues -- -0.43505 -0.43348 -0.42995 -0.42945 -0.42679

Alpha occ. eigenvalues -- -0.42576 -0.42243 -0.42145 -0.42066 -0.41413

Alpha occ. eigenvalues -- -0.39878 -0.39848 -0.39654 -0.39039 -0.38962

Alpha occ. eigenvalues -- -0.38673 -0.37847 -0.37628 -0.37199 -0.36681

Alpha occ. eigenvalues -- -0.35755 -0.35622 -0.35493 -0.35312 -0.34591

Alpha occ. eigenvalues -- -0.34455 -0.34246 -0.34124 -0.33910 -0.33607

Alpha occ. eigenvalues -- -0.33301 -0.32761 -0.32624 -0.32148 -0.31715

Alpha occ. eigenvalues -- -0.31689 -0.30790 -0.30703 -0.29882 -0.29507

Alpha occ. eigenvalues -- -0.29356 -0.27982 -0.27833 -0.26623 -0.26353

Alpha occ. eigenvalues -- -0.25446 -0.25336 -0.25252 -0.25213 -0.24786

Alpha occ. eigenvalues -- -0.24708 -0.23044 -0.23018 -0.22935 -0.18552

Alpha occ. eigenvalues -- -0.14226

Alpha virt. eigenvalues -- -0.09988 -0.06625 -0.06206 -0.05930 -0.05711

Alpha virt. eigenvalues -- -0.04926 -0.00360 -0.00344 -0.00226 0.00370

Alpha virt. eigenvalues -- 0.00562 0.01002 0.01222 0.02034 0.02438

Alpha virt. eigenvalues -- 0.04325 0.04966 0.04999 0.05923 0.06250

Alpha virt. eigenvalues -- 0.06277 0.06291 0.06372 0.07094 0.07328

Alpha virt. eigenvalues -- 0.07348 0.07766 0.08338 0.08865 0.08876

Alpha virt. eigenvalues -- 0.09689 0.09695 0.10543 0.10915 0.11118

Alpha virt. eigenvalues -- 0.11646 0.11663 0.11925 0.12045 0.12321

Alpha virt. eigenvalues -- 0.12479 0.12591 0.12652 0.13349 0.13380

Alpha virt. eigenvalues -- 0.14412 0.14619 0.16363 0.16459 0.17872

Alpha virt. eigenvalues -- 0.18217 0.18219 0.18350 0.18644 0.18667

Alpha virt. eigenvalues -- 0.18808 0.18848 0.18892 0.19397 0.20532

Alpha virt. eigenvalues -- 0.21393 0.21696 0.22315 0.22377 0.22998

Alpha virt. eigenvalues -- 0.23041 0.23131 0.24217 0.24460 0.24712

Alpha virt. eigenvalues -- 0.25724 0.25890 0.26152 0.26432 0.26706

Alpha virt. eigenvalues -- 0.27608 0.27859 0.27897 0.27916 0.28043

Alpha virt. eigenvalues -- 0.28169 0.28346 0.28577 0.28696 0.29096

Alpha virt. eigenvalues -- 0.29125 0.29634 0.30438 0.30613 0.30713

Alpha virt. eigenvalues -- 0.30752 0.31056 0.31213 0.31252 0.31850

Alpha virt. eigenvalues -- 0.31879 0.32717 0.32724 0.33140 0.34617

Alpha virt. eigenvalues -- 0.34653 0.35039 0.35058 0.35596 0.35911

Alpha virt. eigenvalues -- 0.36153 0.36460 0.36774 0.37059 0.37282

Alpha virt. eigenvalues -- 0.37304 0.37610 0.37851 0.37876 0.37930

Alpha virt. eigenvalues -- 0.38271 0.38357 0.38510 0.38833 0.39099

Alpha virt. eigenvalues -- 0.39172 0.39180 0.39609 0.39729 0.40064

Alpha virt. eigenvalues -- 0.40150 0.40186 0.40305 0.40685 0.40688

Alpha virt. eigenvalues -- 0.40989 0.41191 0.41483 0.41715 0.42005

Alpha virt. eigenvalues -- 0.42588 0.42693 0.42809 0.42992 0.43077

Alpha virt. eigenvalues -- 0.43220 0.43250 0.43355 0.43372 0.43511

Alpha virt. eigenvalues -- 0.43607 0.43662 0.43995 0.44053 0.44333

Alpha virt. eigenvalues -- 0.44445 0.44588 0.44710 0.44980 0.45144

Alpha virt. eigenvalues -- 0.45221 0.46068 0.46073 0.46093 0.46260

Alpha virt. eigenvalues -- 0.46499 0.46579 0.46609 0.46947 0.47214

Alpha virt. eigenvalues -- 0.47320 0.47490 0.47510 0.47523 0.48137

Alpha virt. eigenvalues -- 0.48431 0.48730 0.48786 0.49154 0.49380

Alpha virt. eigenvalues -- 0.49612 0.50371 0.50669 0.50844 0.50846

Alpha virt. eigenvalues -- 0.51295 0.51530 0.51564 0.52015 0.52247

Alpha virt. eigenvalues -- 0.53022 0.53196 0.53270 0.53303 0.53649

Alpha virt. eigenvalues -- 0.53865 0.54637 0.54921 0.55385 0.55785

Alpha virt. eigenvalues -- 0.56407 0.56548 0.56651 0.57833 0.58129

Alpha virt. eigenvalues -- 0.58823 0.58838 0.59387 0.59991 0.60245

Alpha virt. eigenvalues -- 0.60574 0.60706 0.60852 0.61077 0.61293

Alpha virt. eigenvalues -- 0.61541 0.61803 0.61803 0.62152 0.62257

Alpha virt. eigenvalues -- 0.62417 0.62689 0.62897 0.62942 0.63032

Alpha virt. eigenvalues -- 0.63144 0.63438 0.63568 0.64304 0.64391

Alpha virt. eigenvalues -- 0.64400 0.64503 0.65388 0.65754 0.65810

Alpha virt. eigenvalues -- 0.66285 0.67246 0.67456 0.67490 0.67980

Alpha virt. eigenvalues -- 0.68025 0.68196 0.68306 0.68959 0.68973

Alpha virt. eigenvalues -- 0.69285 0.69340 0.69352 0.69883 0.69940

Alpha virt. eigenvalues -- 0.70760 0.70774 0.71032 0.72044 0.72673

Alpha virt. eigenvalues -- 0.73025 0.73128 0.73203 0.73371 0.73456

Alpha virt. eigenvalues -- 0.73930 0.74487 0.74742 0.75293 0.75302

Alpha virt. eigenvalues -- 0.75936 0.75986 0.76341 0.76658 0.76866

Alpha virt. eigenvalues -- 0.78299 0.78535 0.78664 0.78853 0.79138

Alpha virt. eigenvalues -- 0.79383 0.79436 0.79758 0.80267 0.80489

Alpha virt. eigenvalues -- 0.80490 0.80638 0.80812 0.81370 0.81389

Alpha virt. eigenvalues -- 0.81669 0.82066 0.82171 0.82638 0.82821

Alpha virt. eigenvalues -- 0.83006 0.84162 0.84183 0.84353 0.84863

Alpha virt. eigenvalues -- 0.85057 0.85156 0.85768 0.85978 0.86242

Alpha virt. eigenvalues -- 0.87712 0.87800 0.87818 0.88191 0.88592

Alpha virt. eigenvalues -- 0.88707 0.89943 0.91612 0.91743 0.92120

Alpha virt. eigenvalues -- 0.92470 0.93599 0.93869 0.94339 0.94803

Alpha virt. eigenvalues -- 0.94833 0.95699 0.95962 0.96406 0.96863

Alpha virt. eigenvalues -- 0.96988 0.97362 0.97495 0.97556 0.97896

Alpha virt. eigenvalues -- 0.98038 0.98238 0.98363 0.98791 0.98869

Alpha virt. eigenvalues -- 0.99499 0.99761 0.99784 1.00231 1.01251

Alpha virt. eigenvalues -- 1.01977 1.02365 1.02403 1.02654 1.03415

Alpha virt. eigenvalues -- 1.03677 1.03728 1.05141 1.05492 1.06098

Alpha virt. eigenvalues -- 1.06349 1.06975 1.07112 1.07368 1.08464

Alpha virt. eigenvalues -- 1.09701 1.09792 1.09940 1.10231 1.10372

Alpha virt. eigenvalues -- 1.10878 1.11192 1.11377 1.11426 1.11640

Alpha virt. eigenvalues -- 1.11685 1.12306 1.12363 1.12395 1.12473

Alpha virt. eigenvalues -- 1.12516 1.13617 1.14103 1.14163 1.14606

Alpha virt. eigenvalues -- 1.14700 1.16521 1.16594 1.16660 1.16973

Alpha virt. eigenvalues -- 1.17095 1.17463 1.17701 1.18310 1.18738

Alpha virt. eigenvalues -- 1.19380 1.19572 1.21046 1.21527 1.21535

Alpha virt. eigenvalues -- 1.21736 1.21741 1.21809 1.22366 1.22550

Alpha virt. eigenvalues -- 1.22581 1.23301 1.24717 1.24840 1.25056

Alpha virt. eigenvalues -- 1.25435 1.25862 1.26717 1.26842 1.27232

Alpha virt. eigenvalues -- 1.27660 1.27683 1.28010 1.28757 1.29099

Alpha virt. eigenvalues -- 1.29740 1.30178 1.30219 1.30699 1.33063

Alpha virt. eigenvalues -- 1.34186 1.34375 1.34637 1.35119 1.35277

Alpha virt. eigenvalues -- 1.36321 1.38000 1.38483 1.38952 1.39152

Alpha virt. eigenvalues -- 1.39185 1.39735 1.39836 1.40352 1.42657

Alpha virt. eigenvalues -- 1.42901 1.42937 1.44605 1.44675 1.44767

Alpha virt. eigenvalues -- 1.44777 1.44975 1.45734 1.45766 1.46297

Alpha virt. eigenvalues -- 1.47167 1.48306 1.48669 1.48837 1.51210

Alpha virt. eigenvalues -- 1.51448 1.51526 1.51676 1.51705 1.51746

Alpha virt. eigenvalues -- 1.51830 1.51940 1.51984 1.52070 1.52436

Alpha virt. eigenvalues -- 1.52540 1.53039 1.53051 1.53053 1.53064

Alpha virt. eigenvalues -- 1.54035 1.54277 1.54341 1.54920 1.56225

Alpha virt. eigenvalues -- 1.56441 1.56620 1.57626 1.58157 1.60600

Alpha virt. eigenvalues -- 1.60790 1.63907 1.64419 1.64912 1.64972

Alpha virt. eigenvalues -- 1.65019 1.65160 1.66941 1.68220 1.68230

Alpha virt. eigenvalues -- 1.69147 1.69432 1.69608 1.70552 1.70682

Alpha virt. eigenvalues -- 1.71490 1.71558 1.72116 1.72555 1.73753

Alpha virt. eigenvalues -- 1.73867 1.74335 1.75254 1.75650 1.76539

Alpha virt. eigenvalues -- 1.76804 1.77139 1.77776 1.77958 1.77983

Alpha virt. eigenvalues -- 1.79109 1.79928 1.80166 1.81303 1.81884

Alpha virt. eigenvalues -- 1.82012 1.82060 1.82160 1.82687 1.82854

Alpha virt. eigenvalues -- 1.83267 1.83585 1.84533 1.84995 1.85952

Alpha virt. eigenvalues -- 1.86331 1.86420 1.86531 1.87173 1.87206

Alpha virt. eigenvalues -- 1.88170 1.88520 1.88760 1.88848 1.89083

Alpha virt. eigenvalues -- 1.89493 1.89662 1.90074 1.90408 1.91279

Alpha virt. eigenvalues -- 1.91445 1.91597 1.92119 1.92124 1.92170

Alpha virt. eigenvalues -- 1.92406 1.92584 1.92602 1.92607 1.92747

Alpha virt. eigenvalues -- 1.94234 1.94630 1.94822 1.94846 1.95074

Alpha virt. eigenvalues -- 1.95113 1.95226 1.95689 1.96112 1.96663

Alpha virt. eigenvalues -- 1.97020 1.97170 1.97335 1.97475 1.97607

Alpha virt. eigenvalues -- 1.97821 1.99274 1.99583 1.99785 2.02037

Alpha virt. eigenvalues -- 2.02828 2.04611 2.04686 2.04875 2.04976

Alpha virt. eigenvalues -- 2.06856 2.07210 2.08604 2.09216 2.12381

Alpha virt. eigenvalues -- 2.12787 2.13592 2.14926 2.15291 2.15377

Alpha virt. eigenvalues -- 2.15553 2.17678 2.18666 2.19100 2.19742

Alpha virt. eigenvalues -- 2.21307 2.21422 2.21725 2.22033 2.22110

Alpha virt. eigenvalues -- 2.22160 2.22329 2.22871 2.23061 2.24604

Alpha virt. eigenvalues -- 2.24759 2.24783 2.25081 2.26183 2.26377

Alpha virt. eigenvalues -- 2.26489 2.27483 2.27849 2.28201 2.28442

Alpha virt. eigenvalues -- 2.30112 2.31029 2.31448 2.31533 2.31740

Alpha virt. eigenvalues -- 2.31899 2.32749 2.33757 2.34207 2.34852

Alpha virt. eigenvalues -- 2.35122 2.35144 2.35285 2.36106 2.36383

Alpha virt. eigenvalues -- 2.36456 2.38324 2.38921 2.40408 2.40436

Alpha virt. eigenvalues -- 2.42973 2.43744 2.44049 2.44421 2.44796

Alpha virt. eigenvalues -- 2.45339 2.45562 2.45656 2.46234 2.47940

Alpha virt. eigenvalues -- 2.49930 2.50624 2.51140 2.51665 2.51868

Alpha virt. eigenvalues -- 2.52367 2.53131 2.53154 2.53423 2.53464

Alpha virt. eigenvalues -- 2.53955 2.55129 2.55206 2.55391 2.55433

Alpha virt. eigenvalues -- 2.55981 2.56143 2.56144 2.57084 2.57394

Alpha virt. eigenvalues -- 2.57439 2.57836 2.58800 2.61082 2.62942

Alpha virt. eigenvalues -- 2.64778 2.64811 2.64831 2.65208 2.65501

Alpha virt. eigenvalues -- 2.67841 2.68786 2.69270 2.69324 2.69550

Alpha virt. eigenvalues -- 2.70574 2.70666 2.70861 2.71215 2.71886

Alpha virt. eigenvalues -- 2.72134 2.72375 2.72947 2.73256 2.73502

Alpha virt. eigenvalues -- 2.73789 2.73858 2.74061 2.74608 2.74664

Alpha virt. eigenvalues -- 2.74678 2.75155 2.75450 2.75800 2.77766

Alpha virt. eigenvalues -- 2.79941 2.80395 2.80509 2.80632 2.81372

Alpha virt. eigenvalues -- 2.82004 2.82086 2.82244 2.82477 2.82595

Alpha virt. eigenvalues -- 2.82728 2.84956 2.86228 2.86420 2.86687

Alpha virt. eigenvalues -- 2.86705 2.87351 2.87392 2.87690 2.87959

Alpha virt. eigenvalues -- 2.87963 2.89351 2.89432 2.89454 2.91142

Alpha virt. eigenvalues -- 2.92577 2.93041 2.93494 2.93861 2.96340

Alpha virt. eigenvalues -- 2.96722 2.98567 3.02450 3.03065 3.03204

Alpha virt. eigenvalues -- 3.03863 3.04202 3.04914 3.05365 3.05558

Alpha virt. eigenvalues -- 3.07502 3.08429 3.08798 3.15120 3.15615

Alpha virt. eigenvalues -- 3.15716 3.15917 3.16547 3.17243 3.17541

Alpha virt. eigenvalues -- 3.18556 3.18617 3.19776 3.19819 3.19992

Alpha virt. eigenvalues -- 3.20108 3.21392 3.21419 3.22500 3.23007

Alpha virt. eigenvalues -- 3.23030 3.23785 3.24453 3.24688 3.26458

Alpha virt. eigenvalues -- 3.26899 3.27160 3.27507 3.28199 3.28227

Alpha virt. eigenvalues -- 3.28365 3.28390 3.28440 3.28552 3.29340

Alpha virt. eigenvalues -- 3.29354 3.31232 3.31262 3.32138 3.32330

Alpha virt. eigenvalues -- 3.32387 3.33859 3.33979 3.34015 3.34882

Alpha virt. eigenvalues -- 3.34952 3.35175 3.37478 3.39789 3.41166

Alpha virt. eigenvalues -- 3.41211 3.42114 3.42194 3.42729 3.42846

Alpha virt. eigenvalues -- 3.43537 3.46772 3.47091 3.47130 3.47680

Alpha virt. eigenvalues -- 3.51440 3.51793 3.51933 3.52709 3.52954

Alpha virt. eigenvalues -- 3.52992 3.53078 3.53247 3.55103 3.59276

Alpha virt. eigenvalues -- 3.60274 3.62463 3.62860 3.63114 3.63276

Alpha virt. eigenvalues -- 3.70489 3.70802 3.71302 3.71993 3.74288

Alpha virt. eigenvalues -- 3.74873 3.75248 3.76019 3.82139 3.83498

Alpha virt. eigenvalues -- 3.84030 3.84232 3.87744 3.88313 3.88930

Alpha virt. eigenvalues -- 3.89305 3.89396 3.90008 3.90154 3.90533

Alpha virt. eigenvalues -- 3.90862 4.00597 4.00901 4.00907 4.02208

Alpha virt. eigenvalues -- 4.02788 4.03276 4.03340 4.05880 4.11270

Alpha virt. eigenvalues -- 4.12224 4.13013 4.20439 4.24656 4.28124

Alpha virt. eigenvalues -- 4.29895 4.38567 4.41744 4.42813 4.45047

Alpha virt. eigenvalues -- 4.45345 4.47696 4.52637 4.53961 4.54408

Alpha virt. eigenvalues -- 4.75807 4.75821 4.75830 4.75846 4.78875

Alpha virt. eigenvalues -- 4.78951 4.78961 4.79108 5.11875 5.12319

Alpha virt. eigenvalues -- 5.12819 5.16076 5.22074 5.35296 5.36027

Alpha virt. eigenvalues -- 5.50377 7.83037 7.87377 7.88235 7.89044

Alpha virt. eigenvalues -- 8.10722 11.10889 23.20499 23.21937 23.22402

Alpha virt. eigenvalues -- 23.23127 23.56086 23.57946 23.58291 23.59143

Alpha virt. eigenvalues -- 23.71999 23.72045 23.73098 23.73124 23.80941

Alpha virt. eigenvalues -- 23.81100 23.81159 23.82015 23.82215 23.82255

Alpha virt. eigenvalues -- 23.82641 23.84172 23.87843 23.88640 23.89346

Alpha virt. eigenvalues -- 23.89834 23.91127 23.91203 23.93129 23.93212

Alpha virt. eigenvalues -- 23.98197 23.98285 23.98331 23.98500 24.05918

Alpha virt. eigenvalues -- 24.05920 24.06773 24.06777 24.09999 24.10046

Alpha virt. eigenvalues -- 24.10730 24.10784 24.13755 24.13763 24.13909

Alpha virt. eigenvalues -- 24.13974 24.14255 24.14285 24.15455 24.15738

Alpha virt. eigenvalues -- 35.56867 35.60009 35.60587 35.61444 35.69622

Alpha virt. eigenvalues -- 35.70289 35.70306 35.70346

Beta occ. eigenvalues -- -14.31972 -14.31972 -14.30814 -14.30814 -14.30814

Beta occ. eigenvalues -- -14.30814 -14.30721 -14.30721 -10.25411 -10.25411

Beta occ. eigenvalues -- -10.25410 -10.25410 -10.24332 -10.24332 -10.24331

Beta occ. eigenvalues -- -10.24331 -10.19387 -10.19387 -10.19348 -10.19348

Beta occ. eigenvalues -- -10.19013 -10.19013 -10.18974 -10.18974 -10.18802

Beta occ. eigenvalues -- -10.18802 -10.18802 -10.18802 -10.18676 -10.18676

Beta occ. eigenvalues -- -10.18634 -10.18634 -10.18450 -10.18450 -10.18449

Beta occ. eigenvalues -- -10.18449 -10.18124 -10.18124 -10.18083 -10.18083

Beta occ. eigenvalues -- -10.17878 -10.17878 -10.17876 -10.17876 -10.17794

Beta occ. eigenvalues -- -10.17794 -10.17751 -10.17751 -10.17680 -10.17680

Beta occ. eigenvalues -- -10.17680 -10.17680 -10.17556 -10.17556 -10.17512

Beta occ. eigenvalues -- -10.17512 -1.00112 -0.98795 -0.98722 -0.96094

Beta occ. eigenvalues -- -0.93904 -0.90347 -0.89701 -0.88482 -0.88067

Beta occ. eigenvalues -- -0.87966 -0.87856 -0.86435 -0.83030 -0.82964

Beta occ. eigenvalues -- -0.82601 -0.82593 -0.78995 -0.78615 -0.78337

Beta occ. eigenvalues -- -0.78328 -0.75586 -0.75551 -0.75290 -0.75247

Beta occ. eigenvalues -- -0.75151 -0.73600 -0.73479 -0.72894 -0.70394

Beta occ. eigenvalues -- -0.68929 -0.68512 -0.65819 -0.65514 -0.65170

Beta occ. eigenvalues -- -0.64915 -0.62927 -0.62343 -0.60960 -0.60825

Beta occ. eigenvalues -- -0.60429 -0.60422 -0.60416 -0.60128 -0.60049

Beta occ. eigenvalues -- -0.59622 -0.57985 -0.56807 -0.56572 -0.56560

Beta occ. eigenvalues -- -0.55818 -0.54360 -0.54262 -0.54078 -0.53519

Beta occ. eigenvalues -- -0.53433 -0.53143 -0.51803 -0.51771 -0.51627

Beta occ. eigenvalues -- -0.51601 -0.51265 -0.51141 -0.50694 -0.50678

Beta occ. eigenvalues -- -0.49013 -0.45768 -0.45763 -0.45609 -0.45550

Beta occ. eigenvalues -- -0.45536 -0.45482 -0.45085 -0.44873 -0.44292

Beta occ. eigenvalues -- -0.44270 -0.44068 -0.43969 -0.43783 -0.43625

Beta occ. eigenvalues -- -0.43431 -0.43302 -0.42936 -0.42817 -0.42526

Beta occ. eigenvalues -- -0.42201 -0.42098 -0.41978 -0.41965 -0.41262

Beta occ. eigenvalues -- -0.39574 -0.39563 -0.39251 -0.38887 -0.38173

Beta occ. eigenvalues -- -0.37792 -0.37746 -0.37590 -0.37157 -0.36636

Beta occ. eigenvalues -- -0.35705 -0.35584 -0.35402 -0.35225 -0.34211

Beta occ. eigenvalues -- -0.34107 -0.33909 -0.33888 -0.33809 -0.33570

Beta occ. eigenvalues -- -0.33050 -0.32592 -0.32506 -0.31752 -0.31266

Beta occ. eigenvalues -- -0.30802 -0.30595 -0.30208 -0.29425 -0.29120

Beta occ. eigenvalues -- -0.28634 -0.27919 -0.27685 -0.26555 -0.26284

Beta occ. eigenvalues -- -0.25323 -0.25051 -0.25043 -0.24816 -0.24517

Beta occ. eigenvalues -- -0.24280 -0.22723 -0.22450 -0.22327

Beta virt. eigenvalues -- -0.13918 -0.09287 -0.08991 -0.05997 -0.05641

Beta virt. eigenvalues -- -0.05456 -0.05159 -0.04130 0.00203 0.00203

Beta virt. eigenvalues -- 0.00401 0.00644 0.01016 0.01387 0.01586

Beta virt. eigenvalues -- 0.02141 0.03458 0.05024 0.05090 0.05729

Beta virt. eigenvalues -- 0.05962 0.06260 0.06288 0.06310 0.06392

Beta virt. eigenvalues -- 0.07153 0.07358 0.07374 0.07799 0.08349

Beta virt. eigenvalues -- 0.09629 0.09657 0.09845 0.09895 0.10556

Beta virt. eigenvalues -- 0.10936 0.11538 0.11663 0.11677 0.12338

Beta virt. eigenvalues -- 0.12397 0.12665 0.13004 0.13324 0.13362

Beta virt. eigenvalues -- 0.13524 0.13574 0.14431 0.14679 0.16415

Beta virt. eigenvalues -- 0.16508 0.17900 0.18321 0.18487 0.18524

Beta virt. eigenvalues -- 0.18871 0.18897 0.18984 0.19209 0.19347

Beta virt. eigenvalues -- 0.19774 0.20633 0.21827 0.21895 0.22682

Beta virt. eigenvalues -- 0.22738 0.23134 0.23144 0.23360 0.24373

Beta virt. eigenvalues -- 0.24599 0.25021 0.25920 0.26106 0.26456

Beta virt. eigenvalues -- 0.26525 0.26933 0.27664 0.27903 0.27935

Beta virt. eigenvalues -- 0.27982 0.28196 0.28310 0.28445 0.28703

Beta virt. eigenvalues -- 0.28802 0.29248 0.29308 0.29702 0.30618

Beta virt. eigenvalues -- 0.30728 0.30833 0.31122 0.31123 0.31319

Beta virt. eigenvalues -- 0.31326 0.31902 0.31927 0.32934 0.33002

Beta virt. eigenvalues -- 0.33287 0.34790 0.34844 0.35122 0.35493

Beta virt. eigenvalues -- 0.35991 0.36181 0.36310 0.36621 0.36952

Beta virt. eigenvalues -- 0.37192 0.37414 0.37513 0.37719 0.38009

Beta virt. eigenvalues -- 0.38030 0.38122 0.38371 0.38484 0.38709

Beta virt. eigenvalues -- 0.39097 0.39335 0.39340 0.39382 0.39803

Beta virt. eigenvalues -- 0.40205 0.40238 0.40292 0.40389 0.40521

Beta virt. eigenvalues -- 0.40911 0.41034 0.41281 0.41340 0.41668

Beta virt. eigenvalues -- 0.41870 0.42052 0.42675 0.42776 0.42936

Beta virt. eigenvalues -- 0.43044 0.43213 0.43297 0.43378 0.43461

Beta virt. eigenvalues -- 0.43583 0.43737 0.43761 0.43820 0.44136

Beta virt. eigenvalues -- 0.44143 0.44524 0.44716 0.44836 0.45095

Beta virt. eigenvalues -- 0.45115 0.45239 0.45728 0.46113 0.46222

Beta virt. eigenvalues -- 0.46290 0.46457 0.46587 0.46681 0.46804

Beta virt. eigenvalues -- 0.47068 0.47338 0.47425 0.47601 0.47622

Beta virt. eigenvalues -- 0.47662 0.48352 0.48581 0.48833 0.49107

Beta virt. eigenvalues -- 0.49325 0.49637 0.49814 0.50464 0.50790

Beta virt. eigenvalues -- 0.50974 0.50992 0.51508 0.51611 0.51658

Beta virt. eigenvalues -- 0.52355 0.52405 0.53242 0.53382 0.53506

Beta virt. eigenvalues -- 0.53539 0.53937 0.53943 0.54708 0.55017

Beta virt. eigenvalues -- 0.55549 0.55951 0.56558 0.56677 0.56838

Beta virt. eigenvalues -- 0.58005 0.58251 0.58896 0.58961 0.59455

Beta virt. eigenvalues -- 0.60064 0.60310 0.60645 0.60924 0.60961

Beta virt. eigenvalues -- 0.61154 0.61347 0.61866 0.61888 0.61910

Beta virt. eigenvalues -- 0.62199 0.62331 0.62622 0.62872 0.62993

Beta virt. eigenvalues -- 0.63079 0.63221 0.63262 0.63583 0.63751

Beta virt. eigenvalues -- 0.64366 0.64428 0.64485 0.64558 0.65540

Beta virt. eigenvalues -- 0.65906 0.65934 0.66350 0.67347 0.67619

Beta virt. eigenvalues -- 0.67781 0.68127 0.68184 0.68339 0.68474

Beta virt. eigenvalues -- 0.69035 0.69072 0.69381 0.69458 0.69464

Beta virt. eigenvalues -- 0.70018 0.70024 0.70807 0.70991 0.71118

Beta virt. eigenvalues -- 0.72262 0.72771 0.73177 0.73194 0.73300

Beta virt. eigenvalues -- 0.73406 0.73595 0.73997 0.74660 0.74823

Beta virt. eigenvalues -- 0.75344 0.75378 0.76024 0.76159 0.76483

Beta virt. eigenvalues -- 0.76861 0.76999 0.78438 0.78635 0.78759

Beta virt. eigenvalues -- 0.79035 0.79290 0.79458 0.79475 0.79817

Beta virt. eigenvalues -- 0.80329 0.80584 0.80639 0.80783 0.80974

Beta virt. eigenvalues -- 0.81442 0.81498 0.81783 0.82152 0.82279

Beta virt. eigenvalues -- 0.82735 0.82906 0.83141 0.84224 0.84273

Beta virt. eigenvalues -- 0.84443 0.84967 0.85130 0.85311 0.85906

Beta virt. eigenvalues -- 0.86062 0.86344 0.87821 0.87856 0.87903

Beta virt. eigenvalues -- 0.88401 0.88718 0.88781 0.90042 0.91695

Beta virt. eigenvalues -- 0.91796 0.92174 0.92609 0.93648 0.93949

Beta virt. eigenvalues -- 0.94525 0.94926 0.94936 0.95870 0.96173

Beta virt. eigenvalues -- 0.96521 0.96949 0.97131 0.97572 0.97582

Beta virt. eigenvalues -- 0.97616 0.97987 0.98147 0.98336 0.98517

Beta virt. eigenvalues -- 0.98836 0.98914 0.99602 0.99884 0.99937

Beta virt. eigenvalues -- 1.00321 1.01343 1.02047 1.02389 1.02542

Beta virt. eigenvalues -- 1.02798 1.03675 1.03896 1.03913 1.05326

Beta virt. eigenvalues -- 1.05564 1.06261 1.06564 1.07225 1.07292

Beta virt. eigenvalues -- 1.07500 1.08718 1.10061 1.10204 1.10340

Beta virt. eigenvalues -- 1.10533 1.10866 1.11139 1.11340 1.11543

Beta virt. eigenvalues -- 1.11583 1.11822 1.11856 1.12442 1.12475

Beta virt. eigenvalues -- 1.12500 1.12728 1.12772 1.13740 1.14164

Beta virt. eigenvalues -- 1.14336 1.14702 1.14741 1.16760 1.16782

Beta virt. eigenvalues -- 1.17106 1.17111 1.17189 1.17720 1.17836

Beta virt. eigenvalues -- 1.18471 1.18852 1.19515 1.20043 1.21207

Beta virt. eigenvalues -- 1.21600 1.21608 1.21884 1.21888 1.21939

Beta virt. eigenvalues -- 1.22558 1.22678 1.22742 1.23415 1.24793

Beta virt. eigenvalues -- 1.25071 1.25444 1.25813 1.25920 1.26802

Beta virt. eigenvalues -- 1.26954 1.27311 1.27779 1.27837 1.28097

Beta virt. eigenvalues -- 1.29155 1.29168 1.29824 1.30299 1.30320

Beta virt. eigenvalues -- 1.30791 1.33181 1.34430 1.34563 1.35042

Beta virt. eigenvalues -- 1.35387 1.35500 1.36458 1.38246 1.38519

Beta virt. eigenvalues -- 1.39325 1.39437 1.39628 1.40105 1.40361

Beta virt. eigenvalues -- 1.40702 1.42823 1.42998 1.43095 1.44645

Beta virt. eigenvalues -- 1.44744 1.44809 1.44830 1.45019 1.45755

Beta virt. eigenvalues -- 1.45804 1.46327 1.47309 1.48351 1.48735

Beta virt. eigenvalues -- 1.48882 1.51413 1.51611 1.51658 1.51802

Beta virt. eigenvalues -- 1.51898 1.51974 1.52059 1.52139 1.52170

Beta virt. eigenvalues -- 1.52284 1.52691 1.52958 1.53141 1.53251

Beta virt. eigenvalues -- 1.53548 1.53563 1.54190 1.54413 1.54427

Beta virt. eigenvalues -- 1.55247 1.56664 1.56826 1.57118 1.58057

Beta virt. eigenvalues -- 1.58353 1.61047 1.61099 1.64034 1.64654

Beta virt. eigenvalues -- 1.64987 1.65080 1.65210 1.65237 1.67081

Beta virt. eigenvalues -- 1.68357 1.68431 1.69350 1.69700 1.69774

Beta virt. eigenvalues -- 1.70783 1.70924 1.71768 1.71934 1.72391

Beta virt. eigenvalues -- 1.72851 1.73837 1.74081 1.74480 1.75389

Beta virt. eigenvalues -- 1.75893 1.76696 1.76982 1.77276 1.77966

Beta virt. eigenvalues -- 1.78054 1.78087 1.79221 1.80084 1.80343

Beta virt. eigenvalues -- 1.81404 1.81945 1.82057 1.82175 1.82277

Beta virt. eigenvalues -- 1.82797 1.82962 1.83377 1.83753 1.84684

Beta virt. eigenvalues -- 1.85282 1.86113 1.86452 1.86517 1.86688

Beta virt. eigenvalues -- 1.87283 1.87466 1.88313 1.88717 1.88866

Beta virt. eigenvalues -- 1.89038 1.89275 1.89651 1.89804 1.90269

Beta virt. eigenvalues -- 1.90580 1.91441 1.91537 1.91771 1.92248

Beta virt. eigenvalues -- 1.92256 1.92267 1.92481 1.92752 1.92843

Beta virt. eigenvalues -- 1.92854 1.92882 1.94370 1.94750 1.94931

Beta virt. eigenvalues -- 1.94937 1.95142 1.95340 1.95347 1.95725

Beta virt. eigenvalues -- 1.96311 1.96941 1.97177 1.97441 1.97485

Beta virt. eigenvalues -- 1.97678 1.98042 1.98318 1.99658 1.99741

Beta virt. eigenvalues -- 1.99924 2.02221 2.03035 2.04821 2.04917

Beta virt. eigenvalues -- 2.05268 2.05306 2.07497 2.08116 2.09016

Beta virt. eigenvalues -- 2.09854 2.12447 2.13044 2.14032 2.14973

Beta virt. eigenvalues -- 2.15349 2.15472 2.15673 2.17808 2.18769

Beta virt. eigenvalues -- 2.19246 2.19807 2.21380 2.21432 2.21793

Beta virt. eigenvalues -- 2.22155 2.22205 2.22265 2.22400 2.22952

Beta virt. eigenvalues -- 2.23353 2.24783 2.24830 2.24867 2.25134

Beta virt. eigenvalues -- 2.26257 2.26596 2.26632 2.27646 2.27873

Beta virt. eigenvalues -- 2.28228 2.28473 2.30151 2.31412 2.31533

Beta virt. eigenvalues -- 2.31600 2.31802 2.31952 2.32878 2.34027

Beta virt. eigenvalues -- 2.34343 2.34931 2.35178 2.35216 2.35339

Beta virt. eigenvalues -- 2.36144 2.36408 2.36497 2.38411 2.39507

Beta virt. eigenvalues -- 2.40696 2.40941 2.43434 2.43951 2.44303

Beta virt. eigenvalues -- 2.44799 2.45008 2.45457 2.45647 2.45751

Beta virt. eigenvalues -- 2.46640 2.48106 2.50059 2.50769 2.51329

Beta virt. eigenvalues -- 2.51784 2.52079 2.52541 2.53167 2.53237

Beta virt. eigenvalues -- 2.53465 2.53488 2.53983 2.55173 2.55257

Beta virt. eigenvalues -- 2.55274 2.55481 2.56183 2.56257 2.56562

Beta virt. eigenvalues -- 2.57302 2.57682 2.57746 2.57910 2.59091

Beta virt. eigenvalues -- 2.61259 2.63324 2.64911 2.65029 2.65039

Beta virt. eigenvalues -- 2.65399 2.65698 2.67943 2.69046 2.69698

Beta virt. eigenvalues -- 2.69721 2.70031 2.70913 2.70930 2.71272

Beta virt. eigenvalues -- 2.71395 2.72114 2.72321 2.72485 2.73271

Beta virt. eigenvalues -- 2.73544 2.73777 2.73864 2.73909 2.74104

Beta virt. eigenvalues -- 2.74701 2.74733 2.75067 2.75214 2.75835

Beta virt. eigenvalues -- 2.76094 2.78150 2.80548 2.80885 2.80953

Beta virt. eigenvalues -- 2.81106 2.81843 2.82279 2.82327 2.82511

Beta virt. eigenvalues -- 2.82810 2.82813 2.82820 2.85019 2.86452

Beta virt. eigenvalues -- 2.86597 2.87018 2.87040 2.87451 2.87483

Beta virt. eigenvalues -- 2.87744 2.88093 2.88217 2.89470 2.89733

Beta virt. eigenvalues -- 2.89756 2.91624 2.92721 2.93162 2.93748

Beta virt. eigenvalues -- 2.94317 2.96967 2.97657 2.99243 3.02563

Beta virt. eigenvalues -- 3.03164 3.03428 3.04058 3.04305 3.05053

Beta virt. eigenvalues -- 3.05447 3.05817 3.07886 3.08550 3.08885

Beta virt. eigenvalues -- 3.15150 3.15642 3.15741 3.15940 3.16591

Beta virt. eigenvalues -- 3.17278 3.17604 3.18599 3.18742 3.19864

Beta virt. eigenvalues -- 3.19924 3.20076 3.20190 3.21491 3.21519

Beta virt. eigenvalues -- 3.22623 3.23074 3.23208 3.23868 3.24515

Beta virt. eigenvalues -- 3.24760 3.26481 3.26953 3.27216 3.27590

Beta virt. eigenvalues -- 3.28222 3.28242 3.28396 3.28424 3.28470

Beta virt. eigenvalues -- 3.28590 3.29407 3.29423 3.31264 3.31291

Beta virt. eigenvalues -- 3.32207 3.32357 3.32449 3.33885 3.34003

Beta virt. eigenvalues -- 3.34071 3.34927 3.35020 3.35221 3.37532

Beta virt. eigenvalues -- 3.39857 3.41225 3.41266 3.42161 3.42264

Beta virt. eigenvalues -- 3.42782 3.42914 3.43582 3.46802 3.47132

Beta virt. eigenvalues -- 3.47150 3.47715 3.51521 3.51864 3.52033

Beta virt. eigenvalues -- 3.52789 3.53023 3.53070 3.53147 3.53331

Beta virt. eigenvalues -- 3.55294 3.59404 3.60430 3.62501 3.62891

Beta virt. eigenvalues -- 3.63151 3.63376 3.70589 3.70928 3.71382

Beta virt. eigenvalues -- 3.72075 3.74442 3.75041 3.75417 3.76226

Beta virt. eigenvalues -- 3.82293 3.83576 3.84059 3.84416 3.87898

Beta virt. eigenvalues -- 3.88376 3.89080 3.89400 3.89428 3.89864

Beta virt. eigenvalues -- 3.90274 3.90922 3.90963 4.00640 4.00941

Beta virt. eigenvalues -- 4.00984 4.02270 4.02905 4.03416 4.03426

Beta virt. eigenvalues -- 4.06026 4.11307 4.12302 4.13077 4.20561

Beta virt. eigenvalues -- 4.24715 4.28246 4.29982 4.38687 4.42018

Beta virt. eigenvalues -- 4.43000 4.45326 4.45565 4.47902 4.52856

Beta virt. eigenvalues -- 4.54062 4.54533 4.75875 4.75891 4.75903

Beta virt. eigenvalues -- 4.75916 4.78941 4.79003 4.79060 4.79192

Beta virt. eigenvalues -- 5.12101 5.12624 5.13054 5.16369 5.22375

Beta virt. eigenvalues -- 5.35614 5.36346 5.50705 7.83036 7.87369

Beta virt. eigenvalues -- 7.88258 7.89046 8.10724 11.10894 23.20530

Beta virt. eigenvalues -- 23.21955 23.22447 23.23160 23.56154 23.57974

Beta virt. eigenvalues -- 23.58383 23.59198 23.72051 23.72098 23.73122

Beta virt. eigenvalues -- 23.73149 23.81180 23.81251 23.81262 23.82067

Beta virt. eigenvalues -- 23.82289 23.82595 23.82854 23.84475 23.88224

Beta virt. eigenvalues -- 23.89053 23.89572 23.90126 23.91136 23.91224

Beta virt. eigenvalues -- 23.93182 23.93271 23.98213 23.98288 23.98362

Beta virt. eigenvalues -- 23.98518 24.05933 24.05935 24.06801 24.06805

Beta virt. eigenvalues -- 24.10060 24.10107 24.10754 24.10808 24.13770

Beta virt. eigenvalues -- 24.13777 24.13948 24.14009 24.14290 24.14321

Beta virt. eigenvalues -- 24.15465 24.15750 35.56867 35.60138 35.60430

Beta virt. eigenvalues -- 35.61415 35.69623 35.70295 35.70328 35.70329

Condensed to atoms (all electrons):

Atomic-Atomic Spin Densities.

Mulliken charges and spin densities:

1 2

1 C 0.381400 0.266653

2 N -0.637012 -0.091740

3 C 0.381400 0.266653

4 C -0.077843 -0.018821

5 C -0.077843 -0.018821

6 N -0.421465 -0.016333

7 C 0.407153 0.123905

8 N -0.682659 0.061687

9 C 0.407153 0.123905

10 C -0.073783 -0.023061

11 C -0.073783 -0.023061

12 N -0.421465 -0.016333

13 C -0.073783 -0.023061

14 C -0.073783 -0.023061

15 C 0.407153 0.123905

16 N -0.682659 0.061687

17 C 0.407153 0.123905

18 N -0.421465 -0.016333

19 N -0.637012 -0.091740

20 C 0.381400 0.266653

21 C -0.077843 -0.018821

22 C -0.077843 -0.018821

23 C 0.381400 0.266653

24 N -0.421465 -0.016333

25 Zn 1.393328 0.000344

26 C -0.200170 0.046919

27 C 0.010528 -0.000171

28 C 0.010528 -0.000171

29 C -0.200170 0.046919

30 C -0.209473 0.081438

31 C 0.007480 0.011450

32 C 0.007480 0.011450

33 C -0.209473 0.081438

34 C -0.200170 0.046919

35 C 0.010528 -0.000171

36 C 0.010528 -0.000171

37 C -0.200170 0.046919

38 C -0.209473 0.081438

39 C 0.007480 0.011450

40 C 0.007480 0.011450

41 C -0.209473 0.081438

42 C -0.228402 0.013860

43 C -0.223059 0.020143

44 C -0.223059 0.020143

45 C -0.228402 0.013860

46 C -0.226241 0.009920

47 C -0.218435 0.008274

48 C -0.218435 0.008274

49 C -0.226241 0.009920

50 C -0.228402 0.013860

51 C -0.223059 0.020143

52 C -0.223059 0.020143

53 C -0.228402 0.013860

54 C -0.226241 0.009920

55 C -0.218435 0.008274

56 C -0.218435 0.008274

57 C -0.226241 0.009920

58 H 0.232895 -0.002250

59 H 0.232895 -0.002250

60 H 0.229811 -0.004078

61 H 0.229811 -0.004078

62 H 0.232895 -0.002250

63 H 0.232895 -0.002250

64 H 0.229811 -0.004078

65 H 0.229811 -0.004078

66 H 0.229923 -0.000569

67 H 0.228282 -0.001329

68 H 0.228282 -0.001329

69 H 0.229923 -0.000569

70 H 0.232380 -0.000466

71 H 0.230522 -0.000545

72 H 0.230522 -0.000545

73 H 0.232380 -0.000466

74 H 0.229923 -0.000569

75 H 0.228282 -0.001329

76 H 0.228282 -0.001329

77 H 0.229923 -0.000569

78 H 0.232380 -0.000466

79 H 0.230522 -0.000545

80 H 0.230522 -0.000545

81 H 0.232380 -0.000466

Sum of Mulliken charges = 0.00000 2.00000

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

1 2

1 C 0.381400 0.266653

2 N -0.637012 -0.091740

3 C 0.381400 0.266653

4 C -0.077843 -0.018821

5 C -0.077843 -0.018821

6 N -0.421465 -0.016333

7 C 0.407153 0.123905

8 N -0.682659 0.061687

9 C 0.407153 0.123905

10 C -0.073783 -0.023061

11 C -0.073783 -0.023061

12 N -0.421465 -0.016333

13 C -0.073783 -0.023061

14 C -0.073783 -0.023061

15 C 0.407153 0.123905

16 N -0.682659 0.061687

17 C 0.407153 0.123905

18 N -0.421465 -0.016333

19 N -0.637012 -0.091740

20 C 0.381400 0.266653

21 C -0.077843 -0.018821

22 C -0.077843 -0.018821

23 C 0.381400 0.266653

24 N -0.421465 -0.016333

25 Zn 1.393328 0.000344

26 C 0.032725 0.044669

27 C 0.010528 -0.000171

28 C 0.010528 -0.000171

29 C 0.032725 0.044669

30 C 0.020338 0.077360

31 C 0.007480 0.011450

32 C 0.007480 0.011450

33 C 0.020338 0.077360

34 C 0.032725 0.044669

35 C 0.010528 -0.000171

36 C 0.010528 -0.000171

37 C 0.032725 0.044669

38 C 0.020338 0.077360

39 C 0.007480 0.011450

40 C 0.007480 0.011450

41 C 0.020338 0.077360

42 C 0.001521 0.013292

43 C 0.005223 0.018814

44 C 0.005223 0.018814

45 C 0.001521 0.013292

46 C 0.006139 0.009454

47 C 0.012087 0.007728

48 C 0.012087 0.007728

49 C 0.006139 0.009454

50 C 0.001521 0.013292

51 C 0.005223 0.018814

52 C 0.005223 0.018814

53 C 0.001521 0.013292

54 C 0.006139 0.009454

55 C 0.012087 0.007728

56 C 0.012087 0.007728

57 C 0.006139 0.009454

Electronic spatial extent (au): <R\*\*2>= 50275.8593

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0000 Y= 0.0000 Z= 2.2512 Tot= 2.2512

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

XX= -243.8152 YY= -273.0570 ZZ= -336.5616

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XX= 40.6627 YY= 11.4209 ZZ= -52.0836

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XXX= 0.0000 YYY= 0.0000 ZZZ= 65.9005 XYY= 0.0000

XXY= 0.0000 XXZ= -11.0098 XZZ= 0.0000 YZZ= 0.0000

YYZ= -93.7525 XYZ= 0.0000

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

XXXX= -26708.8585 YYYY= -28163.0873 ZZZZ= -687.6819 XXXY= 0.0000

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

ZZZY= 0.0000 XXYY= -10219.9075 XXZZ= -6670.1971 YYZZ= -6428.2842

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 6.889497004798D+03 E-N=-1.932241872057D+04 KE= 2.388748248272D+03

Symmetry A1 KE= 6.741335722275D+02

Symmetry A2 KE= 5.317218971740D+02

Symmetry B1 KE= 5.922793821404D+02

Symmetry B2 KE= 5.906133967299D+02

Isotropic Fermi Contact Couplings

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

1 C(13) 0.01961 11.02188 3.93288 3.67650

2 N(14) -0.01730 -2.79557 -0.99753 -0.93250

3 C(13) 0.01961 11.02188 3.93288 3.67650

4 C(13) -0.00963 -5.41357 -1.93170 -1.80577

5 C(13) -0.00963 -5.41357 -1.93170 -1.80577

6 N(14) -0.00558 -0.90113 -0.32155 -0.30058

7 C(13) 0.00763 4.28656 1.52955 1.42984

8 N(14) 0.00560 0.90446 0.32273 0.30170

9 C(13) 0.00763 4.28656 1.52955 1.42984

10 C(13) -0.00556 -3.12806 -1.11617 -1.04341

11 C(13) -0.00556 -3.12806 -1.11617 -1.04341

12 N(14) -0.00558 -0.90113 -0.32155 -0.30058

13 C(13) -0.00556 -3.12806 -1.11617 -1.04341

14 C(13) -0.00556 -3.12806 -1.11617 -1.04341

15 C(13) 0.00763 4.28656 1.52955 1.42984

16 N(14) 0.00560 0.90446 0.32273 0.30170

17 C(13) 0.00763 4.28656 1.52955 1.42984

18 N(14) -0.00558 -0.90113 -0.32155 -0.30058

19 N(14) -0.01730 -2.79557 -0.99753 -0.93250

20 C(13) 0.01961 11.02188 3.93288 3.67650

21 C(13) -0.00963 -5.41357 -1.93170 -1.80577

22 C(13) -0.00963 -5.41357 -1.93170 -1.80577

23 C(13) 0.01961 11.02188 3.93288 3.67650

24 N(14) -0.00558 -0.90113 -0.32155 -0.30058

25 Zn(67) 0.00000 0.00000 0.00000 0.00000

26 C(13) 0.00248 1.39416 0.49747 0.46504

27 C(13) -0.00140 -0.78811 -0.28122 -0.26289

28 C(13) -0.00140 -0.78811 -0.28122 -0.26289

29 C(13) 0.00248 1.39416 0.49747 0.46504

30 C(13) 0.00325 1.82452 0.65103 0.60859

31 C(13) -0.00211 -1.18373 -0.42238 -0.39485

32 C(13) -0.00211 -1.18373 -0.42238 -0.39485

33 C(13) 0.00325 1.82452 0.65103 0.60859

34 C(13) 0.00248 1.39416 0.49747 0.46504

35 C(13) -0.00140 -0.78811 -0.28122 -0.26289

36 C(13) -0.00140 -0.78811 -0.28122 -0.26289

37 C(13) 0.00248 1.39416 0.49747 0.46504

38 C(13) 0.00325 1.82452 0.65103 0.60859

39 C(13) -0.00211 -1.18373 -0.42238 -0.39485

40 C(13) -0.00211 -1.18373 -0.42238 -0.39485

41 C(13) 0.00325 1.82452 0.65103 0.60859

42 C(13) -0.00033 -0.18589 -0.06633 -0.06201

43 C(13) 0.00012 0.07015 0.02503 0.02340

44 C(13) 0.00012 0.07015 0.02503 0.02340

45 C(13) -0.00033 -0.18589 -0.06633 -0.06201

46 C(13) 0.00016 0.08824 0.03149 0.02943

47 C(13) -0.00005 -0.02817 -0.01005 -0.00940

48 C(13) -0.00005 -0.02817 -0.01005 -0.00940

49 C(13) 0.00016 0.08824 0.03149 0.02943

50 C(13) -0.00033 -0.18589 -0.06633 -0.06201

51 C(13) 0.00012 0.07015 0.02503 0.02340

52 C(13) 0.00012 0.07015 0.02503 0.02340

53 C(13) -0.00033 -0.18589 -0.06633 -0.06201

54 C(13) 0.00016 0.08824 0.03149 0.02943

55 C(13) -0.00005 -0.02817 -0.01005 -0.00940

56 C(13) -0.00005 -0.02817 -0.01005 -0.00940

57 C(13) 0.00016 0.08824 0.03149 0.02943

58 H(1) -0.00066 -1.48237 -0.52895 -0.49446

59 H(1) -0.00066 -1.48237 -0.52895 -0.49446

60 H(1) -0.00118 -2.64587 -0.94411 -0.88257

61 H(1) -0.00118 -2.64587 -0.94411 -0.88257

62 H(1) -0.00066 -1.48237 -0.52895 -0.49446

63 H(1) -0.00066 -1.48237 -0.52895 -0.49446

64 H(1) -0.00118 -2.64587 -0.94411 -0.88257

65 H(1) -0.00118 -2.64587 -0.94411 -0.88257

66 H(1) -0.00022 -0.50192 -0.17910 -0.16742

67 H(1) -0.00034 -0.75739 -0.27026 -0.25264

68 H(1) -0.00034 -0.75739 -0.27026 -0.25264

69 H(1) -0.00022 -0.50192 -0.17910 -0.16742

70 H(1) -0.00015 -0.33581 -0.11982 -0.11201

71 H(1) -0.00014 -0.31739 -0.11325 -0.10587

72 H(1) -0.00014 -0.31739 -0.11325 -0.10587

73 H(1) -0.00015 -0.33581 -0.11982 -0.11201

74 H(1) -0.00022 -0.50192 -0.17910 -0.16742

75 H(1) -0.00034 -0.75739 -0.27026 -0.25264

76 H(1) -0.00034 -0.75739 -0.27026 -0.25264

77 H(1) -0.00022 -0.50192 -0.17910 -0.16742

78 H(1) -0.00015 -0.33581 -0.11982 -0.11201

79 H(1) -0.00014 -0.31739 -0.11325 -0.10587

80 H(1) -0.00014 -0.31739 -0.11325 -0.10587

81 H(1) -0.00015 -0.33581 -0.11982 -0.11201

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

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

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

1 Atom -0.174871 -0.158496 0.333367

2 Atom 0.080593 0.063283 -0.143876

3 Atom -0.174871 -0.158496 0.333367

4 Atom -0.006862 0.006031 0.000831

5 Atom -0.006862 0.006031 0.000831

6 Atom -0.014968 -0.007906 0.022874

7 Atom -0.080945 -0.076635 0.157580

8 Atom -0.089097 -0.084026 0.173123

9 Atom -0.080945 -0.076635 0.157580

10 Atom 0.012761 0.005398 -0.018159

11 Atom 0.012761 0.005398 -0.018159

12 Atom -0.014968 -0.007906 0.022874

13 Atom 0.012761 0.005398 -0.018159

14 Atom 0.012761 0.005398 -0.018159

15 Atom -0.080945 -0.076635 0.157580

16 Atom -0.089097 -0.084026 0.173123

17 Atom -0.080945 -0.076635 0.157580

18 Atom -0.014968 -0.007906 0.022874

19 Atom 0.080593 0.063283 -0.143876

20 Atom -0.174871 -0.158496 0.333367

21 Atom -0.006862 0.006031 0.000831

22 Atom -0.006862 0.006031 0.000831

23 Atom -0.174871 -0.158496 0.333367

24 Atom -0.014968 -0.007906 0.022874

25 Atom 0.013225 -0.010316 -0.002910

26 Atom -0.023950 -0.026801 0.050752

27 Atom 0.000141 -0.002572 0.002430

28 Atom 0.000141 -0.002572 0.002430

29 Atom -0.023950 -0.026801 0.050752

30 Atom -0.046620 -0.038183 0.084803

31 Atom -0.011058 -0.006445 0.017502

32 Atom -0.011058 -0.006445 0.017502

33 Atom -0.046620 -0.038183 0.084803

34 Atom -0.023950 -0.026801 0.050752

35 Atom 0.000141 -0.002572 0.002430

36 Atom 0.000141 -0.002572 0.002430

37 Atom -0.023950 -0.026801 0.050752

38 Atom -0.046620 -0.038183 0.084803

39 Atom -0.011058 -0.006445 0.017502

40 Atom -0.011058 -0.006445 0.017502

41 Atom -0.046620 -0.038183 0.084803

42 Atom -0.010094 -0.005251 0.015345

43 Atom -0.012760 -0.010399 0.023159

44 Atom -0.012760 -0.010399 0.023159

45 Atom -0.010094 -0.005251 0.015345

46 Atom -0.004282 -0.006489 0.010770

47 Atom -0.004477 -0.005483 0.009960

48 Atom -0.004477 -0.005483 0.009960

49 Atom -0.004282 -0.006489 0.010770

50 Atom -0.010094 -0.005251 0.015345

51 Atom -0.012760 -0.010399 0.023159

52 Atom -0.012760 -0.010399 0.023159

53 Atom -0.010094 -0.005251 0.015345

54 Atom -0.004282 -0.006489 0.010770

55 Atom -0.004477 -0.005483 0.009960

56 Atom -0.004477 -0.005483 0.009960

57 Atom -0.004282 -0.006489 0.010770

58 Atom -0.000806 0.002997 -0.002191

59 Atom -0.000806 0.002997 -0.002191

60 Atom 0.006121 -0.003089 -0.003032

61 Atom 0.006121 -0.003089 -0.003032

62 Atom -0.000806 0.002997 -0.002191

63 Atom -0.000806 0.002997 -0.002191

64 Atom 0.006121 -0.003089 -0.003032

65 Atom 0.006121 -0.003089 -0.003032

66 Atom 0.001113 0.000481 -0.001595

67 Atom -0.001541 0.002344 -0.000803

68 Atom -0.001541 0.002344 -0.000803

69 Atom 0.001113 0.000481 -0.001595

70 Atom 0.000431 0.000583 -0.001014

71 Atom 0.001265 -0.000690 -0.000575

72 Atom 0.001265 -0.000690 -0.000575

73 Atom 0.000431 0.000583 -0.001014

74 Atom 0.001113 0.000481 -0.001595

75 Atom -0.001541 0.002344 -0.000803

76 Atom -0.001541 0.002344 -0.000803

77 Atom 0.001113 0.000481 -0.001595

78 Atom 0.000431 0.000583 -0.001014

79 Atom 0.001265 -0.000690 -0.000575

80 Atom 0.001265 -0.000690 -0.000575

81 Atom 0.000431 0.000583 -0.001014

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XY XZ YZ

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1 Atom -0.000841 0.016848 0.082851

2 Atom 0.000000 0.000000 -0.046162

3 Atom 0.000841 -0.016848 0.082851

4 Atom -0.002562 0.000249 0.000305

5 Atom 0.002562 -0.000249 0.000305

6 Atom 0.006194 -0.010361 0.015593

7 Atom -0.000125 -0.014544 0.003360

8 Atom 0.000000 -0.027327 0.000000

9 Atom 0.000125 -0.014544 -0.003360

10 Atom 0.001563 0.000849 0.000163

11 Atom -0.001563 0.000849 -0.000163

12 Atom -0.006194 0.010361 0.015593

13 Atom 0.001563 -0.000849 -0.000163

14 Atom -0.001563 -0.000849 0.000163

15 Atom -0.000125 0.014544 -0.003360

16 Atom 0.000000 0.027327 0.000000

17 Atom 0.000125 0.014544 0.003360

18 Atom 0.006194 0.010361 -0.015593

19 Atom 0.000000 0.000000 0.046162

20 Atom 0.000841 0.016848 -0.082851

21 Atom -0.002562 -0.000249 -0.000305

22 Atom 0.002562 0.000249 -0.000305

23 Atom -0.000841 -0.016848 -0.082851

24 Atom -0.006194 -0.010361 -0.015593

25 Atom 0.000000 0.000000 0.000000

26 Atom -0.000133 0.002813 0.001131

27 Atom -0.000389 0.000155 0.000118

28 Atom 0.000389 0.000155 -0.000118

29 Atom 0.000133 0.002813 -0.001131

30 Atom 0.000195 -0.000320 -0.022732

31 Atom -0.000810 -0.000188 -0.004476

32 Atom 0.000810 0.000188 -0.004476

33 Atom -0.000195 0.000320 -0.022732

34 Atom 0.000133 -0.002813 0.001131

35 Atom 0.000389 -0.000155 0.000118

36 Atom -0.000389 -0.000155 -0.000118

37 Atom -0.000133 -0.002813 -0.001131

38 Atom 0.000195 0.000320 0.022732

39 Atom -0.000810 0.000188 0.004476

40 Atom 0.000810 -0.000188 0.004476

41 Atom -0.000195 -0.000320 0.022732

42 Atom 0.000087 0.000025 -0.003790

43 Atom 0.000051 -0.000001 -0.006210

44 Atom -0.000051 0.000001 -0.006210

45 Atom -0.000087 -0.000025 -0.003790

46 Atom 0.000014 0.000676 -0.000071

47 Atom 0.000061 0.000645 -0.000001

48 Atom -0.000061 0.000645 0.000001

49 Atom -0.000014 0.000676 0.000071

50 Atom 0.000087 -0.000025 0.003790

51 Atom 0.000051 0.000001 0.006210

52 Atom -0.000051 -0.000001 0.006210

53 Atom -0.000087 0.000025 0.003790

54 Atom -0.000014 -0.000676 -0.000071

55 Atom -0.000061 -0.000645 -0.000001

56 Atom 0.000061 -0.000645 0.000001

57 Atom 0.000014 -0.000676 0.000071

58 Atom 0.000518 0.000047 -0.000196

59 Atom -0.000518 0.000047 0.000196

60 Atom 0.000593 0.000061 -0.000120

61 Atom -0.000593 -0.000061 -0.000120

62 Atom -0.000518 -0.000047 -0.000196

63 Atom 0.000518 -0.000047 0.000196

64 Atom 0.000593 -0.000061 0.000120

65 Atom -0.000593 0.000061 0.000120

66 Atom -0.000394 -0.000066 0.000337

67 Atom -0.001455 -0.000257 0.000556

68 Atom 0.001455 0.000257 0.000556

69 Atom 0.000394 0.000066 0.000337

70 Atom -0.000300 -0.000030 0.000016

71 Atom -0.000701 -0.000060 0.000028

72 Atom 0.000701 -0.000060 -0.000028

73 Atom 0.000300 -0.000030 -0.000016

74 Atom -0.000394 0.000066 -0.000337

75 Atom -0.001455 0.000257 -0.000556

76 Atom 0.001455 -0.000257 -0.000556

77 Atom 0.000394 -0.000066 -0.000337

78 Atom 0.000300 0.000030 0.000016

79 Atom 0.000701 0.000060 0.000028

80 Atom -0.000701 0.000060 -0.000028

81 Atom -0.000300 0.000030 -0.000016

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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 -0.1777 -23.840 -8.507 -7.952 0.8430 0.5259 -0.1131

1 C(13) Bbb -0.1698 -22.787 -8.131 -7.601 -0.5370 0.8351 -0.1195

Bcc 0.3475 46.627 16.638 15.553 0.0316 0.1615 0.9864

Baa -0.1537 -5.928 -2.115 -1.977 0.0000 0.2081 0.9781

2 N(14) Bbb 0.0731 2.819 1.006 0.940 0.0000 0.9781 -0.2081

Bcc 0.0806 3.108 1.109 1.037 1.0000 0.0000 0.0000

Baa -0.1777 -23.840 -8.507 -7.952 0.8430 -0.5259 0.1131

3 C(13) Bbb -0.1698 -22.787 -8.131 -7.601 0.5370 0.8351 -0.1195

Bcc 0.3475 46.627 16.638 15.553 -0.0316 0.1615 0.9864

Baa -0.0074 -0.988 -0.353 -0.330 0.9814 0.1886 -0.0369

4 C(13) Bbb 0.0008 0.112 0.040 0.037 0.0446 -0.0367 0.9983

Bcc 0.0065 0.877 0.313 0.292 -0.1869 0.9814 0.0444

Baa -0.0074 -0.988 -0.353 -0.330 0.9814 -0.1886 0.0369

5 C(13) Bbb 0.0008 0.112 0.040 0.037 -0.0446 -0.0367 0.9983

Bcc 0.0065 0.877 0.313 0.292 0.1869 0.9814 0.0444

Baa -0.0249 -0.961 -0.343 -0.320 0.7302 -0.5868 0.3498

6 N(14) Bbb -0.0057 -0.219 -0.078 -0.073 0.6635 0.7312 -0.1586

Bcc 0.0306 1.179 0.421 0.393 -0.1627 0.3479 0.9233

Baa -0.0818 -10.981 -3.918 -3.663 0.9980 -0.0153 0.0608

7 C(13) Bbb -0.0767 -10.290 -3.672 -3.432 0.0161 0.9998 -0.0133

Bcc 0.1585 21.271 7.590 7.095 -0.0606 0.0143 0.9981

Baa -0.0919 -3.545 -1.265 -1.182 0.9947 0.0000 0.1026

8 N(14) Bbb -0.0840 -3.241 -1.156 -1.081 0.0000 1.0000 0.0000

Bcc 0.1759 6.786 2.421 2.263 -0.1026 0.0000 0.9947

Baa -0.0818 -10.981 -3.918 -3.663 0.9980 0.0153 0.0608

9 C(13) Bbb -0.0767 -10.290 -3.672 -3.432 -0.0161 0.9998 0.0133

Bcc 0.1585 21.271 7.590 7.095 -0.0606 -0.0143 0.9981

Baa -0.0182 -2.440 -0.871 -0.814 -0.0272 -0.0051 0.9996

10 C(13) Bbb 0.0051 0.682 0.243 0.227 -0.1994 0.9799 -0.0004

Bcc 0.0131 1.758 0.627 0.587 0.9796 0.1993 0.0276

Baa -0.0182 -2.440 -0.871 -0.814 -0.0272 0.0051 0.9996

11 C(13) Bbb 0.0051 0.682 0.243 0.227 0.1994 0.9799 0.0004

Bcc 0.0131 1.758 0.627 0.587 0.9796 -0.1993 0.0276

Baa -0.0249 -0.961 -0.343 -0.320 0.7302 0.5868 -0.3498

12 N(14) Bbb -0.0057 -0.219 -0.078 -0.073 -0.6635 0.7312 -0.1586

Bcc 0.0306 1.179 0.421 0.393 0.1627 0.3479 0.9233

Baa -0.0182 -2.440 -0.871 -0.814 0.0272 0.0051 0.9996

13 C(13) Bbb 0.0051 0.682 0.243 0.227 -0.1994 0.9799 0.0004

Bcc 0.0131 1.758 0.627 0.587 0.9796 0.1993 -0.0276

Baa -0.0182 -2.440 -0.871 -0.814 0.0272 -0.0051 0.9996

14 C(13) Bbb 0.0051 0.682 0.243 0.227 0.1994 0.9799 -0.0004

Bcc 0.0131 1.758 0.627 0.587 0.9796 -0.1993 -0.0276

Baa -0.0818 -10.981 -3.918 -3.663 0.9980 -0.0153 -0.0608

15 C(13) Bbb -0.0767 -10.290 -3.672 -3.432 0.0161 0.9998 0.0133

Bcc 0.1585 21.271 7.590 7.095 0.0606 -0.0143 0.9981

Baa -0.0919 -3.545 -1.265 -1.182 0.9947 0.0000 -0.1026

16 N(14) Bbb -0.0840 -3.241 -1.156 -1.081 0.0000 1.0000 0.0000

Bcc 0.1759 6.786 2.421 2.263 0.1026 0.0000 0.9947

Baa -0.0818 -10.981 -3.918 -3.663 0.9980 0.0153 -0.0608

17 C(13) Bbb -0.0767 -10.290 -3.672 -3.432 -0.0161 0.9998 -0.0133

Bcc 0.1585 21.271 7.590 7.095 0.0606 0.0143 0.9981

Baa -0.0249 -0.961 -0.343 -0.320 0.7302 -0.5868 -0.3498

18 N(14) Bbb -0.0057 -0.219 -0.078 -0.073 0.6635 0.7312 0.1586

Bcc 0.0306 1.179 0.421 0.393 0.1627 -0.3479 0.9233

Baa -0.1537 -5.928 -2.115 -1.977 0.0000 -0.2081 0.9781

19 N(14) Bbb 0.0731 2.819 1.006 0.940 0.0000 0.9781 0.2081

Bcc 0.0806 3.108 1.109 1.037 1.0000 0.0000 0.0000

Baa -0.1777 -23.840 -8.507 -7.952 0.8430 -0.5259 -0.1131

20 C(13) Bbb -0.1698 -22.787 -8.131 -7.601 0.5370 0.8351 0.1195

Bcc 0.3475 46.627 16.638 15.553 0.0316 -0.1615 0.9864

Baa -0.0074 -0.988 -0.353 -0.330 0.9814 0.1886 0.0369

21 C(13) Bbb 0.0008 0.112 0.040 0.037 -0.0446 0.0367 0.9983

Bcc 0.0065 0.877 0.313 0.292 -0.1869 0.9814 -0.0444

Baa -0.0074 -0.988 -0.353 -0.330 0.9814 -0.1886 -0.0369

22 C(13) Bbb 0.0008 0.112 0.040 0.037 0.0446 0.0367 0.9983

Bcc 0.0065 0.877 0.313 0.292 0.1869 0.9814 -0.0444

Baa -0.1777 -23.840 -8.507 -7.952 0.8430 0.5259 0.1131

23 C(13) Bbb -0.1698 -22.787 -8.131 -7.601 -0.5370 0.8351 0.1195

Bcc 0.3475 46.627 16.638 15.553 -0.0316 -0.1615 0.9864

Baa -0.0249 -0.961 -0.343 -0.320 0.7302 0.5868 0.3498

24 N(14) Bbb -0.0057 -0.219 -0.078 -0.073 -0.6635 0.7312 0.1586

Bcc 0.0306 1.179 0.421 0.393 -0.1627 -0.3479 0.9233

Baa -0.0103 -0.345 -0.123 -0.115 0.0000 1.0000 0.0000

25 Zn(67) Bbb -0.0029 -0.097 -0.035 -0.032 0.0000 0.0000 1.0000

Bcc 0.0132 0.442 0.158 0.148 1.0000 0.0000 0.0000

Baa -0.0268 -3.600 -1.285 -1.201 0.0625 0.9979 -0.0168

26 C(13) Bbb -0.0240 -3.227 -1.151 -1.076 0.9973 -0.0631 -0.0366

Bcc 0.0509 6.827 2.436 2.277 0.0375 0.0145 0.9992

Baa -0.0026 -0.353 -0.126 -0.118 0.1405 0.9897 -0.0275

27 C(13) Bbb 0.0002 0.025 0.009 0.008 0.9880 -0.1420 -0.0608

Bcc 0.0024 0.328 0.117 0.109 0.0640 0.0186 0.9978

Baa -0.0026 -0.353 -0.126 -0.118 -0.1405 0.9897 0.0275

28 C(13) Bbb 0.0002 0.025 0.009 0.008 0.9880 0.1420 -0.0608

Bcc 0.0024 0.328 0.117 0.109 0.0640 -0.0186 0.9978

Baa -0.0268 -3.600 -1.285 -1.201 -0.0625 0.9979 0.0168

29 C(13) Bbb -0.0240 -3.227 -1.151 -1.076 0.9973 0.0631 -0.0366

Bcc 0.0509 6.827 2.436 2.277 0.0375 -0.0145 0.9992

Baa -0.0466 -6.257 -2.233 -2.087 0.9995 -0.0310 -0.0029

30 C(13) Bbb -0.0422 -5.669 -2.023 -1.891 0.0310 0.9839 0.1761

Bcc 0.0889 11.926 4.255 3.978 -0.0026 -0.1761 0.9844

Baa -0.0112 -1.507 -0.538 -0.503 0.9789 0.2009 0.0377

31 C(13) Bbb -0.0071 -0.950 -0.339 -0.317 -0.2044 0.9633 0.1738

Bcc 0.0183 2.457 0.877 0.820 -0.0014 -0.1779 0.9841

Baa -0.0112 -1.507 -0.538 -0.503 0.9789 -0.2009 -0.0377

32 C(13) Bbb -0.0071 -0.950 -0.339 -0.317 0.2044 0.9633 0.1738

Bcc 0.0183 2.457 0.877 0.820 0.0014 -0.1779 0.9841

Baa -0.0466 -6.257 -2.233 -2.087 0.9995 0.0310 0.0029

33 C(13) Bbb -0.0422 -5.669 -2.023 -1.891 -0.0310 0.9839 0.1761

Bcc 0.0889 11.926 4.255 3.978 0.0026 -0.1761 0.9844

Baa -0.0268 -3.600 -1.285 -1.201 -0.0625 0.9979 -0.0168

34 C(13) Bbb -0.0240 -3.227 -1.151 -1.076 0.9973 0.0631 0.0366

Bcc 0.0509 6.827 2.436 2.277 -0.0375 0.0145 0.9992

Baa -0.0026 -0.353 -0.126 -0.118 -0.1405 0.9897 -0.0275

35 C(13) Bbb 0.0002 0.025 0.009 0.008 0.9880 0.1420 0.0608

Bcc 0.0024 0.328 0.117 0.109 -0.0640 0.0186 0.9978

Baa -0.0026 -0.353 -0.126 -0.118 0.1405 0.9897 0.0275

36 C(13) Bbb 0.0002 0.025 0.009 0.008 0.9880 -0.1420 0.0608

Bcc 0.0024 0.328 0.117 0.109 -0.0640 -0.0186 0.9978

Baa -0.0268 -3.600 -1.285 -1.201 0.0625 0.9979 0.0168

37 C(13) Bbb -0.0240 -3.227 -1.151 -1.076 0.9973 -0.0631 0.0366

Bcc 0.0509 6.827 2.436 2.277 -0.0375 -0.0145 0.9992

Baa -0.0466 -6.257 -2.233 -2.087 0.9995 -0.0310 0.0029

38 C(13) Bbb -0.0422 -5.669 -2.023 -1.891 0.0310 0.9839 -0.1761

Bcc 0.0889 11.926 4.255 3.978 0.0026 0.1761 0.9844

Baa -0.0112 -1.507 -0.538 -0.503 0.9789 0.2009 -0.0377

39 C(13) Bbb -0.0071 -0.950 -0.339 -0.317 -0.2044 0.9633 -0.1738

Bcc 0.0183 2.457 0.877 0.820 0.0014 0.1779 0.9841

Baa -0.0112 -1.507 -0.538 -0.503 0.9789 -0.2009 0.0377

40 C(13) Bbb -0.0071 -0.950 -0.339 -0.317 0.2044 0.9633 -0.1738

Bcc 0.0183 2.457 0.877 0.820 -0.0014 0.1779 0.9841

Baa -0.0466 -6.257 -2.233 -2.087 0.9995 0.0310 -0.0029

41 C(13) Bbb -0.0422 -5.669 -2.023 -1.891 -0.0310 0.9839 -0.1761

Bcc 0.0889 11.926 4.255 3.978 -0.0026 0.1761 0.9844

Baa -0.0101 -1.355 -0.483 -0.452 0.9998 -0.0212 -0.0041

42 C(13) Bbb -0.0059 -0.795 -0.284 -0.265 0.0216 0.9843 0.1753

Bcc 0.0160 2.150 0.767 0.717 0.0003 -0.1754 0.9845

Baa -0.0128 -1.713 -0.611 -0.571 0.9992 -0.0390 -0.0067

43 C(13) Bbb -0.0115 -1.544 -0.551 -0.515 0.0396 0.9836 0.1762

Bcc 0.0243 3.257 1.162 1.086 -0.0003 -0.1763 0.9843

Baa -0.0128 -1.713 -0.611 -0.571 0.9992 0.0390 0.0067

44 C(13) Bbb -0.0115 -1.544 -0.551 -0.515 -0.0396 0.9836 0.1762

Bcc 0.0243 3.257 1.162 1.086 0.0003 -0.1763 0.9843

Baa -0.0101 -1.355 -0.483 -0.452 0.9998 0.0212 0.0041

45 C(13) Bbb -0.0059 -0.795 -0.284 -0.265 -0.0216 0.9843 0.1753

Bcc 0.0160 2.150 0.767 0.717 -0.0003 -0.1754 0.9845

Baa -0.0065 -0.871 -0.311 -0.290 -0.0076 1.0000 0.0044

46 C(13) Bbb -0.0043 -0.579 -0.206 -0.193 0.9990 0.0078 -0.0448

Bcc 0.0108 1.449 0.517 0.483 0.0448 -0.0040 0.9990

Baa -0.0055 -0.736 -0.263 -0.246 -0.0621 0.9981 0.0026

47 C(13) Bbb -0.0045 -0.604 -0.216 -0.202 0.9971 0.0622 -0.0445

Bcc 0.0100 1.340 0.478 0.447 0.0446 0.0001 0.9990

Baa -0.0055 -0.736 -0.263 -0.246 0.0621 0.9981 -0.0026

48 C(13) Bbb -0.0045 -0.604 -0.216 -0.202 0.9971 -0.0622 -0.0445

Bcc 0.0100 1.340 0.478 0.447 0.0446 -0.0001 0.9990

Baa -0.0065 -0.871 -0.311 -0.290 0.0076 1.0000 -0.0044

49 C(13) Bbb -0.0043 -0.579 -0.206 -0.193 0.9990 -0.0078 -0.0448

Bcc 0.0108 1.449 0.517 0.483 0.0448 0.0040 0.9990

Baa -0.0101 -1.355 -0.483 -0.452 0.9998 -0.0212 0.0041

50 C(13) Bbb -0.0059 -0.795 -0.284 -0.265 0.0216 0.9843 -0.1753

Bcc 0.0160 2.150 0.767 0.717 -0.0003 0.1754 0.9845

Baa -0.0128 -1.713 -0.611 -0.571 0.9992 -0.0390 0.0067

51 C(13) Bbb -0.0115 -1.544 -0.551 -0.515 0.0396 0.9836 -0.1762

Bcc 0.0243 3.257 1.162 1.086 0.0003 0.1763 0.9843

Baa -0.0128 -1.713 -0.611 -0.571 0.9992 0.0390 -0.0067

52 C(13) Bbb -0.0115 -1.544 -0.551 -0.515 -0.0396 0.9836 -0.1762

Bcc 0.0243 3.257 1.162 1.086 -0.0003 0.1763 0.9843

Baa -0.0101 -1.355 -0.483 -0.452 0.9998 0.0212 -0.0041

53 C(13) Bbb -0.0059 -0.795 -0.284 -0.265 -0.0216 0.9843 -0.1753

Bcc 0.0160 2.150 0.767 0.717 0.0003 0.1754 0.9845

Baa -0.0065 -0.871 -0.311 -0.290 0.0076 1.0000 0.0044

54 C(13) Bbb -0.0043 -0.579 -0.206 -0.193 0.9990 -0.0078 0.0448

Bcc 0.0108 1.449 0.517 0.483 -0.0448 -0.0040 0.9990

Baa -0.0055 -0.736 -0.263 -0.246 0.0621 0.9981 0.0026

55 C(13) Bbb -0.0045 -0.604 -0.216 -0.202 0.9971 -0.0622 0.0445

Bcc 0.0100 1.340 0.478 0.447 -0.0446 0.0001 0.9990

Baa -0.0055 -0.736 -0.263 -0.246 -0.0621 0.9981 -0.0026

56 C(13) Bbb -0.0045 -0.604 -0.216 -0.202 0.9971 0.0622 0.0445

Bcc 0.0100 1.340 0.478 0.447 -0.0446 -0.0001 0.9990

Baa -0.0065 -0.871 -0.311 -0.290 -0.0076 1.0000 -0.0044

57 C(13) Bbb -0.0043 -0.579 -0.206 -0.193 0.9990 0.0078 0.0448

Bcc 0.0108 1.449 0.517 0.483 -0.0448 0.0040 0.9990

Baa -0.0022 -1.175 -0.419 -0.392 -0.0495 0.0425 0.9979

58 H(1) Bbb -0.0009 -0.465 -0.166 -0.155 0.9900 -0.1299 0.0546

Bcc 0.0031 1.640 0.585 0.547 0.1319 0.9906 -0.0356

Baa -0.0022 -1.175 -0.419 -0.392 -0.0495 -0.0425 0.9979

59 H(1) Bbb -0.0009 -0.465 -0.166 -0.155 0.9900 0.1299 0.0546

Bcc 0.0031 1.640 0.585 0.547 -0.1319 0.9906 0.0356

Baa -0.0032 -1.714 -0.611 -0.572 -0.0559 0.8220 0.5668

60 H(1) Bbb -0.0029 -1.573 -0.561 -0.525 0.0314 -0.5660 0.8238

Bcc 0.0062 3.286 1.173 1.096 0.9979 0.0639 0.0058

Baa -0.0032 -1.714 -0.611 -0.572 0.0559 0.8220 0.5668

61 H(1) Bbb -0.0029 -1.573 -0.561 -0.525 -0.0314 -0.5660 0.8238

Bcc 0.0062 3.286 1.173 1.096 0.9979 -0.0639 -0.0058

Baa -0.0022 -1.175 -0.419 -0.392 0.0495 0.0425 0.9979

62 H(1) Bbb -0.0009 -0.465 -0.166 -0.155 0.9900 0.1299 -0.0546

Bcc 0.0031 1.640 0.585 0.547 -0.1319 0.9906 -0.0356

Baa -0.0022 -1.175 -0.419 -0.392 0.0495 -0.0425 0.9979

63 H(1) Bbb -0.0009 -0.465 -0.166 -0.155 0.9900 -0.1299 -0.0546

Bcc 0.0031 1.640 0.585 0.547 0.1319 0.9906 0.0356

Baa -0.0032 -1.714 -0.611 -0.572 -0.0559 0.8220 -0.5668

64 H(1) Bbb -0.0029 -1.573 -0.561 -0.525 -0.0314 0.5660 0.8238

Bcc 0.0062 3.286 1.173 1.096 0.9979 0.0639 -0.0058

Baa -0.0032 -1.714 -0.611 -0.572 0.0559 0.8220 -0.5668

65 H(1) Bbb -0.0029 -1.573 -0.561 -0.525 0.0314 0.5660 0.8238

Bcc 0.0062 3.286 1.173 1.096 0.9979 -0.0639 0.0058

Baa -0.0016 -0.879 -0.314 -0.293 0.0014 -0.1561 0.9877

66 H(1) Bbb 0.0003 0.176 0.063 0.059 0.4546 0.8799 0.1384

Bcc 0.0013 0.703 0.251 0.234 0.8907 -0.4489 -0.0722

Baa -0.0020 -1.083 -0.386 -0.361 0.9494 0.3083 0.0590

67 H(1) Bbb -0.0009 -0.479 -0.171 -0.160 -0.0056 -0.1714 0.9852

Bcc 0.0029 1.562 0.557 0.521 -0.3139 0.9357 0.1610

Baa -0.0020 -1.083 -0.386 -0.361 0.9494 -0.3083 -0.0590

68 H(1) Bbb -0.0009 -0.479 -0.171 -0.160 0.0056 -0.1714 0.9852

Bcc 0.0029 1.562 0.557 0.521 0.3139 0.9357 0.1610

Baa -0.0016 -0.879 -0.314 -0.293 -0.0014 -0.1561 0.9877

69 H(1) Bbb 0.0003 0.176 0.063 0.059 -0.4546 0.8799 0.1384

Bcc 0.0013 0.703 0.251 0.234 0.8907 0.4489 0.0722

Baa -0.0010 -0.541 -0.193 -0.181 0.0193 -0.0065 0.9998

70 H(1) Bbb 0.0002 0.106 0.038 0.035 0.7886 0.6148 -0.0112

Bcc 0.0008 0.436 0.155 0.145 -0.6146 0.7886 0.0170

Baa -0.0009 -0.489 -0.174 -0.163 0.3054 0.9519 -0.0258

71 H(1) Bbb -0.0006 -0.308 -0.110 -0.103 0.0381 0.0148 0.9992

Bcc 0.0015 0.796 0.284 0.266 0.9515 -0.3061 -0.0318

Baa -0.0009 -0.489 -0.174 -0.163 -0.3054 0.9519 0.0258

72 H(1) Bbb -0.0006 -0.308 -0.110 -0.103 0.0381 -0.0148 0.9992

Bcc 0.0015 0.796 0.284 0.266 0.9515 0.3061 -0.0318

Baa -0.0010 -0.541 -0.193 -0.181 0.0193 0.0065 0.9998

73 H(1) Bbb 0.0002 0.106 0.038 0.035 0.7886 -0.6148 -0.0112

Bcc 0.0008 0.436 0.155 0.145 0.6146 0.7886 -0.0170

Baa -0.0016 -0.879 -0.314 -0.293 -0.0014 0.1561 0.9877

74 H(1) Bbb 0.0003 0.176 0.063 0.059 0.4546 0.8799 -0.1384

Bcc 0.0013 0.703 0.251 0.234 0.8907 -0.4489 0.0722

Baa -0.0020 -1.083 -0.386 -0.361 0.9494 0.3083 -0.0590

75 H(1) Bbb -0.0009 -0.479 -0.171 -0.160 0.0056 0.1714 0.9852

Bcc 0.0029 1.562 0.557 0.521 -0.3139 0.9357 -0.1610

Baa -0.0020 -1.083 -0.386 -0.361 0.9494 -0.3083 0.0590

76 H(1) Bbb -0.0009 -0.479 -0.171 -0.160 -0.0056 0.1714 0.9852

Bcc 0.0029 1.562 0.557 0.521 0.3139 0.9357 -0.1610

Baa -0.0016 -0.879 -0.314 -0.293 0.0014 0.1561 0.9877

77 H(1) Bbb 0.0003 0.176 0.063 0.059 -0.4546 0.8799 -0.1384

Bcc 0.0013 0.703 0.251 0.234 0.8907 0.4489 -0.0722

Baa -0.0010 -0.541 -0.193 -0.181 -0.0193 -0.0065 0.9998

78 H(1) Bbb 0.0002 0.106 0.038 0.035 0.7886 -0.6148 0.0112

Bcc 0.0008 0.436 0.155 0.145 0.6146 0.7886 0.0170

Baa -0.0009 -0.489 -0.174 -0.163 -0.3054 0.9519 -0.0258

79 H(1) Bbb -0.0006 -0.308 -0.110 -0.103 -0.0381 0.0148 0.9992

Bcc 0.0015 0.796 0.284 0.266 0.9515 0.3061 0.0318

Baa -0.0009 -0.489 -0.174 -0.163 0.3054 0.9519 0.0258

80 H(1) Bbb -0.0006 -0.308 -0.110 -0.103 -0.0381 -0.0148 0.9992

Bcc 0.0015 0.796 0.284 0.266 0.9515 -0.3061 0.0318

Baa -0.0010 -0.541 -0.193 -0.181 -0.0193 0.0065 0.9998

81 H(1) Bbb 0.0002 0.106 0.038 0.035 0.7886 0.6148 0.0112

Bcc 0.0008 0.436 0.155 0.145 -0.6146 0.7886 -0.0170

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

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Sun Jun 30 21:45:48 2019, MaxMem= 1342177280 cpu: 282.9

(Enter /apps/gaussian/g09d01/g09/l9999.exe)

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[C2(Zn1),SGV(N2),SGV'(N2),X(C48H24N4)]\\@

Age does not diminish the extreme disappointment of

having a scoop of ice cream fall from the cone.

-- Jim Fiebig

Job cpu time: 0 days 20 hours 43 minutes 8.8 seconds.

File lengths (MBytes): RWF= 2568 Int= 0 D2E= 0 Chk= 116 Scr= 2

Normal termination of Gaussian 09 at Sun Jun 30 21:45:49 2019.