Entering Gaussian System, Link 0=g09

 Initial command:

 /apps/gaussian/g09d01/g09/l1.exe "/srv/scratch/z5105842/Gau-150928.inp" -scrdir="/srv/scratch/z5105842/"

 Entering Link 1 = /apps/gaussian/g09d01/g09/l1.exe PID= 150947.

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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

 15-Jun-2019

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

 %nprocshared=12

 Will use up to 12 processors via shared memory.

 %mem=10GB

 %chk=ZnPCanion.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 Sat Jun 15 12:04:59 2019, MaxMem= 1342177280 cpu: 3.8

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

 ---------

 ZnPCanion

 ---------

 Symbolic Z-matrix:

 Charge = -1 Multiplicity = 2

 C 2.77772 1.18839 0.00238

 N 1.43982 1.42409 0.02902

 C 1.19044 2.7894 0.00284

 C 2.47021 3.48217 -0.03695

 C 3.4749 2.47654 -0.03787

 N 0. 3.38988 -0.00476

 C -1.19044 2.7894 0.00284

 N -1.43982 1.42409 0.02902

 C -2.77772 1.18839 0.00238

 C -3.4749 2.47654 -0.03787

 C -2.47021 3.48217 -0.03695

 N 3.41035 0. -0.00133

 C 3.4749 -2.47654 -0.03787

 C 2.47021 -3.48217 -0.03695

 C 1.19044 -2.7894 0.00284

 N 1.43982 -1.42409 0.02902

 C 2.77772 -1.18839 0.00238

 N 0. -3.38988 -0.00476

 N -1.43982 -1.42409 0.02902

 C -1.19044 -2.7894 0.00284

 C -2.47021 -3.48217 -0.03695

 C -3.4749 -2.47654 -0.03787

 C -2.77772 -1.18839 0.00238

 N -3.41035 0. -0.00133

 Zn 0. 0. 0.39114

 C 4.8309 -2.81442 -0.07679

 C 5.17488 -4.16759 -0.11147

 C 4.17839 -5.16736 -0.11161

 C 2.82276 -4.83751 -0.07683

 C -4.8309 -2.81442 -0.07679

 C -5.17488 -4.16759 -0.11147

 C -4.17839 -5.16736 -0.11161

 C -2.82276 -4.83751 -0.07683

 C -2.82276 4.83751 -0.07683

 C -4.17839 5.16736 -0.11161

 C -5.17488 4.16759 -0.11147

 C -4.8309 2.81442 -0.07679

 C 4.8309 2.81442 -0.07679

 C 5.17488 4.16759 -0.11147

 C 4.17839 5.16736 -0.11161

 C 2.82276 4.83751 -0.07683

 H 5.59625 -2.04351 -0.07919

 H 2.06073 -5.61165 -0.07925

 H -5.59625 -2.04351 -0.07919

 H -2.06073 -5.61165 -0.07925

 H -2.06073 5.61165 -0.07925

 H -5.59625 2.04351 -0.07919

 H 5.59625 2.04351 -0.07919

 H 2.06073 5.61165 -0.07925

 H -4.4751 6.21221 -0.13972

 H -6.22124 4.45784 -0.13949

 H 4.4751 6.21221 -0.13972

 H 6.22124 4.45784 -0.13949

 H 6.22124 -4.45784 -0.13949

 H 4.4751 -6.21221 -0.13972

 H -4.4751 -6.21221 -0.13972

 H -6.22124 -4.45784 -0.13949

 NAtoms= 57 NQM= 57 NQMF= 0 NMMI= 0 NMMIF= 0

 NMic= 0 NMicF= 0.

 Isotopes and Nuclear Properties:

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

 in nuclear magnetons)

 Atom 1 2 3 4 5 6 7 8 9 10

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

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

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

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

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

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

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

 Atom 11 12 13 14 15 16 17 18 19 20

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

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

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

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

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

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

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

 Atom 21 22 23 24 25 26 27 28 29 30

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

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

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

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

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

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

 AtZNuc= 6.0000000 6.0000000 6.0000000 7.0000000 30.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000

 Atom 31 32 33 34 35 36 37 38 39 40

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

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

 NucSpn= 0 0 0 0 0 0 0 0 0 0

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

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

 NMagM= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

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

 Atom 41 42 43 44 45 46 47 48 49 50

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

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

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

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

 Atom 51 52 53 54 55 56 57

 IAtWgt= 1 1 1 1 1 1 1

 AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

 NucSpn= 1 1 1 1 1 1 1

 AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

 NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

 NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

 AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

 Leave Link 101 at Sat Jun 15 12:04:59 2019, MaxMem= 1342177280 cpu: 5.4

 (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) 1.3588 estimate D2E/DX2 !

 ! R2 R(1,5) 1.4653 estimate D2E/DX2 !

 ! R3 R(1,12) 1.3463 estimate D2E/DX2 !

 ! R4 R(2,3) 1.3881 estimate D2E/DX2 !

 ! R5 R(2,25) 2.0572 estimate D2E/DX2 !

 ! R6 R(3,4) 1.4558 estimate D2E/DX2 !

 ! R7 R(3,6) 1.3333 estimate D2E/DX2 !

 ! R8 R(4,5) 1.4215 estimate D2E/DX2 !

 ! R9 R(4,41) 1.401 estimate D2E/DX2 !

 ! R10 R(5,38) 1.398 estimate D2E/DX2 !

 ! R11 R(6,7) 1.3333 estimate D2E/DX2 !

 ! R12 R(7,8) 1.3881 estimate D2E/DX2 !

 ! R13 R(7,11) 1.4558 estimate D2E/DX2 !

 ! R14 R(8,9) 1.3588 estimate D2E/DX2 !

 ! R15 R(8,25) 2.0572 estimate D2E/DX2 !

 ! R16 R(9,10) 1.4653 estimate D2E/DX2 !

 ! R17 R(9,24) 1.3463 estimate D2E/DX2 !

 ! R18 R(10,11) 1.4215 estimate D2E/DX2 !

 ! R19 R(10,37) 1.398 estimate D2E/DX2 !

 ! R20 R(11,34) 1.401 estimate D2E/DX2 !

 ! R21 R(12,17) 1.3463 estimate D2E/DX2 !

 ! R22 R(13,14) 1.4215 estimate D2E/DX2 !

 ! R23 R(13,17) 1.4653 estimate D2E/DX2 !

 ! R24 R(13,26) 1.398 estimate D2E/DX2 !

 ! R25 R(14,15) 1.4558 estimate D2E/DX2 !

 ! R26 R(14,29) 1.401 estimate D2E/DX2 !

 ! R27 R(15,16) 1.3881 estimate D2E/DX2 !

 ! R28 R(15,18) 1.3333 estimate D2E/DX2 !

 ! R29 R(16,17) 1.3588 estimate D2E/DX2 !

 ! R30 R(16,25) 2.0572 estimate D2E/DX2 !

 ! R31 R(18,20) 1.3333 estimate D2E/DX2 !

 ! R32 R(19,20) 1.3881 estimate D2E/DX2 !

 ! R33 R(19,23) 1.3588 estimate D2E/DX2 !

 ! R34 R(19,25) 2.0572 estimate D2E/DX2 !

 ! R35 R(20,21) 1.4558 estimate D2E/DX2 !

 ! R36 R(21,22) 1.4215 estimate D2E/DX2 !

 ! R37 R(21,33) 1.401 estimate D2E/DX2 !

 ! R38 R(22,23) 1.4653 estimate D2E/DX2 !

 ! R39 R(22,30) 1.398 estimate D2E/DX2 !

 ! R40 R(23,24) 1.3463 estimate D2E/DX2 !

 ! R41 R(26,27) 1.3966 estimate D2E/DX2 !

 ! R42 R(26,42) 1.0863 estimate D2E/DX2 !

 ! R43 R(27,28) 1.4116 estimate D2E/DX2 !

 ! R44 R(27,54) 1.0862 estimate D2E/DX2 !

 ! R45 R(28,29) 1.3956 estimate D2E/DX2 !

 ! R46 R(28,55) 1.0865 estimate D2E/DX2 !

 ! R47 R(29,43) 1.0863 estimate D2E/DX2 !

 ! R48 R(30,31) 1.3966 estimate D2E/DX2 !

 ! R49 R(30,44) 1.0863 estimate D2E/DX2 !

 ! R50 R(31,32) 1.4116 estimate D2E/DX2 !

 ! R51 R(31,57) 1.0862 estimate D2E/DX2 !

 ! R52 R(32,33) 1.3956 estimate D2E/DX2 !

 ! R53 R(32,56) 1.0865 estimate D2E/DX2 !

 ! R54 R(33,45) 1.0863 estimate D2E/DX2 !

 ! R55 R(34,35) 1.3956 estimate D2E/DX2 !

 ! R56 R(34,46) 1.0863 estimate D2E/DX2 !

 ! R57 R(35,36) 1.4116 estimate D2E/DX2 !

 ! R58 R(35,50) 1.0865 estimate D2E/DX2 !

 ! R59 R(36,37) 1.3966 estimate D2E/DX2 !

 ! R60 R(36,51) 1.0862 estimate D2E/DX2 !

 ! R61 R(37,47) 1.0863 estimate D2E/DX2 !

 ! R62 R(38,39) 1.3966 estimate D2E/DX2 !

 ! R63 R(38,48) 1.0863 estimate D2E/DX2 !

 ! R64 R(39,40) 1.4116 estimate D2E/DX2 !

 ! R65 R(39,53) 1.0862 estimate D2E/DX2 !

 ! R66 R(40,41) 1.3956 estimate D2E/DX2 !

 ! R67 R(40,52) 1.0865 estimate D2E/DX2 !

 ! R68 R(41,49) 1.0863 estimate D2E/DX2 !

 ! A1 A(2,1,5) 108.4535 estimate D2E/DX2 !

 ! A2 A(2,1,12) 128.0152 estimate D2E/DX2 !

 ! A3 A(5,1,12) 123.5285 estimate D2E/DX2 !

 ! A4 A(1,2,3) 110.3122 estimate D2E/DX2 !

 ! A5 A(1,2,25) 124.9247 estimate D2E/DX2 !

 ! A6 A(3,2,25) 123.9476 estimate D2E/DX2 !

 ! A7 A(2,3,4) 108.0969 estimate D2E/DX2 !

 ! A8 A(2,3,6) 127.1178 estimate D2E/DX2 !

 ! A9 A(4,3,6) 124.779 estimate D2E/DX2 !

 ! A10 A(3,4,5) 106.5407 estimate D2E/DX2 !

 ! A11 A(3,4,41) 133.027 estimate D2E/DX2 !

 ! A12 A(5,4,41) 120.4315 estimate D2E/DX2 !

 ! A13 A(1,5,4) 106.5958 estimate D2E/DX2 !

 ! A14 A(1,5,38) 132.4343 estimate D2E/DX2 !

 ! A15 A(4,5,38) 120.9696 estimate D2E/DX2 !

 ! A16 A(3,6,7) 126.4617 estimate D2E/DX2 !

 ! A17 A(6,7,8) 127.1178 estimate D2E/DX2 !

 ! A18 A(6,7,11) 124.779 estimate D2E/DX2 !

 ! A19 A(8,7,11) 108.0969 estimate D2E/DX2 !

 ! A20 A(7,8,9) 110.3122 estimate D2E/DX2 !

 ! A21 A(7,8,25) 123.9476 estimate D2E/DX2 !

 ! A22 A(9,8,25) 124.9247 estimate D2E/DX2 !

 ! A23 A(8,9,10) 108.4535 estimate D2E/DX2 !

 ! A24 A(8,9,24) 128.0152 estimate D2E/DX2 !

 ! A25 A(10,9,24) 123.5285 estimate D2E/DX2 !

 ! A26 A(9,10,11) 106.5958 estimate D2E/DX2 !

 ! A27 A(9,10,37) 132.4343 estimate D2E/DX2 !

 ! A28 A(11,10,37) 120.9696 estimate D2E/DX2 !

 ! A29 A(7,11,10) 106.5407 estimate D2E/DX2 !

 ! A30 A(7,11,34) 133.027 estimate D2E/DX2 !

 ! A31 A(10,11,34) 120.4315 estimate D2E/DX2 !

 ! A32 A(1,12,17) 123.9421 estimate D2E/DX2 !

 ! A33 A(14,13,17) 106.5958 estimate D2E/DX2 !

 ! A34 A(14,13,26) 120.9696 estimate D2E/DX2 !

 ! A35 A(17,13,26) 132.4343 estimate D2E/DX2 !

 ! A36 A(13,14,15) 106.5407 estimate D2E/DX2 !

 ! A37 A(13,14,29) 120.4315 estimate D2E/DX2 !

 ! A38 A(15,14,29) 133.027 estimate D2E/DX2 !

 ! A39 A(14,15,16) 108.0969 estimate D2E/DX2 !

 ! A40 A(14,15,18) 124.779 estimate D2E/DX2 !

 ! A41 A(16,15,18) 127.1178 estimate D2E/DX2 !

 ! A42 A(15,16,17) 110.3122 estimate D2E/DX2 !

 ! A43 A(15,16,25) 123.9476 estimate D2E/DX2 !

 ! A44 A(17,16,25) 124.9247 estimate D2E/DX2 !

 ! A45 A(12,17,13) 123.5285 estimate D2E/DX2 !

 ! A46 A(12,17,16) 128.0152 estimate D2E/DX2 !

 ! A47 A(13,17,16) 108.4535 estimate D2E/DX2 !

 ! A48 A(15,18,20) 126.4617 estimate D2E/DX2 !

 ! A49 A(20,19,23) 110.3122 estimate D2E/DX2 !

 ! A50 A(20,19,25) 123.9476 estimate D2E/DX2 !

 ! A51 A(23,19,25) 124.9247 estimate D2E/DX2 !

 ! A52 A(18,20,19) 127.1178 estimate D2E/DX2 !

 ! A53 A(18,20,21) 124.779 estimate D2E/DX2 !

 ! A54 A(19,20,21) 108.0969 estimate D2E/DX2 !

 ! A55 A(20,21,22) 106.5407 estimate D2E/DX2 !

 ! A56 A(20,21,33) 133.027 estimate D2E/DX2 !

 ! A57 A(22,21,33) 120.4315 estimate D2E/DX2 !

 ! A58 A(21,22,23) 106.5958 estimate D2E/DX2 !

 ! A59 A(21,22,30) 120.9696 estimate D2E/DX2 !

 ! A60 A(23,22,30) 132.4343 estimate D2E/DX2 !

 ! A61 A(19,23,22) 108.4535 estimate D2E/DX2 !

 ! A62 A(19,23,24) 128.0152 estimate D2E/DX2 !

 ! A63 A(22,23,24) 123.5285 estimate D2E/DX2 !

 ! A64 A(9,24,23) 123.9421 estimate D2E/DX2 !

 ! A65 A(2,25,8) 88.8342 estimate D2E/DX2 !

 ! A66 A(2,25,16) 87.6145 estimate D2E/DX2 !

 ! A67 A(2,25,19) 159.7235 estimate D2E/DX2 !

 ! A68 A(8,25,16) 159.7235 estimate D2E/DX2 !

 ! A69 A(8,25,19) 87.6145 estimate D2E/DX2 !

 ! A70 A(16,25,19) 88.8342 estimate D2E/DX2 !

 ! A71 A(13,26,27) 118.2777 estimate D2E/DX2 !

 ! A72 A(13,26,42) 120.7915 estimate D2E/DX2 !

 ! A73 A(27,26,42) 120.9307 estimate D2E/DX2 !

 ! A74 A(26,27,28) 120.8215 estimate D2E/DX2 !

 ! A75 A(26,27,54) 119.7877 estimate D2E/DX2 !

 ! A76 A(28,27,54) 119.3908 estimate D2E/DX2 !

 ! A77 A(27,28,29) 121.2194 estimate D2E/DX2 !

 ! A78 A(27,28,55) 119.2308 estimate D2E/DX2 !

 ! A79 A(29,28,55) 119.5498 estimate D2E/DX2 !

 ! A80 A(14,29,28) 118.2796 estimate D2E/DX2 !

 ! A81 A(14,29,43) 120.8617 estimate D2E/DX2 !

 ! A82 A(28,29,43) 120.8587 estimate D2E/DX2 !

 ! A83 A(22,30,31) 118.2777 estimate D2E/DX2 !

 ! A84 A(22,30,44) 120.7915 estimate D2E/DX2 !

 ! A85 A(31,30,44) 120.9307 estimate D2E/DX2 !

 ! A86 A(30,31,32) 120.8215 estimate D2E/DX2 !

 ! A87 A(30,31,57) 119.7877 estimate D2E/DX2 !

 ! A88 A(32,31,57) 119.3908 estimate D2E/DX2 !

 ! A89 A(31,32,33) 121.2194 estimate D2E/DX2 !

 ! A90 A(31,32,56) 119.2308 estimate D2E/DX2 !

 ! A91 A(33,32,56) 119.5498 estimate D2E/DX2 !

 ! A92 A(21,33,32) 118.2796 estimate D2E/DX2 !

 ! A93 A(21,33,45) 120.8617 estimate D2E/DX2 !

 ! A94 A(32,33,45) 120.8587 estimate D2E/DX2 !

 ! A95 A(11,34,35) 118.2796 estimate D2E/DX2 !

 ! A96 A(11,34,46) 120.8617 estimate D2E/DX2 !

 ! A97 A(35,34,46) 120.8587 estimate D2E/DX2 !

 ! A98 A(34,35,36) 121.2194 estimate D2E/DX2 !

 ! A99 A(34,35,50) 119.5498 estimate D2E/DX2 !

 ! A100 A(36,35,50) 119.2308 estimate D2E/DX2 !

 ! A101 A(35,36,37) 120.8215 estimate D2E/DX2 !

 ! A102 A(35,36,51) 119.3908 estimate D2E/DX2 !

 ! A103 A(37,36,51) 119.7877 estimate D2E/DX2 !

 ! A104 A(10,37,36) 118.2777 estimate D2E/DX2 !

 ! A105 A(10,37,47) 120.7915 estimate D2E/DX2 !

 ! A106 A(36,37,47) 120.9307 estimate D2E/DX2 !

 ! A107 A(5,38,39) 118.2777 estimate D2E/DX2 !

 ! A108 A(5,38,48) 120.7915 estimate D2E/DX2 !

 ! A109 A(39,38,48) 120.9307 estimate D2E/DX2 !

 ! A110 A(38,39,40) 120.8215 estimate D2E/DX2 !

 ! A111 A(38,39,53) 119.7877 estimate D2E/DX2 !

 ! A112 A(40,39,53) 119.3908 estimate D2E/DX2 !

 ! A113 A(39,40,41) 121.2194 estimate D2E/DX2 !

 ! A114 A(39,40,52) 119.2308 estimate D2E/DX2 !

 ! A115 A(41,40,52) 119.5498 estimate D2E/DX2 !

 ! A116 A(4,41,40) 118.2796 estimate D2E/DX2 !

 ! A117 A(4,41,49) 120.8617 estimate D2E/DX2 !

 ! A118 A(40,41,49) 120.8587 estimate D2E/DX2 !

 ! D1 D(5,1,2,3) 0.2841 estimate D2E/DX2 !

 ! D2 D(5,1,2,25) -169.687 estimate D2E/DX2 !

 ! D3 D(12,1,2,3) -179.1098 estimate D2E/DX2 !

 ! D4 D(12,1,2,25) 10.9191 estimate D2E/DX2 !

 ! D5 D(2,1,5,4) -0.1514 estimate D2E/DX2 !

 ! D6 D(2,1,5,38) -179.9368 estimate D2E/DX2 !

 ! D7 D(12,1,5,4) 179.2758 estimate D2E/DX2 !

 ! D8 D(12,1,5,38) -0.5097 estimate D2E/DX2 !

 ! D9 D(2,1,12,17) 1.007 estimate D2E/DX2 !

 ! D10 D(5,1,12,17) -178.3033 estimate D2E/DX2 !

 ! D11 D(1,2,3,4) -0.3039 estimate D2E/DX2 !

 ! D12 D(1,2,3,6) 178.8099 estimate D2E/DX2 !

 ! D13 D(25,2,3,4) 169.7849 estimate D2E/DX2 !

 ! D14 D(25,2,3,6) -11.1013 estimate D2E/DX2 !

 ! D15 D(1,2,25,8) -175.6805 estimate D2E/DX2 !

 ! D16 D(1,2,25,16) -15.648 estimate D2E/DX2 !

 ! D17 D(1,2,25,19) -95.7716 estimate D2E/DX2 !

 ! D18 D(3,2,25,8) 15.6736 estimate D2E/DX2 !

 ! D19 D(3,2,25,16) 175.7062 estimate D2E/DX2 !

 ! D20 D(3,2,25,19) 95.5825 estimate D2E/DX2 !

 ! D21 D(2,3,4,5) 0.1991 estimate D2E/DX2 !

 ! D22 D(2,3,4,41) 179.8554 estimate D2E/DX2 !

 ! D23 D(6,3,4,5) -178.9406 estimate D2E/DX2 !

 ! D24 D(6,3,4,41) 0.7157 estimate D2E/DX2 !

 ! D25 D(2,3,6,7) -0.4607 estimate D2E/DX2 !

 ! D26 D(4,3,6,7) 178.5137 estimate D2E/DX2 !

 ! D27 D(3,4,5,1) -0.0309 estimate D2E/DX2 !

 ! D28 D(3,4,5,38) 179.7844 estimate D2E/DX2 !

 ! D29 D(41,4,5,1) -179.7395 estimate D2E/DX2 !

 ! D30 D(41,4,5,38) 0.0758 estimate D2E/DX2 !

 ! D31 D(3,4,41,40) -179.8756 estimate D2E/DX2 !

 ! D32 D(3,4,41,49) 0.2065 estimate D2E/DX2 !

 ! D33 D(5,4,41,40) -0.2578 estimate D2E/DX2 !

 ! D34 D(5,4,41,49) 179.8244 estimate D2E/DX2 !

 ! D35 D(1,5,38,39) 179.9166 estimate D2E/DX2 !

 ! D36 D(1,5,38,48) -0.1291 estimate D2E/DX2 !

 ! D37 D(4,5,38,39) 0.1564 estimate D2E/DX2 !

 ! D38 D(4,5,38,48) -179.8893 estimate D2E/DX2 !

 ! D39 D(3,6,7,8) 0.4607 estimate D2E/DX2 !

 ! D40 D(3,6,7,11) -178.5137 estimate D2E/DX2 !

 ! D41 D(6,7,8,9) -178.8099 estimate D2E/DX2 !

 ! D42 D(6,7,8,25) 11.1013 estimate D2E/DX2 !

 ! D43 D(11,7,8,9) 0.3039 estimate D2E/DX2 !

 ! D44 D(11,7,8,25) -169.7849 estimate D2E/DX2 !

 ! D45 D(6,7,11,10) 178.9406 estimate D2E/DX2 !

 ! D46 D(6,7,11,34) -0.7157 estimate D2E/DX2 !

 ! D47 D(8,7,11,10) -0.1991 estimate D2E/DX2 !

 ! D48 D(8,7,11,34) -179.8554 estimate D2E/DX2 !

 ! D49 D(7,8,9,10) -0.2841 estimate D2E/DX2 !

 ! D50 D(7,8,9,24) 179.1098 estimate D2E/DX2 !

 ! D51 D(25,8,9,10) 169.687 estimate D2E/DX2 !

 ! D52 D(25,8,9,24) -10.9191 estimate D2E/DX2 !

 ! D53 D(7,8,25,2) -15.6736 estimate D2E/DX2 !

 ! D54 D(7,8,25,16) -95.5825 estimate D2E/DX2 !

 ! D55 D(7,8,25,19) -175.7062 estimate D2E/DX2 !

 ! D56 D(9,8,25,2) 175.6805 estimate D2E/DX2 !

 ! D57 D(9,8,25,16) 95.7716 estimate D2E/DX2 !

 ! D58 D(9,8,25,19) 15.648 estimate D2E/DX2 !

 ! D59 D(8,9,10,11) 0.1514 estimate D2E/DX2 !

 ! D60 D(8,9,10,37) 179.9368 estimate D2E/DX2 !

 ! D61 D(24,9,10,11) -179.2758 estimate D2E/DX2 !

 ! D62 D(24,9,10,37) 0.5097 estimate D2E/DX2 !

 ! D63 D(8,9,24,23) -1.007 estimate D2E/DX2 !

 ! D64 D(10,9,24,23) 178.3033 estimate D2E/DX2 !

 ! D65 D(9,10,11,7) 0.0309 estimate D2E/DX2 !

 ! D66 D(9,10,11,34) 179.7395 estimate D2E/DX2 !

 ! D67 D(37,10,11,7) -179.7844 estimate D2E/DX2 !

 ! D68 D(37,10,11,34) -0.0758 estimate D2E/DX2 !

 ! D69 D(9,10,37,36) -179.9166 estimate D2E/DX2 !

 ! D70 D(9,10,37,47) 0.1291 estimate D2E/DX2 !

 ! D71 D(11,10,37,36) -0.1564 estimate D2E/DX2 !

 ! D72 D(11,10,37,47) 179.8893 estimate D2E/DX2 !

 ! D73 D(7,11,34,35) 179.8756 estimate D2E/DX2 !

 ! D74 D(7,11,34,46) -0.2065 estimate D2E/DX2 !

 ! D75 D(10,11,34,35) 0.2578 estimate D2E/DX2 !

 ! D76 D(10,11,34,46) -179.8244 estimate D2E/DX2 !

 ! D77 D(1,12,17,13) 178.3033 estimate D2E/DX2 !

 ! D78 D(1,12,17,16) -1.007 estimate D2E/DX2 !

 ! D79 D(17,13,14,15) 0.0309 estimate D2E/DX2 !

 ! D80 D(17,13,14,29) 179.7395 estimate D2E/DX2 !

 ! D81 D(26,13,14,15) -179.7844 estimate D2E/DX2 !

 ! D82 D(26,13,14,29) -0.0758 estimate D2E/DX2 !

 ! D83 D(14,13,17,12) -179.2758 estimate D2E/DX2 !

 ! D84 D(14,13,17,16) 0.1514 estimate D2E/DX2 !

 ! D85 D(26,13,17,12) 0.5097 estimate D2E/DX2 !

 ! D86 D(26,13,17,16) 179.9368 estimate D2E/DX2 !

 ! D87 D(14,13,26,27) -0.1564 estimate D2E/DX2 !

 ! D88 D(14,13,26,42) 179.8893 estimate D2E/DX2 !

 ! D89 D(17,13,26,27) -179.9166 estimate D2E/DX2 !

 ! D90 D(17,13,26,42) 0.1291 estimate D2E/DX2 !

 ! D91 D(13,14,15,16) -0.1991 estimate D2E/DX2 !

 ! D92 D(13,14,15,18) 178.9406 estimate D2E/DX2 !

 ! D93 D(29,14,15,16) -179.8554 estimate D2E/DX2 !

 ! D94 D(29,14,15,18) -0.7157 estimate D2E/DX2 !

 ! D95 D(13,14,29,28) 0.2578 estimate D2E/DX2 !

 ! D96 D(13,14,29,43) -179.8244 estimate D2E/DX2 !

 ! D97 D(15,14,29,28) 179.8756 estimate D2E/DX2 !

 ! D98 D(15,14,29,43) -0.2065 estimate D2E/DX2 !

 ! D99 D(14,15,16,17) 0.3039 estimate D2E/DX2 !

 ! D100 D(14,15,16,25) -169.7849 estimate D2E/DX2 !

 ! D101 D(18,15,16,17) -178.8099 estimate D2E/DX2 !

 ! D102 D(18,15,16,25) 11.1013 estimate D2E/DX2 !

 ! D103 D(14,15,18,20) -178.5137 estimate D2E/DX2 !

 ! D104 D(16,15,18,20) 0.4607 estimate D2E/DX2 !

 ! D105 D(15,16,17,12) 179.1098 estimate D2E/DX2 !

 ! D106 D(15,16,17,13) -0.2841 estimate D2E/DX2 !

 ! D107 D(25,16,17,12) -10.9191 estimate D2E/DX2 !

 ! D108 D(25,16,17,13) 169.687 estimate D2E/DX2 !

 ! D109 D(15,16,25,2) -175.7062 estimate D2E/DX2 !

 ! D110 D(15,16,25,8) -95.5825 estimate D2E/DX2 !

 ! D111 D(15,16,25,19) -15.6736 estimate D2E/DX2 !

 ! D112 D(17,16,25,2) 15.648 estimate D2E/DX2 !

 ! D113 D(17,16,25,8) 95.7716 estimate D2E/DX2 !

 ! D114 D(17,16,25,19) 175.6805 estimate D2E/DX2 !

 ! D115 D(15,18,20,19) -0.4607 estimate D2E/DX2 !

 ! D116 D(15,18,20,21) 178.5137 estimate D2E/DX2 !

 ! D117 D(23,19,20,18) 178.8099 estimate D2E/DX2 !

 ! D118 D(23,19,20,21) -0.3039 estimate D2E/DX2 !

 ! D119 D(25,19,20,18) -11.1013 estimate D2E/DX2 !

 ! D120 D(25,19,20,21) 169.7849 estimate D2E/DX2 !

 ! D121 D(20,19,23,22) 0.2841 estimate D2E/DX2 !

 ! D122 D(20,19,23,24) -179.1098 estimate D2E/DX2 !

 ! D123 D(25,19,23,22) -169.687 estimate D2E/DX2 !

 ! D124 D(25,19,23,24) 10.9191 estimate D2E/DX2 !

 ! D125 D(20,19,25,2) 95.5825 estimate D2E/DX2 !

 ! D126 D(20,19,25,8) 175.7062 estimate D2E/DX2 !

 ! D127 D(20,19,25,16) 15.6736 estimate D2E/DX2 !

 ! D128 D(23,19,25,2) -95.7716 estimate D2E/DX2 !

 ! D129 D(23,19,25,8) -15.648 estimate D2E/DX2 !

 ! D130 D(23,19,25,16) -175.6805 estimate D2E/DX2 !

 ! D131 D(18,20,21,22) -178.9406 estimate D2E/DX2 !

 ! D132 D(18,20,21,33) 0.7157 estimate D2E/DX2 !

 ! D133 D(19,20,21,22) 0.1991 estimate D2E/DX2 !

 ! D134 D(19,20,21,33) 179.8554 estimate D2E/DX2 !

 ! D135 D(20,21,22,23) -0.0309 estimate D2E/DX2 !

 ! D136 D(20,21,22,30) 179.7844 estimate D2E/DX2 !

 ! D137 D(33,21,22,23) -179.7395 estimate D2E/DX2 !

 ! D138 D(33,21,22,30) 0.0758 estimate D2E/DX2 !

 ! D139 D(20,21,33,32) -179.8756 estimate D2E/DX2 !

 ! D140 D(20,21,33,45) 0.2065 estimate D2E/DX2 !

 ! D141 D(22,21,33,32) -0.2578 estimate D2E/DX2 !

 ! D142 D(22,21,33,45) 179.8244 estimate D2E/DX2 !

 ! D143 D(21,22,23,19) -0.1514 estimate D2E/DX2 !

 ! D144 D(21,22,23,24) 179.2758 estimate D2E/DX2 !

 ! D145 D(30,22,23,19) -179.9368 estimate D2E/DX2 !

 ! D146 D(30,22,23,24) -0.5097 estimate D2E/DX2 !

 ! D147 D(21,22,30,31) 0.1564 estimate D2E/DX2 !

 ! D148 D(21,22,30,44) -179.8893 estimate D2E/DX2 !

 ! D149 D(23,22,30,31) 179.9166 estimate D2E/DX2 !

 ! D150 D(23,22,30,44) -0.1291 estimate D2E/DX2 !

 ! D151 D(19,23,24,9) 1.007 estimate D2E/DX2 !

 ! D152 D(22,23,24,9) -178.3033 estimate D2E/DX2 !

 ! D153 D(13,26,27,28) 0.2038 estimate D2E/DX2 !

 ! D154 D(13,26,27,54) -179.8427 estimate D2E/DX2 !

 ! D155 D(42,26,27,28) -179.842 estimate D2E/DX2 !

 ! D156 D(42,26,27,54) 0.1116 estimate D2E/DX2 !

 ! D157 D(26,27,28,29) -0.0198 estimate D2E/DX2 !

 ! D158 D(26,27,28,55) 179.9579 estimate D2E/DX2 !

 ! D159 D(54,27,28,29) -179.9735 estimate D2E/DX2 !

 ! D160 D(54,27,28,55) 0.0042 estimate D2E/DX2 !

 ! D161 D(27,28,29,14) -0.2121 estimate D2E/DX2 !

 ! D162 D(27,28,29,43) 179.87 estimate D2E/DX2 !

 ! D163 D(55,28,29,14) 179.8102 estimate D2E/DX2 !

 ! D164 D(55,28,29,43) -0.1076 estimate D2E/DX2 !

 ! D165 D(22,30,31,32) -0.2038 estimate D2E/DX2 !

 ! D166 D(22,30,31,57) 179.8427 estimate D2E/DX2 !

 ! D167 D(44,30,31,32) 179.842 estimate D2E/DX2 !

 ! D168 D(44,30,31,57) -0.1116 estimate D2E/DX2 !

 ! D169 D(30,31,32,33) 0.0198 estimate D2E/DX2 !

 ! D170 D(30,31,32,56) -179.9579 estimate D2E/DX2 !

 ! D171 D(57,31,32,33) 179.9735 estimate D2E/DX2 !

 ! D172 D(57,31,32,56) -0.0042 estimate D2E/DX2 !

 ! D173 D(31,32,33,21) 0.2121 estimate D2E/DX2 !

 ! D174 D(31,32,33,45) -179.87 estimate D2E/DX2 !

 ! D175 D(56,32,33,21) -179.8102 estimate D2E/DX2 !

 ! D176 D(56,32,33,45) 0.1076 estimate D2E/DX2 !

 ! D177 D(11,34,35,36) -0.2121 estimate D2E/DX2 !

 ! D178 D(11,34,35,50) 179.8102 estimate D2E/DX2 !

 ! D179 D(46,34,35,36) 179.87 estimate D2E/DX2 !

 ! D180 D(46,34,35,50) -0.1076 estimate D2E/DX2 !

 ! D181 D(34,35,36,37) -0.0198 estimate D2E/DX2 !

 ! D182 D(34,35,36,51) -179.9735 estimate D2E/DX2 !

 ! D183 D(50,35,36,37) 179.9579 estimate D2E/DX2 !

 ! D184 D(50,35,36,51) 0.0042 estimate D2E/DX2 !

 ! D185 D(35,36,37,10) 0.2038 estimate D2E/DX2 !

 ! D186 D(35,36,37,47) -179.842 estimate D2E/DX2 !

 ! D187 D(51,36,37,10) -179.8427 estimate D2E/DX2 !

 ! D188 D(51,36,37,47) 0.1116 estimate D2E/DX2 !

 ! D189 D(5,38,39,40) -0.2038 estimate D2E/DX2 !

 ! D190 D(5,38,39,53) 179.8427 estimate D2E/DX2 !

 ! D191 D(48,38,39,40) 179.842 estimate D2E/DX2 !

 ! D192 D(48,38,39,53) -0.1116 estimate D2E/DX2 !

 ! D193 D(38,39,40,41) 0.0198 estimate D2E/DX2 !

 ! D194 D(38,39,40,52) -179.9579 estimate D2E/DX2 !

 ! D195 D(53,39,40,41) 179.9735 estimate D2E/DX2 !

 ! D196 D(53,39,40,52) -0.0042 estimate D2E/DX2 !

 ! D197 D(39,40,41,4) 0.2121 estimate D2E/DX2 !

 ! D198 D(39,40,41,49) -179.87 estimate D2E/DX2 !

 ! D199 D(52,40,41,4) -179.8102 estimate D2E/DX2 !

 ! D200 D(52,40,41,49) 0.1076 estimate D2E/DX2 !

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

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

 Number of steps in this run= 342 maximum allowed number of steps= 342.

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link 103 at Sat Jun 15 12:05:00 2019, MaxMem= 1342177280 cpu: 0.4

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

 Stoichiometry C32H16N8Zn(1-,2)

 Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C32H16N4)]

 Deg. of freedom 43

 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 2.777717 1.188389 0.002377

 2 7 0 1.439815 1.424093 0.029020

 3 6 0 1.190436 2.789403 0.002839

 4 6 0 2.470212 3.482165 -0.036946

 5 6 0 3.474898 2.476544 -0.037870

 6 7 0 0.000000 3.389883 -0.004761

 7 6 0 -1.190436 2.789403 0.002839

 8 7 0 -1.439815 1.424093 0.029020

 9 6 0 -2.777717 1.188389 0.002377

 10 6 0 -3.474898 2.476544 -0.037870

 11 6 0 -2.470212 3.482165 -0.036946

 12 7 0 3.410354 0.000000 -0.001325

 13 6 0 3.474898 -2.476544 -0.037870

 14 6 0 2.470212 -3.482165 -0.036946

 15 6 0 1.190436 -2.789403 0.002839

 16 7 0 1.439815 -1.424093 0.029020

 17 6 0 2.777717 -1.188389 0.002377

 18 7 0 0.000000 -3.389883 -0.004761

 19 7 0 -1.439815 -1.424093 0.029020

 20 6 0 -1.190436 -2.789403 0.002839

 21 6 0 -2.470212 -3.482165 -0.036946

 22 6 0 -3.474898 -2.476544 -0.037870

 23 6 0 -2.777717 -1.188389 0.002377

 24 7 0 -3.410354 0.000000 -0.001325

 25 30 0 0.000000 0.000000 0.391144

 26 6 0 4.830902 -2.814424 -0.076788

 27 6 0 5.174876 -4.167586 -0.111467

 28 6 0 4.178392 -5.167360 -0.111609

 29 6 0 2.822756 -4.837513 -0.076831

 30 6 0 -4.830902 -2.814424 -0.076788

 31 6 0 -5.174876 -4.167586 -0.111467

 32 6 0 -4.178392 -5.167360 -0.111609

 33 6 0 -2.822756 -4.837513 -0.076831

 34 6 0 -2.822756 4.837513 -0.076831

 35 6 0 -4.178392 5.167360 -0.111609

 36 6 0 -5.174876 4.167586 -0.111467

 37 6 0 -4.830902 2.814424 -0.076788

 38 6 0 4.830902 2.814424 -0.076788

 39 6 0 5.174876 4.167586 -0.111467

 40 6 0 4.178392 5.167360 -0.111609

 41 6 0 2.822756 4.837513 -0.076831

 42 1 0 5.596246 -2.043514 -0.079188

 43 1 0 2.060727 -5.611653 -0.079254

 44 1 0 -5.596246 -2.043514 -0.079188

 45 1 0 -2.060727 -5.611653 -0.079254

 46 1 0 -2.060727 5.611653 -0.079254

 47 1 0 -5.596246 2.043514 -0.079188

 48 1 0 5.596246 2.043514 -0.079188

 49 1 0 2.060727 5.611653 -0.079254

 50 1 0 -4.475100 6.212206 -0.139717

 51 1 0 -6.221236 4.457844 -0.139486

 52 1 0 4.475100 6.212206 -0.139717

 53 1 0 6.221236 4.457844 -0.139486

 54 1 0 6.221236 -4.457844 -0.139486

 55 1 0 4.475100 -6.212206 -0.139717

 56 1 0 -4.475100 -6.212206 -0.139717

 57 1 0 -6.221236 -4.457844 -0.139486

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

 Rotational constants (GHZ): 0.0876884 0.0875743 0.0439064

 Leave Link 202 at Sat Jun 15 12:05:00 2019, MaxMem= 1342177280 cpu: 0.6

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

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

 Centers: 25

 S 1 1.00

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

 S 1 1.00

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

 S 1 1.00

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

 P 1 1.00

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

 P 1 1.00

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

 D 3 1.00

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

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

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

 D 1 1.00

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

 D 1 1.00

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

 \*\*\*\*

 Centers: 42 43 44 45 46 47 48 49 50 51

 Centers: 52 53 54 55 56 57 1 3 4 5

 Centers: 7 9 10 11 13 14 15 17 20 21

 Centers: 22 23 26 27 28 29 30 31 32 33

 Centers: 34 35 36 37 38 39 40 41 2 6

 Centers: 8 12 16 18 19 24

 6-311G\*

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

 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

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 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

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

 There are 225 symmetry adapted cartesian basis functions of A1 symmetry.

 There are 196 symmetry adapted cartesian basis functions of A2 symmetry.

 There are 207 symmetry adapted cartesian basis functions of B1 symmetry.

 There are 207 symmetry adapted cartesian basis functions of B2 symmetry.

 There are 211 symmetry adapted basis functions of A1 symmetry.

 There are 187 symmetry adapted basis functions of A2 symmetry.

 There are 197 symmetry adapted basis functions of B1 symmetry.

 There are 197 symmetry adapted basis functions of B2 symmetry.

 792 basis functions, 1399 primitive gaussians, 835 cartesian basis functions

 139 alpha electrons 138 beta electrons

 nuclear repulsion energy 4365.2036725104 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= 57 NActive= 57 NUniq= 16 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

 Integral buffers will be 131072 words long.

 Raffenetti 2 integral format.

 Two-electron integral symmetry is turned on.

 R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1640381979 Hartrees.

 Nuclear repulsion after empirical dispersion term = 4365.0396343124 Hartrees.

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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= 57.

 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 = 57

 GePol: Total number of spheres = 57

 GePol: Number of exposed spheres = 57 (100.00%)

 GePol: Number of points = 4670

 GePol: Average weight of points = 0.10

 GePol: Minimum weight of points = 0.93D-09

 GePol: Maximum weight of points = 0.18390

 GePol: Number of points with low weight = 312

 GePol: Fraction of low-weight points (<1% of avg) = 6.68%

 GePol: Cavity surface area = 486.913 Ang\*\*2

 GePol: Cavity volume = 505.662 Ang\*\*3

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

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 PCM non-electrostatic energy = -0.0143188439 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 4365.0253154685 Hartrees.

 Leave Link 301 at Sat Jun 15 12:05:00 2019, MaxMem= 1342177280 cpu: 1.1

 (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= 32896 NPrTT= 163506 LenC2= 22819 LenP2D= 61244.

 LDataN: DoStor=T MaxTD1= 5 Len= 102

 NBasis= 792 RedAO= T EigKep= 3.54D-05 NBF= 211 187 197 197

 NBsUse= 792 1.00D-06 EigRej= -1.00D+00 NBFU= 211 187 197 197

 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= 802 802 802 802 802 MxSgAt= 57 MxSgA2= 57.

 Leave Link 302 at Sat Jun 15 12:05:01 2019, MaxMem= 1342177280 cpu: 12.6

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

 DipDrv: MaxL=1.

 Leave Link 303 at Sat Jun 15 12:05:02 2019, MaxMem= 1342177280 cpu: 4.0

 (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= 0

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

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

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

 Petite list used in FoFCou.

 Harris En= -1733.82812209577

 JPrj=0 DoOrth=F DoCkMO=F.

 Initial guess orbital symmetries:

 Alpha Orbitals:

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 The electronic state of the initial guess is 2-B1.

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

 Leave Link 401 at Sat Jun 15 12:05:06 2019, MaxMem= 1342177280 cpu: 43.3

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

 UHF open shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 2129573 IEndB= 2129573 NGot= 1342177280 MDV= 1340762408

 LenX= 1340762408 LenY= 1340064348

 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= 560000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

 Petite list used in FoFCou.

 Inv3: Mode=1 IEnd= 65426700.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 6.99D-15 for 4642.

 Iteration 1 A\*A^-1 deviation from orthogonality is 5.14D-15 for 4664 1194.

 Iteration 1 A^-1\*A deviation from unit magnitude is 6.55D-15 for 4642.

 Iteration 1 A^-1\*A deviation from orthogonality is 6.18D-08 for 2383 2362.

 Iteration 2 A\*A^-1 deviation from unit magnitude is 3.11D-15 for 245.

 Iteration 2 A\*A^-1 deviation from orthogonality is 3.74D-15 for 3610 617.

 Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 306.

 Iteration 2 A^-1\*A deviation from orthogonality is 5.19D-16 for 4642 1163.

 E= -1732.64399178031

 DIIS: error= 9.77D-02 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -1732.64399178031 IErMin= 1 ErrMin= 9.77D-02

 ErrMax= 9.77D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.53D+00 BMatP= 4.53D+00

 IDIUse=3 WtCom= 2.34D-02 WtEn= 9.77D-01

 Coeff-Com: 0.100D+01

 Coeff-En: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.029 Goal= None Shift= 0.000

 Gap= 0.099 Goal= None Shift= 0.000

 GapD= 0.029 DampG=0.250 DampE=0.250 DampFc=0.1250 IDamp=-1.

 Damping current iteration by 1.25D-01

 RMSDP=2.77D-03 MaxDP=9.23D-02 OVMax= 2.36D-01

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 3.46D-04 CP: 9.98D-01

 E= -1732.82423888414 Delta-E= -0.180247103834 Rises=F Damp=T

 DIIS: error= 6.95D-02 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -1732.82423888414 IErMin= 2 ErrMin= 6.95D-02

 ErrMax= 6.95D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.61D+00 BMatP= 4.53D+00

 IDIUse=3 WtCom= 3.05D-01 WtEn= 6.95D-01

 Coeff-Com: -0.288D+01 0.388D+01

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

 Coeff: -0.880D+00 0.188D+01

 Gap= 0.031 Goal= None Shift= 0.000

 Gap= 0.087 Goal= None Shift= 0.000

 RMSDP=1.69D-03 MaxDP=6.00D-02 DE=-1.80D-01 OVMax= 6.64D-02

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 1.03D-03 CP: 9.85D-01 3.00D+00

 E= -1733.30236173797 Delta-E= -0.478122853827 Rises=F Damp=F

 DIIS: error= 5.43D-02 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 3 EnMin= -1733.30236173797 IErMin= 3 ErrMin= 5.43D-02

 ErrMax= 5.43D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D+00 BMatP= 2.61D+00

 IDIUse=3 WtCom= 4.57D-01 WtEn= 5.43D-01

 EnCoef did 100 forward-backward iterations

 Coeff-Com: 0.265D+01-0.281D+01 0.116D+01

 Coeff-En: 0.124D+00 0.322D-02 0.872D+00

 Coeff: 0.128D+01-0.128D+01 0.100D+01

 Gap= 0.035 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=9.33D-04 MaxDP=3.49D-02 DE=-4.78D-01 OVMax= 7.21D-02

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 5.17D-04 CP: 9.86D-01 3.00D+00 2.43D-01

 E= -1733.46908384751 Delta-E= -0.166722109539 Rises=F Damp=F

 DIIS: error= 2.21D-02 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -1733.46908384751 IErMin= 4 ErrMin= 2.21D-02

 ErrMax= 2.21D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.97D-01 BMatP= 1.05D+00

 IDIUse=3 WtCom= 7.79D-01 WtEn= 2.21D-01

 Coeff-Com: -0.900D+00 0.107D+01 0.938D-01 0.733D+00

 Coeff-En: 0.000D+00 0.000D+00 0.116D+00 0.884D+00

 Coeff: -0.701D+00 0.836D+00 0.987D-01 0.766D+00

 Gap= 0.036 Goal= None Shift= 0.000

 Gap= 0.080 Goal= None Shift= 0.000

 RMSDP=2.71D-04 MaxDP=1.10D-02 DE=-1.67D-01 OVMax= 4.17D-02

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 8.75D-05 CP: 9.85D-01 3.00D+00 4.44D-01 7.04D-01

 E= -1733.50429947889 Delta-E= -0.035215631382 Rises=F Damp=F

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

 NSaved= 5 IEnMin= 5 EnMin= -1733.50429947889 IErMin= 5 ErrMin= 2.20D-03

 ErrMax= 2.20D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-02 BMatP= 1.97D-01

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

 Coeff-Com: -0.426D+00 0.497D+00 0.448D-01 0.456D+00 0.428D+00

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

 Coeff: -0.416D+00 0.486D+00 0.438D-01 0.446D+00 0.441D+00

 Gap= 0.036 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=4.86D-05 MaxDP=3.29D-03 DE=-3.52D-02 OVMax= 1.02D-02

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 2.01D-05 CP: 9.86D-01 3.00D+00 4.21D-01 7.46D-01 6.52D-01

 E= -1733.50657532640 Delta-E= -0.002275847509 Rises=F Damp=F

 DIIS: error= 2.75D-04 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -1733.50657532640 IErMin= 6 ErrMin= 2.75D-04

 ErrMax= 2.75D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.30D-04 BMatP= 1.10D-02

 IDIUse=3 WtCom= 9.97D-01 WtEn= 2.75D-03

 Coeff-Com: -0.150D+00 0.172D+00 0.741D-03 0.126D+00 0.143D+00 0.708D+00

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

 Coeff: -0.150D+00 0.171D+00 0.739D-03 0.126D+00 0.143D+00 0.709D+00

 Gap= 0.037 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=1.18D-05 MaxDP=6.05D-04 DE=-2.28D-03 OVMax= 2.01D-03

 Cycle 7 Pass 1 IDiag 1:

 RMSU= 9.97D-06 CP: 9.85D-01 3.00D+00 4.26D-01 7.50D-01 6.68D-01

 CP: 8.55D-01

 E= -1733.50661278333 Delta-E= -0.000037456930 Rises=F Damp=F

 DIIS: error= 1.71D-04 at cycle 7 NSaved= 7.

 NSaved= 7 IEnMin= 7 EnMin= -1733.50661278333 IErMin= 7 ErrMin= 1.71D-04

 ErrMax= 1.71D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.88D-05 BMatP= 1.30D-04

 IDIUse=3 WtCom= 9.98D-01 WtEn= 1.71D-03

 Coeff-Com: -0.690D-02 0.683D-02-0.182D-02 0.169D-03 0.338D-02 0.392D+00

 Coeff-Com: 0.607D+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: -0.689D-02 0.682D-02-0.182D-02 0.169D-03 0.337D-02 0.391D+00

 Coeff: 0.607D+00

 Gap= 0.037 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=6.08D-06 MaxDP=3.10D-04 DE=-3.75D-05 OVMax= 1.70D-03

 Cycle 8 Pass 1 IDiag 1:

 RMSU= 4.38D-06 CP: 9.85D-01 3.00D+00 4.25D-01 7.50D-01 6.87D-01

 CP: 1.04D+00 9.15D-01

 E= -1733.50663156900 Delta-E= -0.000018785676 Rises=F Damp=F

 DIIS: error= 8.41D-05 at cycle 8 NSaved= 8.

 NSaved= 8 IEnMin= 8 EnMin= -1733.50663156900 IErMin= 8 ErrMin= 8.41D-05

 ErrMax= 8.41D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.43D-06 BMatP= 4.88D-05

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

 Coeff-Com: 0.591D-01-0.683D-01-0.650D-03-0.494D-01-0.555D-01-0.132D+00

 Coeff-Com: 0.241D+00 0.101D+01

 Coeff: 0.591D-01-0.683D-01-0.650D-03-0.494D-01-0.555D-01-0.132D+00

 Coeff: 0.241D+00 0.101D+01

 Gap= 0.037 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=4.77D-06 MaxDP=3.24D-04 DE=-1.88D-05 OVMax= 1.51D-03

 Cycle 9 Pass 1 IDiag 1:

 RMSU= 2.68D-06 CP: 9.85D-01 3.00D+00 4.26D-01 7.51D-01 6.93D-01

 CP: 1.14D+00 1.20D+00 1.33D+00

 E= -1733.50663988797 Delta-E= -0.000008318965 Rises=F Damp=F

 DIIS: error= 5.99D-05 at cycle 9 NSaved= 9.

 NSaved= 9 IEnMin= 9 EnMin= -1733.50663988797 IErMin= 9 ErrMin= 5.99D-05

 ErrMax= 5.99D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.69D-06 BMatP= 8.43D-06

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

 Coeff-Com: 0.213D-01-0.244D-01-0.994D-03-0.189D-01-0.200D-01-0.143D+00

 Coeff-Com: 0.199D-01 0.436D+00 0.730D+00

 Coeff: 0.213D-01-0.244D-01-0.994D-03-0.189D-01-0.200D-01-0.143D+00

 Coeff: 0.199D-01 0.436D+00 0.730D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=2.13D-06 MaxDP=1.46D-04 DE=-8.32D-06 OVMax= 5.36D-04

 Cycle 10 Pass 1 IDiag 1:

 RMSU= 1.51D-06 CP: 9.85D-01 3.00D+00 4.26D-01 7.51D-01 6.95D-01

 CP: 1.16D+00 1.29D+00 1.54D+00 1.22D+00

 E= -1733.50664132355 Delta-E= -0.000001435585 Rises=F Damp=F

 DIIS: error= 4.40D-05 at cycle 10 NSaved= 10.

 NSaved=10 IEnMin=10 EnMin= -1733.50664132355 IErMin=10 ErrMin= 4.40D-05

 ErrMax= 4.40D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.58D-06 BMatP= 2.69D-06

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

 Coeff-Com: -0.398D-02 0.480D-02-0.694D-03 0.223D-02 0.477D-02-0.687D-01

 Coeff-Com: -0.636D-01-0.401D-01 0.555D+00 0.610D+00

 Coeff: -0.398D-02 0.480D-02-0.694D-03 0.223D-02 0.477D-02-0.687D-01

 Coeff: -0.636D-01-0.401D-01 0.555D+00 0.610D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=1.38D-06 MaxDP=8.20D-05 DE=-1.44D-06 OVMax= 3.38D-04

 Cycle 11 Pass 1 IDiag 1:

 RMSU= 7.32D-07 CP: 9.85D-01 3.00D+00 4.26D-01 7.51D-01 6.98D-01

 CP: 1.18D+00 1.35D+00 1.67D+00 1.40D+00 7.77D-01

 E= -1733.50664202688 Delta-E= -0.000000703321 Rises=F Damp=F

 DIIS: error= 9.69D-06 at cycle 11 NSaved= 11.

 NSaved=11 IEnMin=11 EnMin= -1733.50664202688 IErMin=11 ErrMin= 9.69D-06

 ErrMax= 9.69D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.88D-08 BMatP= 1.58D-06

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

 Coeff-Com: -0.146D-02 0.168D-02 0.119D-03 0.133D-02 0.161D-02 0.537D-02

 Coeff-Com: -0.101D-01-0.426D-01-0.229D-01 0.579D-01 0.101D+01

 Coeff: -0.146D-02 0.168D-02 0.119D-03 0.133D-02 0.161D-02 0.537D-02

 Coeff: -0.101D-01-0.426D-01-0.229D-01 0.579D-01 0.101D+01

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=5.74D-07 MaxDP=3.40D-05 DE=-7.03D-07 OVMax= 1.45D-04

 Cycle 12 Pass 1 IDiag 1:

 RMSU= 3.59D-07 CP: 9.85D-01 3.00D+00 4.26D-01 7.51D-01 6.98D-01

 CP: 1.18D+00 1.37D+00 1.70D+00 1.47D+00 8.85D-01

 CP: 1.31D+00

 E= -1733.50664213589 Delta-E= -0.000000109015 Rises=F Damp=F

 DIIS: error= 9.10D-06 at cycle 12 NSaved= 12.

 NSaved=12 IEnMin=12 EnMin= -1733.50664213589 IErMin=12 ErrMin= 9.10D-06

 ErrMax= 9.10D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.11D-08 BMatP= 7.88D-08

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

 Coeff-Com: -0.285D-04-0.216D-04 0.317D-03 0.580D-03 0.269D-03 0.219D-01

 Coeff-Com: 0.803D-02-0.184D-01-0.161D+00-0.122D+00 0.627D+00 0.644D+00

 Coeff: -0.285D-04-0.216D-04 0.317D-03 0.580D-03 0.269D-03 0.219D-01

 Coeff: 0.803D-02-0.184D-01-0.161D+00-0.122D+00 0.627D+00 0.644D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=3.38D-07 MaxDP=1.94D-05 DE=-1.09D-07 OVMax= 8.40D-05

 Cycle 13 Pass 1 IDiag 1:

 RMSU= 2.09D-07 CP: 9.85D-01 3.00D+00 4.26D-01 7.51D-01 6.98D-01

 CP: 1.18D+00 1.38D+00 1.72D+00 1.51D+00 9.13D-01

 CP: 1.60D+00 9.56D-01

 E= -1733.50664217836 Delta-E= -0.000000042468 Rises=F Damp=F

 DIIS: error= 5.02D-06 at cycle 13 NSaved= 13.

 NSaved=13 IEnMin=13 EnMin= -1733.50664217836 IErMin=13 ErrMin= 5.02D-06

 ErrMax= 5.02D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.39D-08 BMatP= 6.11D-08

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

 Coeff-Com: 0.280D-03-0.350D-03 0.131D-03 0.129D-03 0.874D-04 0.929D-02

 Coeff-Com: 0.650D-02 0.370D-02-0.678D-01-0.759D-01-0.114D+00 0.313D+00

 Coeff-Com: 0.925D+00

 Coeff: 0.280D-03-0.350D-03 0.131D-03 0.129D-03 0.874D-04 0.929D-02

 Coeff: 0.650D-02 0.370D-02-0.678D-01-0.759D-01-0.114D+00 0.313D+00

 Coeff: 0.925D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=2.53D-07 MaxDP=1.37D-05 DE=-4.25D-08 OVMax= 6.20D-05

 Cycle 14 Pass 1 IDiag 1:

 RMSU= 1.17D-07 CP: 9.85D-01 3.00D+00 4.26D-01 7.51D-01 6.98D-01

 CP: 1.18D+00 1.38D+00 1.73D+00 1.54D+00 9.72D-01

 CP: 1.73D+00 1.38D+00 9.80D-01

 E= -1733.50664219252 Delta-E= -0.000000014164 Rises=F Damp=F

 DIIS: error= 2.39D-06 at cycle 14 NSaved= 14.

 NSaved=14 IEnMin=14 EnMin= -1733.50664219252 IErMin=14 ErrMin= 2.39D-06

 ErrMax= 2.39D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.32D-09 BMatP= 1.39D-08

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

 Coeff-Com: -0.101D-03 0.111D-03-0.178D-04 0.862D-04 0.658D-04 0.157D-02

 Coeff-Com: 0.266D-02 0.441D-02-0.750D-02-0.232D-01-0.215D+00 0.532D-01

 Coeff-Com: 0.604D+00 0.580D+00

 Coeff: -0.101D-03 0.111D-03-0.178D-04 0.862D-04 0.658D-04 0.157D-02

 Coeff: 0.266D-02 0.441D-02-0.750D-02-0.232D-01-0.215D+00 0.532D-01

 Coeff: 0.604D+00 0.580D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=1.00D-07 MaxDP=5.23D-06 DE=-1.42D-08 OVMax= 2.44D-05

 Cycle 15 Pass 1 IDiag 1:

 RMSU= 4.12D-08 CP: 9.85D-01 3.00D+00 4.26D-01 7.51D-01 6.98D-01

 CP: 1.18D+00 1.38D+00 1.73D+00 1.55D+00 9.84D-01

 CP: 1.79D+00 1.41D+00 1.30D+00 8.70D-01

 E= -1733.50664219525 Delta-E= -0.000000002729 Rises=F Damp=F

 DIIS: error= 1.11D-06 at cycle 15 NSaved= 15.

 NSaved=15 IEnMin=15 EnMin= -1733.50664219525 IErMin=15 ErrMin= 1.11D-06

 ErrMax= 1.11D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.99D-10 BMatP= 6.32D-09

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

 Coeff-Com: -0.293D-04 0.375D-04-0.548D-04-0.136D-03-0.251D-03-0.149D-02

 Coeff-Com: 0.455D-03 0.225D-02 0.113D-01 0.241D-02-0.735D-01-0.370D-01

 Coeff-Com: 0.779D-01 0.264D+00 0.754D+00

 Coeff: -0.293D-04 0.375D-04-0.548D-04-0.136D-03-0.251D-03-0.149D-02

 Coeff: 0.455D-03 0.225D-02 0.113D-01 0.241D-02-0.735D-01-0.370D-01

 Coeff: 0.779D-01 0.264D+00 0.754D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=3.23D-08 MaxDP=1.57D-06 DE=-2.73D-09 OVMax= 7.80D-06

 Cycle 16 Pass 1 IDiag 1:

 RMSU= 1.47D-08 CP: 9.85D-01 3.00D+00 4.26D-01 7.51D-01 6.98D-01

 CP: 1.18D+00 1.38D+00 1.73D+00 1.55D+00 9.82D-01

 CP: 1.80D+00 1.46D+00 1.31D+00 9.66D-01 8.91D-01

 E= -1733.50664219564 Delta-E= -0.000000000387 Rises=F Damp=F

 DIIS: error= 2.23D-07 at cycle 16 NSaved= 16.

 NSaved=16 IEnMin=16 EnMin= -1733.50664219564 IErMin=16 ErrMin= 2.23D-07

 ErrMax= 2.23D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.61D-11 BMatP= 6.99D-10

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

 Coeff-Com: 0.159D-04-0.176D-04-0.139D-05-0.281D-04-0.606D-04-0.233D-03

 Coeff-Com: -0.231D-03-0.182D-03 0.169D-02 0.204D-02 0.129D-01-0.751D-02

 Coeff-Com: -0.459D-01-0.319D-01 0.441D-01 0.103D+01

 Coeff: 0.159D-04-0.176D-04-0.139D-05-0.281D-04-0.606D-04-0.233D-03

 Coeff: -0.231D-03-0.182D-03 0.169D-02 0.204D-02 0.129D-01-0.751D-02

 Coeff: -0.459D-01-0.319D-01 0.441D-01 0.103D+01

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=8.30D-09 MaxDP=5.41D-07 DE=-3.87D-10 OVMax= 2.21D-06

 Error on total polarization charges = 0.07601

 SCF Done: E(UB3LYP) = -1733.50664220 A.U. after 16 cycles

 NFock= 16 Conv=0.83D-08 -V/T= 1.9759

 <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7686 S= 0.5092

 <L.S>= 0.000000000000E+00

 KE= 1.776268588325D+03 PE=-1.287684941662D+04 EE= 5.002048870630D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -8.99

 (included in total energy above)

 Annihilation of the first spin contaminant:

 S\*\*2 before annihilation 0.7686, after 0.7503

 Leave Link 502 at Sat Jun 15 12:08:41 2019, MaxMem= 1342177280 cpu: 2505.8

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

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

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

 The electronic state is 2-B1.

 Alpha occ. eigenvalues -- -14.30525 -14.30525 -14.29820 -14.29820 -14.29820

 Alpha occ. eigenvalues -- -14.29820 -14.29225 -14.29225 -10.23232 -10.23232

 Alpha occ. eigenvalues -- -10.23232 -10.23232 -10.22408 -10.22408 -10.22407

 Alpha occ. eigenvalues -- -10.22407 -10.17418 -10.17418 -10.17418 -10.17418

 Alpha occ. eigenvalues -- -10.17352 -10.17352 -10.17352 -10.17352 -10.17296

 Alpha occ. eigenvalues -- -10.17296 -10.17296 -10.17296 -10.17162 -10.17162

 Alpha occ. eigenvalues -- -10.17162 -10.17162 -10.17157 -10.17157 -10.17157

 Alpha occ. eigenvalues -- -10.17157 -10.16996 -10.16996 -10.16996 -10.16996

 Alpha occ. eigenvalues -- -0.98554 -0.97207 -0.97188 -0.94562 -0.92337

 Alpha occ. eigenvalues -- -0.88658 -0.88106 -0.85565 -0.84470 -0.84466

 Alpha occ. eigenvalues -- -0.84433 -0.84120 -0.76405 -0.75170 -0.75084

 Alpha occ. eigenvalues -- -0.74942 -0.74681 -0.74647 -0.74597 -0.74454

 Alpha occ. eigenvalues -- -0.70887 -0.68334 -0.67696 -0.62800 -0.62443

 Alpha occ. eigenvalues -- -0.61905 -0.61883 -0.61575 -0.60820 -0.58618

 Alpha occ. eigenvalues -- -0.58496 -0.58033 -0.57689 -0.56802 -0.55790

 Alpha occ. eigenvalues -- -0.55322 -0.55290 -0.54168 -0.53783 -0.53765

 Alpha occ. eigenvalues -- -0.53591 -0.51736 -0.51435 -0.51351 -0.48668

 Alpha occ. eigenvalues -- -0.48268 -0.47138 -0.47111 -0.46212 -0.45604

 Alpha occ. eigenvalues -- -0.45603 -0.45322 -0.45167 -0.44783 -0.43312

 Alpha occ. eigenvalues -- -0.43306 -0.43251 -0.43236 -0.43224 -0.43183

 Alpha occ. eigenvalues -- -0.42103 -0.41586 -0.41443 -0.40875 -0.40750

 Alpha occ. eigenvalues -- -0.37337 -0.37261 -0.36388 -0.36084 -0.36020

 Alpha occ. eigenvalues -- -0.35849 -0.35824 -0.35706 -0.35304 -0.34572

 Alpha occ. eigenvalues -- -0.33963 -0.33947 -0.33916 -0.33350 -0.31702

 Alpha occ. eigenvalues -- -0.31639 -0.31058 -0.30961 -0.29514 -0.27472

 Alpha occ. eigenvalues -- -0.26775 -0.26605 -0.25557 -0.25455 -0.25347

 Alpha occ. eigenvalues -- -0.25096 -0.24998 -0.24857 -0.24215 -0.24187

 Alpha occ. eigenvalues -- -0.24179 -0.23981 -0.18136 -0.12838

 Alpha virt. eigenvalues -- -0.09075 -0.04368 -0.02738 -0.02272 -0.02042

 Alpha virt. eigenvalues -- -0.01971 0.02573 0.02707 0.03025 0.03120

 Alpha virt. eigenvalues -- 0.05262 0.05272 0.05748 0.05860 0.06066

 Alpha virt. eigenvalues -- 0.07092 0.07094 0.07139 0.07248 0.07701

 Alpha virt. eigenvalues -- 0.09079 0.09089 0.10026 0.10749 0.11580

 Alpha virt. eigenvalues -- 0.11654 0.12050 0.12055 0.12674 0.12952

 Alpha virt. eigenvalues -- 0.14608 0.15274 0.15399 0.16184 0.17439

 Alpha virt. eigenvalues -- 0.18038 0.18097 0.18165 0.19539 0.20582

 Alpha virt. eigenvalues -- 0.20728 0.21466 0.22040 0.22183 0.23029

 Alpha virt. eigenvalues -- 0.24020 0.24034 0.24185 0.24527 0.25127

 Alpha virt. eigenvalues -- 0.25381 0.25761 0.26879 0.27022 0.27435

 Alpha virt. eigenvalues -- 0.27517 0.27962 0.28125 0.28790 0.28816

 Alpha virt. eigenvalues -- 0.28866 0.29007 0.29377 0.30391 0.30635

 Alpha virt. eigenvalues -- 0.30927 0.30988 0.32087 0.33257 0.33488

 Alpha virt. eigenvalues -- 0.34153 0.34645 0.35647 0.35671 0.36252

 Alpha virt. eigenvalues -- 0.36585 0.37065 0.37335 0.38037 0.38189

 Alpha virt. eigenvalues -- 0.38790 0.39011 0.39036 0.39870 0.39875

 Alpha virt. eigenvalues -- 0.40051 0.40750 0.40829 0.40891 0.40926

 Alpha virt. eigenvalues -- 0.41338 0.41628 0.41951 0.42103 0.42411

 Alpha virt. eigenvalues -- 0.42594 0.42792 0.42873 0.43013 0.43426

 Alpha virt. eigenvalues -- 0.43454 0.43491 0.43608 0.43727 0.43748

 Alpha virt. eigenvalues -- 0.43842 0.43979 0.44176 0.44289 0.45742

 Alpha virt. eigenvalues -- 0.45886 0.47066 0.47074 0.47296 0.47364

 Alpha virt. eigenvalues -- 0.47870 0.47882 0.47998 0.48327 0.48840

 Alpha virt. eigenvalues -- 0.50266 0.50408 0.50510 0.51198 0.51511

 Alpha virt. eigenvalues -- 0.51593 0.51904 0.51972 0.52261 0.52262

 Alpha virt. eigenvalues -- 0.52478 0.53592 0.54370 0.54427 0.54684

 Alpha virt. eigenvalues -- 0.55163 0.56160 0.56171 0.57060 0.58995

 Alpha virt. eigenvalues -- 0.60189 0.60372 0.60736 0.60747 0.60836

 Alpha virt. eigenvalues -- 0.60844 0.60927 0.61340 0.61362 0.61389

 Alpha virt. eigenvalues -- 0.61870 0.62227 0.62334 0.63282 0.63350

 Alpha virt. eigenvalues -- 0.63423 0.63470 0.63793 0.64831 0.65067

 Alpha virt. eigenvalues -- 0.65205 0.65269 0.65270 0.66377 0.67156

 Alpha virt. eigenvalues -- 0.67332 0.67394 0.67984 0.68042 0.69849

 Alpha virt. eigenvalues -- 0.70296 0.70338 0.70723 0.70906 0.71084

 Alpha virt. eigenvalues -- 0.71412 0.72177 0.72548 0.73728 0.73966

 Alpha virt. eigenvalues -- 0.74176 0.74537 0.75002 0.75269 0.76619

 Alpha virt. eigenvalues -- 0.77481 0.77546 0.77731 0.77827 0.77893

 Alpha virt. eigenvalues -- 0.78672 0.78803 0.79628 0.80046 0.80048

 Alpha virt. eigenvalues -- 0.80171 0.80403 0.80817 0.81840 0.82215

 Alpha virt. eigenvalues -- 0.82275 0.82413 0.83415 0.83692 0.84471

 Alpha virt. eigenvalues -- 0.84594 0.86670 0.86908 0.87068 0.87321

 Alpha virt. eigenvalues -- 0.87464 0.88697 0.89175 0.89308 0.89868

 Alpha virt. eigenvalues -- 0.90573 0.91110 0.91325 0.91585 0.91804

 Alpha virt. eigenvalues -- 0.92504 0.92769 0.93088 0.94418 0.94991

 Alpha virt. eigenvalues -- 0.96477 0.98045 0.99557 0.99650 0.99710

 Alpha virt. eigenvalues -- 1.00203 1.00408 1.00445 1.00586 1.01087

 Alpha virt. eigenvalues -- 1.02558 1.02594 1.02785 1.03584 1.03663

 Alpha virt. eigenvalues -- 1.06237 1.06338 1.06519 1.07387 1.10940

 Alpha virt. eigenvalues -- 1.11033 1.11309 1.11412 1.11528 1.12042

 Alpha virt. eigenvalues -- 1.12279 1.12371 1.12798 1.14153 1.14421

 Alpha virt. eigenvalues -- 1.14873 1.14928 1.15086 1.15490 1.16144

 Alpha virt. eigenvalues -- 1.17152 1.19056 1.19906 1.21046 1.21075

 Alpha virt. eigenvalues -- 1.21230 1.21304 1.21443 1.21538 1.21551

 Alpha virt. eigenvalues -- 1.21566 1.23396 1.23559 1.25968 1.26209

 Alpha virt. eigenvalues -- 1.26308 1.26649 1.27505 1.27551 1.27712

 Alpha virt. eigenvalues -- 1.28530 1.29236 1.29629 1.30094 1.32438

 Alpha virt. eigenvalues -- 1.34529 1.34794 1.34802 1.35346 1.35586

 Alpha virt. eigenvalues -- 1.36260 1.39038 1.39787 1.42030 1.42271

 Alpha virt. eigenvalues -- 1.42772 1.43173 1.43556 1.43588 1.45564

 Alpha virt. eigenvalues -- 1.45699 1.45741 1.45806 1.45829 1.45870

 Alpha virt. eigenvalues -- 1.48835 1.50248 1.51562 1.51652 1.52220

 Alpha virt. eigenvalues -- 1.53132 1.53384 1.53454 1.53655 1.53656

 Alpha virt. eigenvalues -- 1.54019 1.54116 1.55466 1.56194 1.58310

 Alpha virt. eigenvalues -- 1.58311 1.60193 1.62734 1.62773 1.63163

 Alpha virt. eigenvalues -- 1.63369 1.64063 1.65121 1.66100 1.66298

 Alpha virt. eigenvalues -- 1.67024 1.67871 1.68747 1.69007 1.72531

 Alpha virt. eigenvalues -- 1.72553 1.72898 1.74395 1.74496 1.74683

 Alpha virt. eigenvalues -- 1.74879 1.75241 1.76000 1.76017 1.76035

 Alpha virt. eigenvalues -- 1.81440 1.81563 1.81634 1.81661 1.82199

 Alpha virt. eigenvalues -- 1.82817 1.83092 1.83458 1.83557 1.83870

 Alpha virt. eigenvalues -- 1.84675 1.84929 1.85201 1.86879 1.87034

 Alpha virt. eigenvalues -- 1.87391 1.89453 1.90182 1.91044 1.91170

 Alpha virt. eigenvalues -- 1.91195 1.91256 1.91338 1.91524 1.91557

 Alpha virt. eigenvalues -- 1.91560 1.91768 1.92285 1.92668 1.92784

 Alpha virt. eigenvalues -- 1.93152 1.93379 1.94147 1.95010 1.95406

 Alpha virt. eigenvalues -- 1.95792 1.96681 1.99206 1.99424 1.99611

 Alpha virt. eigenvalues -- 2.00344 2.01560 2.02995 2.03032 2.03533

 Alpha virt. eigenvalues -- 2.04220 2.05039 2.05903 2.06001 2.08373

 Alpha virt. eigenvalues -- 2.12068 2.14249 2.14271 2.16431 2.16434

 Alpha virt. eigenvalues -- 2.18582 2.19910 2.22233 2.23280 2.23817

 Alpha virt. eigenvalues -- 2.24017 2.24422 2.25031 2.25499 2.25875

 Alpha virt. eigenvalues -- 2.26719 2.27145 2.27625 2.27702 2.28095

 Alpha virt. eigenvalues -- 2.28337 2.28409 2.28763 2.29129 2.30528

 Alpha virt. eigenvalues -- 2.30711 2.30741 2.30921 2.33027 2.33327

 Alpha virt. eigenvalues -- 2.33347 2.33906 2.37568 2.38931 2.39193

 Alpha virt. eigenvalues -- 2.39852 2.40109 2.40140 2.41142 2.41869

 Alpha virt. eigenvalues -- 2.43778 2.43888 2.44520 2.45763 2.46644

 Alpha virt. eigenvalues -- 2.49401 2.49475 2.52412 2.53054 2.53854

 Alpha virt. eigenvalues -- 2.53959 2.55143 2.55829 2.56626 2.56830

 Alpha virt. eigenvalues -- 2.57875 2.58168 2.58521 2.58611 2.59728

 Alpha virt. eigenvalues -- 2.61666 2.64692 2.65143 2.65461 2.66145

 Alpha virt. eigenvalues -- 2.66193 2.66629 2.68772 2.68812 2.69277

 Alpha virt. eigenvalues -- 2.69325 2.70639 2.73535 2.74530 2.74569

 Alpha virt. eigenvalues -- 2.74774 2.75071 2.75221 2.75379 2.76067

 Alpha virt. eigenvalues -- 2.77573 2.77704 2.77820 2.78860 2.79579

 Alpha virt. eigenvalues -- 2.79828 2.80060 2.82460 2.82700 2.83017

 Alpha virt. eigenvalues -- 2.83068 2.83136 2.84339 2.85095 2.86049

 Alpha virt. eigenvalues -- 2.86623 2.88580 2.88599 2.88791 2.89072

 Alpha virt. eigenvalues -- 2.92160 2.92274 2.92306 2.92340 2.92548

 Alpha virt. eigenvalues -- 2.97713 2.98022 3.00482 3.04212 3.05247

 Alpha virt. eigenvalues -- 3.05262 3.05527 3.07987 3.08663 3.09779

 Alpha virt. eigenvalues -- 3.15857 3.16691 3.16717 3.16931 3.17734

 Alpha virt. eigenvalues -- 3.18925 3.19766 3.19900 3.20245 3.21733

 Alpha virt. eigenvalues -- 3.22752 3.23113 3.23724 3.26280 3.26527

 Alpha virt. eigenvalues -- 3.26894 3.26918 3.27653 3.27764 3.27963

 Alpha virt. eigenvalues -- 3.28718 3.30540 3.30945 3.31133 3.31203

 Alpha virt. eigenvalues -- 3.31348 3.33234 3.33351 3.36340 3.38034

 Alpha virt. eigenvalues -- 3.40171 3.40219 3.41706 3.46489 3.47349

 Alpha virt. eigenvalues -- 3.47441 3.47764 3.48220 3.48370 3.48477

 Alpha virt. eigenvalues -- 3.49934 3.56774 3.61714 3.62188 3.64523

 Alpha virt. eigenvalues -- 3.64534 3.64637 3.65127 3.72632 3.72809

 Alpha virt. eigenvalues -- 3.73470 3.74490 3.75895 3.76763 3.77372

 Alpha virt. eigenvalues -- 3.77425 3.83116 3.84344 3.84604 3.84889

 Alpha virt. eigenvalues -- 3.88004 3.89079 3.90477 3.90819 3.91716

 Alpha virt. eigenvalues -- 3.95850 3.96582 3.96608 3.97499 4.10987

 Alpha virt. eigenvalues -- 4.12070 4.12664 4.18330 4.18729 4.18842

 Alpha virt. eigenvalues -- 4.20888 4.23676 4.35161 4.40306 4.41180

 Alpha virt. eigenvalues -- 4.41337 4.47111 4.53323 4.55348 4.55433

 Alpha virt. eigenvalues -- 4.78756 4.78915 4.78915 4.79230 5.12571

 Alpha virt. eigenvalues -- 5.13380 5.13995 5.16933 5.21234 5.35161

 Alpha virt. eigenvalues -- 5.37413 5.52616 7.85697 7.85834 7.86332

 Alpha virt. eigenvalues -- 7.92286 8.15793 11.13325 23.28468 23.31532

 Alpha virt. eigenvalues -- 23.31544 23.33298 23.76713 23.78439 23.78640

 Alpha virt. eigenvalues -- 23.78669 23.78901 23.78982 23.79188 23.80795

 Alpha virt. eigenvalues -- 23.88450 23.88732 23.89576 23.89753 23.90880

 Alpha virt. eigenvalues -- 23.90949 23.91002 23.91472 24.02460 24.02722

 Alpha virt. eigenvalues -- 24.02781 24.03331 24.04973 24.04985 24.05032

 Alpha virt. eigenvalues -- 24.05107 24.12786 24.12931 24.12951 24.13292

 Alpha virt. eigenvalues -- 35.57673 35.61108 35.61594 35.62364 35.69512

 Alpha virt. eigenvalues -- 35.70229 35.70274 35.70408

 Beta occ. eigenvalues -- -14.30644 -14.30643 -14.29765 -14.29765 -14.29765

 Beta occ. eigenvalues -- -14.29764 -14.28890 -14.28890 -10.23269 -10.23269

 Beta occ. eigenvalues -- -10.23268 -10.23268 -10.22175 -10.22175 -10.22174

 Beta occ. eigenvalues -- -10.22174 -10.17449 -10.17449 -10.17449 -10.17449

 Beta occ. eigenvalues -- -10.17352 -10.17352 -10.17352 -10.17351 -10.17285

 Beta occ. eigenvalues -- -10.17285 -10.17285 -10.17285 -10.17178 -10.17178

 Beta occ. eigenvalues -- -10.17178 -10.17178 -10.17092 -10.17092 -10.17092

 Beta occ. eigenvalues -- -10.17092 -10.16937 -10.16937 -10.16937 -10.16937

 Beta occ. eigenvalues -- -0.98331 -0.97014 -0.96937 -0.94374 -0.92077

 Beta occ. eigenvalues -- -0.88639 -0.87650 -0.85411 -0.84414 -0.84409

 Beta occ. eigenvalues -- -0.84348 -0.83949 -0.76260 -0.75047 -0.75038

 Beta occ. eigenvalues -- -0.74854 -0.74627 -0.74559 -0.74512 -0.74361

 Beta occ. eigenvalues -- -0.70674 -0.67905 -0.67661 -0.62680 -0.62377

 Beta occ. eigenvalues -- -0.61848 -0.61829 -0.61424 -0.60735 -0.58545

 Beta occ. eigenvalues -- -0.58422 -0.57928 -0.57618 -0.56788 -0.55775

 Beta occ. eigenvalues -- -0.55283 -0.55282 -0.54114 -0.53731 -0.53688

 Beta occ. eigenvalues -- -0.53515 -0.51611 -0.51356 -0.51313 -0.48580

 Beta occ. eigenvalues -- -0.48164 -0.47088 -0.46993 -0.46177 -0.45567

 Beta occ. eigenvalues -- -0.45564 -0.45252 -0.45131 -0.44233 -0.43279

 Beta occ. eigenvalues -- -0.43220 -0.43207 -0.43176 -0.42762 -0.42703

 Beta occ. eigenvalues -- -0.42060 -0.41534 -0.41413 -0.40835 -0.40341

 Beta occ. eigenvalues -- -0.37279 -0.36498 -0.36348 -0.36038 -0.35984

 Beta occ. eigenvalues -- -0.35606 -0.35508 -0.35507 -0.35252 -0.34550

 Beta occ. eigenvalues -- -0.33927 -0.33894 -0.33651 -0.33322 -0.31547

 Beta occ. eigenvalues -- -0.31524 -0.30855 -0.29955 -0.29354 -0.27132

 Beta occ. eigenvalues -- -0.26656 -0.26423 -0.25382 -0.25262 -0.25017

 Beta occ. eigenvalues -- -0.24996 -0.24848 -0.24621 -0.23955 -0.23775

 Beta occ. eigenvalues -- -0.23733 -0.23226 -0.16922

 Beta virt. eigenvalues -- -0.09192 -0.08717 -0.03466 -0.02399 -0.02088

 Beta virt. eigenvalues -- -0.01807 -0.01752 0.02924 0.03173 0.03206

 Beta virt. eigenvalues -- 0.03314 0.05299 0.05302 0.05879 0.06432

 Beta virt. eigenvalues -- 0.06693 0.07108 0.07110 0.07146 0.07285

 Beta virt. eigenvalues -- 0.07708 0.09082 0.09101 0.10041 0.10756

 Beta virt. eigenvalues -- 0.12048 0.12065 0.12335 0.12341 0.12691

 Beta virt. eigenvalues -- 0.13479 0.14617 0.15298 0.15402 0.16193

 Beta virt. eigenvalues -- 0.17702 0.18352 0.18462 0.18491 0.19680

 Beta virt. eigenvalues -- 0.20803 0.20830 0.21477 0.22157 0.22439

 Beta virt. eigenvalues -- 0.23271 0.24073 0.24098 0.24452 0.24671

 Beta virt. eigenvalues -- 0.25179 0.25457 0.25804 0.26964 0.27136

 Beta virt. eigenvalues -- 0.27495 0.27570 0.27999 0.28253 0.28839

 Beta virt. eigenvalues -- 0.28871 0.28926 0.29081 0.29418 0.30560

 Beta virt. eigenvalues -- 0.30703 0.31010 0.31011 0.32302 0.33327

 Beta virt. eigenvalues -- 0.33620 0.34241 0.34668 0.35719 0.35773

 Beta virt. eigenvalues -- 0.36413 0.36697 0.37336 0.37402 0.38093

 Beta virt. eigenvalues -- 0.38282 0.38864 0.39082 0.39157 0.39946

 Beta virt. eigenvalues -- 0.40021 0.40113 0.40836 0.40942 0.40942

 Beta virt. eigenvalues -- 0.40944 0.41566 0.41716 0.42063 0.42240

 Beta virt. eigenvalues -- 0.42494 0.42652 0.42891 0.42976 0.43056

 Beta virt. eigenvalues -- 0.43504 0.43523 0.43534 0.43742 0.43768

 Beta virt. eigenvalues -- 0.43928 0.43973 0.44150 0.44218 0.44388

 Beta virt. eigenvalues -- 0.45812 0.45939 0.47231 0.47234 0.47319

 Beta virt. eigenvalues -- 0.47435 0.47949 0.47971 0.48055 0.48407

 Beta virt. eigenvalues -- 0.48904 0.50454 0.50516 0.50620 0.51351

 Beta virt. eigenvalues -- 0.51540 0.51681 0.51987 0.52155 0.52381

 Beta virt. eigenvalues -- 0.52393 0.52610 0.53660 0.54474 0.54493

 Beta virt. eigenvalues -- 0.54807 0.55258 0.56247 0.56292 0.57176

 Beta virt. eigenvalues -- 0.59143 0.60286 0.60469 0.60753 0.60789

 Beta virt. eigenvalues -- 0.60890 0.60898 0.60964 0.61365 0.61392

 Beta virt. eigenvalues -- 0.61656 0.62049 0.62285 0.62394 0.63336

 Beta virt. eigenvalues -- 0.63418 0.63535 0.63547 0.63864 0.64887

 Beta virt. eigenvalues -- 0.65108 0.65262 0.65327 0.65346 0.66439

 Beta virt. eigenvalues -- 0.67243 0.67457 0.67473 0.68096 0.68106

 Beta virt. eigenvalues -- 0.69948 0.70388 0.70436 0.70784 0.71131

 Beta virt. eigenvalues -- 0.71164 0.71608 0.72349 0.72609 0.73797

 Beta virt. eigenvalues -- 0.74011 0.74275 0.74578 0.75126 0.75304

 Beta virt. eigenvalues -- 0.76799 0.77502 0.77608 0.77744 0.77911

 Beta virt. eigenvalues -- 0.77965 0.78782 0.79155 0.79754 0.80051

 Beta virt. eigenvalues -- 0.80212 0.80247 0.80605 0.80970 0.82085

 Beta virt. eigenvalues -- 0.82309 0.82350 0.82458 0.83468 0.83719

 Beta virt. eigenvalues -- 0.84522 0.84626 0.86716 0.87102 0.87188

 Beta virt. eigenvalues -- 0.87447 0.87479 0.88735 0.89251 0.89351

 Beta virt. eigenvalues -- 0.89920 0.90625 0.91173 0.91343 0.91668

 Beta virt. eigenvalues -- 0.91840 0.92567 0.92925 0.93173 0.94460

 Beta virt. eigenvalues -- 0.95067 0.96528 0.98194 0.99622 0.99707

 Beta virt. eigenvalues -- 0.99820 1.00321 1.00495 1.00495 1.00655

 Beta virt. eigenvalues -- 1.01171 1.02620 1.02633 1.02806 1.03703

 Beta virt. eigenvalues -- 1.03725 1.06399 1.06499 1.06693 1.07457

 Beta virt. eigenvalues -- 1.11051 1.11070 1.11457 1.11599 1.11767

 Beta virt. eigenvalues -- 1.12269 1.12416 1.12536 1.12859 1.14276

 Beta virt. eigenvalues -- 1.14532 1.15032 1.15054 1.15190 1.15665

 Beta virt. eigenvalues -- 1.16302 1.17255 1.19432 1.19977 1.21157

 Beta virt. eigenvalues -- 1.21226 1.21286 1.21419 1.21497 1.21611

 Beta virt. eigenvalues -- 1.21619 1.21664 1.23453 1.23656 1.26013

 Beta virt. eigenvalues -- 1.26355 1.26600 1.26717 1.27548 1.27606

 Beta virt. eigenvalues -- 1.27789 1.28597 1.29273 1.29708 1.30289

 Beta virt. eigenvalues -- 1.32522 1.34657 1.34958 1.34967 1.35477

 Beta virt. eigenvalues -- 1.35718 1.36383 1.39332 1.39989 1.42288

 Beta virt. eigenvalues -- 1.42449 1.43074 1.43201 1.43600 1.43700

 Beta virt. eigenvalues -- 1.45556 1.45730 1.45784 1.45818 1.45858

 Beta virt. eigenvalues -- 1.46070 1.48914 1.50294 1.51579 1.51686

 Beta virt. eigenvalues -- 1.52285 1.53232 1.53608 1.53629 1.53838

 Beta virt. eigenvalues -- 1.53887 1.54084 1.54234 1.55547 1.56329

 Beta virt. eigenvalues -- 1.58407 1.58478 1.60353 1.62905 1.63029

 Beta virt. eigenvalues -- 1.63297 1.63566 1.64180 1.65194 1.66180

 Beta virt. eigenvalues -- 1.66429 1.67114 1.68025 1.68899 1.69091

 Beta virt. eigenvalues -- 1.72645 1.72718 1.72980 1.74455 1.74562

 Beta virt. eigenvalues -- 1.74781 1.74885 1.75335 1.76035 1.76084

 Beta virt. eigenvalues -- 1.76128 1.81557 1.81689 1.81699 1.81740

 Beta virt. eigenvalues -- 1.82307 1.82951 1.83251 1.83532 1.83577

 Beta virt. eigenvalues -- 1.83931 1.84752 1.85021 1.85401 1.86945

 Beta virt. eigenvalues -- 1.87163 1.87523 1.89511 1.90340 1.91157

 Beta virt. eigenvalues -- 1.91252 1.91298 1.91335 1.91466 1.91628

 Beta virt. eigenvalues -- 1.91643 1.91682 1.91908 1.92313 1.92789

 Beta virt. eigenvalues -- 1.92814 1.93292 1.93429 1.94193 1.95062

 Beta virt. eigenvalues -- 1.95453 1.95864 1.96733 1.99390 1.99504

 Beta virt. eigenvalues -- 1.99809 2.00537 2.01711 2.03166 2.03269

 Beta virt. eigenvalues -- 2.03741 2.04553 2.05258 2.06171 2.06331

 Beta virt. eigenvalues -- 2.08583 2.12169 2.14593 2.14597 2.16425

 Beta virt. eigenvalues -- 2.16616 2.18675 2.20053 2.22492 2.23492

 Beta virt. eigenvalues -- 2.23953 2.24159 2.24466 2.25153 2.25547

 Beta virt. eigenvalues -- 2.25907 2.26741 2.27197 2.27677 2.27758

 Beta virt. eigenvalues -- 2.28195 2.28500 2.28609 2.28823 2.29324

 Beta virt. eigenvalues -- 2.30556 2.30736 2.30773 2.30959 2.33058

 Beta virt. eigenvalues -- 2.33340 2.33426 2.33955 2.37782 2.38966

 Beta virt. eigenvalues -- 2.39224 2.40135 2.40191 2.40275 2.41316

 Beta virt. eigenvalues -- 2.42093 2.43934 2.44257 2.44839 2.45907

 Beta virt. eigenvalues -- 2.46940 2.49480 2.49679 2.52714 2.53186

 Beta virt. eigenvalues -- 2.54022 2.54076 2.55282 2.55976 2.56869

 Beta virt. eigenvalues -- 2.56876 2.57916 2.58271 2.58547 2.58830

 Beta virt. eigenvalues -- 2.59791 2.61892 2.64954 2.65430 2.65549

 Beta virt. eigenvalues -- 2.66326 2.66514 2.66724 2.68877 2.69050

 Beta virt. eigenvalues -- 2.69425 2.69595 2.70799 2.73690 2.74842

 Beta virt. eigenvalues -- 2.74871 2.74918 2.75226 2.75365 2.75582

 Beta virt. eigenvalues -- 2.76119 2.77737 2.77739 2.77869 2.78967

 Beta virt. eigenvalues -- 2.79891 2.80103 2.80235 2.82743 2.82840

 Beta virt. eigenvalues -- 2.83121 2.83314 2.83355 2.84384 2.85158

 Beta virt. eigenvalues -- 2.86213 2.86668 2.88663 2.88781 2.89063

 Beta virt. eigenvalues -- 2.89145 2.92235 2.92339 2.92398 2.92536

 Beta virt. eigenvalues -- 2.92893 2.97876 2.98497 3.00731 3.04317

 Beta virt. eigenvalues -- 3.05394 3.05401 3.05600 3.08232 3.08737

 Beta virt. eigenvalues -- 3.09838 3.15879 3.16714 3.16741 3.16955

 Beta virt. eigenvalues -- 3.17793 3.19044 3.19915 3.19924 3.20296

 Beta virt. eigenvalues -- 3.21782 3.22785 3.23155 3.23765 3.26342

 Beta virt. eigenvalues -- 3.26555 3.26932 3.26965 3.27674 3.27784

 Beta virt. eigenvalues -- 3.28004 3.28773 3.30564 3.30974 3.31168

 Beta virt. eigenvalues -- 3.31237 3.31384 3.33255 3.33388 3.36375

 Beta virt. eigenvalues -- 3.38064 3.40201 3.40245 3.41729 3.46521

 Beta virt. eigenvalues -- 3.47381 3.47474 3.47794 3.48249 3.48400

 Beta virt. eigenvalues -- 3.48510 3.49967 3.56872 3.61805 3.62278

 Beta virt. eigenvalues -- 3.64554 3.64560 3.64664 3.65155 3.72707

 Beta virt. eigenvalues -- 3.72871 3.73534 3.74574 3.75948 3.76846

 Beta virt. eigenvalues -- 3.77461 3.77537 3.83538 3.84505 3.84969

 Beta virt. eigenvalues -- 3.85261 3.88299 3.89643 3.90829 3.91278

 Beta virt. eigenvalues -- 3.92076 3.95893 3.96629 3.96649 3.97543

 Beta virt. eigenvalues -- 4.11053 4.12069 4.12822 4.18411 4.18806

 Beta virt. eigenvalues -- 4.18934 4.20982 4.23761 4.35283 4.40481

 Beta virt. eigenvalues -- 4.41340 4.41472 4.47237 4.53410 4.55469

 Beta virt. eigenvalues -- 4.55511 4.78803 4.78964 4.78964 4.79281

 Beta virt. eigenvalues -- 5.12748 5.13508 5.14143 5.17075 5.21421

 Beta virt. eigenvalues -- 5.35355 5.37572 5.52794 7.85701 7.85863

 Beta virt. eigenvalues -- 7.86331 7.92290 8.15797 11.13335 23.28491

 Beta virt. eigenvalues -- 23.31553 23.31566 23.33319 23.76798 23.78454

 Beta virt. eigenvalues -- 23.78655 23.78688 23.78915 23.79040 23.79289

 Beta virt. eigenvalues -- 23.80874 23.88481 23.88781 23.89687 23.89776

 Beta virt. eigenvalues -- 23.90975 23.91010 23.91119 23.91624 24.02487

 Beta virt. eigenvalues -- 24.02747 24.02808 24.03355 24.04989 24.05001

 Beta virt. eigenvalues -- 24.05050 24.05124 24.12803 24.12949 24.12968

 Beta virt. eigenvalues -- 24.13310 35.57755 35.61211 35.61630 35.62423

 Beta virt. eigenvalues -- 35.69601 35.70309 35.70392 35.70538

 Condensed to atoms (all electrons):

 Atomic-Atomic Spin Densities.

 Mulliken charges and spin densities:

 1 2

 1 C 0.361610 -0.019012

 2 N -0.667390 0.023010

 3 C 0.318955 0.142538

 4 C -0.052492 -0.022724

 5 C -0.078615 0.048300

 6 N -0.397137 -0.063862

 7 C 0.318955 0.142538

 8 N -0.667390 0.023010

 9 C 0.361610 -0.019012

 10 C -0.078615 0.048300

 11 C -0.052492 -0.022724

 12 N -0.446002 0.151884

 13 C -0.078615 0.048300

 14 C -0.052492 -0.022724

 15 C 0.318955 0.142538

 16 N -0.667390 0.023010

 17 C 0.361610 -0.019012

 18 N -0.397137 -0.063862

 19 N -0.667390 0.023010

 20 C 0.318955 0.142538

 21 C -0.052492 -0.022724

 22 C -0.078615 0.048300

 23 C 0.361610 -0.019012

 24 N -0.446002 0.151884

 25 Zn 1.363862 -0.002656

 26 C -0.224037 -0.023967

 27 C -0.241531 0.044804

 28 C -0.233396 -0.019027

 29 C -0.231489 0.035242

 30 C -0.224037 -0.023967

 31 C -0.241531 0.044804

 32 C -0.233396 -0.019027

 33 C -0.231489 0.035242

 34 C -0.231489 0.035242

 35 C -0.233396 -0.019027

 36 C -0.241531 0.044804

 37 C -0.224037 -0.023967

 38 C -0.224037 -0.023967

 39 C -0.241531 0.044804

 40 C -0.233396 -0.019027

 41 C -0.231489 0.035242

 42 H 0.216510 0.000796

 43 H 0.216567 -0.001601

 44 H 0.216510 0.000796

 45 H 0.216567 -0.001601

 46 H 0.216567 -0.001601

 47 H 0.216510 0.000796

 48 H 0.216510 0.000796

 49 H 0.216567 -0.001601

 50 H 0.223291 0.000796

 51 H 0.222620 -0.002502

 52 H 0.223291 0.000796

 53 H 0.222620 -0.002502

 54 H 0.222620 -0.002502

 55 H 0.223291 0.000796

 56 H 0.223291 0.000796

 57 H 0.222620 -0.002502

 Sum of Mulliken charges = -1.00000 1.00000

 Mulliken charges and spin densities with hydrogens summed into heavy atoms:

 1 2

 1 C 0.361610 -0.019012

 2 N -0.667390 0.023010

 3 C 0.318955 0.142538

 4 C -0.052492 -0.022724

 5 C -0.078615 0.048300

 6 N -0.397137 -0.063862

 7 C 0.318955 0.142538

 8 N -0.667390 0.023010

 9 C 0.361610 -0.019012

 10 C -0.078615 0.048300

 11 C -0.052492 -0.022724

 12 N -0.446002 0.151884

 13 C -0.078615 0.048300

 14 C -0.052492 -0.022724

 15 C 0.318955 0.142538

 16 N -0.667390 0.023010

 17 C 0.361610 -0.019012

 18 N -0.397137 -0.063862

 19 N -0.667390 0.023010

 20 C 0.318955 0.142538

 21 C -0.052492 -0.022724

 22 C -0.078615 0.048300

 23 C 0.361610 -0.019012

 24 N -0.446002 0.151884

 25 Zn 1.363862 -0.002656

 26 C -0.007527 -0.023171

 27 C -0.018911 0.042302

 28 C -0.010105 -0.018231

 29 C -0.014922 0.033641

 30 C -0.007527 -0.023171

 31 C -0.018911 0.042302

 32 C -0.010105 -0.018231

 33 C -0.014922 0.033641

 34 C -0.014922 0.033641

 35 C -0.010105 -0.018231

 36 C -0.018911 0.042302

 37 C -0.007527 -0.023171

 38 C -0.007527 -0.023171

 39 C -0.018911 0.042302

 40 C -0.010105 -0.018231

 41 C -0.014922 0.033641

 Electronic spatial extent (au): <R\*\*2>= 22467.6999

 Charge= -1.0000 electrons

 Dipole moment (field-independent basis, Debye):

 X= 0.0000 Y= 0.0000 Z= 2.1838 Tot= 2.1838

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

 XX= -260.5370 YY= -257.5731 ZZ= -248.4180

 XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

 XX= -5.0276 YY= -2.0638 ZZ= 7.0914

 XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

 XXX= 0.0000 YYY= 0.0000 ZZZ= 26.7745 XYY= 0.0000

 XXY= 0.0000 XXZ= -1.1024 XZZ= 0.0000 YZZ= 0.0000

 YYZ= -1.0627 XYZ= 0.0000

 Hexadecapole moment (field-independent basis, Debye-Ang\*\*3):

 XXXX= -14826.3820 YYYY= -14709.6939 ZZZZ= -286.4298 XXXY= 0.0000

 XXXZ= 0.0000 YYYX= 0.0000 YYYZ= 0.0000 ZZZX= 0.0000

 ZZZY= 0.0000 XXYY= -4718.9618 XXZZ= -2979.7899 YYZZ= -2975.5466

 XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

 N-N= 4.365025315469D+03 E-N=-1.287684939939D+04 KE= 1.776268588325D+03

 Symmetry A1 KE= 5.097570824818D+02

 Symmetry A2 KE= 3.905693050255D+02

 Symmetry B1 KE= 4.387319917699D+02

 Symmetry B2 KE= 4.372102090481D+02

 Isotropic Fermi Contact Couplings

 Atom a.u. MegaHertz Gauss 10(-4) cm-1

 1 C(13) -0.00735 -8.26118 -2.94779 -2.75563

 2 N(14) 0.00062 0.19944 0.07116 0.06653

 3 C(13) 0.01069 12.01510 4.28729 4.00781

 4 C(13) -0.00696 -7.81906 -2.79003 -2.60816

 5 C(13) 0.00327 3.68137 1.31361 1.22797

 6 N(14) -0.01147 -3.70538 -1.32217 -1.23598

 7 C(13) 0.01069 12.01510 4.28729 4.00781

 8 N(14) 0.00062 0.19944 0.07116 0.06653

 9 C(13) -0.00735 -8.26118 -2.94779 -2.75563

 10 C(13) 0.00327 3.68137 1.31361 1.22797

 11 C(13) -0.00696 -7.81906 -2.79003 -2.60816

 12 N(14) 0.01794 5.79603 2.06817 1.93335

 13 C(13) 0.00327 3.68137 1.31361 1.22797

 14 C(13) -0.00696 -7.81906 -2.79003 -2.60816

 15 C(13) 0.01069 12.01510 4.28729 4.00781

 16 N(14) 0.00062 0.19944 0.07116 0.06653

 17 C(13) -0.00735 -8.26118 -2.94779 -2.75563

 18 N(14) -0.01147 -3.70538 -1.32217 -1.23598

 19 N(14) 0.00062 0.19944 0.07116 0.06653

 20 C(13) 0.01069 12.01510 4.28729 4.00781

 21 C(13) -0.00696 -7.81906 -2.79003 -2.60816

 22 C(13) 0.00327 3.68137 1.31361 1.22797

 23 C(13) -0.00735 -8.26118 -2.94779 -2.75563

 24 N(14) 0.01794 5.79603 2.06817 1.93335

 25 Zn(67) 0.00000 0.00000 0.00000 0.00000

 26 C(13) -0.00348 -3.90959 -1.39504 -1.30410

 27 C(13) 0.00312 3.50870 1.25199 1.17037

 28 C(13) -0.00279 -3.13936 -1.12020 -1.04718

 29 C(13) 0.00227 2.55705 0.91242 0.85294

 30 C(13) -0.00348 -3.90959 -1.39504 -1.30410

 31 C(13) 0.00312 3.50870 1.25199 1.17037

 32 C(13) -0.00279 -3.13936 -1.12020 -1.04718

 33 C(13) 0.00227 2.55705 0.91242 0.85294

 34 C(13) 0.00227 2.55705 0.91242 0.85294

 35 C(13) -0.00279 -3.13936 -1.12020 -1.04718

 36 C(13) 0.00312 3.50870 1.25199 1.17037

 37 C(13) -0.00348 -3.90959 -1.39504 -1.30410

 38 C(13) -0.00348 -3.90959 -1.39504 -1.30410

 39 C(13) 0.00312 3.50870 1.25199 1.17037

 40 C(13) -0.00279 -3.13936 -1.12020 -1.04718

 41 C(13) 0.00227 2.55705 0.91242 0.85294

 42 H(1) 0.00027 1.22897 0.43853 0.40994

 43 H(1) -0.00050 -2.22415 -0.79363 -0.74190

 44 H(1) 0.00027 1.22897 0.43853 0.40994

 45 H(1) -0.00050 -2.22415 -0.79363 -0.74190

 46 H(1) -0.00050 -2.22415 -0.79363 -0.74190

 47 H(1) 0.00027 1.22897 0.43853 0.40994

 48 H(1) 0.00027 1.22897 0.43853 0.40994

 49 H(1) -0.00050 -2.22415 -0.79363 -0.74190

 50 H(1) 0.00020 0.90404 0.32258 0.30155

 51 H(1) -0.00064 -2.87668 -1.02647 -0.95956

 52 H(1) 0.00020 0.90404 0.32258 0.30155

 53 H(1) -0.00064 -2.87668 -1.02647 -0.95956

 54 H(1) -0.00064 -2.87668 -1.02647 -0.95956

 55 H(1) 0.00020 0.90404 0.32258 0.30155

 56 H(1) 0.00020 0.90404 0.32258 0.30155

 57 H(1) -0.00064 -2.87668 -1.02647 -0.95956

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 Center ---- Spin Dipole Couplings ----

 3XX-RR 3YY-RR 3ZZ-RR

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 1 Atom 0.008628 0.012872 -0.021500

 2 Atom -0.035067 -0.036210 0.071277

 3 Atom -0.094514 -0.094472 0.188987

 4 Atom 0.006839 0.007726 -0.014565

 5 Atom -0.027632 -0.027679 0.055312

 6 Atom 0.062169 0.047477 -0.109646

 7 Atom -0.094514 -0.094472 0.188987

 8 Atom -0.035067 -0.036210 0.071277

 9 Atom 0.008628 0.012872 -0.021500

 10 Atom -0.027632 -0.027679 0.055312

 11 Atom 0.006839 0.007726 -0.014565

 12 Atom -0.188497 -0.189914 0.378411

 13 Atom -0.027632 -0.027679 0.055312

 14 Atom 0.006839 0.007726 -0.014565

 15 Atom -0.094514 -0.094472 0.188987

 16 Atom -0.035067 -0.036210 0.071277

 17 Atom 0.008628 0.012872 -0.021500

 18 Atom 0.062169 0.047477 -0.109646

 19 Atom -0.035067 -0.036210 0.071277

 20 Atom -0.094514 -0.094472 0.188987

 21 Atom 0.006839 0.007726 -0.014565

 22 Atom -0.027632 -0.027679 0.055312

 23 Atom 0.008628 0.012872 -0.021500

 24 Atom -0.188497 -0.189914 0.378411

 25 Atom 0.005625 -0.006785 0.001159

 26 Atom 0.011520 0.011296 -0.022817

 27 Atom -0.022736 -0.024477 0.047213

 28 Atom 0.009124 0.007838 -0.016961

 29 Atom -0.017722 -0.016890 0.034612

 30 Atom 0.011520 0.011296 -0.022817

 31 Atom -0.022736 -0.024477 0.047213

 32 Atom 0.009124 0.007838 -0.016961

 33 Atom -0.017722 -0.016890 0.034612

 34 Atom -0.017722 -0.016890 0.034612

 35 Atom 0.009124 0.007838 -0.016961

 36 Atom -0.022736 -0.024477 0.047213

 37 Atom 0.011520 0.011296 -0.022817

 38 Atom 0.011520 0.011296 -0.022817

 39 Atom -0.022736 -0.024477 0.047213

 40 Atom 0.009124 0.007838 -0.016961

 41 Atom -0.017722 -0.016890 0.034612

 42 Atom 0.001109 0.000407 -0.001516

 43 Atom -0.000148 0.001344 -0.001197

 44 Atom 0.001109 0.000407 -0.001516

 45 Atom -0.000148 0.001344 -0.001197

 46 Atom -0.000148 0.001344 -0.001197

 47 Atom 0.001109 0.000407 -0.001516

 48 Atom 0.001109 0.000407 -0.001516

 49 Atom -0.000148 0.001344 -0.001197

 50 Atom 0.000977 -0.000189 -0.000788

 51 Atom 0.002901 -0.002401 -0.000499

 52 Atom 0.000977 -0.000189 -0.000788

 53 Atom 0.002901 -0.002401 -0.000499

 54 Atom 0.002901 -0.002401 -0.000499

 55 Atom 0.000977 -0.000189 -0.000788

 56 Atom 0.000977 -0.000189 -0.000788

 57 Atom 0.002901 -0.002401 -0.000499

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 XY XZ YZ

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 1 Atom -0.006963 -0.000739 -0.000460

 2 Atom -0.001336 0.005906 0.007354

 3 Atom 0.002494 0.003534 0.008144

 4 Atom 0.002757 -0.000991 -0.000647

 5 Atom 0.000572 0.002550 0.003008

 6 Atom 0.000000 0.000000 -0.002847

 7 Atom -0.002494 -0.003534 0.008144

 8 Atom 0.001336 -0.005906 0.007354

 9 Atom 0.006963 0.000739 -0.000460

 10 Atom -0.000572 -0.002550 0.003008

 11 Atom -0.002757 0.000991 -0.000647

 12 Atom 0.000000 0.013574 0.000000

 13 Atom -0.000572 0.002550 -0.003008

 14 Atom -0.002757 -0.000991 0.000647

 15 Atom -0.002494 0.003534 -0.008144

 16 Atom 0.001336 0.005906 -0.007354

 17 Atom 0.006963 -0.000739 0.000460

 18 Atom 0.000000 0.000000 0.002847

 19 Atom -0.001336 -0.005906 -0.007354

 20 Atom 0.002494 -0.003534 -0.008144

 21 Atom 0.002757 0.000991 0.000647

 22 Atom 0.000572 -0.002550 -0.003008

 23 Atom -0.006963 0.000739 0.000460

 24 Atom 0.000000 -0.013574 0.000000

 25 Atom 0.000000 0.000000 0.000000

 26 Atom -0.002145 -0.000771 0.000705

 27 Atom -0.001085 0.001380 -0.001229

 28 Atom -0.000040 -0.000458 0.000500

 29 Atom -0.000824 0.000947 -0.001040

 30 Atom 0.002145 0.000771 0.000705

 31 Atom 0.001085 -0.001380 -0.001229

 32 Atom 0.000040 0.000458 0.000500

 33 Atom 0.000824 -0.000947 -0.001040

 34 Atom -0.000824 -0.000947 0.001040

 35 Atom -0.000040 0.000458 -0.000500

 36 Atom -0.001085 -0.001380 0.001229

 37 Atom -0.002145 0.000771 -0.000705

 38 Atom 0.002145 -0.000771 -0.000705

 39 Atom 0.001085 0.001380 0.001229

 40 Atom 0.000040 -0.000458 -0.000500

 41 Atom 0.000824 0.000947 0.001040

 42 Atom -0.002110 -0.000082 0.000073

 43 Atom 0.001566 0.000030 0.000032

 44 Atom 0.002110 0.000082 0.000073

 45 Atom -0.001566 -0.000030 0.000032

 46 Atom 0.001566 -0.000030 -0.000032

 47 Atom -0.002110 0.000082 -0.000073

 48 Atom 0.002110 -0.000082 -0.000073

 49 Atom -0.001566 0.000030 -0.000032

 50 Atom -0.000199 0.000036 -0.000011

 51 Atom -0.002224 0.000111 -0.000012

 52 Atom 0.000199 -0.000036 -0.000011

 53 Atom 0.002224 -0.000111 -0.000012

 54 Atom -0.002224 -0.000111 0.000012

 55 Atom -0.000199 -0.000036 0.000011

 56 Atom 0.000199 0.000036 0.000011

 57 Atom 0.002224 0.000111 0.000012

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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 -0.0215 -2.889 -1.031 -0.964 0.0289 0.0192 0.9994

 1 C(13) Bbb 0.0035 0.470 0.168 0.157 0.8030 0.5950 -0.0347

 Bcc 0.0180 2.419 0.863 0.807 -0.5953 0.8035 0.0018

 Baa -0.0379 -1.462 -0.522 -0.488 0.5655 0.8202 -0.0858

 2 N(14) Bbb -0.0342 -1.319 -0.471 -0.440 0.8229 -0.5681 -0.0065

 Bcc 0.0721 2.780 0.992 0.927 0.0541 0.0670 0.9963

 Baa -0.0970 -13.020 -4.646 -4.343 -0.6962 0.7178 -0.0118

 3 C(13) Bbb -0.0922 -12.378 -4.417 -4.129 0.7178 0.6957 -0.0292

 Bcc 0.1893 25.398 9.063 8.472 0.0127 0.0288 0.9995

 Baa -0.0146 -1.962 -0.700 -0.655 0.0431 0.0236 0.9988

 4 C(13) Bbb 0.0045 0.603 0.215 0.201 0.7588 -0.6511 -0.0173

 Bcc 0.0101 1.359 0.485 0.453 0.6499 0.7587 -0.0459

 Baa -0.0282 -3.788 -1.352 -1.264 -0.6780 0.7350 -0.0058

 5 C(13) Bbb -0.0273 -3.659 -1.306 -1.221 0.7344 0.6771 -0.0473

 Bcc 0.0555 7.448 2.657 2.484 0.0309 0.0363 0.9989

 Baa -0.1097 -4.231 -1.510 -1.411 0.0000 0.0181 0.9998

 6 N(14) Bbb 0.0475 1.833 0.654 0.611 0.0000 0.9998 -0.0181

 Bcc 0.0622 2.398 0.856 0.800 1.0000 0.0000 0.0000

 Baa -0.0970 -13.020 -4.646 -4.343 0.6962 0.7178 -0.0118

 7 C(13) Bbb -0.0922 -12.378 -4.417 -4.129 0.7178 -0.6957 0.0292

 Bcc 0.1893 25.398 9.063 8.472 -0.0127 0.0288 0.9995

 Baa -0.0379 -1.462 -0.522 -0.488 -0.5655 0.8202 -0.0858

 8 N(14) Bbb -0.0342 -1.319 -0.471 -0.440 0.8229 0.5681 0.0065

 Bcc 0.0721 2.780 0.992 0.927 -0.0541 0.0670 0.9963

 Baa -0.0215 -2.889 -1.031 -0.964 -0.0289 0.0192 0.9994

 9 C(13) Bbb 0.0035 0.470 0.168 0.157 0.8030 -0.5950 0.0347

 Bcc 0.0180 2.419 0.863 0.807 0.5953 0.8035 0.0018

 Baa -0.0282 -3.788 -1.352 -1.264 0.6780 0.7350 -0.0058

 10 C(13) Bbb -0.0273 -3.659 -1.306 -1.221 0.7344 -0.6771 0.0473

 Bcc 0.0555 7.448 2.657 2.484 -0.0309 0.0363 0.9989

 Baa -0.0146 -1.962 -0.700 -0.655 -0.0431 0.0236 0.9988

 11 C(13) Bbb 0.0045 0.603 0.215 0.201 0.7588 0.6511 0.0173

 Bcc 0.0101 1.359 0.485 0.453 -0.6499 0.7587 -0.0459

 Baa -0.1899 -7.325 -2.614 -2.443 0.0000 1.0000 0.0000

 12 N(14) Bbb -0.1888 -7.282 -2.599 -2.429 0.9997 0.0000 -0.0239

 Bcc 0.3787 14.607 5.212 4.872 0.0239 0.0000 0.9997

 Baa -0.0282 -3.788 -1.352 -1.264 0.6780 0.7350 0.0058

 13 C(13) Bbb -0.0273 -3.659 -1.306 -1.221 0.7344 -0.6771 -0.0473

 Bcc 0.0555 7.448 2.657 2.484 0.0309 -0.0363 0.9989

 Baa -0.0146 -1.962 -0.700 -0.655 0.0431 -0.0236 0.9988

 14 C(13) Bbb 0.0045 0.603 0.215 0.201 0.7588 0.6511 -0.0173

 Bcc 0.0101 1.359 0.485 0.453 -0.6499 0.7587 0.0459

 Baa -0.0970 -13.020 -4.646 -4.343 0.6962 0.7178 0.0118

 15 C(13) Bbb -0.0922 -12.378 -4.417 -4.129 0.7178 -0.6957 -0.0292

 Bcc 0.1893 25.398 9.063 8.472 0.0127 -0.0288 0.9995

 Baa -0.0379 -1.462 -0.522 -0.488 -0.5655 0.8202 0.0858

 16 N(14) Bbb -0.0342 -1.319 -0.471 -0.440 0.8229 0.5681 -0.0065

 Bcc 0.0721 2.780 0.992 0.927 0.0541 -0.0670 0.9963

 Baa -0.0215 -2.889 -1.031 -0.964 0.0289 -0.0192 0.9994

 17 C(13) Bbb 0.0035 0.470 0.168 0.157 0.8030 -0.5950 -0.0347

 Bcc 0.0180 2.419 0.863 0.807 0.5953 0.8035 -0.0018

 Baa -0.1097 -4.231 -1.510 -1.411 0.0000 -0.0181 0.9998

 18 N(14) Bbb 0.0475 1.833 0.654 0.611 0.0000 0.9998 0.0181

 Bcc 0.0622 2.398 0.856 0.800 1.0000 0.0000 0.0000

 Baa -0.0379 -1.462 -0.522 -0.488 0.5655 0.8202 0.0858

 19 N(14) Bbb -0.0342 -1.319 -0.471 -0.440 0.8229 -0.5681 0.0065

 Bcc 0.0721 2.780 0.992 0.927 -0.0541 -0.0670 0.9963

 Baa -0.0970 -13.020 -4.646 -4.343 -0.6962 0.7178 0.0118

 20 C(13) Bbb -0.0922 -12.378 -4.417 -4.129 0.7178 0.6957 0.0292

 Bcc 0.1893 25.398 9.063 8.472 -0.0127 -0.0288 0.9995

 Baa -0.0146 -1.962 -0.700 -0.655 -0.0431 -0.0236 0.9988

 21 C(13) Bbb 0.0045 0.603 0.215 0.201 0.7588 -0.6511 0.0173

 Bcc 0.0101 1.359 0.485 0.453 0.6499 0.7587 0.0459

 Baa -0.0282 -3.788 -1.352 -1.264 -0.6780 0.7350 0.0058

 22 C(13) Bbb -0.0273 -3.659 -1.306 -1.221 0.7344 0.6771 0.0473

 Bcc 0.0555 7.448 2.657 2.484 -0.0309 -0.0363 0.9989

 Baa -0.0215 -2.889 -1.031 -0.964 -0.0289 -0.0192 0.9994

 23 C(13) Bbb 0.0035 0.470 0.168 0.157 0.8030 0.5950 0.0347

 Bcc 0.0180 2.419 0.863 0.807 -0.5953 0.8035 -0.0018

 Baa -0.1899 -7.325 -2.614 -2.443 0.0000 1.0000 0.0000

 24 N(14) Bbb -0.1888 -7.282 -2.599 -2.429 0.9997 0.0000 0.0239

 Bcc 0.3787 14.607 5.212 4.872 -0.0239 0.0000 0.9997

 Baa -0.0068 -0.227 -0.081 -0.076 0.0000 1.0000 0.0000

 25 Zn(67) Bbb 0.0012 0.039 0.014 0.013 0.0000 0.0000 1.0000

 Bcc 0.0056 0.188 0.067 0.063 1.0000 0.0000 0.0000

 Baa -0.0228 -3.066 -1.094 -1.023 0.0212 -0.0193 0.9996

 26 C(13) Bbb 0.0093 1.243 0.443 0.414 0.6883 0.7254 -0.0006

 Bcc 0.0136 1.823 0.651 0.608 0.7251 -0.6881 -0.0287

 Baa -0.0250 -3.355 -1.197 -1.119 0.4285 0.9035 0.0072

 27 C(13) Bbb -0.0223 -2.987 -1.066 -0.996 0.9033 -0.4282 -0.0255

 Bcc 0.0473 6.342 2.263 2.116 0.0200 -0.0174 0.9996

 Baa -0.0170 -2.278 -0.813 -0.760 0.0175 -0.0201 0.9996

 28 C(13) Bbb 0.0078 1.053 0.376 0.351 0.0385 0.9991 0.0194

 Bcc 0.0091 1.226 0.437 0.409 0.9991 -0.0381 -0.0183

 Baa -0.0182 -2.446 -0.873 -0.816 0.8535 0.5210 -0.0050

 29 C(13) Bbb -0.0164 -2.203 -0.786 -0.735 -0.5207 0.8533 0.0271

 Bcc 0.0347 4.650 1.659 1.551 0.0184 -0.0205 0.9996

 Baa -0.0228 -3.066 -1.094 -1.023 -0.0212 -0.0193 0.9996

 30 C(13) Bbb 0.0093 1.243 0.443 0.414 -0.6883 0.7254 -0.0006

 Bcc 0.0136 1.823 0.651 0.608 0.7251 0.6881 0.0287

 Baa -0.0250 -3.355 -1.197 -1.119 -0.4285 0.9035 0.0072

 31 C(13) Bbb -0.0223 -2.987 -1.066 -0.996 0.9033 0.4282 0.0255

 Bcc 0.0473 6.342 2.263 2.116 -0.0200 -0.0174 0.9996

 Baa -0.0170 -2.278 -0.813 -0.760 -0.0175 -0.0201 0.9996

 32 C(13) Bbb 0.0078 1.053 0.376 0.351 -0.0385 0.9991 0.0194

 Bcc 0.0091 1.226 0.437 0.409 0.9991 0.0381 0.0183

 Baa -0.0182 -2.446 -0.873 -0.816 0.8535 -0.5210 0.0050

 33 C(13) Bbb -0.0164 -2.203 -0.786 -0.735 0.5207 0.8533 0.0271

 Bcc 0.0347 4.650 1.659 1.551 -0.0184 -0.0205 0.9996

 Baa -0.0182 -2.446 -0.873 -0.816 0.8535 0.5210 0.0050

 34 C(13) Bbb -0.0164 -2.203 -0.786 -0.735 -0.5207 0.8533 -0.0271

 Bcc 0.0347 4.650 1.659 1.551 -0.0184 0.0205 0.9996

 Baa -0.0170 -2.278 -0.813 -0.760 -0.0175 0.0201 0.9996

 35 C(13) Bbb 0.0078 1.053 0.376 0.351 0.0385 0.9991 -0.0194

 Bcc 0.0091 1.226 0.437 0.409 0.9991 -0.0381 0.0183

 Baa -0.0250 -3.355 -1.197 -1.119 0.4285 0.9035 -0.0072

 36 C(13) Bbb -0.0223 -2.987 -1.066 -0.996 0.9033 -0.4282 0.0255

 Bcc 0.0473 6.342 2.263 2.116 -0.0200 0.0174 0.9996

 Baa -0.0228 -3.066 -1.094 -1.023 -0.0212 0.0193 0.9996

 37 C(13) Bbb 0.0093 1.243 0.443 0.414 0.6883 0.7254 0.0006

 Bcc 0.0136 1.823 0.651 0.608 0.7251 -0.6881 0.0287

 Baa -0.0228 -3.066 -1.094 -1.023 0.0212 0.0193 0.9996

 38 C(13) Bbb 0.0093 1.243 0.443 0.414 -0.6883 0.7254 0.0006

 Bcc 0.0136 1.823 0.651 0.608 0.7251 0.6881 -0.0287

 Baa -0.0250 -3.355 -1.197 -1.119 -0.4285 0.9035 -0.0072

 39 C(13) Bbb -0.0223 -2.987 -1.066 -0.996 0.9033 0.4282 -0.0255

 Bcc 0.0473 6.342 2.263 2.116 0.0200 0.0174 0.9996

 Baa -0.0170 -2.278 -0.813 -0.760 0.0175 0.0201 0.9996

 40 C(13) Bbb 0.0078 1.053 0.376 0.351 -0.0385 0.9991 -0.0194

 Bcc 0.0091 1.226 0.437 0.409 0.9991 0.0381 -0.0183

 Baa -0.0182 -2.446 -0.873 -0.816 0.8535 -0.5210 -0.0050

 41 C(13) Bbb -0.0164 -2.203 -0.786 -0.735 0.5207 0.8533 -0.0271

 Bcc 0.0347 4.650 1.659 1.551 0.0184 0.0205 0.9996

 Baa -0.0015 -0.810 -0.289 -0.270 0.0046 -0.0330 0.9994

 42 H(1) Bbb -0.0014 -0.737 -0.263 -0.246 0.6467 0.7624 0.0222

 Bcc 0.0029 1.547 0.552 0.516 0.7627 -0.6462 -0.0249

 Baa -0.0012 -0.639 -0.228 -0.213 -0.1170 0.0596 0.9913

 43 H(1) Bbb -0.0011 -0.606 -0.216 -0.202 0.8375 -0.5306 0.1308

 Bcc 0.0023 1.245 0.444 0.415 0.5338 0.8455 0.0122

 Baa -0.0015 -0.810 -0.289 -0.270 -0.0046 -0.0330 0.9994

 44 H(1) Bbb -0.0014 -0.737 -0.263 -0.246 -0.6467 0.7624 0.0222

 Bcc 0.0029 1.547 0.552 0.516 0.7627 0.6462 0.0249

 Baa -0.0012 -0.639 -0.228 -0.213 0.1170 0.0596 0.9913

 45 H(1) Bbb -0.0011 -0.606 -0.216 -0.202 0.8375 0.5306 -0.1308

 Bcc 0.0023 1.245 0.444 0.415 -0.5338 0.8455 0.0122

 Baa -0.0012 -0.639 -0.228 -0.213 0.1170 -0.0596 0.9913

 46 H(1) Bbb -0.0011 -0.606 -0.216 -0.202 0.8375 -0.5306 -0.1308

 Bcc 0.0023 1.245 0.444 0.415 0.5338 0.8455 -0.0122

 Baa -0.0015 -0.810 -0.289 -0.270 -0.0046 0.0330 0.9994

 47 H(1) Bbb -0.0014 -0.737 -0.263 -0.246 0.6467 0.7624 -0.0222

 Bcc 0.0029 1.547 0.552 0.516 0.7627 -0.6462 0.0249

 Baa -0.0015 -0.810 -0.289 -0.270 0.0046 0.0330 0.9994

 48 H(1) Bbb -0.0014 -0.737 -0.263 -0.246 -0.6467 0.7624 -0.0222

 Bcc 0.0029 1.547 0.552 0.516 0.7627 0.6462 -0.0249

 Baa -0.0012 -0.639 -0.228 -0.213 -0.1170 -0.0596 0.9913

 49 H(1) Bbb -0.0011 -0.606 -0.216 -0.202 0.8375 0.5306 0.1308

 Bcc 0.0023 1.245 0.444 0.415 -0.5338 0.8455 -0.0122

 Baa -0.0008 -0.421 -0.150 -0.140 -0.0188 0.0126 0.9997

 50 H(1) Bbb -0.0002 -0.119 -0.042 -0.040 0.1636 0.9865 -0.0094

 Bcc 0.0010 0.539 0.192 0.180 0.9863 -0.1634 0.0206

 Baa -0.0032 -1.713 -0.611 -0.572 0.3421 0.9396 -0.0098

 51 H(1) Bbb -0.0005 -0.268 -0.096 -0.089 -0.0208 0.0180 0.9996

 Bcc 0.0037 1.981 0.707 0.661 0.9394 -0.3418 0.0257

 Baa -0.0008 -0.421 -0.150 -0.140 0.0188 0.0126 0.9997

 52 H(1) Bbb -0.0002 -0.119 -0.042 -0.040 -0.1636 0.9865 -0.0094

 Bcc 0.0010 0.539 0.192 0.180 0.9863 0.1634 -0.0206

 Baa -0.0032 -1.713 -0.611 -0.572 -0.3421 0.9396 -0.0098

 53 H(1) Bbb -0.0005 -0.268 -0.096 -0.089 0.0208 0.0180 0.9996

 Bcc 0.0037 1.981 0.707 0.661 0.9394 0.3418 -0.0257

 Baa -0.0032 -1.713 -0.611 -0.572 0.3421 0.9396 0.0098

 54 H(1) Bbb -0.0005 -0.268 -0.096 -0.089 0.0208 -0.0180 0.9996

 Bcc 0.0037 1.981 0.707 0.661 0.9394 -0.3418 -0.0257

 Baa -0.0008 -0.421 -0.150 -0.140 0.0188 -0.0126 0.9997

 55 H(1) Bbb -0.0002 -0.119 -0.042 -0.040 0.1636 0.9865 0.0094

 Bcc 0.0010 0.539 0.192 0.180 0.9863 -0.1634 -0.0206

 Baa -0.0008 -0.421 -0.150 -0.140 -0.0188 -0.0126 0.9997

 56 H(1) Bbb -0.0002 -0.119 -0.042 -0.040 -0.1636 0.9865 0.0094

 Bcc 0.0010 0.539 0.192 0.180 0.9863 0.1634 0.0206

 Baa -0.0032 -1.713 -0.611 -0.572 -0.3421 0.9396 0.0098

 57 H(1) Bbb -0.0005 -0.268 -0.096 -0.089 -0.0208 -0.0180 0.9996

 Bcc 0.0037 1.981 0.707 0.661 0.9394 0.3418 0.0257

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

 No NMR shielding tensors so no spin-rotation constants.

 Leave Link 601 at Sat Jun 15 12:08:46 2019, MaxMem= 1342177280 cpu: 50.3

 (Enter /apps/gaussian/g09d01/g09/l701.exe)

 Compute integral first derivatives.

 ... and contract with generalized density number 0.

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

 4 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22819 LenP2D= 61244.

 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 = 199

 Leave Link 701 at Sat Jun 15 12:08:55 2019, MaxMem= 1342177280 cpu: 103.7

 (Enter /apps/gaussian/g09d01/g09/l702.exe)

 L702 exits ... SP integral derivatives will be done elsewhere.

 Leave Link 702 at Sat Jun 15 12:08:56 2019, MaxMem= 1342177280 cpu: 3.5

 (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= 800

 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 Sat Jun 15 12:09:16 2019, MaxMem= 1342177280 cpu: 228.4

 (Enter /apps/gaussian/g09d01/g09/l716.exe)

 Dipole = 9.94759830D-14 5.86197757D-14 8.59163674D-01

 \*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

 Center Atomic Forces (Hartrees/Bohr)

 Number Number X Y Z

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

 1 6 -0.000732653 -0.002885362 -0.000215846

 2 7 0.003259801 0.002327264 0.000353437

 3 6 -0.002835104 0.000295573 -0.000269478

 4 6 0.000898563 0.000140601 -0.000006199

 5 6 0.000346196 0.001110114 -0.000038030

 6 7 0.000000000 -0.002048515 0.000145739

 7 6 0.002835104 0.000295573 -0.000269478

 8 7 -0.003259801 0.002327264 0.000353437

 9 6 0.000732653 -0.002885362 -0.000215846

 10 6 -0.000346196 0.001110114 -0.000038030

 11 6 -0.000898563 0.000140601 -0.000006199

 12 7 -0.002122903 0.000000000 0.000126010

 13 6 0.000346196 -0.001110114 -0.000038030

 14 6 0.000898563 -0.000140601 -0.000006199

 15 6 -0.002835104 -0.000295573 -0.000269478

 16 7 0.003259801 -0.002327264 0.000353437

 17 6 -0.000732653 0.002885362 -0.000215846

 18 7 0.000000000 0.002048515 0.000145739

 19 7 -0.003259801 -0.002327264 0.000353437

 20 6 0.002835104 -0.000295573 -0.000269478

 21 6 -0.000898563 -0.000140601 -0.000006199

 22 6 -0.000346196 -0.001110114 -0.000038030

 23 6 0.000732653 0.002885362 -0.000215846

 24 7 0.002122903 0.000000000 0.000126010

 25 30 0.000000000 0.000000000 -0.000414524

 26 6 -0.001563186 -0.002683409 -0.000050872

 27 6 -0.002614276 0.001317930 0.000086257

 28 6 -0.001386188 0.002621208 0.000081426

 29 6 0.002715168 0.001522812 -0.000033604

 30 6 0.001563186 -0.002683409 -0.000050872

 31 6 0.002614276 0.001317930 0.000086257

 32 6 0.001386188 0.002621208 0.000081426

 33 6 -0.002715168 0.001522812 -0.000033604

 34 6 -0.002715168 -0.001522812 -0.000033604

 35 6 0.001386188 -0.002621208 0.000081426

 36 6 0.002614276 -0.001317930 0.000086257

 37 6 0.001563186 0.002683409 -0.000050872

 38 6 -0.001563186 0.002683409 -0.000050872

 39 6 -0.002614276 -0.001317930 0.000086257

 40 6 -0.001386188 -0.002621208 0.000081426

 41 6 0.002715168 -0.001522812 -0.000033604

 42 1 -0.000757864 -0.000561397 0.000011928

 43 1 0.000562505 0.000732660 0.000007331

 44 1 0.000757864 -0.000561397 0.000011928

 45 1 -0.000562505 0.000732660 0.000007331

 46 1 -0.000562505 -0.000732660 0.000007331

 47 1 0.000757864 0.000561397 0.000011928

 48 1 -0.000757864 0.000561397 0.000011928

 49 1 0.000562505 -0.000732660 0.000007331

 50 1 0.000248291 -0.000929702 0.000020473

 51 1 0.000936160 -0.000247015 0.000020932

 52 1 -0.000248291 -0.000929702 0.000020473

 53 1 -0.000936160 -0.000247015 0.000020932

 54 1 -0.000936160 0.000247015 0.000020932

 55 1 -0.000248291 0.000929702 0.000020473

 56 1 0.000248291 0.000929702 0.000020473

 57 1 0.000936160 0.000247015 0.000020932

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 Cartesian Forces: Max 0.003259801 RMS 0.001369610

 Leave Link 716 at Sat Jun 15 12:09:19 2019, MaxMem= 1342177280 cpu: 8.0

 (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 0.004195477 RMS 0.001174592

 Search for a local minimum.

 Step number 1 out of a maximum of 342

 All quantities printed in internal units (Hartrees-Bohrs-Radians)

 RMS Force = .11746D-02 SwitMx=.10000D-02 MixMth= 1

 Mixed Optimization -- RFO/linear search

 Second derivative matrix not updated -- first step.

 ITU= 0

 Eigenvalues --- 0.01571 0.01587 0.01610 0.01614 0.01624

 Eigenvalues --- 0.01645 0.01681 0.01697 0.01763 0.01768

 Eigenvalues --- 0.01776 0.01780 0.01781 0.01783 0.01783

 Eigenvalues --- 0.01794 0.01835 0.01846 0.01891 0.01894

 Eigenvalues --- 0.01903 0.01957 0.01958 0.02008 0.02008

 Eigenvalues --- 0.02008 0.02008 0.02051 0.02051 0.02051

 Eigenvalues --- 0.02051 0.02053 0.02053 0.02053 0.02053

 Eigenvalues --- 0.02077 0.02113 0.02113 0.02113 0.02113

 Eigenvalues --- 0.02119 0.02119 0.02119 0.02119 0.02124

 Eigenvalues --- 0.02124 0.02124 0.02124 0.02245 0.02249

 Eigenvalues --- 0.02324 0.02335 0.03347 0.03901 0.03919

 Eigenvalues --- 0.07464 0.15215 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 0.16238 0.16348

 Eigenvalues --- 0.17211 0.22000 0.22000 0.22000 0.22000

 Eigenvalues --- 0.22599 0.22600 0.22600 0.22606 0.24075

 Eigenvalues --- 0.24274 0.24508 0.24509 0.24521 0.24530

 Eigenvalues --- 0.24597 0.24605 0.24825 0.24946 0.24947

 Eigenvalues --- 0.24955 0.24984 0.24998 0.24998 0.24998

 Eigenvalues --- 0.24998 0.33739 0.34078 0.34263 0.34315

 Eigenvalues --- 0.34822 0.34872 0.35074 0.35218 0.35218

 Eigenvalues --- 0.35218 0.35218 0.35231 0.35243 0.35243

 Eigenvalues --- 0.35243 0.35243 0.35247 0.35247 0.35247

 Eigenvalues --- 0.35247 0.35252 0.35252 0.35252 0.35252

 Eigenvalues --- 0.37368 0.37390 0.37553 0.37567 0.40819

 Eigenvalues --- 0.40903 0.41950 0.41951 0.41966 0.41979

 Eigenvalues --- 0.41986 0.42301 0.43209 0.43248 0.44583

 Eigenvalues --- 0.45129 0.45211 0.45217 0.45344 0.45791

 Eigenvalues --- 0.45910 0.45911 0.45919 0.45942 0.46127

 Eigenvalues --- 0.46178 0.46180 0.46180 0.46184 0.46684

 Eigenvalues --- 0.48980 0.50406 0.50867 0.51351 0.53511

 Eigenvalues --- 0.55376 0.55383 0.55601 0.58016 0.58041

 RFO step: Lambda=-1.23532379D-03 EMin= 1.57050720D-02

 Linear search not attempted -- first point.

 Iteration 1 RMS(Cart)= 0.01102000 RMS(Int)= 0.00000829

 Iteration 2 RMS(Cart)= 0.00002053 RMS(Int)= 0.00000215

 Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000215

 ITry= 1 IFail=0 DXMaxC= 3.03D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

 ClnCor: largest displacement from symmetrization is 1.23D-11 for atom 54.

 Variable Old X -DE/DX Delta X Delta X Delta X New X

 (Linear) (Quad) (Total)

 R1 2.56770 -0.00295 0.00000 -0.00542 -0.00542 2.56228

 R2 2.76896 -0.00182 0.00000 -0.00526 -0.00526 2.76370

 R3 2.54413 -0.00308 0.00000 -0.00677 -0.00677 2.53736

 R4 2.62321 -0.00202 0.00000 -0.00406 -0.00406 2.61915

 R5 3.88762 -0.00180 0.00000 -0.00549 -0.00549 3.88213

 R6 2.75105 -0.00212 0.00000 -0.00578 -0.00578 2.74527

 R7 2.51963 -0.00317 0.00000 -0.00660 -0.00661 2.51302

 R8 2.68625 -0.00236 0.00000 -0.00602 -0.00602 2.68023

 R9 2.64754 -0.00346 0.00000 -0.00750 -0.00750 2.64004

 R10 2.64185 -0.00354 0.00000 -0.00761 -0.00761 2.63424

 R11 2.51963 -0.00317 0.00000 -0.00660 -0.00661 2.51302

 R12 2.62321 -0.00202 0.00000 -0.00406 -0.00406 2.61915

 R13 2.75105 -0.00212 0.00000 -0.00578 -0.00578 2.74527

 R14 2.56770 -0.00295 0.00000 -0.00542 -0.00542 2.56228

 R15 3.88762 -0.00180 0.00000 -0.00549 -0.00549 3.88213

 R16 2.76896 -0.00182 0.00000 -0.00526 -0.00526 2.76370

 R17 2.54413 -0.00308 0.00000 -0.00677 -0.00677 2.53736

 R18 2.68625 -0.00236 0.00000 -0.00602 -0.00602 2.68023

 R19 2.64185 -0.00354 0.00000 -0.00761 -0.00761 2.63424

 R20 2.64754 -0.00346 0.00000 -0.00750 -0.00750 2.64004

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 R23 2.76896 -0.00182 0.00000 -0.00526 -0.00526 2.76370

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 D110 -1.66823 0.00013 0.00000 0.00359 0.00359 -1.66464

 D111 -0.27356 -0.00006 0.00000 0.00271 0.00270 -0.27085

 D112 0.27311 0.00005 0.00000 -0.00296 -0.00296 0.27015

 D113 1.67153 -0.00014 0.00000 -0.00389 -0.00388 1.66765

 D114 3.06620 -0.00033 0.00000 -0.00477 -0.00477 3.06143

 D115 -0.00804 -0.00008 0.00000 -0.00198 -0.00198 -0.01002

 D116 3.11565 -0.00012 0.00000 -0.00256 -0.00256 3.11309

 D117 3.12082 -0.00007 0.00000 -0.00336 -0.00337 3.11745

 D118 -0.00530 -0.00005 0.00000 -0.00287 -0.00287 -0.00818

 D119 -0.19375 -0.00004 0.00000 0.00274 0.00274 -0.19101

 D120 2.96331 -0.00002 0.00000 0.00323 0.00324 2.96654

 D121 0.00496 0.00004 0.00000 0.00265 0.00266 0.00762

 D122 -3.12606 0.00007 0.00000 0.00321 0.00322 -3.12284

 D123 -2.96160 0.00000 0.00000 -0.00359 -0.00359 -2.96518

 D124 0.19057 0.00003 0.00000 -0.00303 -0.00303 0.18755

 D125 1.66823 -0.00013 0.00000 -0.00359 -0.00359 1.66464

 D126 3.06665 -0.00033 0.00000 -0.00452 -0.00452 3.06213

 D127 0.27356 0.00006 0.00000 -0.00271 -0.00270 0.27085

 D128 -1.67153 0.00014 0.00000 0.00389 0.00388 -1.66765

 D129 -0.27311 -0.00005 0.00000 0.00296 0.00296 -0.27015

 D130 -3.06620 0.00033 0.00000 0.00477 0.00477 -3.06143

 D131 -3.12310 0.00004 0.00000 0.00233 0.00233 -3.12077

 D132 0.01249 0.00001 0.00000 0.00085 0.00085 0.01334

 D133 0.00347 0.00003 0.00000 0.00190 0.00190 0.00538

 D134 3.13907 0.00000 0.00000 0.00042 0.00042 3.13949

 D135 -0.00054 -0.00001 0.00000 -0.00034 -0.00034 -0.00088

 D136 3.13783 -0.00003 0.00000 -0.00131 -0.00131 3.13652

 D137 -3.13705 0.00002 0.00000 0.00092 0.00092 -3.13613

 D138 0.00132 0.00000 0.00000 -0.00005 -0.00005 0.00128

 D139 -3.13942 0.00003 0.00000 0.00136 0.00136 -3.13806

 D140 0.00360 0.00002 0.00000 0.00119 0.00119 0.00479

 D141 -0.00450 0.00000 0.00000 -0.00028 -0.00028 -0.00478

 D142 3.13853 -0.00001 0.00000 -0.00046 -0.00046 3.13807

 D143 -0.00264 -0.00002 0.00000 -0.00138 -0.00138 -0.00402

 D144 3.12895 -0.00004 0.00000 -0.00187 -0.00187 3.12709

 D145 -3.14049 0.00001 0.00000 -0.00025 -0.00025 -3.14074

 D146 -0.00890 -0.00002 0.00000 -0.00075 -0.00074 -0.00964

 D147 0.00273 0.00001 0.00000 0.00038 0.00038 0.00311

 D148 -3.13966 0.00001 0.00000 0.00029 0.00029 -3.13937

 D149 3.14014 -0.00002 0.00000 -0.00088 -0.00087 3.13926

 D150 -0.00225 -0.00002 0.00000 -0.00096 -0.00096 -0.00321

 D151 0.01758 0.00008 0.00000 0.00200 0.00200 0.01957

 D152 -3.11198 0.00012 0.00000 0.00264 0.00264 -3.10934

 D153 0.00356 0.00001 0.00000 0.00038 0.00038 0.00393

 D154 -3.13885 0.00000 0.00000 0.00002 0.00002 -3.13883

 D155 -3.13883 0.00001 0.00000 0.00029 0.00029 -3.13854

 D156 0.00195 0.00000 0.00000 -0.00007 -0.00007 0.00188

 D157 -0.00035 0.00000 0.00000 -0.00005 -0.00005 -0.00039

 D158 3.14086 -0.00001 0.00000 -0.00039 -0.00039 3.14047

 D159 -3.14113 0.00001 0.00000 0.00031 0.00031 -3.14082

 D160 0.00007 0.00000 0.00000 -0.00003 -0.00003 0.00004

 D161 -0.00370 -0.00001 0.00000 -0.00029 -0.00029 -0.00399

 D162 3.13932 -0.00001 0.00000 -0.00046 -0.00046 3.13886

 D163 3.13828 0.00000 0.00000 0.00006 0.00006 3.13834

 D164 -0.00188 0.00000 0.00000 -0.00011 -0.00011 -0.00199

 D165 -0.00356 -0.00001 0.00000 -0.00038 -0.00038 -0.00393

 D166 3.13885 0.00000 0.00000 -0.00002 -0.00002 3.13883

 D167 3.13883 -0.00001 0.00000 -0.00029 -0.00029 3.13854

 D168 -0.00195 0.00000 0.00000 0.00007 0.00007 -0.00188

 D169 0.00035 0.00000 0.00000 0.00005 0.00005 0.00039

 D170 -3.14086 0.00001 0.00000 0.00039 0.00039 -3.14047

 D171 3.14113 -0.00001 0.00000 -0.00031 -0.00031 3.14082

 D172 -0.00007 0.00000 0.00000 0.00003 0.00003 -0.00004

 D173 0.00370 0.00001 0.00000 0.00029 0.00029 0.00399

 D174 -3.13932 0.00001 0.00000 0.00046 0.00046 -3.13886

 D175 -3.13828 0.00000 0.00000 -0.00006 -0.00006 -3.13834

 D176 0.00188 0.00000 0.00000 0.00011 0.00011 0.00199

 D177 -0.00370 -0.00001 0.00000 -0.00029 -0.00029 -0.00399

 D178 3.13828 0.00000 0.00000 0.00006 0.00006 3.13834

 D179 3.13932 -0.00001 0.00000 -0.00046 -0.00046 3.13886

 D180 -0.00188 0.00000 0.00000 -0.00011 -0.00011 -0.00199

 D181 -0.00035 0.00000 0.00000 -0.00005 -0.00005 -0.00039

 D182 -3.14113 0.00001 0.00000 0.00031 0.00031 -3.14082

 D183 3.14086 -0.00001 0.00000 -0.00039 -0.00039 3.14047

 D184 0.00007 0.00000 0.00000 -0.00003 -0.00003 0.00004

 D185 0.00356 0.00001 0.00000 0.00038 0.00038 0.00393

 D186 -3.13883 0.00001 0.00000 0.00029 0.00029 -3.13854

 D187 -3.13885 0.00000 0.00000 0.00002 0.00002 -3.13883

 D188 0.00195 0.00000 0.00000 -0.00007 -0.00007 0.00188

 D189 -0.00356 -0.00001 0.00000 -0.00038 -0.00038 -0.00393

 D190 3.13885 0.00000 0.00000 -0.00002 -0.00002 3.13883

 D191 3.13883 -0.00001 0.00000 -0.00029 -0.00029 3.13854

 D192 -0.00195 0.00000 0.00000 0.00007 0.00007 -0.00188

 D193 0.00035 0.00000 0.00000 0.00005 0.00005 0.00039

 D194 -3.14086 0.00001 0.00000 0.00039 0.00039 -3.14047

 D195 3.14113 -0.00001 0.00000 -0.00031 -0.00031 3.14082

 D196 -0.00007 0.00000 0.00000 0.00003 0.00003 -0.00004

 D197 0.00370 0.00001 0.00000 0.00029 0.00029 0.00399

 D198 -3.13932 0.00001 0.00000 0.00046 0.00046 -3.13886

 D199 -3.13828 0.00000 0.00000 -0.00006 -0.00006 -3.13834

 D200 0.00188 0.00000 0.00000 0.00011 0.00011 0.00199

 Item Value Threshold Converged?

 Maximum Force 0.004195 0.000450 NO

 RMS Force 0.001175 0.000300 NO

 Maximum Displacement 0.030277 0.001800 NO

 RMS Displacement 0.011030 0.001200 NO

 Predicted change in Energy=-6.199131D-04

 Lowest energy point so far. Saving SCF results.

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link 103 at Sat Jun 15 12:09:19 2019, MaxMem= 1342177280 cpu: 4.9

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

 Stoichiometry C32H16N8Zn(1-,2)

 Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C32H16N4)]

 Deg. of freedom 43

 Full point group C2V NOp 4

 RotChk: IX=0 Diff= 1.95D-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 2.771922 1.184079 0.006670

 2 7 0 1.437416 1.421962 0.037829

 3 6 0 1.186139 2.784646 0.007179

 4 6 0 2.464118 3.474046 -0.036761

 5 6 0 3.466305 2.470434 -0.038033

 6 7 0 0.000000 3.385862 -0.001472

 7 6 0 -1.186139 2.784646 0.007179

 8 7 0 -1.437416 1.421962 0.037829

 9 6 0 -2.771922 1.184079 0.006670

 10 6 0 -3.466305 2.470434 -0.038033

 11 6 0 -2.464118 3.474046 -0.036761

 12 7 0 3.405016 0.000000 0.001776

 13 6 0 3.466305 -2.470434 -0.038033

 14 6 0 2.464118 -3.474046 -0.036761

 15 6 0 1.186139 -2.784646 0.007179

 16 7 0 1.437416 -1.421962 0.037829

 17 6 0 2.771922 -1.184079 0.006670

 18 7 0 0.000000 -3.385862 -0.001472

 19 7 0 -1.437416 -1.421962 0.037829

 20 6 0 -1.186139 -2.784646 0.007179

 21 6 0 -2.464118 -3.474046 -0.036761

 22 6 0 -3.466305 -2.470434 -0.038033

 23 6 0 -2.771922 -1.184079 0.006670

 24 7 0 -3.405016 0.000000 0.001776

 25 30 0 0.000000 0.000000 0.401365

 26 6 0 4.818197 -2.807511 -0.082151

 27 6 0 5.160857 -4.155937 -0.121197

 28 6 0 4.167592 -5.152964 -0.120998

 29 6 0 2.816546 -4.825170 -0.081479

 30 6 0 -4.818197 -2.807511 -0.082151

 31 6 0 -5.160857 -4.155937 -0.121197

 32 6 0 -4.167592 -5.152964 -0.120998

 33 6 0 -2.816546 -4.825170 -0.081479

 34 6 0 -2.816546 4.825170 -0.081479

 35 6 0 -4.167592 5.152964 -0.120998

 36 6 0 -5.160857 4.155937 -0.121197

 37 6 0 -4.818197 2.807511 -0.082151

 38 6 0 4.818197 2.807511 -0.082151

 39 6 0 5.160857 4.155937 -0.121197

 40 6 0 4.167592 5.152964 -0.120998

 41 6 0 2.816546 4.825170 -0.081479

 42 1 0 5.581934 -2.036974 -0.085054

 43 1 0 2.055429 -5.598283 -0.084079

 44 1 0 -5.581934 -2.036974 -0.085054

 45 1 0 -2.055429 -5.598283 -0.084079

 46 1 0 -2.055429 5.598283 -0.084079

 47 1 0 -5.581934 2.036974 -0.085054

 48 1 0 5.581934 2.036974 -0.085054

 49 1 0 2.055429 5.598283 -0.084079

 50 1 0 -4.464352 6.196184 -0.153012

 51 1 0 -6.205735 4.445688 -0.153339

 52 1 0 4.464352 6.196184 -0.153012

 53 1 0 6.205735 4.445688 -0.153339

 54 1 0 6.205735 -4.445688 -0.153339

 55 1 0 4.464352 -6.196184 -0.153012

 56 1 0 -4.464352 -6.196184 -0.153012

 57 1 0 -6.205735 -4.445688 -0.153339

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

 Rotational constants (GHZ): 0.0881084 0.0879953 0.0441243

 Leave Link 202 at Sat Jun 15 12:09:19 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 225 symmetry adapted cartesian basis functions of A1 symmetry.

 There are 196 symmetry adapted cartesian basis functions of A2 symmetry.

 There are 207 symmetry adapted cartesian basis functions of B1 symmetry.

 There are 207 symmetry adapted cartesian basis functions of B2 symmetry.

 There are 211 symmetry adapted basis functions of A1 symmetry.

 There are 187 symmetry adapted basis functions of A2 symmetry.

 There are 197 symmetry adapted basis functions of B1 symmetry.

 There are 197 symmetry adapted basis functions of B2 symmetry.

 792 basis functions, 1399 primitive gaussians, 835 cartesian basis functions

 139 alpha electrons 138 beta electrons

 nuclear repulsion energy 4375.5745292560 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= 57 NActive= 57 NUniq= 16 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

 Integral buffers will be 131072 words long.

 Raffenetti 2 integral format.

 Two-electron integral symmetry is turned on.

 R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1642878855 Hartrees.

 Nuclear repulsion after empirical dispersion term = 4375.4102413704 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= 57.

 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 = 57

 GePol: Total number of spheres = 57

 GePol: Number of exposed spheres = 57 (100.00%)

 GePol: Number of points = 4674

 GePol: Average weight of points = 0.10

 GePol: Minimum weight of points = 0.12D-08

 GePol: Maximum weight of points = 0.18390

 GePol: Number of points with low weight = 348

 GePol: Fraction of low-weight points (<1% of avg) = 7.45%

 GePol: Cavity surface area = 485.253 Ang\*\*2

 GePol: Cavity volume = 504.105 Ang\*\*3

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

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 PCM non-electrostatic energy = -0.0144581783 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 4375.3957831921 Hartrees.

 Leave Link 301 at Sat Jun 15 12:09:20 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= 32896 NPrTT= 163506 LenC2= 22879 LenP2D= 61392.

 LDataN: DoStor=T MaxTD1= 5 Len= 102

 NBasis= 792 RedAO= T EigKep= 3.42D-05 NBF= 211 187 197 197

 NBsUse= 792 1.00D-06 EigRej= -1.00D+00 NBFU= 211 187 197 197

 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= 802 802 802 802 802 MxSgAt= 57 MxSgA2= 57.

 Leave Link 302 at Sat Jun 15 12:09:21 2019, MaxMem= 1342177280 cpu: 14.3

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

 DipDrv: MaxL=1.

 Leave Link 303 at Sat Jun 15 12:09:22 2019, MaxMem= 1342177280 cpu: 3.3

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

 Initial guess from the checkpoint file: "ZnPCanion.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) (A2) (B1) (B2) (A1) (B1) (A1) (B1) (A2)

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 The electronic state of the initial guess is 2-B1.

 Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7685 S= 0.5092

 Generating alternative initial guess.

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

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

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

 ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

 Petite list used in FoFCou.

 Harris En= -1733.84204742460

 Leave Link 401 at Sat Jun 15 12:09:32 2019, MaxMem= 1342177280 cpu: 103.6

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

 UHF open shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 2129573 IEndB= 2129573 NGot= 1342177280 MDV= 1340762408

 LenX= 1340762408 LenY= 1340064348

 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= 560000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

 Petite list used in FoFCou.

 Inv3: Mode=1 IEnd= 65538828.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 6.66D-15 for 4660.

 Iteration 1 A\*A^-1 deviation from orthogonality is 4.31D-15 for 4665 3778.

 Iteration 1 A^-1\*A deviation from unit magnitude is 6.00D-15 for 4660.

 Iteration 1 A^-1\*A deviation from orthogonality is 2.15D-08 for 1935 1916.

 Iteration 2 A\*A^-1 deviation from unit magnitude is 3.77D-15 for 16.

 Iteration 2 A\*A^-1 deviation from orthogonality is 4.31D-15 for 3404 1148.

 Iteration 2 A^-1\*A deviation from unit magnitude is 1.11D-15 for 1120.

 Iteration 2 A^-1\*A deviation from orthogonality is 4.44D-16 for 2690 2315.

 E= -1733.50684949072

 DIIS: error= 4.98D-04 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -1733.50684949072 IErMin= 1 ErrMin= 4.98D-04

 ErrMax= 4.98D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.12D-03 BMatP= 1.12D-03

 IDIUse=3 WtCom= 9.95D-01 WtEn= 4.98D-03

 Coeff-Com: 0.100D+01

 Coeff-En: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.368 Goal= None Shift= 0.000

 Gap= 0.409 Goal= None Shift= 0.000

 RMSDP=5.18D-05 MaxDP=1.63D-03 OVMax= 2.47D-03

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 5.11D-05 CP: 1.00D+00

 E= -1733.50716816977 Delta-E= -0.000318679049 Rises=F Damp=F

 DIIS: error= 2.14D-04 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -1733.50716816977 IErMin= 2 ErrMin= 2.14D-04

 ErrMax= 2.14D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.01D-04 BMatP= 1.12D-03

 IDIUse=3 WtCom= 9.98D-01 WtEn= 2.14D-03

 Coeff-Com: 0.120D+00 0.880D+00

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

 Coeff: 0.120D+00 0.880D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=1.32D-05 MaxDP=5.36D-04 DE=-3.19D-04 OVMax= 1.25D-03

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 1.28D-05 CP: 1.00D+00 1.06D+00

 E= -1733.50717543381 Delta-E= -0.000007264038 Rises=F Damp=F

 DIIS: error= 2.29D-04 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 3 EnMin= -1733.50717543381 IErMin= 2 ErrMin= 2.14D-04

 ErrMax= 2.29D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.07D-05 BMatP= 1.01D-04

 IDIUse=3 WtCom= 9.98D-01 WtEn= 2.29D-03

 Coeff-Com: -0.685D-02 0.471D+00 0.536D+00

 Coeff-En: 0.000D+00 0.417D+00 0.583D+00

 Coeff: -0.683D-02 0.471D+00 0.536D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=6.23D-06 MaxDP=2.41D-04 DE=-7.26D-06 OVMax= 9.84D-04

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 3.72D-06 CP: 1.00D+00 1.05D+00 6.13D-01

 E= -1733.50719275660 Delta-E= -0.000017322790 Rises=F Damp=F

 DIIS: error= 9.18D-05 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -1733.50719275660 IErMin= 4 ErrMin= 9.18D-05

 ErrMax= 9.18D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.18D-06 BMatP= 8.07D-05

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

 Coeff-Com: -0.122D-01 0.226D+00 0.327D+00 0.459D+00

 Coeff: -0.122D-01 0.226D+00 0.327D+00 0.459D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=1.87D-06 MaxDP=8.98D-05 DE=-1.73D-05 OVMax= 3.45D-04

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 1.17D-06 CP: 1.00D+00 1.05D+00 6.21D-01 6.14D-01

 E= -1733.50719486897 Delta-E= -0.000002112371 Rises=F Damp=F

 DIIS: error= 1.61D-05 at cycle 5 NSaved= 5.

 NSaved= 5 IEnMin= 5 EnMin= -1733.50719486897 IErMin= 5 ErrMin= 1.61D-05

 ErrMax= 1.61D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.21D-07 BMatP= 9.18D-06

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

 Coeff-Com: -0.521D-02 0.657D-01 0.110D+00 0.223D+00 0.607D+00

 Coeff: -0.521D-02 0.657D-01 0.110D+00 0.223D+00 0.607D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=5.06D-07 MaxDP=2.46D-05 DE=-2.11D-06 OVMax= 9.26D-05

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 4.43D-07 CP: 1.00D+00 1.05D+00 6.12D-01 6.18D-01 8.66D-01

 E= -1733.50719494192 Delta-E= -0.000000072952 Rises=F Damp=F

 DIIS: error= 9.56D-06 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -1733.50719494192 IErMin= 6 ErrMin= 9.56D-06

 ErrMax= 9.56D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.68D-08 BMatP= 4.21D-07

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

 Coeff-Com: -0.679D-03-0.223D-02 0.541D-02 0.472D-01 0.345D+00 0.605D+00

 Coeff: -0.679D-03-0.223D-02 0.541D-02 0.472D-01 0.345D+00 0.605D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=2.74D-07 MaxDP=1.23D-05 DE=-7.30D-08 OVMax= 4.27D-05

 Cycle 7 Pass 1 IDiag 1:

 RMSU= 1.52D-07 CP: 1.00D+00 1.05D+00 6.21D-01 6.25D-01 8.87D-01

 CP: 6.69D-01

 E= -1733.50719496152 Delta-E= -0.000000019592 Rises=F Damp=F

 DIIS: error= 2.05D-06 at cycle 7 NSaved= 7.

 NSaved= 7 IEnMin= 7 EnMin= -1733.50719496152 IErMin= 7 ErrMin= 2.05D-06

 ErrMax= 2.05D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.77D-09 BMatP= 8.68D-08

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

 Coeff-Com: -0.206D-04-0.547D-02-0.455D-02 0.847D-02 0.127D+00 0.298D+00

 Coeff-Com: 0.576D+00

 Coeff: -0.206D-04-0.547D-02-0.455D-02 0.847D-02 0.127D+00 0.298D+00

 Coeff: 0.576D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=8.18D-08 MaxDP=3.53D-06 DE=-1.96D-08 OVMax= 1.73D-05

 Cycle 8 Pass 1 IDiag 1:

 RMSU= 6.08D-08 CP: 1.00D+00 1.05D+00 6.20D-01 6.32D-01 9.02D-01

 CP: 7.23D-01 7.67D-01

 E= -1733.50719496334 Delta-E= -0.000000001828 Rises=F Damp=F

 DIIS: error= 1.24D-06 at cycle 8 NSaved= 8.

 NSaved= 8 IEnMin= 8 EnMin= -1733.50719496334 IErMin= 8 ErrMin= 1.24D-06

 ErrMax= 1.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.81D-09 BMatP= 6.77D-09

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

 Coeff-Com: 0.140D-03-0.310D-02-0.429D-02-0.545D-02 0.475D-02 0.528D-01

 Coeff-Com: 0.333D+00 0.622D+00

 Coeff: 0.140D-03-0.310D-02-0.429D-02-0.545D-02 0.475D-02 0.528D-01

 Coeff: 0.333D+00 0.622D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=4.24D-08 MaxDP=2.02D-06 DE=-1.83D-09 OVMax= 9.66D-06

 Cycle 9 Pass 1 IDiag 1:

 RMSU= 3.28D-08 CP: 1.00D+00 1.05D+00 6.20D-01 6.32D-01 9.08D-01

 CP: 7.30D-01 9.23D-01 8.58D-01

 E= -1733.50719496437 Delta-E= -0.000000001027 Rises=F Damp=F

 DIIS: error= 5.52D-07 at cycle 9 NSaved= 9.

 NSaved= 9 IEnMin= 9 EnMin= -1733.50719496437 IErMin= 9 ErrMin= 5.52D-07

 ErrMax= 5.52D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.95D-10 BMatP= 1.81D-09

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

 Coeff-Com: 0.524D-04 0.490D-03-0.875D-04-0.408D-02-0.314D-01-0.626D-01

 Coeff-Com: -0.610D-01 0.164D+00 0.995D+00

 Coeff: 0.524D-04 0.490D-03-0.875D-04-0.408D-02-0.314D-01-0.626D-01

 Coeff: -0.610D-01 0.164D+00 0.995D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=3.33D-08 MaxDP=1.64D-06 DE=-1.03D-09 OVMax= 8.78D-06

 Cycle 10 Pass 1 IDiag 1:

 RMSU= 1.79D-08 CP: 1.00D+00 1.05D+00 6.21D-01 6.32D-01 9.09D-01

 CP: 7.42D-01 9.82D-01 1.27D+00 1.15D+00

 E= -1733.50719496463 Delta-E= -0.000000000258 Rises=F Damp=F

 DIIS: error= 4.57D-07 at cycle 10 NSaved= 10.

 NSaved=10 IEnMin=10 EnMin= -1733.50719496463 IErMin=10 ErrMin= 4.57D-07

 ErrMax= 4.57D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.42D-10 BMatP= 2.95D-10

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

 Coeff-Com: -0.148D-04 0.158D-02 0.161D-02-0.112D-02-0.259D-01-0.677D-01

 Coeff-Com: -0.158D+00-0.991D-01 0.730D+00 0.620D+00

 Coeff: -0.148D-04 0.158D-02 0.161D-02-0.112D-02-0.259D-01-0.677D-01

 Coeff: -0.158D+00-0.991D-01 0.730D+00 0.620D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=2.14D-08 MaxDP=9.91D-07 DE=-2.58D-10 OVMax= 5.70D-06

 Cycle 11 Pass 1 IDiag 1:

 RMSU= 9.08D-09 CP: 1.00D+00 1.05D+00 6.20D-01 6.32D-01 9.12D-01

 CP: 7.45D-01 1.04D+00 1.34D+00 1.63D+00 8.76D-01

 E= -1733.50719496462 Delta-E= 0.000000000008 Rises=F Damp=F

 DIIS: error= 1.50D-07 at cycle 11 NSaved= 11.

 NSaved=11 IEnMin=10 EnMin= -1733.50719496463 IErMin=11 ErrMin= 1.50D-07

 ErrMax= 1.50D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.51D-11 BMatP= 2.42D-10

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

 Coeff-Com: -0.194D-04 0.202D-03 0.403D-03 0.985D-03 0.417D-02 0.434D-02

 Coeff-Com: -0.901D-02-0.824D-01-0.175D+00 0.171D+00 0.108D+01

 Coeff: -0.194D-04 0.202D-03 0.403D-03 0.985D-03 0.417D-02 0.434D-02

 Coeff: -0.901D-02-0.824D-01-0.175D+00 0.171D+00 0.108D+01

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=1.20D-08 MaxDP=6.78D-07 DE= 8.19D-12 OVMax= 3.60D-06

 Cycle 12 Pass 1 IDiag 1:

 RMSU= 3.98D-09 CP: 1.00D+00 1.05D+00 6.20D-01 6.32D-01 9.11D-01

 CP: 7.50D-01 1.06D+00 1.44D+00 1.80D+00 1.23D+00

 CP: 1.24D+00

 E= -1733.50719496458 Delta-E= 0.000000000040 Rises=F Damp=F

 DIIS: error= 7.55D-08 at cycle 12 NSaved= 12.

 NSaved=12 IEnMin=10 EnMin= -1733.50719496463 IErMin=12 ErrMin= 7.55D-08

 ErrMax= 7.55D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.75D-12 BMatP= 2.51D-11

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

 Coeff-Com: -0.746D-05-0.927D-04-0.118D-05 0.606D-03 0.510D-02 0.101D-01

 Coeff-Com: 0.136D-01-0.292D-01-0.174D+00 0.961D-02 0.543D+00 0.622D+00

 Coeff: -0.746D-05-0.927D-04-0.118D-05 0.606D-03 0.510D-02 0.101D-01

 Coeff: 0.136D-01-0.292D-01-0.174D+00 0.961D-02 0.543D+00 0.622D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=3.51D-09 MaxDP=1.74D-07 DE= 4.00D-11 OVMax= 9.54D-07

 Error on total polarization charges = 0.07592

 SCF Done: E(UB3LYP) = -1733.50719496 A.U. after 12 cycles

 NFock= 12 Conv=0.35D-08 -V/T= 1.9757

 <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5091

 <L.S>= 0.000000000000E+00

 KE= 1.776720461796D+03 PE=-1.289798818767D+04 EE= 5.012364747719D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -9.07

 (included in total energy above)

 Annihilation of the first spin contaminant:

 S\*\*2 before annihilation 0.7682, after 0.7503

 Leave Link 502 at Sat Jun 15 12:12:24 2019, MaxMem= 1342177280 cpu: 1964.3

 (Enter /apps/gaussian/g09d01/g09/l701.exe)

 Compute integral first derivatives.

 ... and contract with generalized density number 0.

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

 4 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22879 LenP2D= 61392.

 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 = 197

 Leave Link 701 at Sat Jun 15 12:12:37 2019, MaxMem= 1342177280 cpu: 128.4

 (Enter /apps/gaussian/g09d01/g09/l702.exe)

 L702 exits ... SP integral derivatives will be done elsewhere.

 Leave Link 702 at Sat Jun 15 12:12:38 2019, MaxMem= 1342177280 cpu: 0.7

 (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= 800

 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 Sat Jun 15 12:12:57 2019, MaxMem= 1342177280 cpu: 220.9

 (Enter /apps/gaussian/g09d01/g09/l716.exe)

 Dipole =-4.51194637D-13-1.19015908D-13 8.48439286D-01

 \*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

 Center Atomic Forces (Hartrees/Bohr)

 Number Number X Y Z

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

 1 6 -0.000213613 -0.000321012 -0.000125160

 2 7 0.000156623 -0.000016311 0.000201353

 3 6 -0.000301913 0.000106157 -0.000060191

 4 6 0.000158717 0.000009966 -0.000029904

 5 6 0.000158227 0.000250512 -0.000016985

 6 7 0.000000000 -0.000571822 0.000085648

 7 6 0.000301913 0.000106157 -0.000060191

 8 7 -0.000156623 -0.000016311 0.000201353

 9 6 0.000213613 -0.000321012 -0.000125160

 10 6 -0.000158227 0.000250512 -0.000016985

 11 6 -0.000158717 0.000009966 -0.000029904

 12 7 -0.000504696 0.000000000 0.000136989

 13 6 0.000158227 -0.000250512 -0.000016985

 14 6 0.000158717 -0.000009966 -0.000029904

 15 6 -0.000301913 -0.000106157 -0.000060191

 16 7 0.000156623 0.000016311 0.000201353

 17 6 -0.000213613 0.000321012 -0.000125160

 18 7 0.000000000 0.000571822 0.000085648

 19 7 -0.000156623 0.000016311 0.000201353

 20 6 0.000301913 -0.000106157 -0.000060191

 21 6 -0.000158717 -0.000009966 -0.000029904

 22 6 -0.000158227 -0.000250512 -0.000016985

 23 6 0.000213613 0.000321012 -0.000125160

 24 7 0.000504696 0.000000000 0.000136989

 25 30 0.000000000 0.000000000 -0.000123741

 26 6 0.000181253 -0.000053702 -0.000018103

 27 6 0.000374169 -0.000038786 -0.000012988

 28 6 0.000028519 -0.000359430 -0.000013600

 29 6 0.000059830 -0.000181563 -0.000024482

 30 6 -0.000181253 -0.000053702 -0.000018103

 31 6 -0.000374169 -0.000038786 -0.000012988

 32 6 -0.000028519 -0.000359430 -0.000013600

 33 6 -0.000059830 -0.000181563 -0.000024482

 34 6 -0.000059830 0.000181563 -0.000024482

 35 6 -0.000028519 0.000359430 -0.000013600

 36 6 -0.000374169 0.000038786 -0.000012988

 37 6 -0.000181253 0.000053702 -0.000018103

 38 6 0.000181253 0.000053702 -0.000018103

 39 6 0.000374169 0.000038786 -0.000012988

 40 6 0.000028519 0.000359430 -0.000013600

 41 6 0.000059830 0.000181563 -0.000024482

 42 1 0.000035153 0.000129896 0.000008673

 43 1 -0.000126218 -0.000041109 0.000009257

 44 1 -0.000035153 0.000129896 0.000008673

 45 1 0.000126218 -0.000041109 0.000009257

 46 1 0.000126218 0.000041109 0.000009257

 47 1 -0.000035153 -0.000129896 0.000008673

 48 1 0.000035153 -0.000129896 0.000008673

 49 1 -0.000126218 0.000041109 0.000009257

 50 1 -0.000065053 0.000105522 0.000001746

 51 1 -0.000103561 0.000064586 0.000000000

 52 1 0.000065053 0.000105522 0.000001746

 53 1 0.000103561 0.000064586 0.000000000

 54 1 0.000103561 -0.000064586 0.000000000

 55 1 0.000065053 -0.000105522 0.000001746

 56 1 -0.000065053 -0.000105522 0.000001746

 57 1 -0.000103561 -0.000064586 0.000000000

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

 Cartesian Forces: Max 0.000571822 RMS 0.000165360

 Leave Link 716 at Sat Jun 15 12:12:57 2019, MaxMem= 1342177280 cpu: 4.4

 (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 0.000763519 RMS 0.000169320

 Search for a local minimum.

 Step number 2 out of a maximum of 342

 All quantities printed in internal units (Hartrees-Bohrs-Radians)

 RMS Force = .16932D-03 SwitMx=.10000D-02 MixMth= 2

 Mixed Optimization -- En-DIIS/RFO-DIIS

 Update second derivatives using D2CorX and points 1 2

 DE= -5.53D-04 DEPred=-6.20D-04 R= 8.92D-01

 TightC=F SS= 1.41D+00 RLast= 6.10D-02 DXNew= 5.0454D-01 1.8307D-01

 Trust test= 8.92D-01 RLast= 6.10D-02 DXMaxT set to 3.00D-01

 ITU= 1 0

 Use linear search instead of GDIIS.

 Eigenvalues --- 0.01570 0.01587 0.01610 0.01610 0.01624

 Eigenvalues --- 0.01645 0.01681 0.01697 0.01762 0.01767

 Eigenvalues --- 0.01775 0.01780 0.01780 0.01782 0.01783

 Eigenvalues --- 0.01788 0.01835 0.01846 0.01892 0.01895

 Eigenvalues --- 0.01905 0.01958 0.01959 0.02008 0.02008

 Eigenvalues --- 0.02008 0.02008 0.02051 0.02051 0.02051

 Eigenvalues --- 0.02051 0.02053 0.02053 0.02053 0.02053

 Eigenvalues --- 0.02077 0.02113 0.02113 0.02113 0.02113

 Eigenvalues --- 0.02119 0.02119 0.02119 0.02119 0.02124

 Eigenvalues --- 0.02124 0.02124 0.02124 0.02243 0.02249

 Eigenvalues --- 0.02323 0.02331 0.03341 0.03920 0.03939

 Eigenvalues --- 0.07479 0.15228 0.15973 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 0.16256 0.16364

 Eigenvalues --- 0.17348 0.22000 0.22000 0.22000 0.22000

 Eigenvalues --- 0.22566 0.22598 0.22600 0.22600 0.24114

 Eigenvalues --- 0.24298 0.24510 0.24510 0.24519 0.24529

 Eigenvalues --- 0.24612 0.24618 0.24833 0.24948 0.24956

 Eigenvalues --- 0.24985 0.24995 0.24997 0.24997 0.24998

 Eigenvalues --- 0.25446 0.33725 0.34067 0.34312 0.34354

 Eigenvalues --- 0.34800 0.34846 0.35155 0.35214 0.35218

 Eigenvalues --- 0.35218 0.35218 0.35227 0.35243 0.35243

 Eigenvalues --- 0.35243 0.35245 0.35247 0.35247 0.35247

 Eigenvalues --- 0.35250 0.35252 0.35252 0.35252 0.35615

 Eigenvalues --- 0.37367 0.37388 0.37564 0.38013 0.40798

 Eigenvalues --- 0.40886 0.41928 0.41932 0.41947 0.41960

 Eigenvalues --- 0.41970 0.42394 0.43207 0.43246 0.44575

 Eigenvalues --- 0.45210 0.45216 0.45266 0.45342 0.45777

 Eigenvalues --- 0.45910 0.45911 0.45918 0.46020 0.46122

 Eigenvalues --- 0.46178 0.46179 0.46184 0.46689 0.48460

 Eigenvalues --- 0.49756 0.50396 0.50600 0.51365 0.53527

 Eigenvalues --- 0.55372 0.55378 0.55559 0.58008 0.58035

 RFO step: Lambda=-1.76559293D-05 EMin= 1.57037402D-02

 Quartic linear search produced a step of -0.09739.

 Iteration 1 RMS(Cart)= 0.00241686 RMS(Int)= 0.00000093

 Iteration 2 RMS(Cart)= 0.00000228 RMS(Int)= 0.00000025

 Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000025

 ITry= 1 IFail=0 DXMaxC= 8.78D-03 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

 ClnCor: largest displacement from symmetrization is 1.27D-11 for atom 48.

 Variable Old X -DE/DX Delta X Delta X Delta X New X

 (Linear) (Quad) (Total)

 R1 2.56228 -0.00003 0.00053 -0.00072 -0.00019 2.56209

 R2 2.76370 0.00076 0.00051 0.00133 0.00185 2.76555

 R3 2.53736 0.00003 0.00066 -0.00061 0.00005 2.53741

 R4 2.61915 0.00016 0.00040 -0.00022 0.00018 2.61933

 R5 3.88213 0.00037 0.00053 0.00137 0.00190 3.88404

 R6 2.74527 0.00068 0.00056 0.00104 0.00160 2.74687

 R7 2.51302 0.00002 0.00064 -0.00060 0.00004 2.51307

 R8 2.68023 0.00015 0.00059 -0.00026 0.00033 2.68056

 R9 2.64004 0.00049 0.00073 0.00012 0.00085 2.64089

 R10 2.63424 0.00048 0.00074 0.00009 0.00083 2.63507

 R11 2.51302 0.00002 0.00064 -0.00060 0.00004 2.51307

 R12 2.61915 0.00016 0.00040 -0.00022 0.00018 2.61933

 R13 2.74527 0.00068 0.00056 0.00104 0.00160 2.74687

 R14 2.56228 -0.00003 0.00053 -0.00072 -0.00019 2.56209

 R15 3.88213 0.00037 0.00053 0.00137 0.00190 3.88404

 R16 2.76370 0.00076 0.00051 0.00133 0.00185 2.76555

 R17 2.53736 0.00003 0.00066 -0.00061 0.00005 2.53741

 R18 2.68023 0.00015 0.00059 -0.00026 0.00033 2.68056

 R19 2.63424 0.00048 0.00074 0.00009 0.00083 2.63507

 R20 2.64004 0.00049 0.00073 0.00012 0.00085 2.64089

 R21 2.53736 0.00003 0.00066 -0.00061 0.00005 2.53741

 R22 2.68023 0.00015 0.00059 -0.00026 0.00033 2.68056

 R23 2.76370 0.00076 0.00051 0.00133 0.00185 2.76555

 R24 2.63424 0.00048 0.00074 0.00009 0.00083 2.63507

 R25 2.74527 0.00068 0.00056 0.00104 0.00160 2.74687

 R26 2.64004 0.00049 0.00073 0.00012 0.00085 2.64089

 R27 2.61915 0.00016 0.00040 -0.00022 0.00018 2.61933

 R28 2.51302 0.00002 0.00064 -0.00060 0.00004 2.51307

 R29 2.56228 -0.00003 0.00053 -0.00072 -0.00019 2.56209

 R30 3.88213 0.00037 0.00053 0.00137 0.00190 3.88404

 R31 2.51302 0.00002 0.00064 -0.00060 0.00004 2.51307

 R32 2.61915 0.00016 0.00040 -0.00022 0.00018 2.61933

 R33 2.56228 -0.00003 0.00053 -0.00072 -0.00019 2.56209

 R34 3.88213 0.00037 0.00053 0.00137 0.00190 3.88404

 R35 2.74527 0.00068 0.00056 0.00104 0.00160 2.74687

 R36 2.68023 0.00015 0.00059 -0.00026 0.00033 2.68056

 R37 2.64004 0.00049 0.00073 0.00012 0.00085 2.64089

 R38 2.76370 0.00076 0.00051 0.00133 0.00185 2.76555

 R39 2.63424 0.00048 0.00074 0.00009 0.00083 2.63507

 R40 2.53736 0.00003 0.00066 -0.00061 0.00005 2.53741

 R41 2.63018 0.00040 0.00088 -0.00022 0.00066 2.63084

 R42 2.05018 0.00012 0.00026 0.00000 0.00026 2.05044

 R43 2.65951 0.00037 0.00078 -0.00012 0.00066 2.66017

 R44 2.04995 0.00012 0.00027 -0.00001 0.00026 2.05021

 R45 2.62824 0.00040 0.00089 -0.00024 0.00065 2.62889

 R46 2.05050 0.00012 0.00027 0.00000 0.00026 2.05077

 R47 2.05016 0.00012 0.00025 0.00001 0.00026 2.05043

 R48 2.63018 0.00040 0.00088 -0.00022 0.00066 2.63084

 R49 2.05018 0.00012 0.00026 0.00000 0.00026 2.05044

 R50 2.65951 0.00037 0.00078 -0.00012 0.00066 2.66017

 R51 2.04995 0.00012 0.00027 -0.00001 0.00026 2.05021

 R52 2.62824 0.00040 0.00089 -0.00024 0.00065 2.62889

 R53 2.05050 0.00012 0.00027 0.00000 0.00026 2.05077

 R54 2.05016 0.00012 0.00025 0.00001 0.00026 2.05043

 R55 2.62824 0.00040 0.00089 -0.00024 0.00065 2.62889

 R56 2.05016 0.00012 0.00025 0.00001 0.00026 2.05043

 R57 2.65951 0.00037 0.00078 -0.00012 0.00066 2.66017

 R58 2.05050 0.00012 0.00027 0.00000 0.00026 2.05077

 R59 2.63018 0.00040 0.00088 -0.00022 0.00066 2.63084

 R60 2.04995 0.00012 0.00027 -0.00001 0.00026 2.05021

 R61 2.05018 0.00012 0.00026 0.00000 0.00026 2.05044

 R62 2.63018 0.00040 0.00088 -0.00022 0.00066 2.63084

 R63 2.05018 0.00012 0.00026 0.00000 0.00026 2.05044

 R64 2.65951 0.00037 0.00078 -0.00012 0.00066 2.66017

 R65 2.04995 0.00012 0.00027 -0.00001 0.00026 2.05021

 R66 2.62824 0.00040 0.00089 -0.00024 0.00065 2.62889

 R67 2.05050 0.00012 0.00027 0.00000 0.00026 2.05077

 R68 2.05016 0.00012 0.00025 0.00001 0.00026 2.05043

 A1 1.88988 0.00013 0.00029 -0.00012 0.00017 1.89005

 A2 2.23809 -0.00022 -0.00037 -0.00032 -0.00069 2.23740

 A3 2.15516 0.00010 0.00008 0.00044 0.00052 2.15569

 A4 1.92882 -0.00002 -0.00034 0.00052 0.00018 1.92900

 A5 2.17887 -0.00001 0.00014 -0.00013 0.00002 2.17889

 A6 2.16228 0.00004 0.00010 0.00010 0.00020 2.16248

 A7 1.88363 0.00008 0.00029 -0.00025 0.00004 1.88367

 A8 2.22225 -0.00024 -0.00035 -0.00042 -0.00078 2.22148

 A9 2.17719 0.00016 0.00006 0.00067 0.00073 2.17792

 A10 1.86067 -0.00006 -0.00012 0.00003 -0.00008 1.86059

 A11 2.32108 0.00013 0.00007 0.00034 0.00041 2.32148

 A12 2.10142 -0.00007 0.00005 -0.00038 -0.00033 2.10109

 A13 1.86175 -0.00012 -0.00013 -0.00019 -0.00032 1.86144

 A14 2.31056 0.00016 0.00008 0.00044 0.00052 2.31108

 A15 2.11086 -0.00004 0.00004 -0.00025 -0.00021 2.11065

 A16 2.20325 0.00043 0.00038 0.00131 0.00169 2.20494

 A17 2.22225 -0.00024 -0.00035 -0.00042 -0.00078 2.22148

 A18 2.17719 0.00016 0.00006 0.00067 0.00073 2.17792

 A19 1.88363 0.00008 0.00029 -0.00025 0.00004 1.88367

 A20 1.92882 -0.00002 -0.00034 0.00052 0.00018 1.92900

 A21 2.16228 0.00004 0.00010 0.00010 0.00020 2.16248

 A22 2.17887 -0.00001 0.00014 -0.00013 0.00002 2.17889

 A23 1.88988 0.00013 0.00029 -0.00012 0.00017 1.89005

 A24 2.23809 -0.00022 -0.00037 -0.00032 -0.00069 2.23740

 A25 2.15516 0.00010 0.00008 0.00044 0.00052 2.15569

 A26 1.86175 -0.00012 -0.00013 -0.00019 -0.00032 1.86144

 A27 2.31056 0.00016 0.00008 0.00044 0.00052 2.31108

 A28 2.11086 -0.00004 0.00004 -0.00025 -0.00021 2.11065

 A29 1.86067 -0.00006 -0.00012 0.00003 -0.00008 1.86059

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 D3 -3.12284 0.00001 -0.00031 0.00107 0.00076 -3.12208

 D4 0.18755 -0.00004 0.00029 -0.00213 -0.00183 0.18571

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 D6 -3.14074 0.00000 0.00002 -0.00030 -0.00028 -3.14102

 D7 3.12709 -0.00001 0.00018 -0.00081 -0.00062 3.12646

 D8 -0.00964 0.00000 0.00007 -0.00037 -0.00030 -0.00994

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 D10 -3.10934 0.00003 -0.00026 0.00169 0.00143 -3.10791

 D11 -0.00818 0.00000 0.00028 -0.00087 -0.00059 -0.00877

 D12 3.11745 -0.00001 0.00033 -0.00152 -0.00119 3.11626

 D13 2.96654 0.00004 -0.00032 0.00227 0.00195 2.96850

 D14 -0.19101 0.00003 -0.00027 0.00162 0.00135 -0.18966

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 D17 -1.66765 0.00003 -0.00038 0.00196 0.00158 -1.66607

 D18 0.27085 -0.00004 0.00026 -0.00168 -0.00142 0.26944

 D19 3.06213 -0.00001 0.00044 -0.00174 -0.00130 3.06083

 D20 1.66464 -0.00002 0.00035 -0.00169 -0.00134 1.66330

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 D24 0.01334 0.00001 -0.00008 0.00074 0.00066 0.01400

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 D36 -0.00321 -0.00001 0.00009 -0.00053 -0.00044 -0.00365

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 D182 -3.14082 0.00000 -0.00003 -0.00006 -0.00009 -3.14091

 D183 3.14047 0.00000 0.00004 0.00008 0.00012 3.14058

 D184 0.00004 0.00000 0.00000 0.00005 0.00005 0.00009

 D185 0.00393 0.00000 -0.00004 0.00019 0.00015 0.00409

 D186 -3.13854 0.00000 -0.00003 -0.00001 -0.00003 -3.13857

 D187 -3.13883 0.00001 0.00000 0.00022 0.00022 -3.13861

 D188 0.00188 0.00000 0.00001 0.00003 0.00003 0.00191

 D189 -0.00393 0.00000 0.00004 -0.00019 -0.00015 -0.00409

 D190 3.13883 -0.00001 0.00000 -0.00022 -0.00022 3.13861

 D191 3.13854 0.00000 0.00003 0.00001 0.00003 3.13857

 D192 -0.00188 0.00000 -0.00001 -0.00003 -0.00003 -0.00191

 D193 0.00039 0.00000 0.00000 0.00003 0.00002 0.00041

 D194 -3.14047 0.00000 -0.00004 -0.00008 -0.00012 -3.14058

 D195 3.14082 0.00000 0.00003 0.00006 0.00009 3.14091

 D196 -0.00004 0.00000 0.00000 -0.00005 -0.00005 -0.00009

 D197 0.00399 0.00000 -0.00003 0.00018 0.00015 0.00414

 D198 -3.13886 0.00000 -0.00004 -0.00012 -0.00016 -3.13903

 D199 -3.13834 0.00001 0.00001 0.00029 0.00029 -3.13805

 D200 0.00199 0.00000 -0.00001 -0.00001 -0.00002 0.00197

 Item Value Threshold Converged?

 Maximum Force 0.000764 0.000450 NO

 RMS Force 0.000169 0.000300 YES

 Maximum Displacement 0.008781 0.001800 NO

 RMS Displacement 0.002416 0.001200 NO

 Predicted change in Energy=-1.531747D-05

 Lowest energy point so far. Saving SCF results.

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link 103 at Sat Jun 15 12:13:00 2019, MaxMem= 1342177280 cpu: 23.5

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

 Stoichiometry C32H16N8Zn(1-,2)

 Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C32H16N4)]

 Deg. of freedom 43

 Full point group C2V NOp 4

 RotChk: IX=0 Diff= 4.33D-17

 Largest Abelian subgroup C2V NOp 4

 Largest concise Abelian subgroup C2V NOp 4

 Standard orientation:

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 2.772382 1.184648 0.008457

 2 7 0 1.438057 1.422754 0.041297

 3 6 0 1.186666 2.785477 0.009128

 4 6 0 2.465285 3.475337 -0.036926

 5 6 0 3.467595 2.471600 -0.038100

 6 7 0 0.000000 3.385697 0.000207

 7 6 0 -1.186666 2.785477 0.009128

 8 7 0 -1.438057 1.422754 0.041297

 9 6 0 -2.772382 1.184648 0.008457

 10 6 0 -3.467595 2.471600 -0.038100

 11 6 0 -2.465285 3.475337 -0.036926

 12 7 0 3.404464 0.000000 0.003492

 13 6 0 3.467595 -2.471600 -0.038100

 14 6 0 2.465285 -3.475337 -0.036926

 15 6 0 1.186666 -2.785477 0.009128

 16 7 0 1.438057 -1.422754 0.041297

 17 6 0 2.772382 -1.184648 0.008457

 18 7 0 0.000000 -3.385697 0.000207

 19 7 0 -1.438057 -1.422754 0.041297

 20 6 0 -1.186666 -2.785477 0.009128

 21 6 0 -2.465285 -3.475337 -0.036926

 22 6 0 -3.467595 -2.471600 -0.038100

 23 6 0 -2.772382 -1.184648 0.008457

 24 7 0 -3.404464 0.000000 0.003492

 25 30 0 0.000000 0.000000 0.404889

 26 6 0 4.819796 -2.809016 -0.084046

 27 6 0 5.162967 -4.157619 -0.124884

 28 6 0 4.169472 -5.154910 -0.124841

 29 6 0 2.818217 -4.826727 -0.083669

 30 6 0 -4.819796 -2.809016 -0.084046

 31 6 0 -5.162967 -4.157619 -0.124884

 32 6 0 -4.169472 -5.154910 -0.124841

 33 6 0 -2.818217 -4.826727 -0.083669

 34 6 0 -2.818217 4.826727 -0.083669

 35 6 0 -4.169472 5.154910 -0.124841

 36 6 0 -5.162967 4.157619 -0.124884

 37 6 0 -4.819796 2.809016 -0.084046

 38 6 0 4.819796 2.809016 -0.084046

 39 6 0 5.162967 4.157619 -0.124884

 40 6 0 4.169472 5.154910 -0.124841

 41 6 0 2.818217 4.826727 -0.083669

 42 1 0 5.583268 -2.038022 -0.086778

 43 1 0 2.056745 -5.599685 -0.086233

 44 1 0 -5.583268 -2.038022 -0.086778

 45 1 0 -2.056745 -5.599685 -0.086233

 46 1 0 -2.056745 5.599685 -0.086233

 47 1 0 -5.583268 2.038022 -0.086778

 48 1 0 5.583268 2.038022 -0.086778

 49 1 0 2.056745 5.599685 -0.086233

 50 1 0 -4.466320 6.198210 -0.158151

 51 1 0 -6.207941 4.447394 -0.158251

 52 1 0 4.466320 6.198210 -0.158151

 53 1 0 6.207941 4.447394 -0.158251

 54 1 0 6.207941 -4.447394 -0.158251

 55 1 0 4.466320 -6.198210 -0.158151

 56 1 0 -4.466320 -6.198210 -0.158151

 57 1 0 -6.207941 -4.447394 -0.158251

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 Rotational constants (GHZ): 0.0880404 0.0879268 0.0440926

 Leave Link 202 at Sat Jun 15 12:13:01 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 225 symmetry adapted cartesian basis functions of A1 symmetry.

 There are 196 symmetry adapted cartesian basis functions of A2 symmetry.

 There are 207 symmetry adapted cartesian basis functions of B1 symmetry.

 There are 207 symmetry adapted cartesian basis functions of B2 symmetry.

 There are 211 symmetry adapted basis functions of A1 symmetry.

 There are 187 symmetry adapted basis functions of A2 symmetry.

 There are 197 symmetry adapted basis functions of B1 symmetry.

 There are 197 symmetry adapted basis functions of B2 symmetry.

 792 basis functions, 1399 primitive gaussians, 835 cartesian basis functions

 139 alpha electrons 138 beta electrons

 nuclear repulsion energy 4374.1508503224 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= 57 NActive= 57 NUniq= 16 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

 Integral buffers will be 131072 words long.

 Raffenetti 2 integral format.

 Two-electron integral symmetry is turned on.

 R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1642503273 Hartrees.

 Nuclear repulsion after empirical dispersion term = 4373.9865999951 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= 57.

 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 = 57

 GePol: Total number of spheres = 57

 GePol: Number of exposed spheres = 57 (100.00%)

 GePol: Number of points = 4678

 GePol: Average weight of points = 0.10

 GePol: Minimum weight of points = 0.76D-10

 GePol: Maximum weight of points = 0.18390

 GePol: Number of points with low weight = 352

 GePol: Fraction of low-weight points (<1% of avg) = 7.52%

 GePol: Cavity surface area = 485.605 Ang\*\*2

 GePol: Cavity volume = 504.329 Ang\*\*3

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

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 PCM non-electrostatic energy = -0.0144431087 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 4373.9721568865 Hartrees.

 Leave Link 301 at Sat Jun 15 12:13:01 2019, MaxMem= 1342177280 cpu: 0.6

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

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

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

 One-electron integrals computed using PRISM.

 One-electron integral symmetry used in STVInt

 4 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22879 LenP2D= 61376.

 LDataN: DoStor=T MaxTD1= 5 Len= 102

 NBasis= 792 RedAO= T EigKep= 3.44D-05 NBF= 211 187 197 197

 NBsUse= 792 1.00D-06 EigRej= -1.00D+00 NBFU= 211 187 197 197

 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= 802 802 802 802 802 MxSgAt= 57 MxSgA2= 57.

 Leave Link 302 at Sat Jun 15 12:13:02 2019, MaxMem= 1342177280 cpu: 12.4

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

 DipDrv: MaxL=1.

 Leave Link 303 at Sat Jun 15 12:13:02 2019, MaxMem= 1342177280 cpu: 1.9

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

 Initial guess from the checkpoint file: "ZnPCanion.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) (A2) (B1) (B2) (A1) (B1) (A1) (B1) (A2)

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 The electronic state of the initial guess is 2-B1.

 Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5091

 Leave Link 401 at Sat Jun 15 12:13:09 2019, MaxMem= 1342177280 cpu: 73.3

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

 UHF open shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 2129573 IEndB= 2129573 NGot= 1342177280 MDV= 1340762408

 LenX= 1340762408 LenY= 1340064348

 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= 560000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

 Petite list used in FoFCou.

 Inv3: Mode=1 IEnd= 65651052.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 8.22D-15 for 4670.

 Iteration 1 A\*A^-1 deviation from orthogonality is 8.22D-15 for 4670 3783.

 Iteration 1 A^-1\*A deviation from unit magnitude is 9.10D-15 for 4670.

 Iteration 1 A^-1\*A deviation from orthogonality is 2.69D-12 for 3734 3724.

 E= -1733.50718313904

 DIIS: error= 1.57D-04 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -1733.50718313904 IErMin= 1 ErrMin= 1.57D-04

 ErrMax= 1.57D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.97D-05 BMatP= 6.97D-05

 IDIUse=3 WtCom= 9.98D-01 WtEn= 1.57D-03

 Coeff-Com: 0.100D+01

 Coeff-En: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.368 Goal= None Shift= 0.000

 Gap= 0.409 Goal= None Shift= 0.000

 RMSDP=1.09D-05 MaxDP=2.99D-04 OVMax= 8.99D-04

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 1.08D-05 CP: 1.00D+00

 E= -1733.50721210302 Delta-E= -0.000028963978 Rises=F Damp=F

 DIIS: error= 4.05D-05 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -1733.50721210302 IErMin= 2 ErrMin= 4.05D-05

 ErrMax= 4.05D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.89D-06 BMatP= 6.97D-05

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

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

 Coeff: -0.202D-01 0.102D+01

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=1.73D-06 MaxDP=7.47D-05 DE=-2.90D-05 OVMax= 2.00D-04

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 1.71D-06 CP: 1.00D+00 1.02D+00

 E= -1733.50721214503 Delta-E= -0.000000042019 Rises=F Damp=F

 DIIS: error= 6.31D-05 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 3 EnMin= -1733.50721214503 IErMin= 2 ErrMin= 4.05D-05

 ErrMax= 6.31D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.99D-06 BMatP= 1.89D-06

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

 Coeff-Com: -0.340D-01 0.591D+00 0.443D+00

 Coeff: -0.340D-01 0.591D+00 0.443D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=1.19D-06 MaxDP=5.98D-05 DE=-4.20D-08 OVMax= 1.60D-04

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 7.85D-07 CP: 1.00D+00 1.05D+00 5.41D-01

 E= -1733.50721273943 Delta-E= -0.000000594391 Rises=F Damp=F

 DIIS: error= 1.79D-05 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -1733.50721273943 IErMin= 4 ErrMin= 1.79D-05

 ErrMax= 1.79D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.69D-07 BMatP= 1.89D-06

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

 Coeff-Com: -0.142D-01 0.187D+00 0.227D+00 0.600D+00

 Coeff: -0.142D-01 0.187D+00 0.227D+00 0.600D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=3.80D-07 MaxDP=1.96D-05 DE=-5.94D-07 OVMax= 4.42D-05

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 2.56D-07 CP: 1.00D+00 1.05D+00 6.04D-01 7.00D-01

 E= -1733.50721277134 Delta-E= -0.000000031914 Rises=F Damp=F

 DIIS: error= 6.23D-06 at cycle 5 NSaved= 5.

 NSaved= 5 IEnMin= 5 EnMin= -1733.50721277134 IErMin= 5 ErrMin= 6.23D-06

 ErrMax= 6.23D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.22D-08 BMatP= 1.69D-07

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

 Coeff-Com: -0.335D-02 0.301D-01 0.694D-01 0.320D+00 0.584D+00

 Coeff: -0.335D-02 0.301D-01 0.694D-01 0.320D+00 0.584D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=1.19D-07 MaxDP=4.24D-06 DE=-3.19D-08 OVMax= 2.15D-05

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 9.44D-08 CP: 1.00D+00 1.05D+00 6.10D-01 7.22D-01 7.37D-01

 E= -1733.50721277560 Delta-E= -0.000000004257 Rises=F Damp=F

 DIIS: error= 1.93D-06 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -1733.50721277560 IErMin= 6 ErrMin= 1.93D-06

 ErrMax= 1.93D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.90D-09 BMatP= 2.22D-08

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

 Coeff-Com: -0.129D-03-0.816D-02 0.885D-02 0.958D-01 0.318D+00 0.585D+00

 Coeff: -0.129D-03-0.816D-02 0.885D-02 0.958D-01 0.318D+00 0.585D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=4.63D-08 MaxDP=2.50D-06 DE=-4.26D-09 OVMax= 1.01D-05

 Cycle 7 Pass 1 IDiag 1:

 RMSU= 2.51D-08 CP: 1.00D+00 1.05D+00 6.13D-01 7.53D-01 7.54D-01

 CP: 7.05D-01

 E= -1733.50721277598 Delta-E= -0.000000000387 Rises=F Damp=F

 DIIS: error= 4.25D-07 at cycle 7 NSaved= 7.

 NSaved= 7 IEnMin= 7 EnMin= -1733.50721277598 IErMin= 7 ErrMin= 4.25D-07

 ErrMax= 4.25D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.07D-10 BMatP= 2.90D-09

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

 Coeff-Com: 0.323D-03-0.839D-02-0.313D-02 0.183D-01 0.115D+00 0.307D+00

 Coeff-Com: 0.571D+00

 Coeff: 0.323D-03-0.839D-02-0.313D-02 0.183D-01 0.115D+00 0.307D+00

 Coeff: 0.571D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=1.17D-08 MaxDP=7.67D-07 DE=-3.87D-10 OVMax= 2.62D-06

 Cycle 8 Pass 1 IDiag 1:

 RMSU= 9.56D-09 CP: 1.00D+00 1.05D+00 6.14D-01 7.51D-01 7.66D-01

 CP: 7.43D-01 8.33D-01

 E= -1733.50721277631 Delta-E= -0.000000000326 Rises=F Damp=F

 DIIS: error= 2.70D-07 at cycle 8 NSaved= 8.

 NSaved= 8 IEnMin= 8 EnMin= -1733.50721277631 IErMin= 8 ErrMin= 2.70D-07

 ErrMax= 2.70D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.08D-11 BMatP= 3.07D-10

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

 Coeff-Com: 0.172D-03-0.336D-02-0.264D-02-0.161D-02 0.217D-01 0.875D-01

 Coeff-Com: 0.304D+00 0.595D+00

 Coeff: 0.172D-03-0.336D-02-0.264D-02-0.161D-02 0.217D-01 0.875D-01

 Coeff: 0.304D+00 0.595D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=5.76D-09 MaxDP=2.49D-07 DE=-3.26D-10 OVMax= 1.72D-06

 Error on total polarization charges = 0.07593

 SCF Done: E(UB3LYP) = -1733.50721278 A.U. after 8 cycles

 NFock= 8 Conv=0.58D-08 -V/T= 1.9757

 <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5091

 <L.S>= 0.000000000000E+00

 KE= 1.776676988943D+03 PE=-1.289509720518D+04 EE= 5.010940846570D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -9.06

 (included in total energy above)

 Annihilation of the first spin contaminant:

 S\*\*2 before annihilation 0.7682, after 0.7503

 Leave Link 502 at Sat Jun 15 12:15:10 2019, MaxMem= 1342177280 cpu: 1379.5

 (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= 32896 NPrTT= 163506 LenC2= 22879 LenP2D= 61376.

 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 = 197

 Leave Link 701 at Sat Jun 15 12:15:20 2019, MaxMem= 1342177280 cpu: 105.8

 (Enter /apps/gaussian/g09d01/g09/l702.exe)

 L702 exits ... SP integral derivatives will be done elsewhere.

 Leave Link 702 at Sat Jun 15 12:15:23 2019, MaxMem= 1342177280 cpu: 1.7

 (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= 800

 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 Sat Jun 15 12:15:41 2019, MaxMem= 1342177280 cpu: 217.4

 (Enter /apps/gaussian/g09d01/g09/l716.exe)

 Dipole =-2.34479103D-13-5.68434189D-14 8.44082161D-01

 \*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

 Center Atomic Forces (Hartrees/Bohr)

 Number Number X Y Z

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

 1 6 -0.000074499 -0.000255518 -0.000061691

 2 7 0.000164742 0.000070164 0.000137124

 3 6 -0.000222869 0.000130778 -0.000052901

 4 6 0.000063309 -0.000052636 -0.000004968

 5 6 0.000024070 0.000110536 -0.000024448

 6 7 0.000000000 -0.000223664 0.000045359

 7 6 0.000222869 0.000130778 -0.000052901

 8 7 -0.000164742 0.000070164 0.000137124

 9 6 0.000074499 -0.000255518 -0.000061691

 10 6 -0.000024070 0.000110536 -0.000024448

 11 6 -0.000063309 -0.000052636 -0.000004968

 12 7 -0.000135114 0.000000000 0.000080324

 13 6 0.000024070 -0.000110536 -0.000024448

 14 6 0.000063309 0.000052636 -0.000004968

 15 6 -0.000222869 -0.000130778 -0.000052901

 16 7 0.000164742 -0.000070164 0.000137124

 17 6 -0.000074499 0.000255518 -0.000061691

 18 7 0.000000000 0.000223664 0.000045359

 19 7 -0.000164742 -0.000070164 0.000137124

 20 6 0.000222869 -0.000130778 -0.000052901

 21 6 -0.000063309 0.000052636 -0.000004968

 22 6 -0.000024070 -0.000110536 -0.000024448

 23 6 0.000074499 0.000255518 -0.000061691

 24 7 0.000135114 0.000000000 0.000080324

 25 30 0.000000000 0.000000000 -0.000193837

 26 6 0.000014091 -0.000040225 -0.000006406

 27 6 0.000058872 0.000050444 -0.000001087

 28 6 -0.000057768 -0.000057354 -0.000000296

 29 6 0.000050825 -0.000031804 0.000000312

 30 6 -0.000014091 -0.000040225 -0.000006406

 31 6 -0.000058872 0.000050444 -0.000001087

 32 6 0.000057768 -0.000057354 -0.000000296

 33 6 -0.000050825 -0.000031804 0.000000312

 34 6 -0.000050825 0.000031804 0.000000312

 35 6 0.000057768 0.000057354 -0.000000296

 36 6 -0.000058872 -0.000050444 -0.000001087

 37 6 -0.000014091 0.000040225 -0.000006406

 38 6 0.000014091 0.000040225 -0.000006406

 39 6 0.000058872 -0.000050444 -0.000001087

 40 6 -0.000057768 0.000057354 -0.000000296

 41 6 0.000050825 0.000031804 0.000000312

 42 1 0.000007498 0.000036305 0.000000651

 43 1 -0.000033355 -0.000010082 -0.000000696

 44 1 -0.000007498 0.000036305 0.000000651

 45 1 0.000033355 -0.000010082 -0.000000696

 46 1 0.000033355 0.000010082 -0.000000696

 47 1 -0.000007498 -0.000036305 0.000000651

 48 1 0.000007498 -0.000036305 0.000000651

 49 1 -0.000033355 0.000010082 -0.000000696

 50 1 -0.000001968 0.000009991 -0.000000738

 51 1 -0.000009037 0.000002326 0.000000761

 52 1 0.000001968 0.000009991 -0.000000738

 53 1 0.000009037 0.000002326 0.000000761

 54 1 0.000009037 -0.000002326 0.000000761

 55 1 0.000001968 -0.000009991 -0.000000738

 56 1 -0.000001968 -0.000009991 -0.000000738

 57 1 -0.000009037 -0.000002326 0.000000761

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

 Cartesian Forces: Max 0.000255518 RMS 0.000081498

 Leave Link 716 at Sat Jun 15 12:15:43 2019, MaxMem= 1342177280 cpu: 5.2

 (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 0.000130808 RMS 0.000031821

 Search for a local minimum.

 Step number 3 out of a maximum of 342

 All quantities printed in internal units (Hartrees-Bohrs-Radians)

 RMS Force = .31821D-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= -1.78D-05 DEPred=-1.53D-05 R= 1.16D+00

 TightC=F SS= 1.41D+00 RLast= 1.53D-02 DXNew= 5.0454D-01 4.5799D-02

 Trust test= 1.16D+00 RLast= 1.53D-02 DXMaxT set to 3.00D-01

 ITU= 1 1 0

 Eigenvalues --- 0.01512 0.01572 0.01587 0.01609 0.01624

 Eigenvalues --- 0.01645 0.01681 0.01697 0.01703 0.01761

 Eigenvalues --- 0.01772 0.01775 0.01780 0.01780 0.01782

 Eigenvalues --- 0.01787 0.01834 0.01846 0.01892 0.01894

 Eigenvalues --- 0.01903 0.01958 0.01959 0.02008 0.02008

 Eigenvalues --- 0.02008 0.02008 0.02051 0.02051 0.02051

 Eigenvalues --- 0.02051 0.02053 0.02053 0.02053 0.02053

 Eigenvalues --- 0.02077 0.02113 0.02113 0.02113 0.02113

 Eigenvalues --- 0.02119 0.02119 0.02119 0.02119 0.02124

 Eigenvalues --- 0.02124 0.02124 0.02124 0.02188 0.02249

 Eigenvalues --- 0.02305 0.02323 0.03339 0.03920 0.03938

 Eigenvalues --- 0.07488 0.15227 0.15765 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 0.16013 0.16259 0.16366

 Eigenvalues --- 0.16791 0.22000 0.22000 0.22000 0.22000

 Eigenvalues --- 0.22578 0.22598 0.22600 0.22600 0.24131

 Eigenvalues --- 0.24270 0.24510 0.24510 0.24512 0.24529

 Eigenvalues --- 0.24619 0.24624 0.24836 0.24885 0.24948

 Eigenvalues --- 0.24956 0.24992 0.24997 0.24997 0.24997

 Eigenvalues --- 0.25900 0.33727 0.34031 0.34069 0.34313

 Eigenvalues --- 0.34804 0.34851 0.35184 0.35201 0.35218

 Eigenvalues --- 0.35218 0.35218 0.35218 0.35241 0.35243

 Eigenvalues --- 0.35243 0.35243 0.35245 0.35247 0.35247

 Eigenvalues --- 0.35247 0.35252 0.35252 0.35252 0.35865

 Eigenvalues --- 0.36254 0.37367 0.37388 0.37565 0.40802

 Eigenvalues --- 0.40889 0.41930 0.41932 0.41947 0.41960

 Eigenvalues --- 0.41972 0.42323 0.43207 0.43247 0.44577

 Eigenvalues --- 0.44736 0.45211 0.45217 0.45343 0.45785

 Eigenvalues --- 0.45910 0.45911 0.45919 0.45994 0.46122

 Eigenvalues --- 0.46178 0.46180 0.46184 0.46700 0.46903

 Eigenvalues --- 0.50021 0.50393 0.51367 0.52915 0.53527

 Eigenvalues --- 0.55373 0.55380 0.55777 0.58011 0.58038

 En-DIIS/RFO-DIIS IScMMF= 0 using points: 3 2

 RFO step: Lambda=-8.52201928D-07.

 NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 1.78D-05 SmlDif= 1.00D-05

 RMS Error= 0.8610503354D-04 NUsed= 2 EDIIS=F

 DidBck=F Rises=F RFO-DIIS coefs: 1.19530 -0.19530

 Iteration 1 RMS(Cart)= 0.00163864 RMS(Int)= 0.00000059

 Iteration 2 RMS(Cart)= 0.00000174 RMS(Int)= 0.00000022

 Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000022

 ITry= 1 IFail=0 DXMaxC= 7.05D-03 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

 ClnCor: largest displacement from symmetrization is 1.49D-11 for atom 57.

 Variable Old X -DE/DX Delta X Delta X Delta X New X

 (Linear) (Quad) (Total)

 R1 2.56209 -0.00008 -0.00004 -0.00021 -0.00024 2.56185

 R2 2.76555 0.00013 0.00036 0.00016 0.00052 2.76608

 R3 2.53741 -0.00010 0.00001 -0.00030 -0.00029 2.53712

 R4 2.61933 0.00003 0.00003 0.00002 0.00006 2.61939

 R5 3.88404 0.00003 0.00037 0.00017 0.00055 3.88458

 R6 2.74687 0.00008 0.00031 0.00002 0.00034 2.74720

 R7 2.51307 -0.00012 0.00001 -0.00032 -0.00031 2.51275

 R8 2.68056 0.00000 0.00006 -0.00008 -0.00002 2.68054

 R9 2.64089 0.00005 0.00017 -0.00002 0.00015 2.64104

 R10 2.63507 0.00003 0.00016 -0.00007 0.00009 2.63516

 R11 2.51307 -0.00012 0.00001 -0.00032 -0.00031 2.51275

 R12 2.61933 0.00003 0.00003 0.00002 0.00006 2.61939

 R13 2.74687 0.00008 0.00031 0.00002 0.00034 2.74720

 R14 2.56209 -0.00008 -0.00004 -0.00021 -0.00024 2.56185

 R15 3.88404 0.00003 0.00037 0.00017 0.00055 3.88458

 R16 2.76555 0.00013 0.00036 0.00016 0.00052 2.76608

 R17 2.53741 -0.00010 0.00001 -0.00030 -0.00029 2.53712

 R18 2.68056 0.00000 0.00006 -0.00008 -0.00002 2.68054

 R19 2.63507 0.00003 0.00016 -0.00007 0.00009 2.63516

 R20 2.64089 0.00005 0.00017 -0.00002 0.00015 2.64104

 R21 2.53741 -0.00010 0.00001 -0.00030 -0.00029 2.53712

 R22 2.68056 0.00000 0.00006 -0.00008 -0.00002 2.68054

 R23 2.76555 0.00013 0.00036 0.00016 0.00052 2.76608

 R24 2.63507 0.00003 0.00016 -0.00007 0.00009 2.63516

 R25 2.74687 0.00008 0.00031 0.00002 0.00034 2.74720

 R26 2.64089 0.00005 0.00017 -0.00002 0.00015 2.64104

 R27 2.61933 0.00003 0.00003 0.00002 0.00006 2.61939

 R28 2.51307 -0.00012 0.00001 -0.00032 -0.00031 2.51275

 R29 2.56209 -0.00008 -0.00004 -0.00021 -0.00024 2.56185

 R30 3.88404 0.00003 0.00037 0.00017 0.00055 3.88458

 R31 2.51307 -0.00012 0.00001 -0.00032 -0.00031 2.51275

 R32 2.61933 0.00003 0.00003 0.00002 0.00006 2.61939

 R33 2.56209 -0.00008 -0.00004 -0.00021 -0.00024 2.56185

 R34 3.88404 0.00003 0.00037 0.00017 0.00055 3.88458

 R35 2.74687 0.00008 0.00031 0.00002 0.00034 2.74720

 R36 2.68056 0.00000 0.00006 -0.00008 -0.00002 2.68054

 R37 2.64089 0.00005 0.00017 -0.00002 0.00015 2.64104

 R38 2.76555 0.00013 0.00036 0.00016 0.00052 2.76608

 R39 2.63507 0.00003 0.00016 -0.00007 0.00009 2.63516

 R40 2.53741 -0.00010 0.00001 -0.00030 -0.00029 2.53712

 R41 2.63084 0.00001 0.00013 -0.00010 0.00003 2.63087

 R42 2.05044 0.00003 0.00005 0.00006 0.00011 2.05055

 R43 2.66017 0.00009 0.00013 0.00011 0.00024 2.66041

 R44 2.05021 0.00001 0.00005 -0.00002 0.00003 2.05024

 R45 2.62889 0.00001 0.00013 -0.00012 0.00001 2.62889

 R46 2.05077 0.00001 0.00005 -0.00002 0.00004 2.05080

 R47 2.05043 0.00003 0.00005 0.00006 0.00011 2.05053

 R48 2.63084 0.00001 0.00013 -0.00010 0.00003 2.63087

 R49 2.05044 0.00003 0.00005 0.00006 0.00011 2.05055

 R50 2.66017 0.00009 0.00013 0.00011 0.00024 2.66041

 R51 2.05021 0.00001 0.00005 -0.00002 0.00003 2.05024

 R52 2.62889 0.00001 0.00013 -0.00012 0.00001 2.62889

 R53 2.05077 0.00001 0.00005 -0.00002 0.00004 2.05080

 R54 2.05043 0.00003 0.00005 0.00006 0.00011 2.05053

 R55 2.62889 0.00001 0.00013 -0.00012 0.00001 2.62889

 R56 2.05043 0.00003 0.00005 0.00006 0.00011 2.05053

 R57 2.66017 0.00009 0.00013 0.00011 0.00024 2.66041

 R58 2.05077 0.00001 0.00005 -0.00002 0.00004 2.05080

 R59 2.63084 0.00001 0.00013 -0.00010 0.00003 2.63087

 R60 2.05021 0.00001 0.00005 -0.00002 0.00003 2.05024

 R61 2.05044 0.00003 0.00005 0.00006 0.00011 2.05055

 R62 2.63084 0.00001 0.00013 -0.00010 0.00003 2.63087

 R63 2.05044 0.00003 0.00005 0.00006 0.00011 2.05055

 R64 2.66017 0.00009 0.00013 0.00011 0.00024 2.66041

 R65 2.05021 0.00001 0.00005 -0.00002 0.00003 2.05024

 R66 2.62889 0.00001 0.00013 -0.00012 0.00001 2.62889

 R67 2.05077 0.00001 0.00005 -0.00002 0.00004 2.05080

 R68 2.05043 0.00003 0.00005 0.00006 0.00011 2.05053

 A1 1.89005 -0.00003 0.00003 -0.00020 -0.00017 1.88988

 A2 2.23740 0.00001 -0.00014 0.00021 0.00007 2.23747

 A3 2.15569 0.00001 0.00010 -0.00001 0.00009 2.15578

 A4 1.92900 0.00007 0.00004 0.00030 0.00034 1.92934

 A5 2.17889 -0.00005 0.00000 -0.00009 -0.00009 2.17880

 A6 2.16248 -0.00002 0.00004 0.00004 0.00007 2.16256

 A7 1.88367 -0.00004 0.00001 -0.00023 -0.00022 1.88345

 A8 2.22148 -0.00002 -0.00015 0.00006 -0.00010 2.22138

 A9 2.17792 0.00006 0.00014 0.00017 0.00031 2.17822

 A10 1.86059 0.00001 -0.00002 0.00008 0.00007 1.86065

 A11 2.32148 0.00000 0.00008 -0.00009 -0.00001 2.32147

 A12 2.10109 0.00000 -0.00006 0.00001 -0.00005 2.10104

 A13 1.86144 -0.00001 -0.00006 0.00004 -0.00002 1.86142

 A14 2.31108 0.00000 0.00010 -0.00008 0.00002 2.31111

 A15 2.11065 0.00001 -0.00004 0.00004 0.00000 2.11065

 A16 2.20494 0.00008 0.00033 0.00014 0.00047 2.20542

 A17 2.22148 -0.00002 -0.00015 0.00006 -0.00010 2.22138

 A18 2.17792 0.00006 0.00014 0.00017 0.00031 2.17822

 A19 1.88367 -0.00004 0.00001 -0.00023 -0.00022 1.88345

 A20 1.92900 0.00007 0.00004 0.00030 0.00034 1.92934

 A21 2.16248 -0.00002 0.00004 0.00004 0.00007 2.16256

 A22 2.17889 -0.00005 0.00000 -0.00009 -0.00009 2.17880

 A23 1.89005 -0.00003 0.00003 -0.00020 -0.00017 1.88988

 A24 2.23740 0.00001 -0.00014 0.00021 0.00007 2.23747

 A25 2.15569 0.00001 0.00010 -0.00001 0.00009 2.15578

 A26 1.86144 -0.00001 -0.00006 0.00004 -0.00002 1.86142

 A27 2.31108 0.00000 0.00010 -0.00008 0.00002 2.31111

 A28 2.11065 0.00001 -0.00004 0.00004 0.00000 2.11065

 A29 1.86059 0.00001 -0.00002 0.00008 0.00007 1.86065

 A30 2.32148 0.00000 0.00008 -0.00009 -0.00001 2.32147

 A31 2.10109 0.00000 -0.00006 0.00001 -0.00005 2.10104

 A32 2.16130 0.00006 0.00034 -0.00001 0.00033 2.16163

 A33 1.86144 -0.00001 -0.00006 0.00004 -0.00002 1.86142

 A34 2.11065 0.00001 -0.00004 0.00004 0.00000 2.11065

 A35 2.31108 0.00000 0.00010 -0.00008 0.00002 2.31111

 A36 1.86059 0.00001 -0.00002 0.00008 0.00007 1.86065

 A37 2.10109 0.00000 -0.00006 0.00001 -0.00005 2.10104

 A38 2.32148 0.00000 0.00008 -0.00009 -0.00001 2.32147

 A39 1.88367 -0.00004 0.00001 -0.00023 -0.00022 1.88345

 A40 2.17792 0.00006 0.00014 0.00017 0.00031 2.17822

 A41 2.22148 -0.00002 -0.00015 0.00006 -0.00010 2.22138

 A42 1.92900 0.00007 0.00004 0.00030 0.00034 1.92934

 A43 2.16248 -0.00002 0.00004 0.00004 0.00007 2.16256

 A44 2.17889 -0.00005 0.00000 -0.00009 -0.00009 2.17880

 A45 2.15569 0.00001 0.00010 -0.00001 0.00009 2.15578

 A46 2.23740 0.00001 -0.00014 0.00021 0.00007 2.23747

 A47 1.89005 -0.00003 0.00003 -0.00020 -0.00017 1.88988

 A48 2.20494 0.00008 0.00033 0.00014 0.00047 2.20542

 A49 1.92900 0.00007 0.00004 0.00030 0.00034 1.92934

 A50 2.16248 -0.00002 0.00004 0.00004 0.00007 2.16256

 A51 2.17889 -0.00005 0.00000 -0.00009 -0.00009 2.17880

 A52 2.22148 -0.00002 -0.00015 0.00006 -0.00010 2.22138

 A53 2.17792 0.00006 0.00014 0.00017 0.00031 2.17822

 A54 1.88367 -0.00004 0.00001 -0.00023 -0.00022 1.88345

 A55 1.86059 0.00001 -0.00002 0.00008 0.00007 1.86065

 A56 2.32148 0.00000 0.00008 -0.00009 -0.00001 2.32147

 A57 2.10109 0.00000 -0.00006 0.00001 -0.00005 2.10104

 A58 1.86144 -0.00001 -0.00006 0.00004 -0.00002 1.86142

 A59 2.11065 0.00001 -0.00004 0.00004 0.00000 2.11065

 A60 2.31108 0.00000 0.00010 -0.00008 0.00002 2.31111

 A61 1.89005 -0.00003 0.00003 -0.00020 -0.00017 1.88988

 A62 2.23740 0.00001 -0.00014 0.00021 0.00007 2.23747

 A63 2.15569 0.00001 0.00010 -0.00001 0.00009 2.15578

 A64 2.16130 0.00006 0.00034 -0.00001 0.00033 2.16163

 A65 1.54986 -0.00001 -0.00002 0.00001 -0.00001 1.54985

 A66 1.52913 0.00001 0.00003 0.00008 0.00010 1.52923

 A67 2.78592 0.00001 0.00002 0.00025 0.00027 2.78619

 A68 2.78592 0.00001 0.00002 0.00025 0.00027 2.78619

 A69 1.52913 0.00001 0.00003 0.00008 0.00010 1.52923

 A70 1.54986 -0.00001 -0.00002 0.00001 -0.00001 1.54985

 A71 2.06508 0.00001 0.00011 -0.00002 0.00009 2.06517

 A72 2.10653 -0.00003 -0.00013 -0.00010 -0.00023 2.10629

 A73 2.11157 0.00002 0.00002 0.00012 0.00015 2.11172

 A74 2.10867 -0.00001 -0.00006 0.00000 -0.00007 2.10860

 A75 2.09100 0.00001 0.00007 -0.00003 0.00005 2.09105

 A76 2.08352 0.00001 -0.00001 0.00003 0.00002 2.08354

 A77 2.11576 -0.00001 -0.00005 0.00000 -0.00006 2.11570

 A78 2.08063 0.00001 -0.00001 0.00003 0.00002 2.08066

 A79 2.08679 0.00000 0.00007 -0.00003 0.00004 2.08682

 A80 2.06510 0.00001 0.00011 -0.00002 0.00010 2.06519

 A81 2.10798 -0.00002 -0.00013 -0.00008 -0.00021 2.10777

 A82 2.11010 0.00001 0.00001 0.00010 0.00011 2.11022

 A83 2.06508 0.00001 0.00011 -0.00002 0.00009 2.06517

 A84 2.10653 -0.00003 -0.00013 -0.00010 -0.00023 2.10629

 A85 2.11157 0.00002 0.00002 0.00012 0.00015 2.11172

 A86 2.10867 -0.00001 -0.00006 0.00000 -0.00007 2.10860

 A87 2.09100 0.00001 0.00007 -0.00003 0.00005 2.09105

 A88 2.08352 0.00001 -0.00001 0.00003 0.00002 2.08354

 A89 2.11576 -0.00001 -0.00005 0.00000 -0.00006 2.11570

 A90 2.08063 0.00001 -0.00001 0.00003 0.00002 2.08066

 A91 2.08679 0.00000 0.00007 -0.00003 0.00004 2.08682

 A92 2.06510 0.00001 0.00011 -0.00002 0.00010 2.06519

 A93 2.10798 -0.00002 -0.00013 -0.00008 -0.00021 2.10777

 A94 2.11010 0.00001 0.00001 0.00010 0.00011 2.11022

 A95 2.06510 0.00001 0.00011 -0.00002 0.00010 2.06519

 A96 2.10798 -0.00002 -0.00013 -0.00008 -0.00021 2.10777

 A97 2.11010 0.00001 0.00001 0.00010 0.00011 2.11022

 A98 2.11576 -0.00001 -0.00005 0.00000 -0.00006 2.11570

 A99 2.08679 0.00000 0.00007 -0.00003 0.00004 2.08682

 A100 2.08063 0.00001 -0.00001 0.00003 0.00002 2.08066

 A101 2.10867 -0.00001 -0.00006 0.00000 -0.00007 2.10860

 A102 2.08352 0.00001 -0.00001 0.00003 0.00002 2.08354

 A103 2.09100 0.00001 0.00007 -0.00003 0.00005 2.09105

 A104 2.06508 0.00001 0.00011 -0.00002 0.00009 2.06517

 A105 2.10653 -0.00003 -0.00013 -0.00010 -0.00023 2.10629

 A106 2.11157 0.00002 0.00002 0.00012 0.00015 2.11172

 A107 2.06508 0.00001 0.00011 -0.00002 0.00009 2.06517

 A108 2.10653 -0.00003 -0.00013 -0.00010 -0.00023 2.10629

 A109 2.11157 0.00002 0.00002 0.00012 0.00015 2.11172

 A110 2.10867 -0.00001 -0.00006 0.00000 -0.00007 2.10860

 A111 2.09100 0.00001 0.00007 -0.00003 0.00005 2.09105

 A112 2.08352 0.00001 -0.00001 0.00003 0.00002 2.08354

 A113 2.11576 -0.00001 -0.00005 0.00000 -0.00006 2.11570

 A114 2.08063 0.00001 -0.00001 0.00003 0.00002 2.08066

 A115 2.08679 0.00000 0.00007 -0.00003 0.00004 2.08682

 A116 2.06510 0.00001 0.00011 -0.00002 0.00010 2.06519

 A117 2.10798 -0.00002 -0.00013 -0.00008 -0.00021 2.10777

 A118 2.11010 0.00001 0.00001 0.00010 0.00011 2.11022

 D1 0.00836 0.00000 0.00014 0.00022 0.00036 0.00872

 D2 -2.96703 -0.00003 -0.00036 -0.00137 -0.00173 -2.96876

 D3 -3.12208 0.00000 0.00015 0.00044 0.00059 -3.12150

 D4 0.18571 -0.00002 -0.00036 -0.00114 -0.00150 0.18421

 D5 -0.00462 0.00000 -0.00012 0.00003 -0.00009 -0.00471

 D6 -3.14102 0.00000 -0.00005 0.00008 0.00003 -3.14099

 D7 3.12646 0.00000 -0.00012 -0.00018 -0.00030 3.12616

 D8 -0.00994 0.00000 -0.00006 -0.00013 -0.00019 -0.01013

 D9 0.02098 0.00002 0.00028 0.00088 0.00115 0.02214

 D10 -3.10791 0.00002 0.00028 0.00113 0.00141 -3.10649

 D11 -0.00877 0.00000 -0.00011 -0.00037 -0.00049 -0.00925

 D12 3.11626 0.00000 -0.00023 -0.00059 -0.00082 3.11544

 D13 2.96850 0.00002 0.00038 0.00118 0.00156 2.97006

 D14 -0.18966 0.00002 0.00026 0.00096 0.00123 -0.18843

 D15 -3.05993 0.00001 0.00029 0.00077 0.00106 -3.05887

 D16 -0.26853 0.00002 0.00032 0.00101 0.00132 -0.26721

 D17 -1.66607 0.00002 0.00031 0.00089 0.00120 -1.66486

 D18 0.26944 -0.00002 -0.00028 -0.00104 -0.00132 0.26812

 D19 3.06083 -0.00001 -0.00025 -0.00081 -0.00106 3.05977

 D20 1.66330 -0.00002 -0.00026 -0.00092 -0.00118 1.66212

 D21 0.00556 0.00000 0.00004 0.00038 0.00041 0.00598

 D22 3.13955 0.00000 0.00001 0.00008 0.00010 3.13965

 D23 -3.11998 0.00001 0.00015 0.00059 0.00074 -3.11924

 D24 0.01400 0.00000 0.00013 0.00030 0.00043 0.01443

 D25 -0.01080 -0.00001 -0.00015 -0.00048 -0.00064 -0.01144

 D26 3.11160 -0.00001 -0.00029 -0.00074 -0.00103 3.11057

 D27 -0.00064 0.00000 0.00005 -0.00025 -0.00020 -0.00084

 D28 3.13649 0.00000 -0.00001 -0.00029 -0.00030 3.13619

 D29 -3.13578 0.00000 0.00007 0.00000 0.00007 -3.13572

 D30 0.00134 0.00000 0.00001 -0.00004 -0.00003 0.00131

 D31 -3.13812 0.00000 -0.00001 0.00031 0.00030 -3.13782

 D32 0.00505 0.00000 0.00005 0.00019 0.00024 0.00528

 D33 -0.00498 0.00000 -0.00004 -0.00001 -0.00005 -0.00503

 D34 3.13819 0.00000 0.00002 -0.00014 -0.00012 3.13808

 D35 3.13901 0.00000 -0.00005 0.00001 -0.00004 3.13898

 D36 -0.00365 0.00000 -0.00009 -0.00001 -0.00010 -0.00374

 D37 0.00322 0.00000 0.00002 0.00007 0.00009 0.00331

 D38 -3.13944 0.00000 -0.00002 0.00005 0.00003 -3.13941

 D39 0.01080 0.00001 0.00015 0.00048 0.00064 0.01144

 D40 -3.11160 0.00001 0.00029 0.00074 0.00103 -3.11057

 D41 -3.11626 0.00000 0.00023 0.00059 0.00082 -3.11544

 D42 0.18966 -0.00002 -0.00026 -0.00096 -0.00123 0.18843

 D43 0.00877 0.00000 0.00011 0.00037 0.00049 0.00925

 D44 -2.96850 -0.00002 -0.00038 -0.00118 -0.00156 -2.97006

 D45 3.11998 -0.00001 -0.00015 -0.00059 -0.00074 3.11924

 D46 -0.01400 0.00000 -0.00013 -0.00030 -0.00043 -0.01443

 D47 -0.00556 0.00000 -0.00004 -0.00038 -0.00041 -0.00598

 D48 -3.13955 0.00000 -0.00001 -0.00008 -0.00010 -3.13965

 D49 -0.00836 0.00000 -0.00014 -0.00022 -0.00036 -0.00872

 D50 3.12208 0.00000 -0.00015 -0.00044 -0.00059 3.12150

 D51 2.96703 0.00003 0.00036 0.00137 0.00173 2.96876

 D52 -0.18571 0.00002 0.00036 0.00114 0.00150 -0.18421

 D53 -0.26944 0.00002 0.00028 0.00104 0.00132 -0.26812

 D54 -1.66330 0.00002 0.00026 0.00092 0.00118 -1.66212

 D55 -3.06083 0.00001 0.00025 0.00081 0.00106 -3.05977

 D56 3.05993 -0.00001 -0.00029 -0.00077 -0.00106 3.05887

 D57 1.66607 -0.00002 -0.00031 -0.00089 -0.00120 1.66486

 D58 0.26853 -0.00002 -0.00032 -0.00101 -0.00132 0.26721

 D59 0.00462 0.00000 0.00012 -0.00003 0.00009 0.00471

 D60 3.14102 0.00000 0.00005 -0.00008 -0.00003 3.14099

 D61 -3.12646 0.00000 0.00012 0.00018 0.00030 -3.12616

 D62 0.00994 0.00000 0.00006 0.00013 0.00019 0.01013

 D63 -0.02098 -0.00002 -0.00028 -0.00088 -0.00115 -0.02214

 D64 3.10791 -0.00002 -0.00028 -0.00113 -0.00141 3.10649

 D65 0.00064 0.00000 -0.00005 0.00025 0.00020 0.00084

 D66 3.13578 0.00000 -0.00007 0.00000 -0.00007 3.13572

 D67 -3.13649 0.00000 0.00001 0.00029 0.00030 -3.13619

 D68 -0.00134 0.00000 -0.00001 0.00004 0.00003 -0.00131

 D69 -3.13901 0.00000 0.00005 -0.00001 0.00004 -3.13898

 D70 0.00365 0.00000 0.00009 0.00001 0.00010 0.00374

 D71 -0.00322 0.00000 -0.00002 -0.00007 -0.00009 -0.00331

 D72 3.13944 0.00000 0.00002 -0.00005 -0.00003 3.13941

 D73 3.13812 0.00000 0.00001 -0.00031 -0.00030 3.13782

 D74 -0.00505 0.00000 -0.00005 -0.00019 -0.00024 -0.00528

 D75 0.00498 0.00000 0.00004 0.00001 0.00005 0.00503

 D76 -3.13819 0.00000 -0.00002 0.00014 0.00012 -3.13808

 D77 3.10791 -0.00002 -0.00028 -0.00113 -0.00141 3.10649

 D78 -0.02098 -0.00002 -0.00028 -0.00088 -0.00115 -0.02214

 D79 0.00064 0.00000 -0.00005 0.00025 0.00020 0.00084

 D80 3.13578 0.00000 -0.00007 0.00000 -0.00007 3.13572

 D81 -3.13649 0.00000 0.00001 0.00029 0.00030 -3.13619

 D82 -0.00134 0.00000 -0.00001 0.00004 0.00003 -0.00131

 D83 -3.12646 0.00000 0.00012 0.00018 0.00030 -3.12616

 D84 0.00462 0.00000 0.00012 -0.00003 0.00009 0.00471

 D85 0.00994 0.00000 0.00006 0.00013 0.00019 0.01013

 D86 3.14102 0.00000 0.00005 -0.00008 -0.00003 3.14099

 D87 -0.00322 0.00000 -0.00002 -0.00007 -0.00009 -0.00331

 D88 3.13944 0.00000 0.00002 -0.00005 -0.00003 3.13941

 D89 -3.13901 0.00000 0.00005 -0.00001 0.00004 -3.13898

 D90 0.00365 0.00000 0.00009 0.00001 0.00010 0.00374

 D91 -0.00556 0.00000 -0.00004 -0.00038 -0.00041 -0.00598

 D92 3.11998 -0.00001 -0.00015 -0.00059 -0.00074 3.11924

 D93 -3.13955 0.00000 -0.00001 -0.00008 -0.00010 -3.13965

 D94 -0.01400 0.00000 -0.00013 -0.00030 -0.00043 -0.01443

 D95 0.00498 0.00000 0.00004 0.00001 0.00005 0.00503

 D96 -3.13819 0.00000 -0.00002 0.00014 0.00012 -3.13808

 D97 3.13812 0.00000 0.00001 -0.00031 -0.00030 3.13782

 D98 -0.00505 0.00000 -0.00005 -0.00019 -0.00024 -0.00528

 D99 0.00877 0.00000 0.00011 0.00037 0.00049 0.00925

 D100 -2.96850 -0.00002 -0.00038 -0.00118 -0.00156 -2.97006

 D101 -3.11626 0.00000 0.00023 0.00059 0.00082 -3.11544

 D102 0.18966 -0.00002 -0.00026 -0.00096 -0.00123 0.18843

 D103 -3.11160 0.00001 0.00029 0.00074 0.00103 -3.11057

 D104 0.01080 0.00001 0.00015 0.00048 0.00064 0.01144

 D105 3.12208 0.00000 -0.00015 -0.00044 -0.00059 3.12150

 D106 -0.00836 0.00000 -0.00014 -0.00022 -0.00036 -0.00872

 D107 -0.18571 0.00002 0.00036 0.00114 0.00150 -0.18421

 D108 2.96703 0.00003 0.00036 0.00137 0.00173 2.96876

 D109 -3.06083 0.00001 0.00025 0.00081 0.00106 -3.05977

 D110 -1.66330 0.00002 0.00026 0.00092 0.00118 -1.66212

 D111 -0.26944 0.00002 0.00028 0.00104 0.00132 -0.26812

 D112 0.26853 -0.00002 -0.00032 -0.00101 -0.00132 0.26721

 D113 1.66607 -0.00002 -0.00031 -0.00089 -0.00120 1.66486

 D114 3.05993 -0.00001 -0.00029 -0.00077 -0.00106 3.05887

 D115 -0.01080 -0.00001 -0.00015 -0.00048 -0.00064 -0.01144

 D116 3.11160 -0.00001 -0.00029 -0.00074 -0.00103 3.11057

 D117 3.11626 0.00000 -0.00023 -0.00059 -0.00082 3.11544

 D118 -0.00877 0.00000 -0.00011 -0.00037 -0.00049 -0.00925

 D119 -0.18966 0.00002 0.00026 0.00096 0.00123 -0.18843

 D120 2.96850 0.00002 0.00038 0.00118 0.00156 2.97006

 D121 0.00836 0.00000 0.00014 0.00022 0.00036 0.00872

 D122 -3.12208 0.00000 0.00015 0.00044 0.00059 -3.12150

 D123 -2.96703 -0.00003 -0.00036 -0.00137 -0.00173 -2.96876

 D124 0.18571 -0.00002 -0.00036 -0.00114 -0.00150 0.18421

 D125 1.66330 -0.00002 -0.00026 -0.00092 -0.00118 1.66212

 D126 3.06083 -0.00001 -0.00025 -0.00081 -0.00106 3.05977

 D127 0.26944 -0.00002 -0.00028 -0.00104 -0.00132 0.26812

 D128 -1.66607 0.00002 0.00031 0.00089 0.00120 -1.66486

 D129 -0.26853 0.00002 0.00032 0.00101 0.00132 -0.26721

 D130 -3.05993 0.00001 0.00029 0.00077 0.00106 -3.05887

 D131 -3.11998 0.00001 0.00015 0.00059 0.00074 -3.11924

 D132 0.01400 0.00000 0.00013 0.00030 0.00043 0.01443

 D133 0.00556 0.00000 0.00004 0.00038 0.00041 0.00598

 D134 3.13955 0.00000 0.00001 0.00008 0.00010 3.13965

 D135 -0.00064 0.00000 0.00005 -0.00025 -0.00020 -0.00084

 D136 3.13649 0.00000 -0.00001 -0.00029 -0.00030 3.13619

 D137 -3.13578 0.00000 0.00007 0.00000 0.00007 -3.13572

 D138 0.00134 0.00000 0.00001 -0.00004 -0.00003 0.00131

 D139 -3.13812 0.00000 -0.00001 0.00031 0.00030 -3.13782

 D140 0.00505 0.00000 0.00005 0.00019 0.00024 0.00528

 D141 -0.00498 0.00000 -0.00004 -0.00001 -0.00005 -0.00503

 D142 3.13819 0.00000 0.00002 -0.00014 -0.00012 3.13808

 D143 -0.00462 0.00000 -0.00012 0.00003 -0.00009 -0.00471

 D144 3.12646 0.00000 -0.00012 -0.00018 -0.00030 3.12616

 D145 -3.14102 0.00000 -0.00005 0.00008 0.00003 -3.14099

 D146 -0.00994 0.00000 -0.00006 -0.00013 -0.00019 -0.01013

 D147 0.00322 0.00000 0.00002 0.00007 0.00009 0.00331

 D148 -3.13944 0.00000 -0.00002 0.00005 0.00003 -3.13941

 D149 3.13901 0.00000 -0.00005 0.00001 -0.00004 3.13898

 D150 -0.00365 0.00000 -0.00009 -0.00001 -0.00010 -0.00374

 D151 0.02098 0.00002 0.00028 0.00088 0.00115 0.02214

 D152 -3.10791 0.00002 0.00028 0.00113 0.00141 -3.10649

 D153 0.00409 0.00000 0.00003 0.00005 0.00008 0.00417

 D154 -3.13861 0.00000 0.00004 0.00003 0.00007 -3.13854

 D155 -3.13857 0.00000 -0.00001 0.00002 0.00002 -3.13856

 D156 0.00191 0.00000 0.00001 0.00000 0.00001 0.00192

 D157 -0.00041 0.00000 0.00000 0.00000 0.00000 -0.00041

 D158 3.14058 0.00000 0.00002 -0.00008 -0.00006 3.14053

 D159 -3.14091 0.00000 -0.00002 0.00002 0.00001 -3.14090

 D160 0.00009 0.00000 0.00001 -0.00006 -0.00005 0.00004

 D161 -0.00414 0.00000 -0.00003 -0.00003 -0.00006 -0.00421

 D162 3.13903 0.00000 0.00003 -0.00016 -0.00013 3.13890

 D163 3.13805 0.00000 -0.00006 0.00005 -0.00001 3.13804

 D164 -0.00197 0.00000 0.00000 -0.00008 -0.00007 -0.00204

 D165 -0.00409 0.00000 -0.00003 -0.00005 -0.00008 -0.00417

 D166 3.13861 0.00000 -0.00004 -0.00003 -0.00007 3.13854

 D167 3.13857 0.00000 0.00001 -0.00002 -0.00002 3.13856

 D168 -0.00191 0.00000 -0.00001 0.00000 -0.00001 -0.00192

 D169 0.00041 0.00000 0.00000 0.00000 0.00000 0.00041

 D170 -3.14058 0.00000 -0.00002 0.00008 0.00006 -3.14053

 D171 3.14091 0.00000 0.00002 -0.00002 -0.00001 3.14090

 D172 -0.00009 0.00000 -0.00001 0.00006 0.00005 -0.00004

 D173 0.00414 0.00000 0.00003 0.00003 0.00006 0.00421

 D174 -3.13903 0.00000 -0.00003 0.00016 0.00013 -3.13890

 D175 -3.13805 0.00000 0.00006 -0.00005 0.00001 -3.13804

 D176 0.00197 0.00000 0.00000 0.00008 0.00007 0.00204

 D177 -0.00414 0.00000 -0.00003 -0.00003 -0.00006 -0.00421

 D178 3.13805 0.00000 -0.00006 0.00005 -0.00001 3.13804

 D179 3.13903 0.00000 0.00003 -0.00016 -0.00013 3.13890

 D180 -0.00197 0.00000 0.00000 -0.00008 -0.00007 -0.00204

 D181 -0.00041 0.00000 0.00000 0.00000 0.00000 -0.00041

 D182 -3.14091 0.00000 -0.00002 0.00002 0.00001 -3.14090

 D183 3.14058 0.00000 0.00002 -0.00008 -0.00006 3.14053

 D184 0.00009 0.00000 0.00001 -0.00006 -0.00005 0.00004

 D185 0.00409 0.00000 0.00003 0.00005 0.00008 0.00417

 D186 -3.13857 0.00000 -0.00001 0.00002 0.00002 -3.13856

 D187 -3.13861 0.00000 0.00004 0.00003 0.00007 -3.13854

 D188 0.00191 0.00000 0.00001 0.00000 0.00001 0.00192

 D189 -0.00409 0.00000 -0.00003 -0.00005 -0.00008 -0.00417

 D190 3.13861 0.00000 -0.00004 -0.00003 -0.00007 3.13854

 D191 3.13857 0.00000 0.00001 -0.00002 -0.00002 3.13856

 D192 -0.00191 0.00000 -0.00001 0.00000 -0.00001 -0.00192

 D193 0.00041 0.00000 0.00000 0.00000 0.00000 0.00041

 D194 -3.14058 0.00000 -0.00002 0.00008 0.00006 -3.14053

 D195 3.14091 0.00000 0.00002 -0.00002 -0.00001 3.14090

 D196 -0.00009 0.00000 -0.00001 0.00006 0.00005 -0.00004

 D197 0.00414 0.00000 0.00003 0.00003 0.00006 0.00421

 D198 -3.13903 0.00000 -0.00003 0.00016 0.00013 -3.13890

 D199 -3.13805 0.00000 0.00006 -0.00005 0.00001 -3.13804

 D200 0.00197 0.00000 0.00000 0.00008 0.00007 0.00204

 Item Value Threshold Converged?

 Maximum Force 0.000131 0.000450 YES

 RMS Force 0.000032 0.000300 YES

 Maximum Displacement 0.007053 0.001800 NO

 RMS Displacement 0.001639 0.001200 NO

 Predicted change in Energy=-1.430943D-06

 Lowest energy point so far. Saving SCF results.

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link 103 at Sat Jun 15 12:15:46 2019, MaxMem= 1342177280 cpu: 15.7

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

 Stoichiometry C32H16N8Zn(1-,2)

 Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C32H16N4)]

 Deg. of freedom 43

 Full point group C2V NOp 4

 RotChk: IX=0 Diff= 3.74D-17

 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 2.772362 1.184618 0.010082

 2 7 0 1.438252 1.423032 0.044100

 3 6 0 1.186660 2.785720 0.010687

 4 6 0 2.465469 3.475502 -0.036865

 5 6 0 3.467735 2.471737 -0.038181

 6 7 0 0.000000 3.385581 0.001533

 7 6 0 -1.186660 2.785720 0.010687

 8 7 0 -1.438252 1.423032 0.044100

 9 6 0 -2.772362 1.184618 0.010082

 10 6 0 -3.467735 2.471737 -0.038181

 11 6 0 -2.465469 3.475502 -0.036865

 12 7 0 3.404179 0.000000 0.005141

 13 6 0 3.467735 -2.471737 -0.038181

 14 6 0 2.465469 -3.475502 -0.036865

 15 6 0 1.186660 -2.785720 0.010687

 16 7 0 1.438252 -1.423032 0.044100

 17 6 0 2.772362 -1.184618 0.010082

 18 7 0 0.000000 -3.385581 0.001533

 19 7 0 -1.438252 -1.423032 0.044100

 20 6 0 -1.186660 -2.785720 0.010687

 21 6 0 -2.465469 -3.475502 -0.036865

 22 6 0 -3.467735 -2.471737 -0.038181

 23 6 0 -2.772362 -1.184618 0.010082

 24 7 0 -3.404179 0.000000 0.005141

 25 30 0 0.000000 0.000000 0.407466

 26 6 0 4.819945 -2.809078 -0.085801

 27 6 0 5.163240 -4.157621 -0.128059

 28 6 0 4.169708 -5.155055 -0.127859

 29 6 0 2.818493 -4.826897 -0.085118

 30 6 0 -4.819945 -2.809078 -0.085801

 31 6 0 -5.163240 -4.157621 -0.128059

 32 6 0 -4.169708 -5.155055 -0.127859

 33 6 0 -2.818493 -4.826897 -0.085118

 34 6 0 -2.818493 4.826897 -0.085118

 35 6 0 -4.169708 5.155055 -0.127859

 36 6 0 -5.163240 4.157621 -0.128059

 37 6 0 -4.819945 2.809078 -0.085801

 38 6 0 4.819945 2.809078 -0.085801

 39 6 0 5.163240 4.157621 -0.128059

 40 6 0 4.169708 5.155055 -0.127859

 41 6 0 2.818493 4.826897 -0.085118

 42 1 0 5.583248 -2.037838 -0.088656

 43 1 0 2.056885 -5.599800 -0.087685

 44 1 0 -5.583248 -2.037838 -0.088656

 45 1 0 -2.056885 -5.599800 -0.087685

 46 1 0 -2.056885 5.599800 -0.087685

 47 1 0 -5.583248 2.037838 -0.088656

 48 1 0 5.583248 2.037838 -0.088656

 49 1 0 2.056885 5.599800 -0.087685

 50 1 0 -4.466560 6.198335 -0.162351

 51 1 0 -6.208220 4.447297 -0.162673

 52 1 0 4.466560 6.198335 -0.162351

 53 1 0 6.208220 4.447297 -0.162673

 54 1 0 6.208220 -4.447297 -0.162673

 55 1 0 4.466560 -6.198335 -0.162351

 56 1 0 -4.466560 -6.198335 -0.162351

 57 1 0 -6.208220 -4.447297 -0.162673

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

 Rotational constants (GHZ): 0.0880311 0.0879157 0.0440895

 Leave Link 202 at Sat Jun 15 12:15:46 2019, MaxMem= 1342177280 cpu: 0.8

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

 Basis read from rwf: (5D, 7F)

 Pseudo-potential data read from rwf file.

 There are 225 symmetry adapted cartesian basis functions of A1 symmetry.

 There are 196 symmetry adapted cartesian basis functions of A2 symmetry.

 There are 207 symmetry adapted cartesian basis functions of B1 symmetry.

 There are 207 symmetry adapted cartesian basis functions of B2 symmetry.

 There are 211 symmetry adapted basis functions of A1 symmetry.

 There are 187 symmetry adapted basis functions of A2 symmetry.

 There are 197 symmetry adapted basis functions of B1 symmetry.

 There are 197 symmetry adapted basis functions of B2 symmetry.

 792 basis functions, 1399 primitive gaussians, 835 cartesian basis functions

 139 alpha electrons 138 beta electrons

 nuclear repulsion energy 4373.9663799788 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= 57 NActive= 57 NUniq= 16 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

 Integral buffers will be 131072 words long.

 Raffenetti 2 integral format.

 Two-electron integral symmetry is turned on.

 R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1642464194 Hartrees.

 Nuclear repulsion after empirical dispersion term = 4373.8021335593 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= 57.

 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 = 57

 GePol: Total number of spheres = 57

 GePol: Number of exposed spheres = 57 (100.00%)

 GePol: Number of points = 4682

 GePol: Average weight of points = 0.10

 GePol: Minimum weight of points = 0.99D-09

 GePol: Maximum weight of points = 0.18390

 GePol: Number of points with low weight = 364

 GePol: Fraction of low-weight points (<1% of avg) = 7.77%

 GePol: Cavity surface area = 485.735 Ang\*\*2

 GePol: Cavity volume = 504.402 Ang\*\*3

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

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 PCM non-electrostatic energy = -0.0144374419 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 4373.7876961174 Hartrees.

 Leave Link 301 at Sat Jun 15 12:15:48 2019, MaxMem= 1342177280 cpu: 15.3

 (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= 32896 NPrTT= 163506 LenC2= 22875 LenP2D= 61368.

 LDataN: DoStor=T MaxTD1= 5 Len= 102

 NBasis= 792 RedAO= T EigKep= 3.44D-05 NBF= 211 187 197 197

 NBsUse= 792 1.00D-06 EigRej= -1.00D+00 NBFU= 211 187 197 197

 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= 802 802 802 802 802 MxSgAt= 57 MxSgA2= 57.

 Leave Link 302 at Sat Jun 15 12:15:51 2019, MaxMem= 1342177280 cpu: 15.9

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

 DipDrv: MaxL=1.

 Leave Link 303 at Sat Jun 15 12:15:51 2019, MaxMem= 1342177280 cpu: 1.6

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

 Initial guess from the checkpoint file: "ZnPCanion.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) (A2) (B1) (B2) (A1) (B1) (A1) (B1) (A2)

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

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

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

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

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

 Virtual (A1) (A1) (A1) (A1) (A1) (A1) (A1) (A1) (A1) (A1)

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 The electronic state of the initial guess is 2-B1.

 Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5091

 Leave Link 401 at Sat Jun 15 12:15:57 2019, MaxMem= 1342177280 cpu: 66.9

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

 UHF open shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 2129573 IEndB= 2129573 NGot= 1342177280 MDV= 1340762408

 LenX= 1340762408 LenY= 1340064348

 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= 560000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

 Petite list used in FoFCou.

 Inv3: Mode=1 IEnd= 65763372.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 7.99D-15 for 385.

 Iteration 1 A\*A^-1 deviation from orthogonality is 6.42D-15 for 4674 3787.

 Iteration 1 A^-1\*A deviation from unit magnitude is 9.10D-15 for 780.

 Iteration 1 A^-1\*A deviation from orthogonality is 2.00D-12 for 3873 3831.

 E= -1733.50719689647

 DIIS: error= 1.32D-04 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -1733.50719689647 IErMin= 1 ErrMin= 1.32D-04

 ErrMax= 1.32D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.57D-05 BMatP= 3.57D-05

 IDIUse=3 WtCom= 9.99D-01 WtEn= 1.32D-03

 Coeff-Com: 0.100D+01

 Coeff-En: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.368 Goal= None Shift= 0.000

 Gap= 0.409 Goal= None Shift= 0.000

 RMSDP=5.80D-06 MaxDP=1.15D-04 OVMax= 6.92D-04

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 5.79D-06 CP: 1.00D+00

 E= -1733.50721414533 Delta-E= -0.000017248861 Rises=F Damp=F

 DIIS: error= 2.71D-05 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -1733.50721414533 IErMin= 2 ErrMin= 2.71D-05

 ErrMax= 2.71D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.16D-07 BMatP= 3.57D-05

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

 Coeff-Com: -0.486D-01 0.105D+01

 Coeff: -0.486D-01 0.105D+01

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=1.36D-06 MaxDP=7.70D-05 DE=-1.72D-05 OVMax= 1.61D-04

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 1.31D-06 CP: 1.00D+00 1.05D+00

 E= -1733.50721415550 Delta-E= -0.000000010162 Rises=F Damp=F

 DIIS: error= 5.71D-05 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 3 EnMin= -1733.50721415550 IErMin= 2 ErrMin= 2.71D-05

 ErrMax= 5.71D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.60D-06 BMatP= 8.16D-07

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

 Coeff-Com: -0.465D-01 0.646D+00 0.401D+00

 Coeff: -0.465D-01 0.646D+00 0.401D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=9.27D-07 MaxDP=5.25D-05 DE=-1.02D-08 OVMax= 1.22D-04

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 4.48D-07 CP: 1.00D+00 1.08D+00 4.09D-01

 E= -1733.50721447544 Delta-E= -0.000000319948 Rises=F Damp=F

 DIIS: error= 8.14D-06 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -1733.50721447544 IErMin= 4 ErrMin= 8.14D-06

 ErrMax= 8.14D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.40D-08 BMatP= 8.16D-07

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

 Coeff-Com: -0.104D-01 0.116D+00 0.165D+00 0.729D+00

 Coeff: -0.104D-01 0.116D+00 0.165D+00 0.729D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=1.65D-07 MaxDP=7.07D-06 DE=-3.20D-07 OVMax= 2.59D-05

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 1.31D-07 CP: 1.00D+00 1.08D+00 4.71D-01 8.76D-01

 E= -1733.50721448383 Delta-E= -0.000000008391 Rises=F Damp=F

 DIIS: error= 2.25D-06 at cycle 5 NSaved= 5.

 NSaved= 5 IEnMin= 5 EnMin= -1733.50721448383 IErMin= 5 ErrMin= 2.25D-06

 ErrMax= 2.25D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.69D-09 BMatP= 4.40D-08

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

 Coeff-Com: -0.209D-02 0.125D-01 0.603D-01 0.408D+00 0.521D+00

 Coeff: -0.209D-02 0.125D-01 0.603D-01 0.408D+00 0.521D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=7.50D-08 MaxDP=3.77D-06 DE=-8.39D-09 OVMax= 1.60D-05

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 5.03D-08 CP: 1.00D+00 1.08D+00 4.89D-01 8.94D-01 6.25D-01

 E= -1733.50721448590 Delta-E= -0.000000002065 Rises=F Damp=F

 DIIS: error= 6.63D-07 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -1733.50721448590 IErMin= 6 ErrMin= 6.63D-07

 ErrMax= 6.63D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.66D-10 BMatP= 8.69D-09

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

 Coeff-Com: 0.720D-03-0.167D-01 0.113D-02 0.858D-01 0.283D+00 0.646D+00

 Coeff: 0.720D-03-0.167D-01 0.113D-02 0.858D-01 0.283D+00 0.646D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=2.27D-08 MaxDP=1.12D-06 DE=-2.07D-09 OVMax= 4.62D-06

 Cycle 7 Pass 1 IDiag 1:

 RMSU= 1.19D-08 CP: 1.00D+00 1.08D+00 4.87D-01 9.15D-01 6.85D-01

 CP: 7.16D-01

 E= -1733.50721448588 Delta-E= 0.000000000023 Rises=F Damp=F

 DIIS: error= 3.59D-07 at cycle 7 NSaved= 7.

 NSaved= 7 IEnMin= 6 EnMin= -1733.50721448590 IErMin= 7 ErrMin= 3.59D-07

 ErrMax= 3.59D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.01D-11 BMatP= 9.66D-10

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

 Coeff-Com: 0.480D-03-0.967D-02-0.195D-02 0.298D-01 0.133D+00 0.347D+00

 Coeff-Com: 0.501D+00

 Coeff: 0.480D-03-0.967D-02-0.195D-02 0.298D-01 0.133D+00 0.347D+00

 Coeff: 0.501D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=7.35D-09 MaxDP=3.10D-07 DE= 2.27D-11 OVMax= 1.36D-06

 Error on total polarization charges = 0.07593

 SCF Done: E(UB3LYP) = -1733.50721449 A.U. after 7 cycles

 NFock= 7 Conv=0.74D-08 -V/T= 1.9757

 <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5091

 <L.S>= 0.000000000000E+00

 KE= 1.776672915522D+03 PE=-1.289472316322D+04 EE= 5.010755337096D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -9.06

 (included in total energy above)

 Annihilation of the first spin contaminant:

 S\*\*2 before annihilation 0.7682, after 0.7503

 Leave Link 502 at Sat Jun 15 12:17:46 2019, MaxMem= 1342177280 cpu: 1232.2

 (Enter /apps/gaussian/g09d01/g09/l701.exe)

 Compute integral first derivatives.

 ... and contract with generalized density number 0.

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

 4 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22875 LenP2D= 61368.

 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 = 197

 Leave Link 701 at Sat Jun 15 12:17:55 2019, MaxMem= 1342177280 cpu: 104.2

 (Enter /apps/gaussian/g09d01/g09/l702.exe)

 L702 exits ... SP integral derivatives will be done elsewhere.

 Leave Link 702 at Sat Jun 15 12:17:56 2019, MaxMem= 1342177280 cpu: 3.3

 (Enter /apps/gaussian/g09d01/g09/l703.exe)

 Compute integral first derivatives, UseDBF=F ICtDFT= 0.

 Integral derivatives from FoFJK, PRISM(SPDF).

 Calling FoFJK, ICntrl= 2127 FMM=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= 800

 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 Sat Jun 15 12:18:16 2019, MaxMem= 1342177280 cpu: 221.0

 (Enter /apps/gaussian/g09d01/g09/l716.exe)

 Dipole = 2.66453526D-13-2.84217094D-14 8.38647083D-01

 \*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

 Center Atomic Forces (Hartrees/Bohr)

 Number Number X Y Z

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

 1 6 -0.000027824 -0.000012756 -0.000048814

 2 7 0.000012906 -0.000013193 0.000093509

 3 6 -0.000011169 0.000048747 -0.000021990

 4 6 0.000022630 -0.000039864 -0.000009221

 5 6 -0.000017905 0.000036754 0.000005216

 6 7 0.000000000 -0.000033243 0.000019651

 7 6 0.000011169 0.000048747 -0.000021990

 8 7 -0.000012906 -0.000013193 0.000093509

 9 6 0.000027824 -0.000012756 -0.000048814

 10 6 0.000017905 0.000036754 0.000005216

 11 6 -0.000022630 -0.000039864 -0.000009221

 12 7 0.000018207 0.000000000 0.000037601

 13 6 -0.000017905 -0.000036754 0.000005216

 14 6 0.000022630 0.000039864 -0.000009221

 15 6 -0.000011169 -0.000048747 -0.000021990

 16 7 0.000012906 0.000013193 0.000093509

 17 6 -0.000027824 0.000012756 -0.000048814

 18 7 0.000000000 0.000033243 0.000019651

 19 7 -0.000012906 0.000013193 0.000093509

 20 6 0.000011169 -0.000048747 -0.000021990

 21 6 -0.000022630 0.000039864 -0.000009221

 22 6 0.000017905 -0.000036754 0.000005216

 23 6 0.000027824 0.000012756 -0.000048814

 24 7 -0.000018207 0.000000000 0.000037601

 25 30 0.000000000 0.000000000 -0.000183749

 26 6 -0.000002261 0.000002826 0.000002048

 27 6 -0.000008908 0.000006513 0.000000096

 28 6 -0.000008890 0.000010187 0.000000138

 29 6 0.000000143 -0.000004436 -0.000003951

 30 6 0.000002261 0.000002826 0.000002048

 31 6 0.000008908 0.000006513 0.000000096

 32 6 0.000008890 0.000010187 0.000000138

 33 6 -0.000000143 -0.000004436 -0.000003951

 34 6 -0.000000143 0.000004436 -0.000003951

 35 6 0.000008890 -0.000010187 0.000000138

 36 6 0.000008908 -0.000006513 0.000000096

 37 6 0.000002261 -0.000002826 0.000002048

 38 6 -0.000002261 -0.000002826 0.000002048

 39 6 -0.000008908 -0.000006513 0.000000096

 40 6 -0.000008890 -0.000010187 0.000000138

 41 6 0.000000143 0.000004436 -0.000003951

 42 1 -0.000002054 -0.000005568 -0.000001286

 43 1 0.000004953 0.000002562 0.000000268

 44 1 0.000002054 -0.000005568 -0.000001286

 45 1 -0.000004953 0.000002562 0.000000268

 46 1 -0.000004953 -0.000002562 0.000000268

 47 1 0.000002054 0.000005568 -0.000001286

 48 1 -0.000002054 0.000005568 -0.000001286

 49 1 0.000004953 -0.000002562 0.000000268

 50 1 0.000000659 -0.000004620 0.000001259

 51 1 0.000004326 -0.000000610 0.000000039

 52 1 -0.000000659 -0.000004620 0.000001259

 53 1 -0.000004326 -0.000000610 0.000000039

 54 1 -0.000004326 0.000000610 0.000000039

 55 1 -0.000000659 0.000004620 0.000001259

 56 1 0.000000659 0.000004620 0.000001259

 57 1 0.000004326 0.000000610 0.000000039

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

 Cartesian Forces: Max 0.000183749 RMS 0.000026403

 Leave Link 716 at Sat Jun 15 12:18:18 2019, MaxMem= 1342177280 cpu: 12.8

 (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.

 GSVD: received Info= 1 from GESDD.

 Internal Forces: Max 0.000032578 RMS 0.000008660

 Search for a local minimum.

 Step number 4 out of a maximum of 342

 All quantities printed in internal units (Hartrees-Bohrs-Radians)

 RMS Force = .86599D-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

 DE= -1.71D-06 DEPred=-1.43D-06 R= 1.19D+00

 TightC=F SS= 1.41D+00 RLast= 1.04D-02 DXNew= 5.0454D-01 3.1224D-02

 Trust test= 1.19D+00 RLast= 1.04D-02 DXMaxT set to 3.00D-01

 ITU= 1 1 1 0

 Eigenvalues --- 0.01128 0.01576 0.01586 0.01609 0.01624

 Eigenvalues --- 0.01645 0.01667 0.01681 0.01697 0.01761

 Eigenvalues --- 0.01772 0.01774 0.01779 0.01780 0.01782

 Eigenvalues --- 0.01804 0.01834 0.01846 0.01892 0.01894

 Eigenvalues --- 0.01923 0.01958 0.01959 0.02008 0.02008

 Eigenvalues --- 0.02008 0.02009 0.02051 0.02051 0.02051

 Eigenvalues --- 0.02051 0.02052 0.02053 0.02053 0.02053

 Eigenvalues --- 0.02076 0.02110 0.02113 0.02113 0.02113

 Eigenvalues --- 0.02113 0.02119 0.02119 0.02119 0.02124

 Eigenvalues --- 0.02124 0.02124 0.02124 0.02128 0.02249

 Eigenvalues --- 0.02299 0.02323 0.03338 0.03916 0.03934

 Eigenvalues --- 0.07429 0.15227 0.15990 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 0.16028 0.16261 0.16367

 Eigenvalues --- 0.17674 0.22000 0.22000 0.22000 0.22000

 Eigenvalues --- 0.22598 0.22600 0.22600 0.22851 0.24145

 Eigenvalues --- 0.24203 0.24511 0.24511 0.24512 0.24529

 Eigenvalues --- 0.24625 0.24629 0.24761 0.24839 0.24948

 Eigenvalues --- 0.24956 0.24993 0.24997 0.24997 0.24997

 Eigenvalues --- 0.26067 0.33728 0.34070 0.34120 0.34313

 Eigenvalues --- 0.34804 0.34851 0.35214 0.35218 0.35218

 Eigenvalues --- 0.35218 0.35218 0.35243 0.35243 0.35243

 Eigenvalues --- 0.35245 0.35247 0.35247 0.35247 0.35247

 Eigenvalues --- 0.35252 0.35252 0.35252 0.35279 0.35660

 Eigenvalues --- 0.37367 0.37388 0.37565 0.37881 0.40803

 Eigenvalues --- 0.40890 0.41920 0.41932 0.41946 0.41959

 Eigenvalues --- 0.41973 0.42585 0.43208 0.43247 0.44578

 Eigenvalues --- 0.45042 0.45211 0.45217 0.45343 0.45862

 Eigenvalues --- 0.45910 0.45911 0.45919 0.46025 0.46122

 Eigenvalues --- 0.46178 0.46180 0.46184 0.46706 0.48326

 Eigenvalues --- 0.49387 0.50393 0.51092 0.51369 0.53530

 Eigenvalues --- 0.55373 0.55380 0.55508 0.58012 0.58038

 En-DIIS/RFO-DIIS IScMMF= 0 using points: 4 3 2

 RFO step: Lambda=-8.63227565D-08.

 NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=F DC= 1.78D-05 SmlDif= 1.00D-05

 RMS Error= 0.3473985802D-04 NUsed= 3 EDIIS=F

 DidBck=F Rises=F RFO-DIIS coefs: 1.32771 -0.36664 0.03892

 Iteration 1 RMS(Cart)= 0.00062700 RMS(Int)= 0.00000012

 Iteration 2 RMS(Cart)= 0.00000029 RMS(Int)= 0.00000008

 ITry= 1 IFail=0 DXMaxC= 2.88D-03 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

 ClnCor: largest displacement from symmetrization is 1.84D-11 for atom 56.

 Variable Old X -DE/DX Delta X Delta X Delta X New X

 (Linear) (Quad) (Total)

 R1 2.56185 -0.00002 -0.00007 -0.00002 -0.00009 2.56175

 R2 2.76608 0.00000 0.00010 0.00001 0.00011 2.76619

 R3 2.53712 0.00000 -0.00010 0.00004 -0.00005 2.53707

 R4 2.61939 0.00001 0.00001 0.00003 0.00004 2.61943

 R5 3.88458 -0.00003 0.00011 -0.00017 -0.00006 3.88452

 R6 2.74720 -0.00002 0.00005 -0.00003 0.00002 2.74722

 R7 2.51275 -0.00002 -0.00010 0.00000 -0.00011 2.51265

 R8 2.68054 -0.00003 -0.00002 -0.00009 -0.00011 2.68043

 R9 2.64104 -0.00001 0.00002 0.00000 0.00001 2.64105

 R10 2.63516 -0.00001 0.00000 0.00000 -0.00001 2.63515

 R11 2.51275 -0.00002 -0.00010 0.00000 -0.00011 2.51265

 R12 2.61939 0.00001 0.00001 0.00003 0.00004 2.61943

 R13 2.74720 -0.00002 0.00005 -0.00003 0.00002 2.74722

 R14 2.56185 -0.00002 -0.00007 -0.00002 -0.00009 2.56175

 R15 3.88458 -0.00003 0.00011 -0.00017 -0.00006 3.88452

 R16 2.76608 0.00000 0.00010 0.00001 0.00011 2.76619

 R17 2.53712 0.00000 -0.00010 0.00004 -0.00005 2.53707

 R18 2.68054 -0.00003 -0.00002 -0.00009 -0.00011 2.68043

 R19 2.63516 -0.00001 0.00000 0.00000 -0.00001 2.63515

 R20 2.64104 -0.00001 0.00002 0.00000 0.00001 2.64105

 R21 2.53712 0.00000 -0.00010 0.00004 -0.00005 2.53707

 R22 2.68054 -0.00003 -0.00002 -0.00009 -0.00011 2.68043

 R23 2.76608 0.00000 0.00010 0.00001 0.00011 2.76619

 R24 2.63516 -0.00001 0.00000 0.00000 -0.00001 2.63515

 R25 2.74720 -0.00002 0.00005 -0.00003 0.00002 2.74722

 R26 2.64104 -0.00001 0.00002 0.00000 0.00001 2.64105

 R27 2.61939 0.00001 0.00001 0.00003 0.00004 2.61943

 R28 2.51275 -0.00002 -0.00010 0.00000 -0.00011 2.51265

 R29 2.56185 -0.00002 -0.00007 -0.00002 -0.00009 2.56175

 R30 3.88458 -0.00003 0.00011 -0.00017 -0.00006 3.88452

 R31 2.51275 -0.00002 -0.00010 0.00000 -0.00011 2.51265

 R32 2.61939 0.00001 0.00001 0.00003 0.00004 2.61943

 R33 2.56185 -0.00002 -0.00007 -0.00002 -0.00009 2.56175

 R34 3.88458 -0.00003 0.00011 -0.00017 -0.00006 3.88452

 R35 2.74720 -0.00002 0.00005 -0.00003 0.00002 2.74722

 R36 2.68054 -0.00003 -0.00002 -0.00009 -0.00011 2.68043

 R37 2.64104 -0.00001 0.00002 0.00000 0.00001 2.64105

 R38 2.76608 0.00000 0.00010 0.00001 0.00011 2.76619

 R39 2.63516 -0.00001 0.00000 0.00000 -0.00001 2.63515

 R40 2.53712 0.00000 -0.00010 0.00004 -0.00005 2.53707

 R41 2.63087 -0.00002 -0.00002 -0.00001 -0.00003 2.63084

 R42 2.05055 -0.00001 0.00003 -0.00003 0.00000 2.05055

 R43 2.66041 -0.00001 0.00005 -0.00004 0.00001 2.66042

 R44 2.05024 0.00000 0.00000 -0.00001 -0.00001 2.05023

 R45 2.62889 -0.00002 -0.00002 -0.00002 -0.00004 2.62885

 R46 2.05080 0.00000 0.00000 -0.00001 -0.00001 2.05080

 R47 2.05053 -0.00001 0.00002 -0.00003 0.00000 2.05053

 R48 2.63087 -0.00002 -0.00002 -0.00001 -0.00003 2.63084

 R49 2.05055 -0.00001 0.00003 -0.00003 0.00000 2.05055

 R50 2.66041 -0.00001 0.00005 -0.00004 0.00001 2.66042

 R51 2.05024 0.00000 0.00000 -0.00001 -0.00001 2.05023

 R52 2.62889 -0.00002 -0.00002 -0.00002 -0.00004 2.62885

 R53 2.05080 0.00000 0.00000 -0.00001 -0.00001 2.05080

 R54 2.05053 -0.00001 0.00002 -0.00003 0.00000 2.05053

 R55 2.62889 -0.00002 -0.00002 -0.00002 -0.00004 2.62885

 R56 2.05053 -0.00001 0.00002 -0.00003 0.00000 2.05053

 R57 2.66041 -0.00001 0.00005 -0.00004 0.00001 2.66042

 R58 2.05080 0.00000 0.00000 -0.00001 -0.00001 2.05080

 R59 2.63087 -0.00002 -0.00002 -0.00001 -0.00003 2.63084

 R60 2.05024 0.00000 0.00000 -0.00001 -0.00001 2.05023

 R61 2.05055 -0.00001 0.00003 -0.00003 0.00000 2.05055

 R62 2.63087 -0.00002 -0.00002 -0.00001 -0.00003 2.63084

 R63 2.05055 -0.00001 0.00003 -0.00003 0.00000 2.05055

 R64 2.66041 -0.00001 0.00005 -0.00004 0.00001 2.66042

 R65 2.05024 0.00000 0.00000 -0.00001 -0.00001 2.05023

 R66 2.62889 -0.00002 -0.00002 -0.00002 -0.00004 2.62885

 R67 2.05080 0.00000 0.00000 -0.00001 -0.00001 2.05080

 R68 2.05053 -0.00001 0.00002 -0.00003 0.00000 2.05053

 A1 1.88988 -0.00001 -0.00006 0.00002 -0.00004 1.88984

 A2 2.23747 0.00001 0.00005 0.00000 0.00005 2.23752

 A3 2.15578 0.00000 0.00001 -0.00001 0.00000 2.15578

 A4 1.92934 0.00000 0.00010 -0.00005 0.00005 1.92939

 A5 2.17880 0.00000 -0.00003 0.00006 0.00003 2.17882

 A6 2.16256 0.00001 0.00002 0.00009 0.00011 2.16266

 A7 1.88345 -0.00001 -0.00007 0.00002 -0.00006 1.88339

 A8 2.22138 0.00000 0.00000 -0.00004 -0.00004 2.22134

 A9 2.17822 0.00001 0.00007 0.00003 0.00010 2.17832

 A10 1.86065 0.00001 0.00002 0.00001 0.00004 1.86069

 A11 2.32147 -0.00001 -0.00002 -0.00002 -0.00004 2.32143

 A12 2.10104 0.00000 0.00000 0.00001 0.00000 2.10104

 A13 1.86142 0.00000 0.00001 0.00000 0.00000 1.86142

 A14 2.31111 -0.00001 -0.00001 -0.00001 -0.00002 2.31109

 A15 2.11065 0.00000 0.00001 0.00001 0.00001 2.11067

 A16 2.20542 0.00000 0.00009 0.00003 0.00012 2.20554

 A17 2.22138 0.00000 0.00000 -0.00004 -0.00004 2.22134

 A18 2.17822 0.00001 0.00007 0.00003 0.00010 2.17832

 A19 1.88345 -0.00001 -0.00007 0.00002 -0.00006 1.88339

 A20 1.92934 0.00000 0.00010 -0.00005 0.00005 1.92939

 A21 2.16256 0.00001 0.00002 0.00009 0.00011 2.16266

 A22 2.17880 0.00000 -0.00003 0.00006 0.00003 2.17882

 A23 1.88988 -0.00001 -0.00006 0.00002 -0.00004 1.88984

 A24 2.23747 0.00001 0.00005 0.00000 0.00005 2.23752

 A25 2.15578 0.00000 0.00001 -0.00001 0.00000 2.15578

 A26 1.86142 0.00000 0.00001 0.00000 0.00000 1.86142

 A27 2.31111 -0.00001 -0.00001 -0.00001 -0.00002 2.31109

 A28 2.11065 0.00000 0.00001 0.00001 0.00001 2.11067

 A29 1.86065 0.00001 0.00002 0.00001 0.00004 1.86069

 A30 2.32147 -0.00001 -0.00002 -0.00002 -0.00004 2.32143

 A31 2.10104 0.00000 0.00000 0.00001 0.00000 2.10104

 A32 2.16163 -0.00001 0.00004 -0.00002 0.00002 2.16165

 A33 1.86142 0.00000 0.00001 0.00000 0.00000 1.86142

 A34 2.11065 0.00000 0.00001 0.00001 0.00001 2.11067

 A35 2.31111 -0.00001 -0.00001 -0.00001 -0.00002 2.31109

 A36 1.86065 0.00001 0.00002 0.00001 0.00004 1.86069

 A37 2.10104 0.00000 0.00000 0.00001 0.00000 2.10104

 A38 2.32147 -0.00001 -0.00002 -0.00002 -0.00004 2.32143

 A39 1.88345 -0.00001 -0.00007 0.00002 -0.00006 1.88339

 A40 2.17822 0.00001 0.00007 0.00003 0.00010 2.17832

 A41 2.22138 0.00000 0.00000 -0.00004 -0.00004 2.22134

 A42 1.92934 0.00000 0.00010 -0.00005 0.00005 1.92939

 A43 2.16256 0.00001 0.00002 0.00009 0.00011 2.16266

 A44 2.17880 0.00000 -0.00003 0.00006 0.00003 2.17882

 A45 2.15578 0.00000 0.00001 -0.00001 0.00000 2.15578

 A46 2.23747 0.00001 0.00005 0.00000 0.00005 2.23752

 A47 1.88988 -0.00001 -0.00006 0.00002 -0.00004 1.88984

 A48 2.20542 0.00000 0.00009 0.00003 0.00012 2.20554

 A49 1.92934 0.00000 0.00010 -0.00005 0.00005 1.92939

 A50 2.16256 0.00001 0.00002 0.00009 0.00011 2.16266

 A51 2.17880 0.00000 -0.00003 0.00006 0.00003 2.17882

 A52 2.22138 0.00000 0.00000 -0.00004 -0.00004 2.22134

 A53 2.17822 0.00001 0.00007 0.00003 0.00010 2.17832

 A54 1.88345 -0.00001 -0.00007 0.00002 -0.00006 1.88339

 A55 1.86065 0.00001 0.00002 0.00001 0.00004 1.86069

 A56 2.32147 -0.00001 -0.00002 -0.00002 -0.00004 2.32143

 A57 2.10104 0.00000 0.00000 0.00001 0.00000 2.10104

 A58 1.86142 0.00000 0.00001 0.00000 0.00000 1.86142

 A59 2.11065 0.00000 0.00001 0.00001 0.00001 2.11067

 A60 2.31111 -0.00001 -0.00001 -0.00001 -0.00002 2.31109

 A61 1.88988 -0.00001 -0.00006 0.00002 -0.00004 1.88984

 A62 2.23747 0.00001 0.00005 0.00000 0.00005 2.23752

 A63 2.15578 0.00000 0.00001 -0.00001 0.00000 2.15578

 A64 2.16163 -0.00001 0.00004 -0.00002 0.00002 2.16165

 A65 1.54985 0.00000 0.00000 0.00005 0.00005 1.54990

 A66 1.52923 0.00001 0.00003 0.00008 0.00011 1.52934

 A67 2.78619 0.00002 0.00008 0.00038 0.00047 2.78666

 A68 2.78619 0.00002 0.00008 0.00038 0.00047 2.78666

 A69 1.52923 0.00001 0.00003 0.00008 0.00011 1.52934

 A70 1.54985 0.00000 0.00000 0.00005 0.00005 1.54990

 A71 2.06517 -0.00001 0.00001 -0.00001 0.00000 2.06517

 A72 2.10629 0.00001 -0.00005 0.00003 -0.00002 2.10628

 A73 2.11172 0.00000 0.00004 -0.00003 0.00002 2.11174

 A74 2.10860 0.00000 -0.00001 0.00000 -0.00001 2.10859

 A75 2.09105 0.00000 0.00000 0.00002 0.00002 2.09107

 A76 2.08354 0.00000 0.00001 -0.00002 -0.00001 2.08353

 A77 2.11570 0.00000 -0.00001 0.00000 -0.00001 2.11570

 A78 2.08066 0.00000 0.00001 -0.00002 -0.00001 2.08064

 A79 2.08682 0.00000 0.00000 0.00002 0.00002 2.08684

 A80 2.06519 -0.00001 0.00001 -0.00001 0.00000 2.06519

 A81 2.10777 0.00000 -0.00004 0.00002 -0.00002 2.10776

 A82 2.11022 0.00000 0.00003 -0.00002 0.00002 2.11023

 A83 2.06517 -0.00001 0.00001 -0.00001 0.00000 2.06517

 A84 2.10629 0.00001 -0.00005 0.00003 -0.00002 2.10628

 A85 2.11172 0.00000 0.00004 -0.00003 0.00002 2.11174

 A86 2.10860 0.00000 -0.00001 0.00000 -0.00001 2.10859

 A87 2.09105 0.00000 0.00000 0.00002 0.00002 2.09107

 A88 2.08354 0.00000 0.00001 -0.00002 -0.00001 2.08353

 A89 2.11570 0.00000 -0.00001 0.00000 -0.00001 2.11570

 A90 2.08066 0.00000 0.00001 -0.00002 -0.00001 2.08064

 A91 2.08682 0.00000 0.00000 0.00002 0.00002 2.08684

 A92 2.06519 -0.00001 0.00001 -0.00001 0.00000 2.06519

 A93 2.10777 0.00000 -0.00004 0.00002 -0.00002 2.10776

 A94 2.11022 0.00000 0.00003 -0.00002 0.00002 2.11023

 A95 2.06519 -0.00001 0.00001 -0.00001 0.00000 2.06519

 A96 2.10777 0.00000 -0.00004 0.00002 -0.00002 2.10776

 A97 2.11022 0.00000 0.00003 -0.00002 0.00002 2.11023

 A98 2.11570 0.00000 -0.00001 0.00000 -0.00001 2.11570

 A99 2.08682 0.00000 0.00000 0.00002 0.00002 2.08684

 A100 2.08066 0.00000 0.00001 -0.00002 -0.00001 2.08064

 A101 2.10860 0.00000 -0.00001 0.00000 -0.00001 2.10859

 A102 2.08354 0.00000 0.00001 -0.00002 -0.00001 2.08353

 A103 2.09105 0.00000 0.00000 0.00002 0.00002 2.09107

 A104 2.06517 -0.00001 0.00001 -0.00001 0.00000 2.06517

 A105 2.10629 0.00001 -0.00005 0.00003 -0.00002 2.10628

 A106 2.11172 0.00000 0.00004 -0.00003 0.00002 2.11174

 A107 2.06517 -0.00001 0.00001 -0.00001 0.00000 2.06517

 A108 2.10629 0.00001 -0.00005 0.00003 -0.00002 2.10628

 A109 2.11172 0.00000 0.00004 -0.00003 0.00002 2.11174

 A110 2.10860 0.00000 -0.00001 0.00000 -0.00001 2.10859

 A111 2.09105 0.00000 0.00000 0.00002 0.00002 2.09107

 A112 2.08354 0.00000 0.00001 -0.00002 -0.00001 2.08353

 A113 2.11570 0.00000 -0.00001 0.00000 -0.00001 2.11570

 A114 2.08066 0.00000 0.00001 -0.00002 -0.00001 2.08064

 A115 2.08682 0.00000 0.00000 0.00002 0.00002 2.08684

 A116 2.06519 -0.00001 0.00001 -0.00001 0.00000 2.06519

 A117 2.10777 0.00000 -0.00004 0.00002 -0.00002 2.10776

 A118 2.11022 0.00000 0.00003 -0.00002 0.00002 2.11023

 D1 0.00872 0.00000 0.00009 0.00035 0.00044 0.00915

 D2 -2.96876 -0.00001 -0.00049 -0.00030 -0.00080 -2.96956

 D3 -3.12150 0.00000 0.00016 0.00004 0.00020 -3.12129

 D4 0.18421 -0.00002 -0.00042 -0.00061 -0.00103 0.18318

 D5 -0.00471 0.00000 -0.00001 -0.00041 -0.00041 -0.00512

 D6 -3.14099 0.00000 0.00002 -0.00021 -0.00019 -3.14118

 D7 3.12616 0.00000 -0.00007 -0.00012 -0.00019 3.12597

 D8 -0.01013 0.00000 -0.00005 0.00008 0.00003 -0.01010

 D9 0.02214 0.00001 0.00032 0.00043 0.00076 0.02289

 D10 -3.10649 0.00000 0.00041 0.00008 0.00049 -3.10601

 D11 -0.00925 0.00000 -0.00014 -0.00015 -0.00029 -0.00954

 D12 3.11544 0.00000 -0.00022 -0.00018 -0.00041 3.11504

 D13 2.97006 0.00001 0.00044 0.00049 0.00092 2.97098

 D14 -0.18843 0.00001 0.00035 0.00045 0.00080 -0.18763

 D15 -3.05887 0.00000 0.00029 0.00018 0.00047 -3.05840

 D16 -0.26721 0.00002 0.00037 0.00055 0.00092 -0.26629

 D17 -1.66486 0.00001 0.00033 0.00037 0.00070 -1.66416

 D18 0.26812 -0.00002 -0.00038 -0.00054 -0.00091 0.26720

 D19 3.05977 0.00000 -0.00030 -0.00017 -0.00047 3.05930

 D20 1.66212 -0.00001 -0.00033 -0.00035 -0.00068 1.66144

 D21 0.00598 0.00000 0.00013 -0.00011 0.00002 0.00599

 D22 3.13965 0.00000 0.00003 0.00000 0.00003 3.13968

 D23 -3.11924 0.00000 0.00021 -0.00008 0.00013 -3.11911

 D24 0.01443 0.00000 0.00011 0.00004 0.00015 0.01458

 D25 -0.01144 0.00000 -0.00018 -0.00014 -0.00032 -0.01176

 D26 3.11057 0.00000 -0.00028 -0.00018 -0.00046 3.11012

 D27 -0.00084 0.00000 -0.00007 0.00031 0.00023 -0.00060

 D28 3.13619 0.00000 -0.00010 0.00014 0.00004 3.13623

 D29 -3.13572 0.00000 0.00001 0.00021 0.00022 -3.13549

 D30 0.00131 0.00000 -0.00001 0.00004 0.00003 0.00134

 D31 -3.13782 0.00000 0.00010 -0.00020 -0.00009 -3.13792

 D32 0.00528 0.00000 0.00007 -0.00007 0.00000 0.00528

 D33 -0.00503 0.00000 -0.00001 -0.00007 -0.00008 -0.00511

 D34 3.13808 0.00000 -0.00004 0.00006 0.00001 3.13809

 D35 3.13898 0.00000 0.00000 -0.00021 -0.00021 3.13876

 D36 -0.00374 0.00000 -0.00001 -0.00015 -0.00016 -0.00390

 D37 0.00331 0.00000 0.00003 0.00001 0.00004 0.00335

 D38 -3.13941 0.00000 0.00001 0.00008 0.00009 -3.13932

 D39 0.01144 0.00000 0.00018 0.00014 0.00032 0.01176

 D40 -3.11057 0.00000 0.00028 0.00018 0.00046 -3.11012

 D41 -3.11544 0.00000 0.00022 0.00018 0.00041 -3.11504

 D42 0.18843 -0.00001 -0.00035 -0.00045 -0.00080 0.18763

 D43 0.00925 0.00000 0.00014 0.00015 0.00029 0.00954

 D44 -2.97006 -0.00001 -0.00044 -0.00049 -0.00092 -2.97098

 D45 3.11924 0.00000 -0.00021 0.00008 -0.00013 3.11911

 D46 -0.01443 0.00000 -0.00011 -0.00004 -0.00015 -0.01458

 D47 -0.00598 0.00000 -0.00013 0.00011 -0.00002 -0.00599

 D48 -3.13965 0.00000 -0.00003 0.00000 -0.00003 -3.13968

 D49 -0.00872 0.00000 -0.00009 -0.00035 -0.00044 -0.00915

 D50 3.12150 0.00000 -0.00016 -0.00004 -0.00020 3.12129

 D51 2.96876 0.00001 0.00049 0.00030 0.00080 2.96956

 D52 -0.18421 0.00002 0.00042 0.00061 0.00103 -0.18318

 D53 -0.26812 0.00002 0.00038 0.00054 0.00091 -0.26720

 D54 -1.66212 0.00001 0.00033 0.00035 0.00068 -1.66144

 D55 -3.05977 0.00000 0.00030 0.00017 0.00047 -3.05930

 D56 3.05887 0.00000 -0.00029 -0.00018 -0.00047 3.05840

 D57 1.66486 -0.00001 -0.00033 -0.00037 -0.00070 1.66416

 D58 0.26721 -0.00002 -0.00037 -0.00055 -0.00092 0.26629

 D59 0.00471 0.00000 0.00001 0.00041 0.00041 0.00512

 D60 3.14099 0.00000 -0.00002 0.00021 0.00019 3.14118

 D61 -3.12616 0.00000 0.00007 0.00012 0.00019 -3.12597

 D62 0.01013 0.00000 0.00005 -0.00008 -0.00003 0.01010

 D63 -0.02214 -0.00001 -0.00032 -0.00043 -0.00076 -0.02289

 D64 3.10649 0.00000 -0.00041 -0.00008 -0.00049 3.10601

 D65 0.00084 0.00000 0.00007 -0.00031 -0.00023 0.00060

 D66 3.13572 0.00000 -0.00001 -0.00021 -0.00022 3.13549

 D67 -3.13619 0.00000 0.00010 -0.00014 -0.00004 -3.13623

 D68 -0.00131 0.00000 0.00001 -0.00004 -0.00003 -0.00134

 D69 -3.13898 0.00000 0.00000 0.00021 0.00021 -3.13876

 D70 0.00374 0.00000 0.00001 0.00015 0.00016 0.00390

 D71 -0.00331 0.00000 -0.00003 -0.00001 -0.00004 -0.00335

 D72 3.13941 0.00000 -0.00001 -0.00008 -0.00009 3.13932

 D73 3.13782 0.00000 -0.00010 0.00020 0.00009 3.13792

 D74 -0.00528 0.00000 -0.00007 0.00007 0.00000 -0.00528

 D75 0.00503 0.00000 0.00001 0.00007 0.00008 0.00511

 D76 -3.13808 0.00000 0.00004 -0.00006 -0.00001 -3.13809

 D77 3.10649 0.00000 -0.00041 -0.00008 -0.00049 3.10601

 D78 -0.02214 -0.00001 -0.00032 -0.00043 -0.00076 -0.02289

 D79 0.00084 0.00000 0.00007 -0.00031 -0.00023 0.00060

 D80 3.13572 0.00000 -0.00001 -0.00021 -0.00022 3.13549

 D81 -3.13619 0.00000 0.00010 -0.00014 -0.00004 -3.13623

 D82 -0.00131 0.00000 0.00001 -0.00004 -0.00003 -0.00134

 D83 -3.12616 0.00000 0.00007 0.00012 0.00019 -3.12597

 D84 0.00471 0.00000 0.00001 0.00041 0.00041 0.00512

 D85 0.01013 0.00000 0.00005 -0.00008 -0.00003 0.01010

 D86 3.14099 0.00000 -0.00002 0.00021 0.00019 3.14118

 D87 -0.00331 0.00000 -0.00003 -0.00001 -0.00004 -0.00335

 D88 3.13941 0.00000 -0.00001 -0.00008 -0.00009 3.13932

 D89 -3.13898 0.00000 0.00000 0.00021 0.00021 -3.13876

 D90 0.00374 0.00000 0.00001 0.00015 0.00016 0.00390

 D91 -0.00598 0.00000 -0.00013 0.00011 -0.00002 -0.00599

 D92 3.11924 0.00000 -0.00021 0.00008 -0.00013 3.11911

 D93 -3.13965 0.00000 -0.00003 0.00000 -0.00003 -3.13968

 D94 -0.01443 0.00000 -0.00011 -0.00004 -0.00015 -0.01458

 D95 0.00503 0.00000 0.00001 0.00007 0.00008 0.00511

 D96 -3.13808 0.00000 0.00004 -0.00006 -0.00001 -3.13809

 D97 3.13782 0.00000 -0.00010 0.00020 0.00009 3.13792

 D98 -0.00528 0.00000 -0.00007 0.00007 0.00000 -0.00528

 D99 0.00925 0.00000 0.00014 0.00015 0.00029 0.00954

 D100 -2.97006 -0.00001 -0.00044 -0.00049 -0.00092 -2.97098

 D101 -3.11544 0.00000 0.00022 0.00018 0.00041 -3.11504

 D102 0.18843 -0.00001 -0.00035 -0.00045 -0.00080 0.18763

 D103 -3.11057 0.00000 0.00028 0.00018 0.00046 -3.11012

 D104 0.01144 0.00000 0.00018 0.00014 0.00032 0.01176

 D105 3.12150 0.00000 -0.00016 -0.00004 -0.00020 3.12129

 D106 -0.00872 0.00000 -0.00009 -0.00035 -0.00044 -0.00915

 D107 -0.18421 0.00002 0.00042 0.00061 0.00103 -0.18318

 D108 2.96876 0.00001 0.00049 0.00030 0.00080 2.96956

 D109 -3.05977 0.00000 0.00030 0.00017 0.00047 -3.05930

 D110 -1.66212 0.00001 0.00033 0.00035 0.00068 -1.66144

 D111 -0.26812 0.00002 0.00038 0.00054 0.00091 -0.26720

 D112 0.26721 -0.00002 -0.00037 -0.00055 -0.00092 0.26629

 D113 1.66486 -0.00001 -0.00033 -0.00037 -0.00070 1.66416

 D114 3.05887 0.00000 -0.00029 -0.00018 -0.00047 3.05840

 D115 -0.01144 0.00000 -0.00018 -0.00014 -0.00032 -0.01176

 D116 3.11057 0.00000 -0.00028 -0.00018 -0.00046 3.11012

 D117 3.11544 0.00000 -0.00022 -0.00018 -0.00041 3.11504

 D118 -0.00925 0.00000 -0.00014 -0.00015 -0.00029 -0.00954

 D119 -0.18843 0.00001 0.00035 0.00045 0.00080 -0.18763

 D120 2.97006 0.00001 0.00044 0.00049 0.00092 2.97098

 D121 0.00872 0.00000 0.00009 0.00035 0.00044 0.00915

 D122 -3.12150 0.00000 0.00016 0.00004 0.00020 -3.12129

 D123 -2.96876 -0.00001 -0.00049 -0.00030 -0.00080 -2.96956

 D124 0.18421 -0.00002 -0.00042 -0.00061 -0.00103 0.18318

 D125 1.66212 -0.00001 -0.00033 -0.00035 -0.00068 1.66144

 D126 3.05977 0.00000 -0.00030 -0.00017 -0.00047 3.05930

 D127 0.26812 -0.00002 -0.00038 -0.00054 -0.00091 0.26720

 D128 -1.66486 0.00001 0.00033 0.00037 0.00070 -1.66416

 D129 -0.26721 0.00002 0.00037 0.00055 0.00092 -0.26629

 D130 -3.05887 0.00000 0.00029 0.00018 0.00047 -3.05840

 D131 -3.11924 0.00000 0.00021 -0.00008 0.00013 -3.11911

 D132 0.01443 0.00000 0.00011 0.00004 0.00015 0.01458

 D133 0.00598 0.00000 0.00013 -0.00011 0.00002 0.00599

 D134 3.13965 0.00000 0.00003 0.00000 0.00003 3.13968

 D135 -0.00084 0.00000 -0.00007 0.00031 0.00023 -0.00060

 D136 3.13619 0.00000 -0.00010 0.00014 0.00004 3.13623

 D137 -3.13572 0.00000 0.00001 0.00021 0.00022 -3.13549

 D138 0.00131 0.00000 -0.00001 0.00004 0.00003 0.00134

 D139 -3.13782 0.00000 0.00010 -0.00020 -0.00009 -3.13792

 D140 0.00528 0.00000 0.00007 -0.00007 0.00000 0.00528

 D141 -0.00503 0.00000 -0.00001 -0.00007 -0.00008 -0.00511

 D142 3.13808 0.00000 -0.00004 0.00006 0.00001 3.13809

 D143 -0.00471 0.00000 -0.00001 -0.00041 -0.00041 -0.00512

 D144 3.12616 0.00000 -0.00007 -0.00012 -0.00019 3.12597

 D145 -3.14099 0.00000 0.00002 -0.00021 -0.00019 -3.14118

 D146 -0.01013 0.00000 -0.00005 0.00008 0.00003 -0.01010

 D147 0.00331 0.00000 0.00003 0.00001 0.00004 0.00335

 D148 -3.13941 0.00000 0.00001 0.00008 0.00009 -3.13932

 D149 3.13898 0.00000 0.00000 -0.00021 -0.00021 3.13876

 D150 -0.00374 0.00000 -0.00001 -0.00015 -0.00016 -0.00390

 D151 0.02214 0.00001 0.00032 0.00043 0.00076 0.02289

 D152 -3.10649 0.00000 0.00041 0.00008 0.00049 -3.10601

 D153 0.00417 0.00000 0.00002 0.00003 0.00005 0.00422

 D154 -3.13854 0.00000 0.00001 0.00000 0.00002 -3.13852

 D155 -3.13856 0.00000 0.00001 0.00010 0.00010 -3.13845

 D156 0.00192 0.00000 0.00000 0.00007 0.00007 0.00200

 D157 -0.00041 0.00000 0.00000 0.00000 0.00000 -0.00041

 D158 3.14053 0.00000 -0.00002 0.00004 0.00002 3.14054

 D159 -3.14090 0.00000 0.00001 0.00003 0.00003 -3.14087

 D160 0.00004 0.00000 -0.00002 0.00007 0.00005 0.00009

 D161 -0.00421 0.00000 -0.00002 -0.00005 -0.00006 -0.00427

 D162 3.13890 0.00000 -0.00005 0.00008 0.00003 3.13893

 D163 3.13804 0.00000 0.00001 -0.00009 -0.00008 3.13796

 D164 -0.00204 0.00000 -0.00002 0.00003 0.00001 -0.00203

 D165 -0.00417 0.00000 -0.00002 -0.00003 -0.00005 -0.00422

 D166 3.13854 0.00000 -0.00001 0.00000 -0.00002 3.13852

 D167 3.13856 0.00000 -0.00001 -0.00010 -0.00010 3.13845

 D168 -0.00192 0.00000 0.00000 -0.00007 -0.00007 -0.00200

 D169 0.00041 0.00000 0.00000 0.00000 0.00000 0.00041

 D170 -3.14053 0.00000 0.00002 -0.00004 -0.00002 -3.14054

 D171 3.14090 0.00000 -0.00001 -0.00003 -0.00003 3.14087

 D172 -0.00004 0.00000 0.00002 -0.00007 -0.00005 -0.00009

 D173 0.00421 0.00000 0.00002 0.00005 0.00006 0.00427

 D174 -3.13890 0.00000 0.00005 -0.00008 -0.00003 -3.13893

 D175 -3.13804 0.00000 -0.00001 0.00009 0.00008 -3.13796

 D176 0.00204 0.00000 0.00002 -0.00003 -0.00001 0.00203

 D177 -0.00421 0.00000 -0.00002 -0.00005 -0.00006 -0.00427

 D178 3.13804 0.00000 0.00001 -0.00009 -0.00008 3.13796

 D179 3.13890 0.00000 -0.00005 0.00008 0.00003 3.13893

 D180 -0.00204 0.00000 -0.00002 0.00003 0.00001 -0.00203

 D181 -0.00041 0.00000 0.00000 0.00000 0.00000 -0.00041

 D182 -3.14090 0.00000 0.00001 0.00003 0.00003 -3.14087

 D183 3.14053 0.00000 -0.00002 0.00004 0.00002 3.14054

 D184 0.00004 0.00000 -0.00002 0.00007 0.00005 0.00009

 D185 0.00417 0.00000 0.00002 0.00003 0.00005 0.00422

 D186 -3.13856 0.00000 0.00001 0.00010 0.00010 -3.13845

 D187 -3.13854 0.00000 0.00001 0.00000 0.00002 -3.13852

 D188 0.00192 0.00000 0.00000 0.00007 0.00007 0.00200

 D189 -0.00417 0.00000 -0.00002 -0.00003 -0.00005 -0.00422

 D190 3.13854 0.00000 -0.00001 0.00000 -0.00002 3.13852

 D191 3.13856 0.00000 -0.00001 -0.00010 -0.00010 3.13845

 D192 -0.00192 0.00000 0.00000 -0.00007 -0.00007 -0.00200

 D193 0.00041 0.00000 0.00000 0.00000 0.00000 0.00041

 D194 -3.14053 0.00000 0.00002 -0.00004 -0.00002 -3.14054

 D195 3.14090 0.00000 -0.00001 -0.00003 -0.00003 3.14087

 D196 -0.00004 0.00000 0.00002 -0.00007 -0.00005 -0.00009

 D197 0.00421 0.00000 0.00002 0.00005 0.00006 0.00427

 D198 -3.13890 0.00000 0.00005 -0.00008 -0.00003 -3.13893

 D199 -3.13804 0.00000 -0.00001 0.00009 0.00008 -3.13796

 D200 0.00204 0.00000 0.00002 -0.00003 -0.00001 0.00203

 Item Value Threshold Converged?

 Maximum Force 0.000033 0.000450 YES

 RMS Force 0.000009 0.000300 YES

 Maximum Displacement 0.002884 0.001800 NO

 RMS Displacement 0.000627 0.001200 YES

 Predicted change in Energy=-2.320375D-07

 Lowest energy point so far. Saving SCF results.

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link 103 at Sat Jun 15 12:18:20 2019, MaxMem= 1342177280 cpu: 7.6

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

 Stoichiometry C32H16N8Zn(1-,2)

 Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C32H16N4)]

 Deg. of freedom 43

 Full point group C2V NOp 4

 RotChk: IX=0 Diff= 7.43D-18

 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 2.772294 1.184601 0.010690

 2 7 0 1.438265 1.423092 0.045298

 3 6 0 1.186646 2.785782 0.011266

 4 6 0 2.465483 3.475486 -0.036964

 5 6 0 3.467698 2.471751 -0.038060

 6 7 0 0.000000 3.385545 0.001996

 7 6 0 -1.186646 2.785782 0.011266

 8 7 0 -1.438265 1.423092 0.045298

 9 6 0 -2.772294 1.184601 0.010690

 10 6 0 -3.467698 2.471751 -0.038060

 11 6 0 -2.465483 3.475486 -0.036964

 12 7 0 3.404086 0.000000 0.005849

 13 6 0 3.467698 -2.471751 -0.038060

 14 6 0 2.465483 -3.475486 -0.036964

 15 6 0 1.186646 -2.785782 0.011266

 16 7 0 1.438265 -1.423092 0.045298

 17 6 0 2.772294 -1.184601 0.010690

 18 7 0 0.000000 -3.385545 0.001996

 19 7 0 -1.438265 -1.423092 0.045298

 20 6 0 -1.186646 -2.785782 0.011266

 21 6 0 -2.465483 -3.475486 -0.036964

 22 6 0 -3.467698 -2.471751 -0.038060

 23 6 0 -2.772294 -1.184601 0.010690

 24 7 0 -3.404086 0.000000 0.005849

 25 30 0 0.000000 0.000000 0.408186

 26 6 0 4.819902 -2.809036 -0.086159

 27 6 0 5.163218 -4.157537 -0.129072

 28 6 0 4.169696 -5.154986 -0.129109

 29 6 0 2.818507 -4.826862 -0.085957

 30 6 0 -4.819902 -2.809036 -0.086159

 31 6 0 -5.163218 -4.157537 -0.129072

 32 6 0 -4.169696 -5.154986 -0.129109

 33 6 0 -2.818507 -4.826862 -0.085957

 34 6 0 -2.818507 4.826862 -0.085957

 35 6 0 -4.169696 5.154986 -0.129109

 36 6 0 -5.163218 4.157537 -0.129072

 37 6 0 -4.819902 2.809036 -0.086159

 38 6 0 4.819902 2.809036 -0.086159

 39 6 0 5.163218 4.157537 -0.129072

 40 6 0 4.169696 5.154986 -0.129109

 41 6 0 2.818507 4.826862 -0.085957

 42 1 0 5.583169 -2.037761 -0.088926

 43 1 0 2.056891 -5.599756 -0.088682

 44 1 0 -5.583169 -2.037761 -0.088926

 45 1 0 -2.056891 -5.599756 -0.088682

 46 1 0 -2.056891 5.599756 -0.088682

 47 1 0 -5.583169 2.037761 -0.088926

 48 1 0 5.583169 2.037761 -0.088926

 49 1 0 2.056891 5.599756 -0.088682

 50 1 0 -4.466566 6.198241 -0.164097

 51 1 0 -6.208188 4.447190 -0.164051

 52 1 0 4.466566 6.198241 -0.164097

 53 1 0 6.208188 4.447190 -0.164051

 54 1 0 6.208188 -4.447190 -0.164051

 55 1 0 4.466566 -6.198241 -0.164097

 56 1 0 -4.466566 -6.198241 -0.164097

 57 1 0 -6.208188 -4.447190 -0.164051

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 Rotational constants (GHZ): 0.0880312 0.0879156 0.0440902

 Leave Link 202 at Sat Jun 15 12:18:20 2019, MaxMem= 1342177280 cpu: 0.1

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

 Basis read from rwf: (5D, 7F)

 Pseudo-potential data read from rwf file.

 There are 225 symmetry adapted cartesian basis functions of A1 symmetry.

 There are 196 symmetry adapted cartesian basis functions of A2 symmetry.

 There are 207 symmetry adapted cartesian basis functions of B1 symmetry.

 There are 207 symmetry adapted cartesian basis functions of B2 symmetry.

 There are 211 symmetry adapted basis functions of A1 symmetry.

 There are 187 symmetry adapted basis functions of A2 symmetry.

 There are 197 symmetry adapted basis functions of B1 symmetry.

 There are 197 symmetry adapted basis functions of B2 symmetry.

 792 basis functions, 1399 primitive gaussians, 835 cartesian basis functions

 139 alpha electrons 138 beta electrons

 nuclear repulsion energy 4373.9833173677 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= 57 NActive= 57 NUniq= 16 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

 Integral buffers will be 131072 words long.

 Raffenetti 2 integral format.

 Two-electron integral symmetry is turned on.

 R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1642463430 Hartrees.

 Nuclear repulsion after empirical dispersion term = 4373.8190710248 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= 57.

 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 = 57

 GePol: Total number of spheres = 57

 GePol: Number of exposed spheres = 57 (100.00%)

 GePol: Number of points = 4682

 GePol: Average weight of points = 0.10

 GePol: Minimum weight of points = 0.35D-08

 GePol: Maximum weight of points = 0.18390

 GePol: Number of points with low weight = 364

 GePol: Fraction of low-weight points (<1% of avg) = 7.77%

 GePol: Cavity surface area = 485.766 Ang\*\*2

 GePol: Cavity volume = 504.419 Ang\*\*3

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

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 PCM non-electrostatic energy = -0.0144354355 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 4373.8046355893 Hartrees.

 Leave Link 301 at Sat Jun 15 12:18:20 2019, MaxMem= 1342177280 cpu: 1.2

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

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

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

 One-electron integrals computed using PRISM.

 One-electron integral symmetry used in STVInt

 4 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22875 LenP2D= 61368.

 LDataN: DoStor=T MaxTD1= 5 Len= 102

 NBasis= 792 RedAO= T EigKep= 3.44D-05 NBF= 211 187 197 197

 NBsUse= 792 1.00D-06 EigRej= -1.00D+00 NBFU= 211 187 197 197

 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= 802 802 802 802 802 MxSgAt= 57 MxSgA2= 57.

 Leave Link 302 at Sat Jun 15 12:18:22 2019, MaxMem= 1342177280 cpu: 15.6

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

 DipDrv: MaxL=1.

 Leave Link 303 at Sat Jun 15 12:18:23 2019, MaxMem= 1342177280 cpu: 4.0

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

 Initial guess from the checkpoint file: "ZnPCanion.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 2-B1.

 Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5090

 Leave Link 401 at Sat Jun 15 12:18:29 2019, MaxMem= 1342177280 cpu: 67.7

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

 UHF open shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 2129573 IEndB= 2129573 NGot= 1342177280 MDV= 1340762408

 LenX= 1340762408 LenY= 1340064348

 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= 560000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

 Petite list used in FoFCou.

 Inv3: Mode=1 IEnd= 65763372.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 7.33D-15 for 758.

 Iteration 1 A\*A^-1 deviation from orthogonality is 7.66D-15 for 4442 762.

 Iteration 1 A^-1\*A deviation from unit magnitude is 7.66D-15 for 1925.

 Iteration 1 A^-1\*A deviation from orthogonality is 1.42D-12 for 2037 2025.

 E= -1733.50721191982

 DIIS: error= 5.03D-05 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -1733.50721191982 IErMin= 1 ErrMin= 5.03D-05

 ErrMax= 5.03D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.87D-06 BMatP= 5.87D-06

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

 Coeff-Com: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.368 Goal= None Shift= 0.000

 Gap= 0.409 Goal= None Shift= 0.000

 RMSDP=2.96D-06 MaxDP=7.21D-05 OVMax= 3.01D-04

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 2.96D-06 CP: 1.00D+00

 E= -1733.50721475260 Delta-E= -0.000002832776 Rises=F Damp=F

 DIIS: error= 7.41D-06 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -1733.50721475260 IErMin= 2 ErrMin= 7.41D-06

 ErrMax= 7.41D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.58D-08 BMatP= 5.87D-06

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

 Coeff-Com: -0.626D-01 0.106D+01

 Coeff: -0.626D-01 0.106D+01

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=4.46D-07 MaxDP=2.31D-05 DE=-2.83D-06 OVMax= 5.43D-05

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 4.05D-07 CP: 1.00D+00 1.06D+00

 E= -1733.50721478151 Delta-E= -0.000000028911 Rises=F Damp=F

 DIIS: error= 1.13D-05 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 3 EnMin= -1733.50721478151 IErMin= 2 ErrMin= 7.41D-06

 ErrMax= 1.13D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.13D-08 BMatP= 9.58D-08

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

 Coeff-Com: -0.419D-01 0.566D+00 0.476D+00

 Coeff: -0.419D-01 0.566D+00 0.476D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=2.77D-07 MaxDP=1.80D-05 DE=-2.89D-08 OVMax= 3.72D-05

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 1.86D-07 CP: 1.00D+00 1.07D+00 5.00D-01

 E= -1733.50721479724 Delta-E= -0.000000015732 Rises=F Damp=F

 DIIS: error= 3.40D-06 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -1733.50721479724 IErMin= 4 ErrMin= 3.40D-06

 ErrMax= 3.40D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.44D-09 BMatP= 9.13D-08

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

 Coeff-Com: -0.988D-02 0.113D+00 0.255D+00 0.642D+00

 Coeff: -0.988D-02 0.113D+00 0.255D+00 0.642D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=9.48D-08 MaxDP=5.05D-06 DE=-1.57D-08 OVMax= 1.52D-05

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 6.05D-08 CP: 1.00D+00 1.07D+00 6.24D-01 7.19D-01

 E= -1733.50721479940 Delta-E= -0.000000002160 Rises=F Damp=F

 DIIS: error= 1.65D-06 at cycle 5 NSaved= 5.

 NSaved= 5 IEnMin= 5 EnMin= -1733.50721479940 IErMin= 5 ErrMin= 1.65D-06

 ErrMax= 1.65D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.31D-09 BMatP= 9.44D-09

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

 Coeff-Com: -0.161D-02 0.776D-02 0.977D-01 0.364D+00 0.532D+00

 Coeff: -0.161D-02 0.776D-02 0.977D-01 0.364D+00 0.532D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=3.65D-08 MaxDP=1.59D-06 DE=-2.16D-09 OVMax= 5.77D-06

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 2.07D-08 CP: 1.00D+00 1.07D+00 6.20D-01 8.00D-01 5.72D-01

 E= -1733.50721479944 Delta-E= -0.000000000043 Rises=F Damp=F

 DIIS: error= 4.23D-07 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -1733.50721479944 IErMin= 6 ErrMin= 4.23D-07

 ErrMax= 4.23D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.48D-10 BMatP= 1.31D-09

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

 Coeff-Com: 0.733D-03-0.165D-01 0.111D-01 0.975D-01 0.295D+00 0.613D+00

 Coeff: 0.733D-03-0.165D-01 0.111D-01 0.975D-01 0.295D+00 0.613D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=1.16D-08 MaxDP=5.75D-07 DE=-4.27D-11 OVMax= 2.01D-06

 Cycle 7 Pass 1 IDiag 1:

 RMSU= 5.01D-09 CP: 1.00D+00 1.07D+00 6.26D-01 7.98D-01 6.77D-01

 CP: 6.21D-01

 E= -1733.50721479990 Delta-E= -0.000000000458 Rises=F Damp=F

 DIIS: error= 1.47D-07 at cycle 7 NSaved= 7.

 NSaved= 7 IEnMin= 7 EnMin= -1733.50721479990 IErMin= 7 ErrMin= 1.47D-07

 ErrMax= 1.47D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.36D-11 BMatP= 1.48D-10

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

 Coeff-Com: 0.506D-03-0.990D-02 0.495D-03 0.341D-01 0.135D+00 0.344D+00

 Coeff-Com: 0.496D+00

 Coeff: 0.506D-03-0.990D-02 0.495D-03 0.341D-01 0.135D+00 0.344D+00

 Coeff: 0.496D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=3.11D-09 MaxDP=1.71D-07 DE=-4.58D-10 OVMax= 5.52D-07

 Error on total polarization charges = 0.07593

 SCF Done: E(UB3LYP) = -1733.50721480 A.U. after 7 cycles

 NFock= 7 Conv=0.31D-08 -V/T= 1.9757

 <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5090

 <L.S>= 0.000000000000E+00

 KE= 1.776674233683D+03 PE=-1.289475850790D+04 EE= 5.010772423823D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -9.06

 (included in total energy above)

 Annihilation of the first spin contaminant:

 S\*\*2 before annihilation 0.7682, after 0.7503

 Leave Link 502 at Sat Jun 15 12:20:15 2019, MaxMem= 1342177280 cpu: 1210.7

 (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= 32896 NPrTT= 163506 LenC2= 22875 LenP2D= 61368.

 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 = 197

 Leave Link 701 at Sat Jun 15 12:20:25 2019, MaxMem= 1342177280 cpu: 104.7

 (Enter /apps/gaussian/g09d01/g09/l702.exe)

 L702 exits ... SP integral derivatives will be done elsewhere.

 Leave Link 702 at Sat Jun 15 12:20:26 2019, MaxMem= 1342177280 cpu: 2.0

 (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= 800

 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 Sat Jun 15 12:20:45 2019, MaxMem= 1342177280 cpu: 226.3

 (Enter /apps/gaussian/g09d01/g09/l716.exe)

 Dipole =-4.26325641D-14-6.25277607D-13 8.35411948D-01

 \*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

 Center Atomic Forces (Hartrees/Bohr)

 Number Number X Y Z

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

 1 6 0.000003114 0.000035324 0.000008549

 2 7 -0.000019268 -0.000016483 0.000041697

 3 6 0.000027892 0.000008254 -0.000010983

 4 6 -0.000006408 -0.000009788 0.000006173

 5 6 -0.000009922 -0.000011040 -0.000013595

 6 7 0.000000000 0.000026114 0.000001392

 7 6 -0.000027892 0.000008254 -0.000010983

 8 7 0.000019268 -0.000016483 0.000041697

 9 6 -0.000003114 0.000035324 0.000008549

 10 6 0.000009922 -0.000011040 -0.000013595

 11 6 0.000006408 -0.000009788 0.000006173

 12 7 0.000038096 0.000000000 0.000004509

 13 6 -0.000009922 0.000011040 -0.000013595

 14 6 -0.000006408 0.000009788 0.000006173

 15 6 0.000027892 -0.000008254 -0.000010983

 16 7 -0.000019268 0.000016483 0.000041697

 17 6 0.000003114 -0.000035324 0.000008549

 18 7 0.000000000 -0.000026114 0.000001392

 19 7 0.000019268 0.000016483 0.000041697

 20 6 -0.000027892 -0.000008254 -0.000010983

 21 6 0.000006408 0.000009788 0.000006173

 22 6 0.000009922 0.000011040 -0.000013595

 23 6 -0.000003114 -0.000035324 0.000008549

 24 7 -0.000038096 0.000000000 0.000004509

 25 30 0.000000000 0.000000000 -0.000140689

 26 6 -0.000000346 0.000012560 -0.000003952

 27 6 -0.000008718 -0.000003837 0.000000264

 28 6 0.000003832 0.000008679 0.000000219

 29 6 -0.000011779 -0.000001275 0.000004698

 30 6 0.000000346 0.000012560 -0.000003952

 31 6 0.000008718 -0.000003837 0.000000264

 32 6 -0.000003832 0.000008679 0.000000219

 33 6 0.000011779 -0.000001275 0.000004698

 34 6 0.000011779 0.000001275 0.000004698

 35 6 -0.000003832 -0.000008679 0.000000219

 36 6 0.000008718 0.000003837 0.000000264

 37 6 0.000000346 -0.000012560 -0.000003952

 38 6 -0.000000346 -0.000012560 -0.000003952

 39 6 -0.000008718 0.000003837 0.000000264

 40 6 0.000003832 -0.000008679 0.000000219

 41 6 -0.000011779 0.000001275 0.000004698

 42 1 0.000000162 -0.000006182 0.000000423

 43 1 0.000005742 0.000000464 -0.000001456

 44 1 -0.000000162 -0.000006182 0.000000423

 45 1 -0.000005742 0.000000464 -0.000001456

 46 1 -0.000005742 -0.000000464 -0.000001456

 47 1 -0.000000162 0.000006182 0.000000423

 48 1 0.000000162 0.000006182 0.000000423

 49 1 0.000005742 -0.000000464 -0.000001456

 50 1 0.000000903 -0.000001598 -0.000000722

 51 1 0.000001577 -0.000001013 0.000000908

 52 1 -0.000000903 -0.000001598 -0.000000722

 53 1 -0.000001577 -0.000001013 0.000000908

 54 1 -0.000001577 0.000001013 0.000000908

 55 1 -0.000000903 0.000001598 -0.000000722

 56 1 0.000000903 0.000001598 -0.000000722

 57 1 0.000001577 0.000001013 0.000000908

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

 Cartesian Forces: Max 0.000140689 RMS 0.000016673

 Leave Link 716 at Sat Jun 15 12:20:45 2019, MaxMem= 1342177280 cpu: 1.1

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

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Berny optimization.

 Using GEDIIS/GDIIS optimizer.

 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

 GSVD: received Info= 1 from GESDD.

 Internal Forces: Max 0.000024884 RMS 0.000006881

 Search for a local minimum.

 Step number 5 out of a maximum of 342

 All quantities printed in internal units (Hartrees-Bohrs-Radians)

 RMS Force = .68807D-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

 DE= -3.14D-07 DEPred=-2.32D-07 R= 1.35D+00

 Trust test= 1.35D+00 RLast= 5.87D-03 DXMaxT set to 3.00D-01

 ITU= 0 1 1 1 0

 Eigenvalues --- 0.00718 0.01580 0.01586 0.01609 0.01624

 Eigenvalues --- 0.01645 0.01658 0.01681 0.01697 0.01761

 Eigenvalues --- 0.01772 0.01774 0.01779 0.01780 0.01782

 Eigenvalues --- 0.01834 0.01846 0.01853 0.01891 0.01894

 Eigenvalues --- 0.01958 0.01959 0.02004 0.02008 0.02008

 Eigenvalues --- 0.02008 0.02047 0.02051 0.02051 0.02051

 Eigenvalues --- 0.02052 0.02053 0.02053 0.02053 0.02074

 Eigenvalues --- 0.02076 0.02105 0.02113 0.02113 0.02113

 Eigenvalues --- 0.02119 0.02119 0.02119 0.02122 0.02123

 Eigenvalues --- 0.02124 0.02124 0.02124 0.02215 0.02249

 Eigenvalues --- 0.02298 0.02323 0.03337 0.03910 0.03928

 Eigenvalues --- 0.06819 0.15227 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 0.16030 0.16073 0.16261 0.16367

 Eigenvalues --- 0.17687 0.22000 0.22000 0.22000 0.22000

 Eigenvalues --- 0.22598 0.22600 0.22600 0.22830 0.24153

 Eigenvalues --- 0.24250 0.24511 0.24511 0.24514 0.24530

 Eigenvalues --- 0.24629 0.24632 0.24841 0.24848 0.24948

 Eigenvalues --- 0.24956 0.24997 0.24997 0.24997 0.24997

 Eigenvalues --- 0.26100 0.33728 0.34071 0.34313 0.34482

 Eigenvalues --- 0.34804 0.34852 0.35207 0.35218 0.35218

 Eigenvalues --- 0.35218 0.35219 0.35243 0.35243 0.35243

 Eigenvalues --- 0.35244 0.35245 0.35247 0.35247 0.35247

 Eigenvalues --- 0.35252 0.35252 0.35252 0.35377 0.35564

 Eigenvalues --- 0.37367 0.37389 0.37565 0.39144 0.40803

 Eigenvalues --- 0.40890 0.41918 0.41932 0.41946 0.41959

 Eigenvalues --- 0.41973 0.42611 0.43208 0.43248 0.44577

 Eigenvalues --- 0.45211 0.45217 0.45287 0.45343 0.45909

 Eigenvalues --- 0.45910 0.45911 0.45919 0.46041 0.46122

 Eigenvalues --- 0.46178 0.46180 0.46184 0.46709 0.48680

 Eigenvalues --- 0.50032 0.50393 0.51371 0.53532 0.53863

 Eigenvalues --- 0.55373 0.55380 0.55891 0.58012 0.58039

 En-DIIS/RFO-DIIS IScMMF= 0 using points: 5 4 3 2

 RFO step: Lambda=-4.99027086D-08.

 NNeg= 0 NP= 4 Switch= 2.50D-03 Rises=F DC= 1.78D-05 SmlDif= 1.00D-05

 RMS Error= 0.2543290775D-04 NUsed= 4 EDIIS=F

 DidBck=F Rises=F RFO-DIIS coefs: 1.22537 -0.08194 -0.17840 0.03496

 Iteration 1 RMS(Cart)= 0.00045052 RMS(Int)= 0.00000007

 Iteration 2 RMS(Cart)= 0.00000017 RMS(Int)= 0.00000006

 ITry= 1 IFail=0 DXMaxC= 1.95D-03 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

 ClnCor: largest displacement from symmetrization is 1.53D-11 for atom 57.

 Variable Old X -DE/DX Delta X Delta X Delta X New X

 (Linear) (Quad) (Total)

 R1 2.56175 0.00001 -0.00005 0.00002 -0.00003 2.56172

 R2 2.76619 -0.00002 0.00004 -0.00002 0.00001 2.76620

 R3 2.53707 0.00002 -0.00005 0.00006 0.00001 2.53708

 R4 2.61943 0.00001 0.00001 0.00003 0.00004 2.61948

 R5 3.88452 -0.00002 0.00000 -0.00014 -0.00015 3.88437

 R6 2.74722 -0.00002 0.00000 -0.00002 -0.00002 2.74720

 R7 2.51265 0.00001 -0.00007 0.00004 -0.00003 2.51262

 R8 2.68043 0.00000 -0.00004 -0.00001 -0.00005 2.68038

 R9 2.64105 -0.00001 -0.00001 0.00001 0.00001 2.64106

 R10 2.63515 -0.00001 -0.00002 0.00001 -0.00001 2.63515

 R11 2.51265 0.00001 -0.00007 0.00004 -0.00003 2.51262

 R12 2.61943 0.00001 0.00001 0.00003 0.00004 2.61948

 R13 2.74722 -0.00002 0.00000 -0.00002 -0.00002 2.74720

 R14 2.56175 0.00001 -0.00005 0.00002 -0.00003 2.56172

 R15 3.88452 -0.00002 0.00000 -0.00014 -0.00015 3.88437

 R16 2.76619 -0.00002 0.00004 -0.00002 0.00001 2.76620

 R17 2.53707 0.00002 -0.00005 0.00006 0.00001 2.53708

 R18 2.68043 0.00000 -0.00004 -0.00001 -0.00005 2.68038

 R19 2.63515 -0.00001 -0.00002 0.00001 -0.00001 2.63515

 R20 2.64105 -0.00001 -0.00001 0.00001 0.00001 2.64106

 R21 2.53707 0.00002 -0.00005 0.00006 0.00001 2.53708

 R22 2.68043 0.00000 -0.00004 -0.00001 -0.00005 2.68038

 R23 2.76619 -0.00002 0.00004 -0.00002 0.00001 2.76620

 R24 2.63515 -0.00001 -0.00002 0.00001 -0.00001 2.63515

 R25 2.74722 -0.00002 0.00000 -0.00002 -0.00002 2.74720

 R26 2.64105 -0.00001 -0.00001 0.00001 0.00001 2.64106

 R27 2.61943 0.00001 0.00001 0.00003 0.00004 2.61948

 R28 2.51265 0.00001 -0.00007 0.00004 -0.00003 2.51262

 R29 2.56175 0.00001 -0.00005 0.00002 -0.00003 2.56172

 R30 3.88452 -0.00002 0.00000 -0.00014 -0.00015 3.88437

 R31 2.51265 0.00001 -0.00007 0.00004 -0.00003 2.51262

 R32 2.61943 0.00001 0.00001 0.00003 0.00004 2.61948

 R33 2.56175 0.00001 -0.00005 0.00002 -0.00003 2.56172

 R34 3.88452 -0.00002 0.00000 -0.00014 -0.00015 3.88437

 R35 2.74722 -0.00002 0.00000 -0.00002 -0.00002 2.74720

 R36 2.68043 0.00000 -0.00004 -0.00001 -0.00005 2.68038

 R37 2.64105 -0.00001 -0.00001 0.00001 0.00001 2.64106

 R38 2.76619 -0.00002 0.00004 -0.00002 0.00001 2.76620

 R39 2.63515 -0.00001 -0.00002 0.00001 -0.00001 2.63515

 R40 2.53707 0.00002 -0.00005 0.00006 0.00001 2.53708

 R41 2.63084 0.00000 -0.00003 0.00001 -0.00002 2.63082

 R42 2.05055 0.00000 0.00001 -0.00001 -0.00001 2.05054

 R43 2.66042 -0.00001 0.00001 -0.00002 0.00000 2.66041

 R44 2.05023 0.00000 -0.00001 0.00000 0.00000 2.05023

 R45 2.62885 0.00000 -0.00003 0.00001 -0.00002 2.62883

 R46 2.05080 0.00000 -0.00001 0.00000 0.00000 2.05079

 R47 2.05053 0.00000 0.00001 -0.00001 -0.00001 2.05052

 R48 2.63084 0.00000 -0.00003 0.00001 -0.00002 2.63082

 R49 2.05055 0.00000 0.00001 -0.00001 -0.00001 2.05054

 R50 2.66042 -0.00001 0.00001 -0.00002 0.00000 2.66041

 R51 2.05023 0.00000 -0.00001 0.00000 0.00000 2.05023

 R52 2.62885 0.00000 -0.00003 0.00001 -0.00002 2.62883

 R53 2.05080 0.00000 -0.00001 0.00000 0.00000 2.05079

 R54 2.05053 0.00000 0.00001 -0.00001 -0.00001 2.05052

 R55 2.62885 0.00000 -0.00003 0.00001 -0.00002 2.62883

 R56 2.05053 0.00000 0.00001 -0.00001 -0.00001 2.05052

 R57 2.66042 -0.00001 0.00001 -0.00002 0.00000 2.66041

 R58 2.05080 0.00000 -0.00001 0.00000 0.00000 2.05079

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 R68 2.05053 0.00000 0.00001 -0.00001 -0.00001 2.05052

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 A3 2.15578 -0.00001 -0.00001 -0.00001 -0.00002 2.15576

 A4 1.92939 -0.00001 0.00005 -0.00003 0.00002 1.92941

 A5 2.17882 0.00000 -0.00001 0.00003 0.00002 2.17885

 A6 2.16266 0.00001 0.00003 0.00006 0.00008 2.16275

 A7 1.88339 0.00000 -0.00005 0.00001 -0.00004 1.88336

 A8 2.22134 0.00000 0.00000 -0.00002 -0.00002 2.22132

 A9 2.17832 0.00000 0.00004 0.00001 0.00005 2.17838

 A10 1.86069 0.00000 0.00002 0.00001 0.00003 1.86072

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 A13 1.86142 0.00000 0.00001 0.00000 0.00001 1.86143

 A14 2.31109 -0.00001 -0.00002 0.00000 -0.00002 2.31106

 A15 2.11067 0.00000 0.00001 0.00001 0.00002 2.11068

 A16 2.20554 -0.00001 0.00004 0.00000 0.00004 2.20558

 A17 2.22134 0.00000 0.00000 -0.00002 -0.00002 2.22132

 A18 2.17832 0.00000 0.00004 0.00001 0.00005 2.17838

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 A24 2.23752 0.00000 0.00005 -0.00001 0.00004 2.23755

 A25 2.15578 -0.00001 -0.00001 -0.00001 -0.00002 2.15576

 A26 1.86142 0.00000 0.00001 0.00000 0.00001 1.86143

 A27 2.31109 -0.00001 -0.00002 0.00000 -0.00002 2.31106

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 A32 2.16165 -0.00002 -0.00001 -0.00001 -0.00002 2.16163

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 A42 1.92939 -0.00001 0.00005 -0.00003 0.00002 1.92941

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 A53 2.17832 0.00000 0.00004 0.00001 0.00005 2.17838

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 A55 1.86069 0.00000 0.00002 0.00001 0.00003 1.86072

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 A72 2.10628 0.00001 -0.00001 0.00003 0.00002 2.10630

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 A75 2.09107 0.00000 0.00000 0.00001 0.00000 2.09107

 A76 2.08353 0.00000 0.00000 -0.00001 -0.00001 2.08352

 A77 2.11570 0.00000 0.00000 0.00001 0.00001 2.11570

 A78 2.08064 0.00000 0.00000 -0.00001 -0.00001 2.08064

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 A80 2.06519 -0.00001 -0.00001 -0.00001 -0.00002 2.06518

 A81 2.10776 0.00001 -0.00001 0.00003 0.00002 2.10777

 A82 2.11023 0.00000 0.00002 -0.00002 0.00000 2.11023

 A83 2.06517 -0.00001 -0.00001 -0.00001 -0.00002 2.06515

 A84 2.10628 0.00001 -0.00001 0.00003 0.00002 2.10630

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 A87 2.09107 0.00000 0.00000 0.00001 0.00000 2.09107

 A88 2.08353 0.00000 0.00000 -0.00001 -0.00001 2.08352

 A89 2.11570 0.00000 0.00000 0.00001 0.00001 2.11570

 A90 2.08064 0.00000 0.00000 -0.00001 -0.00001 2.08064

 A91 2.08684 0.00000 0.00000 0.00001 0.00000 2.08684

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 A105 2.10628 0.00001 -0.00001 0.00003 0.00002 2.10630

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 A107 2.06517 -0.00001 -0.00001 -0.00001 -0.00002 2.06515

 A108 2.10628 0.00001 -0.00001 0.00003 0.00002 2.10630

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 A117 2.10776 0.00001 -0.00001 0.00003 0.00002 2.10777

 A118 2.11023 0.00000 0.00002 -0.00002 0.00000 2.11023

 D1 0.00915 -0.00001 0.00012 -0.00011 0.00001 0.00917

 D2 -2.96956 -0.00001 -0.00036 -0.00046 -0.00082 -2.97038

 D3 -3.12129 0.00000 0.00010 0.00006 0.00017 -3.12113

 D4 0.18318 -0.00001 -0.00038 -0.00029 -0.00067 0.18251

 D5 -0.00512 0.00001 -0.00009 0.00019 0.00010 -0.00502

 D6 -3.14118 0.00000 -0.00003 0.00011 0.00008 -3.14111

 D7 3.12597 0.00000 -0.00006 0.00002 -0.00004 3.12592

 D8 -0.01010 0.00000 -0.00001 -0.00006 -0.00007 -0.01016

 D9 0.02289 0.00000 0.00029 0.00005 0.00034 0.02323

 D10 -3.10601 0.00000 0.00026 0.00025 0.00051 -3.10550

 D11 -0.00954 0.00000 -0.00011 -0.00001 -0.00012 -0.00966

 D12 3.11504 0.00000 -0.00017 0.00000 -0.00017 3.11487

 D13 2.97098 0.00001 0.00036 0.00034 0.00070 2.97168

 D14 -0.18763 0.00001 0.00031 0.00034 0.00065 -0.18698

 D15 -3.05840 -0.00001 0.00021 -0.00007 0.00014 -3.05826

 D16 -0.26629 0.00001 0.00034 0.00036 0.00069 -0.26560

 D17 -1.66416 0.00000 0.00028 0.00015 0.00042 -1.66374

 D18 0.26720 -0.00002 -0.00035 -0.00046 -0.00080 0.26640

 D19 3.05930 0.00001 -0.00021 -0.00003 -0.00025 3.05906

 D20 1.66144 0.00000 -0.00028 -0.00024 -0.00052 1.66092

 D21 0.00599 0.00000 0.00006 0.00013 0.00018 0.00617

 D22 3.13968 0.00000 0.00002 0.00003 0.00005 3.13972

 D23 -3.11911 0.00000 0.00011 0.00012 0.00023 -3.11888

 D24 0.01458 0.00000 0.00007 0.00002 0.00009 0.01467

 D25 -0.01176 0.00000 -0.00014 -0.00002 -0.00016 -0.01191

 D26 3.11012 0.00001 -0.00020 -0.00001 -0.00021 3.10990

 D27 -0.00060 0.00000 0.00002 -0.00019 -0.00017 -0.00077

 D28 3.13623 0.00000 -0.00003 -0.00012 -0.00015 3.13608

 D29 -3.13549 0.00000 0.00005 -0.00010 -0.00005 -3.13555

 D30 0.00134 0.00000 0.00000 -0.00003 -0.00003 0.00131

 D31 -3.13792 0.00000 0.00002 0.00012 0.00014 -3.13778

 D32 0.00528 0.00000 0.00002 0.00007 0.00009 0.00537

 D33 -0.00511 0.00000 -0.00002 0.00001 -0.00001 -0.00512

 D34 3.13809 0.00000 -0.00002 -0.00004 -0.00006 3.13803

 D35 3.13876 0.00000 -0.00004 0.00013 0.00009 3.13885

 D36 -0.00390 0.00000 -0.00003 0.00005 0.00002 -0.00389

 D37 0.00335 0.00000 0.00002 0.00004 0.00006 0.00341

 D38 -3.13932 0.00000 0.00003 -0.00003 -0.00001 -3.13933

 D39 0.01176 0.00000 0.00014 0.00002 0.00016 0.01191

 D40 -3.11012 -0.00001 0.00020 0.00001 0.00021 -3.10990

 D41 -3.11504 0.00000 0.00017 0.00000 0.00017 -3.11487

 D42 0.18763 -0.00001 -0.00031 -0.00034 -0.00065 0.18698

 D43 0.00954 0.00000 0.00011 0.00001 0.00012 0.00966

 D44 -2.97098 -0.00001 -0.00036 -0.00034 -0.00070 -2.97168

 D45 3.11911 0.00000 -0.00011 -0.00012 -0.00023 3.11888

 D46 -0.01458 0.00000 -0.00007 -0.00002 -0.00009 -0.01467

 D47 -0.00599 0.00000 -0.00006 -0.00013 -0.00018 -0.00617

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 D49 -0.00915 0.00001 -0.00012 0.00011 -0.00001 -0.00917

 D50 3.12129 0.00000 -0.00010 -0.00006 -0.00017 3.12113

 D51 2.96956 0.00001 0.00036 0.00046 0.00082 2.97038

 D52 -0.18318 0.00001 0.00038 0.00029 0.00067 -0.18251

 D53 -0.26720 0.00002 0.00035 0.00046 0.00080 -0.26640

 D54 -1.66144 0.00000 0.00028 0.00024 0.00052 -1.66092

 D55 -3.05930 -0.00001 0.00021 0.00003 0.00025 -3.05906

 D56 3.05840 0.00001 -0.00021 0.00007 -0.00014 3.05826

 D57 1.66416 0.00000 -0.00028 -0.00015 -0.00042 1.66374

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 D61 -3.12597 0.00000 0.00006 -0.00002 0.00004 -3.12592

 D62 0.01010 0.00000 0.00001 0.00006 0.00007 0.01016

 D63 -0.02289 0.00000 -0.00029 -0.00005 -0.00034 -0.02323

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 D65 0.00060 0.00000 -0.00002 0.00019 0.00017 0.00077

 D66 3.13549 0.00000 -0.00005 0.00010 0.00005 3.13555

 D67 -3.13623 0.00000 0.00003 0.00012 0.00015 -3.13608

 D68 -0.00134 0.00000 0.00000 0.00003 0.00003 -0.00131

 D69 -3.13876 0.00000 0.00004 -0.00013 -0.00009 -3.13885

 D70 0.00390 0.00000 0.00003 -0.00005 -0.00002 0.00389

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 D73 3.13792 0.00000 -0.00002 -0.00012 -0.00014 3.13778

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 D75 0.00511 0.00000 0.00002 -0.00001 0.00001 0.00512

 D76 -3.13809 0.00000 0.00002 0.00004 0.00006 -3.13803

 D77 3.10601 0.00000 -0.00026 -0.00025 -0.00051 3.10550

 D78 -0.02289 0.00000 -0.00029 -0.00005 -0.00034 -0.02323

 D79 0.00060 0.00000 -0.00002 0.00019 0.00017 0.00077

 D80 3.13549 0.00000 -0.00005 0.00010 0.00005 3.13555

 D81 -3.13623 0.00000 0.00003 0.00012 0.00015 -3.13608

 D82 -0.00134 0.00000 0.00000 0.00003 0.00003 -0.00131

 D83 -3.12597 0.00000 0.00006 -0.00002 0.00004 -3.12592

 D84 0.00512 -0.00001 0.00009 -0.00019 -0.00010 0.00502

 D85 0.01010 0.00000 0.00001 0.00006 0.00007 0.01016

 D86 3.14118 0.00000 0.00003 -0.00011 -0.00008 3.14111

 D87 -0.00335 0.00000 -0.00002 -0.00004 -0.00006 -0.00341

 D88 3.13932 0.00000 -0.00003 0.00003 0.00001 3.13933

 D89 -3.13876 0.00000 0.00004 -0.00013 -0.00009 -3.13885

 D90 0.00390 0.00000 0.00003 -0.00005 -0.00002 0.00389

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 D93 -3.13968 0.00000 -0.00002 -0.00003 -0.00005 -3.13972

 D94 -0.01458 0.00000 -0.00007 -0.00002 -0.00009 -0.01467

 D95 0.00511 0.00000 0.00002 -0.00001 0.00001 0.00512

 D96 -3.13809 0.00000 0.00002 0.00004 0.00006 -3.13803

 D97 3.13792 0.00000 -0.00002 -0.00012 -0.00014 3.13778

 D98 -0.00528 0.00000 -0.00002 -0.00007 -0.00009 -0.00537

 D99 0.00954 0.00000 0.00011 0.00001 0.00012 0.00966

 D100 -2.97098 -0.00001 -0.00036 -0.00034 -0.00070 -2.97168

 D101 -3.11504 0.00000 0.00017 0.00000 0.00017 -3.11487

 D102 0.18763 -0.00001 -0.00031 -0.00034 -0.00065 0.18698

 D103 -3.11012 -0.00001 0.00020 0.00001 0.00021 -3.10990

 D104 0.01176 0.00000 0.00014 0.00002 0.00016 0.01191

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 D107 -0.18318 0.00001 0.00038 0.00029 0.00067 -0.18251

 D108 2.96956 0.00001 0.00036 0.00046 0.00082 2.97038

 D109 -3.05930 -0.00001 0.00021 0.00003 0.00025 -3.05906

 D110 -1.66144 0.00000 0.00028 0.00024 0.00052 -1.66092

 D111 -0.26720 0.00002 0.00035 0.00046 0.00080 -0.26640

 D112 0.26629 -0.00001 -0.00034 -0.00036 -0.00069 0.26560

 D113 1.66416 0.00000 -0.00028 -0.00015 -0.00042 1.66374

 D114 3.05840 0.00001 -0.00021 0.00007 -0.00014 3.05826

 D115 -0.01176 0.00000 -0.00014 -0.00002 -0.00016 -0.01191

 D116 3.11012 0.00001 -0.00020 -0.00001 -0.00021 3.10990

 D117 3.11504 0.00000 -0.00017 0.00000 -0.00017 3.11487

 D118 -0.00954 0.00000 -0.00011 -0.00001 -0.00012 -0.00966

 D119 -0.18763 0.00001 0.00031 0.00034 0.00065 -0.18698

 D120 2.97098 0.00001 0.00036 0.00034 0.00070 2.97168

 D121 0.00915 -0.00001 0.00012 -0.00011 0.00001 0.00917

 D122 -3.12129 0.00000 0.00010 0.00006 0.00017 -3.12113

 D123 -2.96956 -0.00001 -0.00036 -0.00046 -0.00082 -2.97038

 D124 0.18318 -0.00001 -0.00038 -0.00029 -0.00067 0.18251

 D125 1.66144 0.00000 -0.00028 -0.00024 -0.00052 1.66092

 D126 3.05930 0.00001 -0.00021 -0.00003 -0.00025 3.05906

 D127 0.26720 -0.00002 -0.00035 -0.00046 -0.00080 0.26640

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 D130 -3.05840 -0.00001 0.00021 -0.00007 0.00014 -3.05826

 D131 -3.11911 0.00000 0.00011 0.00012 0.00023 -3.11888

 D132 0.01458 0.00000 0.00007 0.00002 0.00009 0.01467

 D133 0.00599 0.00000 0.00006 0.00013 0.00018 0.00617

 D134 3.13968 0.00000 0.00002 0.00003 0.00005 3.13972

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 D137 -3.13549 0.00000 0.00005 -0.00010 -0.00005 -3.13555

 D138 0.00134 0.00000 0.00000 -0.00003 -0.00003 0.00131

 D139 -3.13792 0.00000 0.00002 0.00012 0.00014 -3.13778

 D140 0.00528 0.00000 0.00002 0.00007 0.00009 0.00537

 D141 -0.00511 0.00000 -0.00002 0.00001 -0.00001 -0.00512

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 D143 -0.00512 0.00001 -0.00009 0.00019 0.00010 -0.00502

 D144 3.12597 0.00000 -0.00006 0.00002 -0.00004 3.12592

 D145 -3.14118 0.00000 -0.00003 0.00011 0.00008 -3.14111

 D146 -0.01010 0.00000 -0.00001 -0.00006 -0.00007 -0.01016

 D147 0.00335 0.00000 0.00002 0.00004 0.00006 0.00341

 D148 -3.13932 0.00000 0.00003 -0.00003 -0.00001 -3.13933

 D149 3.13876 0.00000 -0.00004 0.00013 0.00009 3.13885

 D150 -0.00390 0.00000 -0.00003 0.00005 0.00002 -0.00389

 D151 0.02289 0.00000 0.00029 0.00005 0.00034 0.02323

 D152 -3.10601 0.00000 0.00026 0.00025 0.00051 -3.10550

 D153 0.00422 0.00000 0.00002 0.00003 0.00004 0.00426

 D154 -3.13852 0.00000 0.00001 0.00005 0.00006 -3.13846

 D155 -3.13845 0.00000 0.00003 -0.00005 -0.00002 -3.13848

 D156 0.00200 0.00000 0.00002 -0.00003 -0.00001 0.00198

 D157 -0.00041 0.00000 0.00000 0.00000 0.00000 -0.00042

 D158 3.14054 0.00000 -0.00001 -0.00002 -0.00003 3.14052

 D159 -3.14087 0.00000 0.00001 -0.00003 -0.00001 -3.14088

 D160 0.00009 0.00000 0.00000 -0.00004 -0.00004 0.00005

 D161 -0.00427 0.00000 -0.00002 -0.00001 -0.00003 -0.00430

 D162 3.13893 0.00000 -0.00002 -0.00006 -0.00008 3.13885

 D163 3.13796 0.00000 -0.00001 0.00001 0.00000 3.13796

 D164 -0.00203 0.00000 -0.00001 -0.00004 -0.00005 -0.00208

 D165 -0.00422 0.00000 -0.00002 -0.00003 -0.00004 -0.00426

 D166 3.13852 0.00000 -0.00001 -0.00005 -0.00006 3.13846

 D167 3.13845 0.00000 -0.00003 0.00005 0.00002 3.13848

 D168 -0.00200 0.00000 -0.00002 0.00003 0.00001 -0.00198

 D169 0.00041 0.00000 0.00000 0.00000 0.00000 0.00042

 D170 -3.14054 0.00000 0.00001 0.00002 0.00003 -3.14052

 D171 3.14087 0.00000 -0.00001 0.00003 0.00001 3.14088

 D172 -0.00009 0.00000 0.00000 0.00004 0.00004 -0.00005

 D173 0.00427 0.00000 0.00002 0.00001 0.00003 0.00430

 D174 -3.13893 0.00000 0.00002 0.00006 0.00008 -3.13885

 D175 -3.13796 0.00000 0.00001 -0.00001 0.00000 -3.13796

 D176 0.00203 0.00000 0.00001 0.00004 0.00005 0.00208

 D177 -0.00427 0.00000 -0.00002 -0.00001 -0.00003 -0.00430

 D178 3.13796 0.00000 -0.00001 0.00001 0.00000 3.13796

 D179 3.13893 0.00000 -0.00002 -0.00006 -0.00008 3.13885

 D180 -0.00203 0.00000 -0.00001 -0.00004 -0.00005 -0.00208

 D181 -0.00041 0.00000 0.00000 0.00000 0.00000 -0.00042

 D182 -3.14087 0.00000 0.00001 -0.00003 -0.00001 -3.14088

 D183 3.14054 0.00000 -0.00001 -0.00002 -0.00003 3.14052

 D184 0.00009 0.00000 0.00000 -0.00004 -0.00004 0.00005

 D185 0.00422 0.00000 0.00002 0.00003 0.00004 0.00426

 D186 -3.13845 0.00000 0.00003 -0.00005 -0.00002 -3.13848

 D187 -3.13852 0.00000 0.00001 0.00005 0.00006 -3.13846

 D188 0.00200 0.00000 0.00002 -0.00003 -0.00001 0.00198

 D189 -0.00422 0.00000 -0.00002 -0.00003 -0.00004 -0.00426

 D190 3.13852 0.00000 -0.00001 -0.00005 -0.00006 3.13846

 D191 3.13845 0.00000 -0.00003 0.00005 0.00002 3.13848

 D192 -0.00200 0.00000 -0.00002 0.00003 0.00001 -0.00198

 D193 0.00041 0.00000 0.00000 0.00000 0.00000 0.00042

 D194 -3.14054 0.00000 0.00001 0.00002 0.00003 -3.14052

 D195 3.14087 0.00000 -0.00001 0.00003 0.00001 3.14088

 D196 -0.00009 0.00000 0.00000 0.00004 0.00004 -0.00005

 D197 0.00427 0.00000 0.00002 0.00001 0.00003 0.00430

 D198 -3.13893 0.00000 0.00002 0.00006 0.00008 -3.13885

 D199 -3.13796 0.00000 0.00001 -0.00001 0.00000 -3.13796

 D200 0.00203 0.00000 0.00001 0.00004 0.00005 0.00208

 Item Value Threshold Converged?

 Maximum Force 0.000025 0.000450 YES

 RMS Force 0.000007 0.000300 YES

 Maximum Displacement 0.001953 0.001800 NO

 RMS Displacement 0.000451 0.001200 YES

 Predicted change in Energy=-1.233623D-07

 Lowest energy point so far. Saving SCF results.

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link 103 at Sat Jun 15 12:20:48 2019, MaxMem= 1342177280 cpu: 20.6

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

 Stoichiometry C32H16N8Zn(1-,2)

 Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C32H16N4)]

 Deg. of freedom 43

 Full point group C2V NOp 4

 RotChk: IX=0 Diff= 1.64D-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 2.772273 1.184599 0.011272

 2 7 0 1.438273 1.423126 0.046118

 3 6 0 1.186644 2.785828 0.011707

 4 6 0 2.465490 3.475468 -0.036881

 5 6 0 3.467672 2.471738 -0.038040

 6 7 0 0.000000 3.385559 0.002346

 7 6 0 -1.186644 2.785828 0.011707

 8 7 0 -1.438273 1.423126 0.046118

 9 6 0 -2.772273 1.184599 0.011272

 10 6 0 -3.467672 2.471738 -0.038040

 11 6 0 -2.465490 3.475468 -0.036881

 12 7 0 3.404078 0.000000 0.006486

 13 6 0 3.467672 -2.471738 -0.038040

 14 6 0 2.465490 -3.475468 -0.036881

 15 6 0 1.186644 -2.785828 0.011707

 16 7 0 1.438273 -1.423126 0.046118

 17 6 0 2.772273 -1.184599 0.011272

 18 7 0 0.000000 -3.385559 0.002346

 19 7 0 -1.438273 -1.423126 0.046118

 20 6 0 -1.186644 -2.785828 0.011707

 21 6 0 -2.465490 -3.475468 -0.036881

 22 6 0 -3.467672 -2.471738 -0.038040

 23 6 0 -2.772273 -1.184599 0.011272

 24 7 0 -3.404078 0.000000 0.006486

 25 30 0 0.000000 0.000000 0.408403

 26 6 0 4.819867 -2.808971 -0.086640

 27 6 0 5.163187 -4.157451 -0.129918

 28 6 0 4.169683 -5.154917 -0.129873

 29 6 0 2.818508 -4.826834 -0.086274

 30 6 0 -4.819867 -2.808971 -0.086640

 31 6 0 -5.163187 -4.157451 -0.129918

 32 6 0 -4.169683 -5.154917 -0.129873

 33 6 0 -2.818508 -4.826834 -0.086274

 34 6 0 -2.818508 4.826834 -0.086274

 35 6 0 -4.169683 5.154917 -0.129873

 36 6 0 -5.163187 4.157451 -0.129918

 37 6 0 -4.819867 2.808971 -0.086640

 38 6 0 4.819867 2.808971 -0.086640

 39 6 0 5.163187 4.157451 -0.129918

 40 6 0 4.169683 5.154917 -0.129873

 41 6 0 2.818508 4.826834 -0.086274

 42 1 0 5.583123 -2.037692 -0.089448

 43 1 0 2.056911 -5.599739 -0.089010

 44 1 0 -5.583123 -2.037692 -0.089448

 45 1 0 -2.056911 -5.599739 -0.089010

 46 1 0 -2.056911 5.599739 -0.089010

 47 1 0 -5.583123 2.037692 -0.089448

 48 1 0 5.583123 2.037692 -0.089448

 49 1 0 2.056911 5.599739 -0.089010

 50 1 0 -4.466568 6.198153 -0.165178

 51 1 0 -6.208147 4.447087 -0.165237

 52 1 0 4.466568 6.198153 -0.165178

 53 1 0 6.208147 4.447087 -0.165237

 54 1 0 6.208147 -4.447087 -0.165237

 55 1 0 4.466568 -6.198153 -0.165178

 56 1 0 -4.466568 -6.198153 -0.165178

 57 1 0 -6.208147 -4.447087 -0.165237

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

 Rotational constants (GHZ): 0.0880319 0.0879157 0.0440907

 Leave Link 202 at Sat Jun 15 12:20:48 2019, MaxMem= 1342177280 cpu: 0.0

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

 Basis read from rwf: (5D, 7F)

 Pseudo-potential data read from rwf file.

 There are 225 symmetry adapted cartesian basis functions of A1 symmetry.

 There are 196 symmetry adapted cartesian basis functions of A2 symmetry.

 There are 207 symmetry adapted cartesian basis functions of B1 symmetry.

 There are 207 symmetry adapted cartesian basis functions of B2 symmetry.

 There are 211 symmetry adapted basis functions of A1 symmetry.

 There are 187 symmetry adapted basis functions of A2 symmetry.

 There are 197 symmetry adapted basis functions of B1 symmetry.

 There are 197 symmetry adapted basis functions of B2 symmetry.

 792 basis functions, 1399 primitive gaussians, 835 cartesian basis functions

 139 alpha electrons 138 beta electrons

 nuclear repulsion energy 4373.9994456777 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= 57 NActive= 57 NUniq= 16 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

 Integral buffers will be 131072 words long.

 Raffenetti 2 integral format.

 Two-electron integral symmetry is turned on.

 R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1642466346 Hartrees.

 Nuclear repulsion after empirical dispersion term = 4373.8351990431 Hartrees.

 No density basis found on file 724.

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 Polarizable Continuum Model (PCM)

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

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

 Atomic radii : SMD-Coulomb.

 Polarization charges : Total charges.

 Charge compensation : None.

 Solution method : On-the-fly selection.

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

 Cavity algorithm : GePol (No added spheres)

 Default sphere list used, NSphG= 57.

 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 = 57

 GePol: Total number of spheres = 57

 GePol: Number of exposed spheres = 57 (100.00%)

 GePol: Number of points = 4682

 GePol: Average weight of points = 0.10

 GePol: Minimum weight of points = 0.58D-08

 GePol: Maximum weight of points = 0.18390

 GePol: Number of points with low weight = 364

 GePol: Fraction of low-weight points (<1% of avg) = 7.77%

 GePol: Cavity surface area = 485.786 Ang\*\*2

 GePol: Cavity volume = 504.432 Ang\*\*3

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

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 PCM non-electrostatic energy = -0.0144338412 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 4373.8207652019 Hartrees.

 Leave Link 301 at Sat Jun 15 12:20:48 2019, MaxMem= 1342177280 cpu: 2.3

 (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= 32896 NPrTT= 163506 LenC2= 22875 LenP2D= 61368.

 LDataN: DoStor=T MaxTD1= 5 Len= 102

 NBasis= 792 RedAO= T EigKep= 3.44D-05 NBF= 211 187 197 197

 NBsUse= 792 1.00D-06 EigRej= -1.00D+00 NBFU= 211 187 197 197

 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= 802 802 802 802 802 MxSgAt= 57 MxSgA2= 57.

 Leave Link 302 at Sat Jun 15 12:20:50 2019, MaxMem= 1342177280 cpu: 18.0

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

 DipDrv: MaxL=1.

 Leave Link 303 at Sat Jun 15 12:20:50 2019, MaxMem= 1342177280 cpu: 2.5

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

 Initial guess from the checkpoint file: "ZnPCanion.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) (A2) (B1) (B2) (A1) (B1) (A1) (B1) (A2)

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 The electronic state of the initial guess is 2-B1.

 Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5090

 Leave Link 401 at Sat Jun 15 12:20:56 2019, MaxMem= 1342177280 cpu: 63.9

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

 UHF open shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 2129573 IEndB= 2129573 NGot= 1342177280 MDV= 1340762408

 LenX= 1340762408 LenY= 1340064348

 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= 560000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

 Petite list used in FoFCou.

 Inv3: Mode=1 IEnd= 65763372.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 9.55D-15 for 4681.

 Iteration 1 A\*A^-1 deviation from orthogonality is 6.41D-15 for 4614 761.

 Iteration 1 A^-1\*A deviation from unit magnitude is 9.77D-15 for 4681.

 Iteration 1 A^-1\*A deviation from orthogonality is 1.53D-12 for 3873 3831.

 E= -1733.50721358826

 DIIS: error= 3.62D-05 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -1733.50721358826 IErMin= 1 ErrMin= 3.62D-05

 ErrMax= 3.62D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.80D-06 BMatP= 2.80D-06

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

 Coeff-Com: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.368 Goal= None Shift= 0.000

 Gap= 0.409 Goal= None Shift= 0.000

 RMSDP=2.18D-06 MaxDP=5.19D-05 OVMax= 1.81D-04

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 2.18D-06 CP: 1.00D+00

 E= -1733.50721491967 Delta-E= -0.000001331409 Rises=F Damp=F

 DIIS: error= 1.02D-05 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -1733.50721491967 IErMin= 2 ErrMin= 1.02D-05

 ErrMax= 1.02D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.77D-08 BMatP= 2.80D-06

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

 Coeff-Com: -0.559D-01 0.106D+01

 Coeff: -0.559D-01 0.106D+01

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=2.99D-07 MaxDP=8.56D-06 DE=-1.33D-06 OVMax= 3.51D-05

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 2.77D-07 CP: 1.00D+00 1.05D+00

 E= -1733.50721493228 Delta-E= -0.000000012602 Rises=F Damp=F

 DIIS: error= 1.55D-05 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 3 EnMin= -1733.50721493228 IErMin= 2 ErrMin= 1.02D-05

 ErrMax= 1.55D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.94D-08 BMatP= 4.77D-08

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

 Coeff-Com: -0.421D-01 0.595D+00 0.447D+00

 Coeff: -0.421D-01 0.595D+00 0.447D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=1.70D-07 MaxDP=7.66D-06 DE=-1.26D-08 OVMax= 2.68D-05

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 1.14D-07 CP: 1.00D+00 1.06D+00 5.48D-01

 E= -1733.50721494105 Delta-E= -0.000000008776 Rises=F Damp=F

 DIIS: error= 1.38D-06 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -1733.50721494105 IErMin= 4 ErrMin= 1.38D-06

 ErrMax= 1.38D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.00D-09 BMatP= 4.77D-08

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

 Coeff-Com: -0.126D-01 0.151D+00 0.223D+00 0.639D+00

 Coeff: -0.126D-01 0.151D+00 0.223D+00 0.639D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=6.11D-08 MaxDP=2.48D-06 DE=-8.78D-09 OVMax= 1.21D-05

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 4.50D-08 CP: 1.00D+00 1.06D+00 6.51D-01 7.38D-01

 E= -1733.50721494174 Delta-E= -0.000000000689 Rises=F Damp=F

 DIIS: error= 1.88D-06 at cycle 5 NSaved= 5.

 NSaved= 5 IEnMin= 5 EnMin= -1733.50721494174 IErMin= 4 ErrMin= 1.38D-06

 ErrMax= 1.88D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.19D-09 BMatP= 4.00D-09

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

 Coeff-Com: -0.146D-02 0.191D-02 0.713D-01 0.409D+00 0.519D+00

 Coeff: -0.146D-02 0.191D-02 0.713D-01 0.409D+00 0.519D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=2.78D-08 MaxDP=1.26D-06 DE=-6.89D-10 OVMax= 5.40D-06

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 1.27D-08 CP: 1.00D+00 1.06D+00 6.36D-01 8.55D-01 5.53D-01

 E= -1733.50721494218 Delta-E= -0.000000000442 Rises=F Damp=F

 DIIS: error= 2.35D-07 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -1733.50721494218 IErMin= 6 ErrMin= 2.35D-07

 ErrMax= 2.35D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.05D-11 BMatP= 1.19D-09

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

 Coeff-Com: 0.674D-03-0.163D-01 0.577D-02 0.102D+00 0.222D+00 0.686D+00

 Coeff: 0.674D-03-0.163D-01 0.577D-02 0.102D+00 0.222D+00 0.686D+00

 Gap= 0.038 Goal= None Shift= 0.000

 Gap= 0.078 Goal= None Shift= 0.000

 RMSDP=6.25D-09 MaxDP=2.96D-07 DE=-4.42D-10 OVMax= 9.00D-07

 Error on total polarization charges = 0.07593

 SCF Done: E(UB3LYP) = -1733.50721494 A.U. after 6 cycles

 NFock= 6 Conv=0.63D-08 -V/T= 1.9757

 <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7682 S= 0.5090

 <L.S>= 0.000000000000E+00

 KE= 1.776674872624D+03 PE=-1.289479186592D+04 EE= 5.010789013152D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -9.06

 (included in total energy above)

 Annihilation of the first spin contaminant:

 S\*\*2 before annihilation 0.7682, after 0.7503

 Leave Link 502 at Sat Jun 15 12:22:32 2019, MaxMem= 1342177280 cpu: 1086.2

 (Enter /apps/gaussian/g09d01/g09/l701.exe)

 Compute integral first derivatives.

 ... and contract with generalized density number 0.

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

 4 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22875 LenP2D= 61368.

 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 = 197

 Leave Link 701 at Sat Jun 15 12:22:41 2019, MaxMem= 1342177280 cpu: 102.3

 (Enter /apps/gaussian/g09d01/g09/l702.exe)

 L702 exits ... SP integral derivatives will be done elsewhere.

 Leave Link 702 at Sat Jun 15 12:22:42 2019, MaxMem= 1342177280 cpu: 1.7

 (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= 800

 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 Sat Jun 15 12:23:00 2019, MaxMem= 1342177280 cpu: 216.7

 (Enter /apps/gaussian/g09d01/g09/l716.exe)

 Dipole =-2.91322522D-13 4.76063633D-13 8.32377638D-01

 \*\*\*\*\* Axes restored to original set \*\*\*\*\*

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 Center Atomic Forces (Hartrees/Bohr)

 Number Number X Y Z

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

 1 6 0.000015654 0.000041237 -0.000001665

 2 7 -0.000026880 -0.000008736 0.000020867

 3 6 0.000034796 -0.000018413 0.000003755

 4 6 -0.000017834 0.000011744 -0.000003122

 5 6 -0.000001962 -0.000028252 0.000005566

 6 7 0.000000000 0.000041476 -0.000003507

 7 6 -0.000034796 -0.000018413 0.000003755

 8 7 0.000026880 -0.000008736 0.000020867

 9 6 -0.000015654 0.000041237 -0.000001665

 10 6 0.000001962 -0.000028252 0.000005566

 11 6 0.000017834 0.000011744 -0.000003122

 12 7 0.000027199 0.000000000 -0.000007478

 13 6 -0.000001962 0.000028252 0.000005566

 14 6 -0.000017834 -0.000011744 -0.000003122

 15 6 0.000034796 0.000018413 0.000003755

 16 7 -0.000026880 0.000008736 0.000020867

 17 6 0.000015654 -0.000041237 -0.000001665

 18 7 0.000000000 -0.000041476 -0.000003507

 19 7 0.000026880 0.000008736 0.000020867

 20 6 -0.000034796 0.000018413 0.000003755

 21 6 0.000017834 -0.000011744 -0.000003122

 22 6 0.000001962 0.000028252 0.000005566

 23 6 -0.000015654 -0.000041237 -0.000001665

 24 7 -0.000027199 0.000000000 -0.000007478

 25 30 0.000000000 0.000000000 -0.000089598

 26 6 -0.000000095 0.000009757 0.000003641

 27 6 -0.000005036 -0.000007769 -0.000000392

 28 6 0.000009093 0.000004251 -0.000000035

 29 6 -0.000011632 0.000003048 0.000000215

 30 6 0.000000095 0.000009757 0.000003641

 31 6 0.000005036 -0.000007769 -0.000000392

 32 6 -0.000009093 0.000004251 -0.000000035

 33 6 0.000011632 0.000003048 0.000000215

 34 6 0.000011632 -0.000003048 0.000000215

 35 6 -0.000009093 -0.000004251 -0.000000035

 36 6 0.000005036 0.000007769 -0.000000392

 37 6 0.000000095 -0.000009757 0.000003641

 38 6 -0.000000095 -0.000009757 0.000003641

 39 6 -0.000005036 0.000007769 -0.000000392

 40 6 0.000009093 -0.000004251 -0.000000035

 41 6 -0.000011632 -0.000003048 0.000000215

 42 1 0.000001100 -0.000003862 -0.000000470

 43 1 0.000003339 -0.000000678 0.000000165

 44 1 -0.000001100 -0.000003862 -0.000000470

 45 1 -0.000003339 -0.000000678 0.000000165

 46 1 -0.000003339 0.000000678 0.000000165

 47 1 -0.000001100 0.000003862 -0.000000470

 48 1 0.000001100 0.000003862 -0.000000470

 49 1 0.000003339 0.000000678 0.000000165

 50 1 0.000000632 0.000000404 0.000000009

 51 1 -0.000000348 -0.000000768 -0.000000642

 52 1 -0.000000632 0.000000404 0.000000009

 53 1 0.000000348 -0.000000768 -0.000000642

 54 1 0.000000348 0.000000768 -0.000000642

 55 1 -0.000000632 -0.000000404 0.000000009

 56 1 0.000000632 -0.000000404 0.000000009

 57 1 -0.000000348 0.000000768 -0.000000642

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 Cartesian Forces: Max 0.000089598 RMS 0.000015130

 Leave Link 716 at Sat Jun 15 12:23:01 2019, MaxMem= 1342177280 cpu: 3.2

 (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.

 GSVD: received Info= 1 from GESDD.

 Internal Forces: Max 0.000022867 RMS 0.000006321

 Search for a local minimum.

 Step number 6 out of a maximum of 342

 All quantities printed in internal units (Hartrees-Bohrs-Radians)

 RMS Force = .63210D-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

 DE= -1.42D-07 DEPred=-1.23D-07 R= 1.15D+00

 Trust test= 1.15D+00 RLast= 4.33D-03 DXMaxT set to 3.00D-01

 ITU= 0 0 1 1 1 0

 Eigenvalues --- 0.00617 0.01586 0.01586 0.01609 0.01624

 Eigenvalues --- 0.01645 0.01661 0.01681 0.01697 0.01760

 Eigenvalues --- 0.01772 0.01774 0.01779 0.01780 0.01782

 Eigenvalues --- 0.01834 0.01846 0.01855 0.01891 0.01894

 Eigenvalues --- 0.01958 0.01959 0.02005 0.02008 0.02008

 Eigenvalues --- 0.02008 0.02049 0.02051 0.02051 0.02051

 Eigenvalues --- 0.02052 0.02053 0.02053 0.02053 0.02075

 Eigenvalues --- 0.02076 0.02112 0.02113 0.02113 0.02113

 Eigenvalues --- 0.02119 0.02119 0.02119 0.02122 0.02124

 Eigenvalues --- 0.02124 0.02124 0.02124 0.02249 0.02293

 Eigenvalues --- 0.02323 0.02585 0.03337 0.03903 0.03920

 Eigenvalues --- 0.05674 0.15228 0.15824 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 0.16040 0.16261 0.16367

 Eigenvalues --- 0.16919 0.22000 0.22000 0.22000 0.22001

 Eigenvalues --- 0.22598 0.22600 0.22600 0.22631 0.24159

 Eigenvalues --- 0.24298 0.24511 0.24511 0.24530 0.24530

 Eigenvalues --- 0.24631 0.24635 0.24843 0.24949 0.24956

 Eigenvalues --- 0.24995 0.24997 0.24997 0.24997 0.25087

 Eigenvalues --- 0.26077 0.33728 0.34071 0.34131 0.34313

 Eigenvalues --- 0.34805 0.34851 0.35191 0.35218 0.35218

 Eigenvalues --- 0.35218 0.35219 0.35239 0.35243 0.35243

 Eigenvalues --- 0.35243 0.35245 0.35247 0.35247 0.35247

 Eigenvalues --- 0.35252 0.35252 0.35252 0.35369 0.35752

 Eigenvalues --- 0.37367 0.37389 0.37496 0.37565 0.40803

 Eigenvalues --- 0.40889 0.41932 0.41946 0.41949 0.41959

 Eigenvalues --- 0.41972 0.42766 0.43208 0.43248 0.44577

 Eigenvalues --- 0.45211 0.45217 0.45226 0.45343 0.45824

 Eigenvalues --- 0.45910 0.45911 0.45919 0.46042 0.46122

 Eigenvalues --- 0.46178 0.46180 0.46184 0.46712 0.47614

 Eigenvalues --- 0.50019 0.50394 0.51372 0.53534 0.53685

 Eigenvalues --- 0.55373 0.55380 0.56574 0.58012 0.58039

 En-DIIS/RFO-DIIS IScMMF= 0 using points: 6 5 4 3 2

 RFO step: Lambda=-3.64378458D-08.

 NNeg= 0 NP= 5 Switch= 2.50D-03 Rises=F DC= 1.78D-05 SmlDif= 1.00D-05

 RMS Error= 0.1833966907D-04 NUsed= 5 EDIIS=F

 DidBck=F Rises=F RFO-DIIS coefs: 1.56085 -0.29504 -0.51436 0.27305 -0.02450

 Iteration 1 RMS(Cart)= 0.00010724 RMS(Int)= 0.00000005

 Iteration 2 RMS(Cart)= 0.00000005 RMS(Int)= 0.00000004

 ITry= 1 IFail=0 DXMaxC= 1.50D-03 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

 ClnCor: largest displacement from symmetrization is 2.43D-11 for atom 57.

 Variable Old X -DE/DX Delta X Delta X Delta X New X

 (Linear) (Quad) (Total)

 R1 2.56172 0.00002 0.00001 0.00002 0.00003 2.56175

 R2 2.76620 -0.00002 -0.00005 -0.00002 -0.00007 2.76613

 R3 2.53708 0.00002 0.00006 0.00000 0.00006 2.53714

 R4 2.61948 0.00000 0.00003 0.00000 0.00002 2.61950

 R5 3.88437 -0.00001 -0.00019 -0.00003 -0.00022 3.88415

 R6 2.74720 -0.00001 -0.00005 0.00000 -0.00005 2.74715

 R7 2.51262 0.00002 0.00003 0.00001 0.00005 2.51266

 R8 2.68038 0.00001 -0.00004 0.00007 0.00002 2.68040

 R9 2.64106 0.00000 -0.00001 0.00001 0.00000 2.64105

 R10 2.63515 0.00000 -0.00001 0.00001 0.00000 2.63515

 R11 2.51262 0.00002 0.00003 0.00001 0.00005 2.51266

 R12 2.61948 0.00000 0.00003 0.00000 0.00002 2.61950

 R13 2.74720 -0.00001 -0.00005 0.00000 -0.00005 2.74715

 R14 2.56172 0.00002 0.00001 0.00002 0.00003 2.56175

 R15 3.88437 -0.00001 -0.00019 -0.00003 -0.00022 3.88415

 R16 2.76620 -0.00002 -0.00005 -0.00002 -0.00007 2.76613

 R17 2.53708 0.00002 0.00006 0.00000 0.00006 2.53714

 R18 2.68038 0.00001 -0.00004 0.00007 0.00002 2.68040

 R19 2.63515 0.00000 -0.00001 0.00001 0.00000 2.63515

 R20 2.64106 0.00000 -0.00001 0.00001 0.00000 2.64105

 R21 2.53708 0.00002 0.00006 0.00000 0.00006 2.53714

 R22 2.68038 0.00001 -0.00004 0.00007 0.00002 2.68040

 R23 2.76620 -0.00002 -0.00005 -0.00002 -0.00007 2.76613

 R24 2.63515 0.00000 -0.00001 0.00001 0.00000 2.63515

 R25 2.74720 -0.00001 -0.00005 0.00000 -0.00005 2.74715

 R26 2.64106 0.00000 -0.00001 0.00001 0.00000 2.64105

 R27 2.61948 0.00000 0.00003 0.00000 0.00002 2.61950

 R28 2.51262 0.00002 0.00003 0.00001 0.00005 2.51266

 R29 2.56172 0.00002 0.00001 0.00002 0.00003 2.56175

 R30 3.88437 -0.00001 -0.00019 -0.00003 -0.00022 3.88415

 R31 2.51262 0.00002 0.00003 0.00001 0.00005 2.51266

 R32 2.61948 0.00000 0.00003 0.00000 0.00002 2.61950

 R33 2.56172 0.00002 0.00001 0.00002 0.00003 2.56175

 R34 3.88437 -0.00001 -0.00019 -0.00003 -0.00022 3.88415

 R35 2.74720 -0.00001 -0.00005 0.00000 -0.00005 2.74715

 R36 2.68038 0.00001 -0.00004 0.00007 0.00002 2.68040

 R37 2.64106 0.00000 -0.00001 0.00001 0.00000 2.64105

 R38 2.76620 -0.00002 -0.00005 -0.00002 -0.00007 2.76613

 R39 2.63515 0.00000 -0.00001 0.00001 0.00000 2.63515

 R40 2.53708 0.00002 0.00006 0.00000 0.00006 2.53714

 R41 2.63082 0.00000 -0.00001 0.00001 0.00001 2.63083

 R42 2.05054 0.00000 -0.00003 0.00002 -0.00001 2.05053

 R43 2.66041 -0.00001 -0.00004 0.00003 -0.00001 2.66040

 R44 2.05023 0.00000 -0.00001 0.00001 0.00000 2.05023

 R45 2.62883 0.00000 -0.00001 0.00001 0.00001 2.62884

 R46 2.05079 0.00000 -0.00001 0.00001 0.00000 2.05079

 R47 2.05052 0.00000 -0.00003 0.00002 -0.00001 2.05052

 R48 2.63082 0.00000 -0.00001 0.00001 0.00001 2.63083

 R49 2.05054 0.00000 -0.00003 0.00002 -0.00001 2.05053

 R50 2.66041 -0.00001 -0.00004 0.00003 -0.00001 2.66040

 R51 2.05023 0.00000 -0.00001 0.00001 0.00000 2.05023

 R52 2.62883 0.00000 -0.00001 0.00001 0.00001 2.62884

 R53 2.05079 0.00000 -0.00001 0.00001 0.00000 2.05079

 R54 2.05052 0.00000 -0.00003 0.00002 -0.00001 2.05052

 R55 2.62883 0.00000 -0.00001 0.00001 0.00001 2.62884

 R56 2.05052 0.00000 -0.00003 0.00002 -0.00001 2.05052

 R57 2.66041 -0.00001 -0.00004 0.00003 -0.00001 2.66040

 R58 2.05079 0.00000 -0.00001 0.00001 0.00000 2.05079

 R59 2.63082 0.00000 -0.00001 0.00001 0.00001 2.63083

 R60 2.05023 0.00000 -0.00001 0.00001 0.00000 2.05023

 R61 2.05054 0.00000 -0.00003 0.00002 -0.00001 2.05053

 R62 2.63082 0.00000 -0.00001 0.00001 0.00001 2.63083

 R63 2.05054 0.00000 -0.00003 0.00002 -0.00001 2.05053

 R64 2.66041 -0.00001 -0.00004 0.00003 -0.00001 2.66040

 R65 2.05023 0.00000 -0.00001 0.00001 0.00000 2.05023

 R66 2.62883 0.00000 -0.00001 0.00001 0.00001 2.62884

 R67 2.05079 0.00000 -0.00001 0.00001 0.00000 2.05079

 R68 2.05052 0.00000 -0.00003 0.00002 -0.00001 2.05052

 A1 1.88982 0.00000 0.00003 -0.00003 0.00000 1.88982

 A2 2.23755 0.00000 0.00000 0.00002 0.00001 2.23757

 A3 2.15576 0.00000 -0.00002 0.00001 -0.00001 2.15575

 A4 1.92941 -0.00001 -0.00005 0.00004 -0.00001 1.92940

 A5 2.17885 0.00001 0.00004 -0.00001 0.00003 2.17888

 A6 2.16275 0.00000 0.00006 -0.00001 0.00005 2.16279

 A7 1.88336 0.00001 0.00002 -0.00002 0.00000 1.88335

 A8 2.22132 0.00000 -0.00002 0.00003 0.00001 2.22133

 A9 2.17838 -0.00001 0.00000 -0.00001 -0.00001 2.17837

 A10 1.86072 0.00000 0.00001 0.00000 0.00001 1.86072

 A11 2.32139 0.00000 -0.00002 0.00000 -0.00002 2.32138

 A12 2.10105 0.00000 0.00001 0.00000 0.00001 2.10106

 A13 1.86143 0.00000 0.00000 0.00001 0.00001 1.86144

 A14 2.31106 0.00000 -0.00001 0.00000 -0.00001 2.31105

 A15 2.11068 0.00000 0.00001 0.00000 0.00000 2.11068

 A16 2.20558 -0.00002 -0.00002 -0.00002 -0.00004 2.20554

 A17 2.22132 0.00000 -0.00002 0.00003 0.00001 2.22133

 A18 2.17838 -0.00001 0.00000 -0.00001 -0.00001 2.17837

 A19 1.88336 0.00001 0.00002 -0.00002 0.00000 1.88335

 A20 1.92941 -0.00001 -0.00005 0.00004 -0.00001 1.92940

 A21 2.16275 0.00000 0.00006 -0.00001 0.00005 2.16279

 A22 2.17885 0.00001 0.00004 -0.00001 0.00003 2.17888

 A23 1.88982 0.00000 0.00003 -0.00003 0.00000 1.88982

 A24 2.23755 0.00000 0.00000 0.00002 0.00001 2.23757

 A25 2.15576 0.00000 -0.00002 0.00001 -0.00001 2.15575

 A26 1.86143 0.00000 0.00000 0.00001 0.00001 1.86144

 A27 2.31106 0.00000 -0.00001 0.00000 -0.00001 2.31105

 A28 2.11068 0.00000 0.00001 0.00000 0.00000 2.11068

 A29 1.86072 0.00000 0.00001 0.00000 0.00001 1.86072

 A30 2.32139 0.00000 -0.00002 0.00000 -0.00002 2.32138

 A31 2.10105 0.00000 0.00001 0.00000 0.00001 2.10106

 A32 2.16163 -0.00001 -0.00004 0.00001 -0.00004 2.16159

 A33 1.86143 0.00000 0.00000 0.00001 0.00001 1.86144

 A34 2.11068 0.00000 0.00001 0.00000 0.00000 2.11068

 A35 2.31106 0.00000 -0.00001 0.00000 -0.00001 2.31105

 A36 1.86072 0.00000 0.00001 0.00000 0.00001 1.86072

 A37 2.10105 0.00000 0.00001 0.00000 0.00001 2.10106

 A38 2.32139 0.00000 -0.00002 0.00000 -0.00002 2.32138

 A39 1.88336 0.00001 0.00002 -0.00002 0.00000 1.88335

 A40 2.17838 -0.00001 0.00000 -0.00001 -0.00001 2.17837

 A41 2.22132 0.00000 -0.00002 0.00003 0.00001 2.22133

 A42 1.92941 -0.00001 -0.00005 0.00004 -0.00001 1.92940

 A43 2.16275 0.00000 0.00006 -0.00001 0.00005 2.16279

 A44 2.17885 0.00001 0.00004 -0.00001 0.00003 2.17888

 A45 2.15576 0.00000 -0.00002 0.00001 -0.00001 2.15575

 A46 2.23755 0.00000 0.00000 0.00002 0.00001 2.23757

 A47 1.88982 0.00000 0.00003 -0.00003 0.00000 1.88982

 A48 2.20558 -0.00002 -0.00002 -0.00002 -0.00004 2.20554

 A49 1.92941 -0.00001 -0.00005 0.00004 -0.00001 1.92940

 A50 2.16275 0.00000 0.00006 -0.00001 0.00005 2.16279

 A51 2.17885 0.00001 0.00004 -0.00001 0.00003 2.17888

 A52 2.22132 0.00000 -0.00002 0.00003 0.00001 2.22133

 A53 2.17838 -0.00001 0.00000 -0.00001 -0.00001 2.17837

 A54 1.88336 0.00001 0.00002 -0.00002 0.00000 1.88335

 A55 1.86072 0.00000 0.00001 0.00000 0.00001 1.86072

 A56 2.32139 0.00000 -0.00002 0.00000 -0.00002 2.32138

 A57 2.10105 0.00000 0.00001 0.00000 0.00001 2.10106

 A58 1.86143 0.00000 0.00000 0.00001 0.00001 1.86144

 A59 2.11068 0.00000 0.00001 0.00000 0.00000 2.11068

 A60 2.31106 0.00000 -0.00001 0.00000 -0.00001 2.31105

 A61 1.88982 0.00000 0.00003 -0.00003 0.00000 1.88982

 A62 2.23755 0.00000 0.00000 0.00002 0.00001 2.23757

 A63 2.15576 0.00000 -0.00002 0.00001 -0.00001 2.15575

 A64 2.16163 -0.00001 -0.00004 0.00001 -0.00004 2.16159

 A65 1.54999 0.00000 0.00006 0.00005 0.00012 1.55010

 A66 1.52946 0.00000 0.00007 0.00006 0.00013 1.52959

 A67 2.78724 0.00002 0.00039 0.00032 0.00070 2.78795

 A68 2.78724 0.00002 0.00039 0.00032 0.00070 2.78795

 A69 1.52946 0.00000 0.00007 0.00006 0.00013 1.52959

 A70 1.54999 0.00000 0.00006 0.00005 0.00012 1.55010

 A71 2.06515 0.00000 -0.00002 0.00000 -0.00002 2.06513

 A72 2.10630 0.00000 0.00005 0.00000 0.00005 2.10634

 A73 2.11174 0.00000 -0.00003 0.00001 -0.00002 2.11171

 A74 2.10859 0.00000 0.00001 0.00001 0.00002 2.10861

 A75 2.09107 0.00000 0.00000 -0.00002 -0.00001 2.09106

 A76 2.08352 0.00000 -0.00001 0.00001 0.00000 2.08352

 A77 2.11570 0.00000 0.00001 0.00000 0.00001 2.11572

 A78 2.08064 0.00000 -0.00002 0.00001 0.00000 2.08063

 A79 2.08684 0.00000 0.00001 -0.00002 -0.00001 2.08683

 A80 2.06518 0.00000 -0.00002 0.00000 -0.00002 2.06515

 A81 2.10777 0.00000 0.00004 0.00000 0.00004 2.10781

 A82 2.11023 0.00000 -0.00002 0.00001 -0.00002 2.11022

 A83 2.06515 0.00000 -0.00002 0.00000 -0.00002 2.06513

 A84 2.10630 0.00000 0.00005 0.00000 0.00005 2.10634

 A85 2.11174 0.00000 -0.00003 0.00001 -0.00002 2.11171

 A86 2.10859 0.00000 0.00001 0.00001 0.00002 2.10861

 A87 2.09107 0.00000 0.00000 -0.00002 -0.00001 2.09106

 A88 2.08352 0.00000 -0.00001 0.00001 0.00000 2.08352

 A89 2.11570 0.00000 0.00001 0.00000 0.00001 2.11572

 A90 2.08064 0.00000 -0.00002 0.00001 0.00000 2.08063

 A91 2.08684 0.00000 0.00001 -0.00002 -0.00001 2.08683

 A92 2.06518 0.00000 -0.00002 0.00000 -0.00002 2.06515

 A93 2.10777 0.00000 0.00004 0.00000 0.00004 2.10781

 A94 2.11023 0.00000 -0.00002 0.00001 -0.00002 2.11022

 A95 2.06518 0.00000 -0.00002 0.00000 -0.00002 2.06515

 A96 2.10777 0.00000 0.00004 0.00000 0.00004 2.10781

 A97 2.11023 0.00000 -0.00002 0.00001 -0.00002 2.11022

 A98 2.11570 0.00000 0.00001 0.00000 0.00001 2.11572

 A99 2.08684 0.00000 0.00001 -0.00002 -0.00001 2.08683

 A100 2.08064 0.00000 -0.00002 0.00001 0.00000 2.08063

 A101 2.10859 0.00000 0.00001 0.00001 0.00002 2.10861

 A102 2.08352 0.00000 -0.00001 0.00001 0.00000 2.08352

 A103 2.09107 0.00000 0.00000 -0.00002 -0.00001 2.09106

 A104 2.06515 0.00000 -0.00002 0.00000 -0.00002 2.06513

 A105 2.10630 0.00000 0.00005 0.00000 0.00005 2.10634

 A106 2.11174 0.00000 -0.00003 0.00001 -0.00002 2.11171

 A107 2.06515 0.00000 -0.00002 0.00000 -0.00002 2.06513

 A108 2.10630 0.00000 0.00005 0.00000 0.00005 2.10634

 A109 2.11174 0.00000 -0.00003 0.00001 -0.00002 2.11171

 A110 2.10859 0.00000 0.00001 0.00001 0.00002 2.10861

 A111 2.09107 0.00000 0.00000 -0.00002 -0.00001 2.09106

 A112 2.08352 0.00000 -0.00001 0.00001 0.00000 2.08352

 A113 2.11570 0.00000 0.00001 0.00000 0.00001 2.11572

 A114 2.08064 0.00000 -0.00002 0.00001 0.00000 2.08063

 A115 2.08684 0.00000 0.00001 -0.00002 -0.00001 2.08683

 A116 2.06518 0.00000 -0.00002 0.00000 -0.00002 2.06515

 A117 2.10777 0.00000 0.00004 0.00000 0.00004 2.10781

 A118 2.11023 0.00000 -0.00002 0.00001 -0.00002 2.11022

 D1 0.00917 0.00000 0.00005 0.00002 0.00007 0.00924

 D2 -2.97038 0.00000 -0.00029 -0.00008 -0.00037 -2.97075

 D3 -3.12113 0.00000 0.00002 -0.00003 -0.00001 -3.12113

 D4 0.18251 -0.00001 -0.00032 -0.00012 -0.00045 0.18206

 D5 -0.00502 0.00000 -0.00005 -0.00004 -0.00009 -0.00511

 D6 -3.14111 0.00000 -0.00002 -0.00004 -0.00006 -3.14117

 D7 3.12592 0.00000 -0.00002 0.00000 -0.00001 3.12591

 D8 -0.01016 0.00000 0.00001 0.00001 0.00002 -0.01015

 D9 0.02323 -0.00001 0.00014 -0.00008 0.00006 0.02329

 D10 -3.10550 -0.00001 0.00010 -0.00013 -0.00003 -3.10553

 D11 -0.00966 0.00000 -0.00004 0.00001 -0.00003 -0.00969

 D12 3.11487 0.00000 -0.00003 0.00003 0.00001 3.11487

 D13 2.97168 0.00000 0.00030 0.00011 0.00041 2.97208

 D14 -0.18698 0.00001 0.00031 0.00013 0.00044 -0.18654

 D15 -3.05826 -0.00001 -0.00002 -0.00009 -0.00011 -3.05837

 D16 -0.26560 0.00001 0.00034 0.00022 0.00056 -0.26504

 D17 -1.66374 0.00000 0.00016 0.00007 0.00023 -1.66351

 D18 0.26640 -0.00001 -0.00040 -0.00020 -0.00060 0.26580

 D19 3.05906 0.00001 -0.00003 0.00010 0.00007 3.05913

 D20 1.66092 0.00000 -0.00021 -0.00005 -0.00026 1.66066

 D21 0.00617 0.00000 0.00001 -0.00004 -0.00003 0.00615

 D22 3.13972 0.00000 0.00001 0.00001 0.00002 3.13974

 D23 -3.11888 0.00000 0.00000 -0.00006 -0.00006 -3.11894

 D24 0.01467 0.00000 0.00000 -0.00002 -0.00001 0.01466

 D25 -0.01191 0.00001 -0.00003 0.00004 0.00001 -0.01191

 D26 3.10990 0.00001 -0.00002 0.00007 0.00005 3.10995

 D27 -0.00077 0.00000 0.00002 0.00005 0.00007 -0.00070

 D28 3.13608 0.00000 0.00000 0.00004 0.00004 3.13613

 D29 -3.13555 0.00000 0.00002 0.00001 0.00003 -3.13552

 D30 0.00131 0.00000 0.00000 0.00001 0.00000 0.00131

 D31 -3.13778 0.00000 -0.00002 -0.00001 -0.00004 -3.13781

 D32 0.00537 0.00000 0.00000 -0.00004 -0.00004 0.00533

 D33 -0.00512 0.00000 -0.00002 0.00004 0.00002 -0.00510

 D34 3.13803 0.00000 0.00000 0.00001 0.00001 3.13804

 D35 3.13885 0.00000 -0.00001 -0.00005 -0.00006 3.13879

 D36 -0.00389 0.00000 -0.00002 0.00000 -0.00001 -0.00390

 D37 0.00341 0.00000 0.00002 -0.00005 -0.00002 0.00338

 D38 -3.13933 0.00000 0.00001 0.00001 0.00002 -3.13931

 D39 0.01191 -0.00001 0.00003 -0.00004 -0.00001 0.01191

 D40 -3.10990 -0.00001 0.00002 -0.00007 -0.00005 -3.10995

 D41 -3.11487 0.00000 0.00003 -0.00003 -0.00001 -3.11487

 D42 0.18698 -0.00001 -0.00031 -0.00013 -0.00044 0.18654

 D43 0.00966 0.00000 0.00004 -0.00001 0.00003 0.00969

 D44 -2.97168 0.00000 -0.00030 -0.00011 -0.00041 -2.97208

 D45 3.11888 0.00000 0.00000 0.00006 0.00006 3.11894

 D46 -0.01467 0.00000 0.00000 0.00002 0.00001 -0.01466

 D47 -0.00617 0.00000 -0.00001 0.00004 0.00003 -0.00615

 D48 -3.13972 0.00000 -0.00001 -0.00001 -0.00002 -3.13974

 D49 -0.00917 0.00000 -0.00005 -0.00002 -0.00007 -0.00924

 D50 3.12113 0.00000 -0.00002 0.00003 0.00001 3.12113

 D51 2.97038 0.00000 0.00029 0.00008 0.00037 2.97075

 D52 -0.18251 0.00001 0.00032 0.00012 0.00045 -0.18206

 D53 -0.26640 0.00001 0.00040 0.00020 0.00060 -0.26580

 D54 -1.66092 0.00000 0.00021 0.00005 0.00026 -1.66066

 D55 -3.05906 -0.00001 0.00003 -0.00010 -0.00007 -3.05913

 D56 3.05826 0.00001 0.00002 0.00009 0.00011 3.05837

 D57 1.66374 0.00000 -0.00016 -0.00007 -0.00023 1.66351

 D58 0.26560 -0.00001 -0.00034 -0.00022 -0.00056 0.26504

 D59 0.00502 0.00000 0.00005 0.00004 0.00009 0.00511

 D60 3.14111 0.00000 0.00002 0.00004 0.00006 3.14117

 D61 -3.12592 0.00000 0.00002 0.00000 0.00001 -3.12591

 D62 0.01016 0.00000 -0.00001 -0.00001 -0.00002 0.01015

 D63 -0.02323 0.00001 -0.00014 0.00008 -0.00006 -0.02329

 D64 3.10550 0.00001 -0.00010 0.00013 0.00003 3.10553

 D65 0.00077 0.00000 -0.00002 -0.00005 -0.00007 0.00070

 D66 3.13555 0.00000 -0.00002 -0.00001 -0.00003 3.13552

 D67 -3.13608 0.00000 0.00000 -0.00004 -0.00004 -3.13613

 D68 -0.00131 0.00000 0.00000 -0.00001 0.00000 -0.00131

 D69 -3.13885 0.00000 0.00001 0.00005 0.00006 -3.13879

 D70 0.00389 0.00000 0.00002 0.00000 0.00001 0.00390

 D71 -0.00341 0.00000 -0.00002 0.00005 0.00002 -0.00338

 D72 3.13933 0.00000 -0.00001 -0.00001 -0.00002 3.13931

 D73 3.13778 0.00000 0.00002 0.00001 0.00004 3.13781

 D74 -0.00537 0.00000 0.00000 0.00004 0.00004 -0.00533

 D75 0.00512 0.00000 0.00002 -0.00004 -0.00002 0.00510

 D76 -3.13803 0.00000 0.00000 -0.00001 -0.00001 -3.13804

 D77 3.10550 0.00001 -0.00010 0.00013 0.00003 3.10553

 D78 -0.02323 0.00001 -0.00014 0.00008 -0.00006 -0.02329

 D79 0.00077 0.00000 -0.00002 -0.00005 -0.00007 0.00070

 D80 3.13555 0.00000 -0.00002 -0.00001 -0.00003 3.13552

 D81 -3.13608 0.00000 0.00000 -0.00004 -0.00004 -3.13613

 D82 -0.00131 0.00000 0.00000 -0.00001 0.00000 -0.00131

 D83 -3.12592 0.00000 0.00002 0.00000 0.00001 -3.12591

 D84 0.00502 0.00000 0.00005 0.00004 0.00009 0.00511

 D85 0.01016 0.00000 -0.00001 -0.00001 -0.00002 0.01015

 D86 3.14111 0.00000 0.00002 0.00004 0.00006 3.14117

 D87 -0.00341 0.00000 -0.00002 0.00005 0.00002 -0.00338

 D88 3.13933 0.00000 -0.00001 -0.00001 -0.00002 3.13931

 D89 -3.13885 0.00000 0.00001 0.00005 0.00006 -3.13879

 D90 0.00389 0.00000 0.00002 0.00000 0.00001 0.00390

 D91 -0.00617 0.00000 -0.00001 0.00004 0.00003 -0.00615

 D92 3.11888 0.00000 0.00000 0.00006 0.00006 3.11894

 D93 -3.13972 0.00000 -0.00001 -0.00001 -0.00002 -3.13974

 D94 -0.01467 0.00000 0.00000 0.00002 0.00001 -0.01466

 D95 0.00512 0.00000 0.00002 -0.00004 -0.00002 0.00510

 D96 -3.13803 0.00000 0.00000 -0.00001 -0.00001 -3.13804

 D97 3.13778 0.00000 0.00002 0.00001 0.00004 3.13781

 D98 -0.00537 0.00000 0.00000 0.00004 0.00004 -0.00533

 D99 0.00966 0.00000 0.00004 -0.00001 0.00003 0.00969

 D100 -2.97168 0.00000 -0.00030 -0.00011 -0.00041 -2.97208

 D101 -3.11487 0.00000 0.00003 -0.00003 -0.00001 -3.11487

 D102 0.18698 -0.00001 -0.00031 -0.00013 -0.00044 0.18654

 D103 -3.10990 -0.00001 0.00002 -0.00007 -0.00005 -3.10995

 D104 0.01191 -0.00001 0.00003 -0.00004 -0.00001 0.01191

 D105 3.12113 0.00000 -0.00002 0.00003 0.00001 3.12113

 D106 -0.00917 0.00000 -0.00005 -0.00002 -0.00007 -0.00924

 D107 -0.18251 0.00001 0.00032 0.00012 0.00045 -0.18206

 D108 2.97038 0.00000 0.00029 0.00008 0.00037 2.97075

 D109 -3.05906 -0.00001 0.00003 -0.00010 -0.00007 -3.05913

 D110 -1.66092 0.00000 0.00021 0.00005 0.00026 -1.66066

 D111 -0.26640 0.00001 0.00040 0.00020 0.00060 -0.26580

 D112 0.26560 -0.00001 -0.00034 -0.00022 -0.00056 0.26504

 D113 1.66374 0.00000 -0.00016 -0.00007 -0.00023 1.66351

 D114 3.05826 0.00001 0.00002 0.00009 0.00011 3.05837

 D115 -0.01191 0.00001 -0.00003 0.00004 0.00001 -0.01191

 D116 3.10990 0.00001 -0.00002 0.00007 0.00005 3.10995

 D117 3.11487 0.00000 -0.00003 0.00003 0.00001 3.11487

 D118 -0.00966 0.00000 -0.00004 0.00001 -0.00003 -0.00969

 D119 -0.18698 0.00001 0.00031 0.00013 0.00044 -0.18654

 D120 2.97168 0.00000 0.00030 0.00011 0.00041 2.97208

 D121 0.00917 0.00000 0.00005 0.00002 0.00007 0.00924

 D122 -3.12113 0.00000 0.00002 -0.00003 -0.00001 -3.12113

 D123 -2.97038 0.00000 -0.00029 -0.00008 -0.00037 -2.97075

 D124 0.18251 -0.00001 -0.00032 -0.00012 -0.00045 0.18206

 D125 1.66092 0.00000 -0.00021 -0.00005 -0.00026 1.66066

 D126 3.05906 0.00001 -0.00003 0.00010 0.00007 3.05913

 D127 0.26640 -0.00001 -0.00040 -0.00020 -0.00060 0.26580

 D128 -1.66374 0.00000 0.00016 0.00007 0.00023 -1.66351

 D129 -0.26560 0.00001 0.00034 0.00022 0.00056 -0.26504

 D130 -3.05826 -0.00001 -0.00002 -0.00009 -0.00011 -3.05837

 D131 -3.11888 0.00000 0.00000 -0.00006 -0.00006 -3.11894

 D132 0.01467 0.00000 0.00000 -0.00002 -0.00001 0.01466

 D133 0.00617 0.00000 0.00001 -0.00004 -0.00003 0.00615

 D134 3.13972 0.00000 0.00001 0.00001 0.00002 3.13974

 D135 -0.00077 0.00000 0.00002 0.00005 0.00007 -0.00070

 D136 3.13608 0.00000 0.00000 0.00004 0.00004 3.13613

 D137 -3.13555 0.00000 0.00002 0.00001 0.00003 -3.13552

 D138 0.00131 0.00000 0.00000 0.00001 0.00000 0.00131

 D139 -3.13778 0.00000 -0.00002 -0.00001 -0.00004 -3.13781

 D140 0.00537 0.00000 0.00000 -0.00004 -0.00004 0.00533

 D141 -0.00512 0.00000 -0.00002 0.00004 0.00002 -0.00510

 D142 3.13803 0.00000 0.00000 0.00001 0.00001 3.13804

 D143 -0.00502 0.00000 -0.00005 -0.00004 -0.00009 -0.00511

 D144 3.12592 0.00000 -0.00002 0.00000 -0.00001 3.12591

 D145 -3.14111 0.00000 -0.00002 -0.00004 -0.00006 -3.14117

 D146 -0.01016 0.00000 0.00001 0.00001 0.00002 -0.01015

 D147 0.00341 0.00000 0.00002 -0.00005 -0.00002 0.00338

 D148 -3.13933 0.00000 0.00001 0.00001 0.00002 -3.13931

 D149 3.13885 0.00000 -0.00001 -0.00005 -0.00006 3.13879

 D150 -0.00389 0.00000 -0.00002 0.00000 -0.00001 -0.00390

 D151 0.02323 -0.00001 0.00014 -0.00008 0.00006 0.02329

 D152 -3.10550 -0.00001 0.00010 -0.00013 -0.00003 -3.10553

 D153 0.00426 0.00000 0.00002 -0.00005 -0.00003 0.00424

 D154 -3.13846 0.00000 0.00002 -0.00005 -0.00003 -3.13849

 D155 -3.13848 0.00000 0.00001 0.00001 0.00002 -3.13846

 D156 0.00198 0.00000 0.00001 0.00000 0.00002 0.00200

 D157 -0.00042 0.00000 0.00000 0.00001 0.00001 -0.00041

 D158 3.14052 0.00000 0.00001 0.00000 0.00001 3.14053

 D159 -3.14088 0.00000 0.00000 0.00001 0.00001 -3.14087

 D160 0.00005 0.00000 0.00000 0.00001 0.00001 0.00006

 D161 -0.00430 0.00000 -0.00002 0.00004 0.00002 -0.00428

 D162 3.13885 0.00000 0.00000 0.00001 0.00001 3.13886

 D163 3.13796 0.00000 -0.00003 0.00004 0.00001 3.13797

 D164 -0.00208 0.00000 -0.00001 0.00001 0.00001 -0.00207

 D165 -0.00426 0.00000 -0.00002 0.00005 0.00003 -0.00424

 D166 3.13846 0.00000 -0.00002 0.00005 0.00003 3.13849

 D167 3.13848 0.00000 -0.00001 -0.00001 -0.00002 3.13846

 D168 -0.00198 0.00000 -0.00001 0.00000 -0.00002 -0.00200

 D169 0.00042 0.00000 0.00000 -0.00001 -0.00001 0.00041

 D170 -3.14052 0.00000 -0.00001 0.00000 -0.00001 -3.14053

 D171 3.14088 0.00000 0.00000 -0.00001 -0.00001 3.14087

 D172 -0.00005 0.00000 0.00000 -0.00001 -0.00001 -0.00006

 D173 0.00430 0.00000 0.00002 -0.00004 -0.00002 0.00428

 D174 -3.13885 0.00000 0.00000 -0.00001 -0.00001 -3.13886

 D175 -3.13796 0.00000 0.00003 -0.00004 -0.00001 -3.13797

 D176 0.00208 0.00000 0.00001 -0.00001 -0.00001 0.00207

 D177 -0.00430 0.00000 -0.00002 0.00004 0.00002 -0.00428

 D178 3.13796 0.00000 -0.00003 0.00004 0.00001 3.13797

 D179 3.13885 0.00000 0.00000 0.00001 0.00001 3.13886

 D180 -0.00208 0.00000 -0.00001 0.00001 0.00001 -0.00207

 D181 -0.00042 0.00000 0.00000 0.00001 0.00001 -0.00041

 D182 -3.14088 0.00000 0.00000 0.00001 0.00001 -3.14087

 D183 3.14052 0.00000 0.00001 0.00000 0.00001 3.14053

 D184 0.00005 0.00000 0.00000 0.00001 0.00001 0.00006

 D185 0.00426 0.00000 0.00002 -0.00005 -0.00003 0.00424

 D186 -3.13848 0.00000 0.00001 0.00001 0.00002 -3.13846

 D187 -3.13846 0.00000 0.00002 -0.00005 -0.00003 -3.13849

 D188 0.00198 0.00000 0.00001 0.00000 0.00002 0.00200

 D189 -0.00426 0.00000 -0.00002 0.00005 0.00003 -0.00424

 D190 3.13846 0.00000 -0.00002 0.00005 0.00003 3.13849

 D191 3.13848 0.00000 -0.00001 -0.00001 -0.00002 3.13846

 D192 -0.00198 0.00000 -0.00001 0.00000 -0.00002 -0.00200

 D193 0.00042 0.00000 0.00000 -0.00001 -0.00001 0.00041

 D194 -3.14052 0.00000 -0.00001 0.00000 -0.00001 -3.14053

 D195 3.14088 0.00000 0.00000 -0.00001 -0.00001 3.14087

 D196 -0.00005 0.00000 0.00000 -0.00001 -0.00001 -0.00006

 D197 0.00430 0.00000 0.00002 -0.00004 -0.00002 0.00428

 D198 -3.13885 0.00000 0.00000 -0.00001 -0.00001 -3.13886

 D199 -3.13796 0.00000 0.00003 -0.00004 -0.00001 -3.13797

 D200 0.00208 0.00000 0.00001 -0.00001 -0.00001 0.00207

 Item Value Threshold Converged?

 Maximum Force 0.000023 0.000450 YES

 RMS Force 0.000006 0.000300 YES

 Maximum Displacement 0.001502 0.001800 YES

 RMS Displacement 0.000107 0.001200 YES

 Predicted change in Energy=-6.042976D-08

 Optimization completed.

 -- Stationary point found.

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 ! Optimized Parameters !

 ! (Angstroms and Degrees) !

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 ! Name Definition Value Derivative Info. !

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

 ! R1 R(1,2) 1.3556 -DE/DX = 0.0 !

 ! R2 R(1,5) 1.4638 -DE/DX = 0.0 !

 ! R3 R(1,12) 1.3426 -DE/DX = 0.0 !

 ! R4 R(2,3) 1.3862 -DE/DX = 0.0 !

 ! R5 R(2,25) 2.0555 -DE/DX = 0.0 !

 ! R6 R(3,4) 1.4538 -DE/DX = 0.0 !

 ! R7 R(3,6) 1.3296 -DE/DX = 0.0 !

 ! R8 R(4,5) 1.4184 -DE/DX = 0.0 !

 ! R9 R(4,41) 1.3976 -DE/DX = 0.0 !

 ! R10 R(5,38) 1.3945 -DE/DX = 0.0 !

 ! R11 R(6,7) 1.3296 -DE/DX = 0.0 !

 ! R12 R(7,8) 1.3862 -DE/DX = 0.0 !

 ! R13 R(7,11) 1.4538 -DE/DX = 0.0 !

 ! R14 R(8,9) 1.3556 -DE/DX = 0.0 !

 ! R15 R(8,25) 2.0555 -DE/DX = 0.0 !

 ! R16 R(9,10) 1.4638 -DE/DX = 0.0 !

 ! R17 R(9,24) 1.3426 -DE/DX = 0.0 !

 ! R18 R(10,11) 1.4184 -DE/DX = 0.0 !

 ! R19 R(10,37) 1.3945 -DE/DX = 0.0 !

 ! R20 R(11,34) 1.3976 -DE/DX = 0.0 !

 ! R21 R(12,17) 1.3426 -DE/DX = 0.0 !

 ! R22 R(13,14) 1.4184 -DE/DX = 0.0 !

 ! R23 R(13,17) 1.4638 -DE/DX = 0.0 !

 ! R24 R(13,26) 1.3945 -DE/DX = 0.0 !

 ! R25 R(14,15) 1.4538 -DE/DX = 0.0 !

 ! R26 R(14,29) 1.3976 -DE/DX = 0.0 !

 ! R27 R(15,16) 1.3862 -DE/DX = 0.0 !

 ! R28 R(15,18) 1.3296 -DE/DX = 0.0 !

 ! R29 R(16,17) 1.3556 -DE/DX = 0.0 !

 ! R30 R(16,25) 2.0555 -DE/DX = 0.0 !

 ! R31 R(18,20) 1.3296 -DE/DX = 0.0 !

 ! R32 R(19,20) 1.3862 -DE/DX = 0.0 !

 ! R33 R(19,23) 1.3556 -DE/DX = 0.0 !

 ! R34 R(19,25) 2.0555 -DE/DX = 0.0 !

 ! R35 R(20,21) 1.4538 -DE/DX = 0.0 !

 ! R36 R(21,22) 1.4184 -DE/DX = 0.0 !

 ! R37 R(21,33) 1.3976 -DE/DX = 0.0 !

 ! R38 R(22,23) 1.4638 -DE/DX = 0.0 !

 ! R39 R(22,30) 1.3945 -DE/DX = 0.0 !

 ! R40 R(23,24) 1.3426 -DE/DX = 0.0 !

 ! R41 R(26,27) 1.3922 -DE/DX = 0.0 !

 ! R42 R(26,42) 1.0851 -DE/DX = 0.0 !

 ! R43 R(27,28) 1.4078 -DE/DX = 0.0 !

 ! R44 R(27,54) 1.0849 -DE/DX = 0.0 !

 ! R45 R(28,29) 1.3911 -DE/DX = 0.0 !

 ! R46 R(28,55) 1.0852 -DE/DX = 0.0 !

 ! R47 R(29,43) 1.0851 -DE/DX = 0.0 !

 ! R48 R(30,31) 1.3922 -DE/DX = 0.0 !

 ! R49 R(30,44) 1.0851 -DE/DX = 0.0 !

 ! R50 R(31,32) 1.4078 -DE/DX = 0.0 !

 ! R51 R(31,57) 1.0849 -DE/DX = 0.0 !

 ! R52 R(32,33) 1.3911 -DE/DX = 0.0 !

 ! R53 R(32,56) 1.0852 -DE/DX = 0.0 !

 ! R54 R(33,45) 1.0851 -DE/DX = 0.0 !

 ! R55 R(34,35) 1.3911 -DE/DX = 0.0 !

 ! R56 R(34,46) 1.0851 -DE/DX = 0.0 !

 ! R57 R(35,36) 1.4078 -DE/DX = 0.0 !

 ! R58 R(35,50) 1.0852 -DE/DX = 0.0 !

 ! R59 R(36,37) 1.3922 -DE/DX = 0.0 !

 ! R60 R(36,51) 1.0849 -DE/DX = 0.0 !

 ! R61 R(37,47) 1.0851 -DE/DX = 0.0 !

 ! R62 R(38,39) 1.3922 -DE/DX = 0.0 !

 ! R63 R(38,48) 1.0851 -DE/DX = 0.0 !

 ! R64 R(39,40) 1.4078 -DE/DX = 0.0 !

 ! R65 R(39,53) 1.0849 -DE/DX = 0.0 !

 ! R66 R(40,41) 1.3911 -DE/DX = 0.0 !

 ! R67 R(40,52) 1.0852 -DE/DX = 0.0 !

 ! R68 R(41,49) 1.0851 -DE/DX = 0.0 !

 ! A1 A(2,1,5) 108.2785 -DE/DX = 0.0 !

 ! A2 A(2,1,12) 128.2024 -DE/DX = 0.0 !

 ! A3 A(5,1,12) 123.5158 -DE/DX = 0.0 !

 ! A4 A(1,2,3) 110.5469 -DE/DX = 0.0 !

 ! A5 A(1,2,25) 124.8388 -DE/DX = 0.0 !

 ! A6 A(3,2,25) 123.9163 -DE/DX = 0.0 !

 ! A7 A(2,3,4) 107.9084 -DE/DX = 0.0 !

 ! A8 A(2,3,6) 127.2722 -DE/DX = 0.0 !

 ! A9 A(4,3,6) 124.8117 -DE/DX = 0.0 !

 ! A10 A(3,4,5) 106.6113 -DE/DX = 0.0 !

 ! A11 A(3,4,41) 133.0061 -DE/DX = 0.0 !

 ! A12 A(5,4,41) 120.381 -DE/DX = 0.0 !

 ! A13 A(1,5,4) 106.6519 -DE/DX = 0.0 !

 ! A14 A(1,5,38) 132.4143 -DE/DX = 0.0 !

 ! A15 A(4,5,38) 120.9331 -DE/DX = 0.0 !

 ! A16 A(3,6,7) 126.3702 -DE/DX = 0.0 !

 ! A17 A(6,7,8) 127.2722 -DE/DX = 0.0 !

 ! A18 A(6,7,11) 124.8117 -DE/DX = 0.0 !

 ! A19 A(8,7,11) 107.9084 -DE/DX = 0.0 !

 ! A20 A(7,8,9) 110.5469 -DE/DX = 0.0 !

 ! A21 A(7,8,25) 123.9163 -DE/DX = 0.0 !

 ! A22 A(9,8,25) 124.8388 -DE/DX = 0.0 !

 ! A23 A(8,9,10) 108.2785 -DE/DX = 0.0 !

 ! A24 A(8,9,24) 128.2024 -DE/DX = 0.0 !

 ! A25 A(10,9,24) 123.5158 -DE/DX = 0.0 !

 ! A26 A(9,10,11) 106.6519 -DE/DX = 0.0 !

 ! A27 A(9,10,37) 132.4143 -DE/DX = 0.0 !

 ! A28 A(11,10,37) 120.9331 -DE/DX = 0.0 !

 ! A29 A(7,11,10) 106.6113 -DE/DX = 0.0 !

 ! A30 A(7,11,34) 133.0061 -DE/DX = 0.0 !

 ! A31 A(10,11,34) 120.381 -DE/DX = 0.0 !

 ! A32 A(1,12,17) 123.8522 -DE/DX = 0.0 !

 ! A33 A(14,13,17) 106.6519 -DE/DX = 0.0 !

 ! A34 A(14,13,26) 120.9331 -DE/DX = 0.0 !

 ! A35 A(17,13,26) 132.4143 -DE/DX = 0.0 !

 ! A36 A(13,14,15) 106.6113 -DE/DX = 0.0 !

 ! A37 A(13,14,29) 120.381 -DE/DX = 0.0 !

 ! A38 A(15,14,29) 133.0061 -DE/DX = 0.0 !

 ! A39 A(14,15,16) 107.9084 -DE/DX = 0.0 !

 ! A40 A(14,15,18) 124.8117 -DE/DX = 0.0 !

 ! A41 A(16,15,18) 127.2722 -DE/DX = 0.0 !

 ! A42 A(15,16,17) 110.5469 -DE/DX = 0.0 !

 ! A43 A(15,16,25) 123.9163 -DE/DX = 0.0 !

 ! A44 A(17,16,25) 124.8388 -DE/DX = 0.0 !

 ! A45 A(12,17,13) 123.5158 -DE/DX = 0.0 !

 ! A46 A(12,17,16) 128.2024 -DE/DX = 0.0 !

 ! A47 A(13,17,16) 108.2785 -DE/DX = 0.0 !

 ! A48 A(15,18,20) 126.3702 -DE/DX = 0.0 !

 ! A49 A(20,19,23) 110.5469 -DE/DX = 0.0 !

 ! A50 A(20,19,25) 123.9163 -DE/DX = 0.0 !

 ! A51 A(23,19,25) 124.8388 -DE/DX = 0.0 !

 ! A52 A(18,20,19) 127.2722 -DE/DX = 0.0 !

 ! A53 A(18,20,21) 124.8117 -DE/DX = 0.0 !

 ! A54 A(19,20,21) 107.9084 -DE/DX = 0.0 !

 ! A55 A(20,21,22) 106.6113 -DE/DX = 0.0 !

 ! A56 A(20,21,33) 133.0061 -DE/DX = 0.0 !

 ! A57 A(22,21,33) 120.381 -DE/DX = 0.0 !

 ! A58 A(21,22,23) 106.6519 -DE/DX = 0.0 !

 ! A59 A(21,22,30) 120.9331 -DE/DX = 0.0 !

 ! A60 A(23,22,30) 132.4143 -DE/DX = 0.0 !

 ! A61 A(19,23,22) 108.2785 -DE/DX = 0.0 !

 ! A62 A(19,23,24) 128.2024 -DE/DX = 0.0 !

 ! A63 A(22,23,24) 123.5158 -DE/DX = 0.0 !

 ! A64 A(9,24,23) 123.8522 -DE/DX = 0.0 !

 ! A65 A(2,25,8) 88.8078 -DE/DX = 0.0 !

 ! A66 A(2,25,16) 87.6317 -DE/DX = 0.0 !

 ! A67 A(2,25,19) 159.6972 -DE/DX = 0.0 !

 ! A68 A(8,25,16) 159.6972 -DE/DX = 0.0 !

 ! A69 A(8,25,19) 87.6317 -DE/DX = 0.0 !

 ! A70 A(16,25,19) 88.8078 -DE/DX = 0.0 !

 ! A71 A(13,26,27) 118.3245 -DE/DX = 0.0 !

 ! A72 A(13,26,42) 120.682 -DE/DX = 0.0 !

 ! A73 A(27,26,42) 120.9935 -DE/DX = 0.0 !

 ! A74 A(26,27,28) 120.8135 -DE/DX = 0.0 !

 ! A75 A(26,27,54) 119.8095 -DE/DX = 0.0 !

 ! A76 A(28,27,54) 119.3769 -DE/DX = 0.0 !

 ! A77 A(27,28,29) 121.221 -DE/DX = 0.0 !

 ! A78 A(27,28,55) 119.2116 -DE/DX = 0.0 !

 ! A79 A(29,28,55) 119.5674 -DE/DX = 0.0 !

 ! A80 A(14,29,28) 118.3259 -DE/DX = 0.0 !

 ! A81 A(14,29,43) 120.7665 -DE/DX = 0.0 !

 ! A82 A(28,29,43) 120.9075 -DE/DX = 0.0 !

 ! A83 A(22,30,31) 118.3245 -DE/DX = 0.0 !

 ! A84 A(22,30,44) 120.682 -DE/DX = 0.0 !

 ! A85 A(31,30,44) 120.9935 -DE/DX = 0.0 !

 ! A86 A(30,31,32) 120.8135 -DE/DX = 0.0 !

 ! A87 A(30,31,57) 119.8095 -DE/DX = 0.0 !

 ! A88 A(32,31,57) 119.3769 -DE/DX = 0.0 !

 ! A89 A(31,32,33) 121.221 -DE/DX = 0.0 !

 ! A90 A(31,32,56) 119.2116 -DE/DX = 0.0 !

 ! A91 A(33,32,56) 119.5674 -DE/DX = 0.0 !

 ! A92 A(21,33,32) 118.3259 -DE/DX = 0.0 !

 ! A93 A(21,33,45) 120.7665 -DE/DX = 0.0 !

 ! A94 A(32,33,45) 120.9075 -DE/DX = 0.0 !

 ! A95 A(11,34,35) 118.3259 -DE/DX = 0.0 !

 ! A96 A(11,34,46) 120.7665 -DE/DX = 0.0 !

 ! A97 A(35,34,46) 120.9075 -DE/DX = 0.0 !

 ! A98 A(34,35,36) 121.221 -DE/DX = 0.0 !

 ! A99 A(34,35,50) 119.5674 -DE/DX = 0.0 !

 ! A100 A(36,35,50) 119.2116 -DE/DX = 0.0 !

 ! A101 A(35,36,37) 120.8135 -DE/DX = 0.0 !

 ! A102 A(35,36,51) 119.3769 -DE/DX = 0.0 !

 ! A103 A(37,36,51) 119.8095 -DE/DX = 0.0 !

 ! A104 A(10,37,36) 118.3245 -DE/DX = 0.0 !

 ! A105 A(10,37,47) 120.682 -DE/DX = 0.0 !

 ! A106 A(36,37,47) 120.9935 -DE/DX = 0.0 !

 ! A107 A(5,38,39) 118.3245 -DE/DX = 0.0 !

 ! A108 A(5,38,48) 120.682 -DE/DX = 0.0 !

 ! A109 A(39,38,48) 120.9935 -DE/DX = 0.0 !

 ! A110 A(38,39,40) 120.8135 -DE/DX = 0.0 !

 ! A111 A(38,39,53) 119.8095 -DE/DX = 0.0 !

 ! A112 A(40,39,53) 119.3769 -DE/DX = 0.0 !

 ! A113 A(39,40,41) 121.221 -DE/DX = 0.0 !

 ! A114 A(39,40,52) 119.2116 -DE/DX = 0.0 !

 ! A115 A(41,40,52) 119.5674 -DE/DX = 0.0 !

 ! A116 A(4,41,40) 118.3259 -DE/DX = 0.0 !

 ! A117 A(4,41,49) 120.7665 -DE/DX = 0.0 !

 ! A118 A(40,41,49) 120.9075 -DE/DX = 0.0 !

 ! D1 D(5,1,2,3) 0.5252 -DE/DX = 0.0 !

 ! D2 D(5,1,2,25) -170.1905 -DE/DX = 0.0 !

 ! D3 D(12,1,2,3) -178.8274 -DE/DX = 0.0 !

 ! D4 D(12,1,2,25) 10.4569 -DE/DX = 0.0 !

 ! D5 D(2,1,5,4) -0.2876 -DE/DX = 0.0 !

 ! D6 D(2,1,5,38) -179.9721 -DE/DX = 0.0 !

 ! D7 D(12,1,5,4) 179.1022 -DE/DX = 0.0 !

 ! D8 D(12,1,5,38) -0.5823 -DE/DX = 0.0 !

 ! D9 D(2,1,12,17) 1.3309 -DE/DX = 0.0 !

 ! D10 D(5,1,12,17) -177.9318 -DE/DX = 0.0 !

 ! D11 D(1,2,3,4) -0.5537 -DE/DX = 0.0 !

 ! D12 D(1,2,3,6) 178.4686 -DE/DX = 0.0 !

 ! D13 D(25,2,3,4) 170.2647 -DE/DX = 0.0 !

 ! D14 D(25,2,3,6) -10.7131 -DE/DX = 0.0 !

 ! D15 D(1,2,25,8) -175.2252 -DE/DX = 0.0 !

 ! D16 D(1,2,25,16) -15.2177 -DE/DX = 0.0 !

 ! D17 D(1,2,25,19) -95.3251 -DE/DX = 0.0 !

 ! D18 D(3,2,25,8) 15.2636 -DE/DX = 0.0 !

 ! D19 D(3,2,25,16) 175.2712 -DE/DX = 0.0 !

 ! D20 D(3,2,25,19) 95.1637 -DE/DX = 0.0 !

 ! D21 D(2,3,4,5) 0.3538 -DE/DX = 0.0 !

 ! D22 D(2,3,4,41) 179.893 -DE/DX = 0.0 !

 ! D23 D(6,3,4,5) -178.6986 -DE/DX = 0.0 !

 ! D24 D(6,3,4,41) 0.8406 -DE/DX = 0.0 !

 ! D25 D(2,3,6,7) -0.6826 -DE/DX = 0.0 !

 ! D26 D(4,3,6,7) 178.1842 -DE/DX = 0.0 !

 ! D27 D(3,4,5,1) -0.0443 -DE/DX = 0.0 !

 ! D28 D(3,4,5,38) 179.6842 -DE/DX = 0.0 !

 ! D29 D(41,4,5,1) -179.6537 -DE/DX = 0.0 !

 ! D30 D(41,4,5,38) 0.0748 -DE/DX = 0.0 !

 ! D31 D(3,4,41,40) -179.7813 -DE/DX = 0.0 !

 ! D32 D(3,4,41,49) 0.3077 -DE/DX = 0.0 !

 ! D33 D(5,4,41,40) -0.2931 -DE/DX = 0.0 !

 ! D34 D(5,4,41,49) 179.7958 -DE/DX = 0.0 !

 ! D35 D(1,5,38,39) 179.8429 -DE/DX = 0.0 !

 ! D36 D(1,5,38,48) -0.2226 -DE/DX = 0.0 !

 ! D37 D(4,5,38,39) 0.1952 -DE/DX = 0.0 !

 ! D38 D(4,5,38,48) -179.8703 -DE/DX = 0.0 !

 ! D39 D(3,6,7,8) 0.6826 -DE/DX = 0.0 !

 ! D40 D(3,6,7,11) -178.1842 -DE/DX = 0.0 !

 ! D41 D(6,7,8,9) -178.4686 -DE/DX = 0.0 !

 ! D42 D(6,7,8,25) 10.7131 -DE/DX = 0.0 !

 ! D43 D(11,7,8,9) 0.5537 -DE/DX = 0.0 !

 ! D44 D(11,7,8,25) -170.2647 -DE/DX = 0.0 !

 ! D45 D(6,7,11,10) 178.6986 -DE/DX = 0.0 !

 ! D46 D(6,7,11,34) -0.8406 -DE/DX = 0.0 !

 ! D47 D(8,7,11,10) -0.3538 -DE/DX = 0.0 !

 ! D48 D(8,7,11,34) -179.893 -DE/DX = 0.0 !

 ! D49 D(7,8,9,10) -0.5252 -DE/DX = 0.0 !

 ! D50 D(7,8,9,24) 178.8274 -DE/DX = 0.0 !

 ! D51 D(25,8,9,10) 170.1905 -DE/DX = 0.0 !

 ! D52 D(25,8,9,24) -10.4569 -DE/DX = 0.0 !

 ! D53 D(7,8,25,2) -15.2636 -DE/DX = 0.0 !

 ! D54 D(7,8,25,16) -95.1637 -DE/DX = 0.0 !

 ! D55 D(7,8,25,19) -175.2712 -DE/DX = 0.0 !

 ! D56 D(9,8,25,2) 175.2252 -DE/DX = 0.0 !

 ! D57 D(9,8,25,16) 95.3251 -DE/DX = 0.0 !

 ! D58 D(9,8,25,19) 15.2177 -DE/DX = 0.0 !

 ! D59 D(8,9,10,11) 0.2876 -DE/DX = 0.0 !

 ! D60 D(8,9,10,37) 179.9721 -DE/DX = 0.0 !

 ! D61 D(24,9,10,11) -179.1022 -DE/DX = 0.0 !

 ! D62 D(24,9,10,37) 0.5823 -DE/DX = 0.0 !

 ! D63 D(8,9,24,23) -1.3309 -DE/DX = 0.0 !

 ! D64 D(10,9,24,23) 177.9318 -DE/DX = 0.0 !

 ! D65 D(9,10,11,7) 0.0443 -DE/DX = 0.0 !

 ! D66 D(9,10,11,34) 179.6537 -DE/DX = 0.0 !

 ! D67 D(37,10,11,7) -179.6842 -DE/DX = 0.0 !

 ! D68 D(37,10,11,34) -0.0748 -DE/DX = 0.0 !

 ! D69 D(9,10,37,36) -179.8429 -DE/DX = 0.0 !

 ! D70 D(9,10,37,47) 0.2226 -DE/DX = 0.0 !

 ! D71 D(11,10,37,36) -0.1952 -DE/DX = 0.0 !

 ! D72 D(11,10,37,47) 179.8703 -DE/DX = 0.0 !

 ! D73 D(7,11,34,35) 179.7813 -DE/DX = 0.0 !

 ! D74 D(7,11,34,46) -0.3077 -DE/DX = 0.0 !

 ! D75 D(10,11,34,35) 0.2931 -DE/DX = 0.0 !

 ! D76 D(10,11,34,46) -179.7958 -DE/DX = 0.0 !

 ! D77 D(1,12,17,13) 177.9318 -DE/DX = 0.0 !

 ! D78 D(1,12,17,16) -1.3309 -DE/DX = 0.0 !

 ! D79 D(17,13,14,15) 0.0443 -DE/DX = 0.0 !

 ! D80 D(17,13,14,29) 179.6537 -DE/DX = 0.0 !

 ! D81 D(26,13,14,15) -179.6842 -DE/DX = 0.0 !

 ! D82 D(26,13,14,29) -0.0748 -DE/DX = 0.0 !

 ! D83 D(14,13,17,12) -179.1022 -DE/DX = 0.0 !

 ! D84 D(14,13,17,16) 0.2876 -DE/DX = 0.0 !

 ! D85 D(26,13,17,12) 0.5823 -DE/DX = 0.0 !

 ! D86 D(26,13,17,16) 179.9721 -DE/DX = 0.0 !

 ! D87 D(14,13,26,27) -0.1952 -DE/DX = 0.0 !

 ! D88 D(14,13,26,42) 179.8703 -DE/DX = 0.0 !

 ! D89 D(17,13,26,27) -179.8429 -DE/DX = 0.0 !

 ! D90 D(17,13,26,42) 0.2226 -DE/DX = 0.0 !

 ! D91 D(13,14,15,16) -0.3538 -DE/DX = 0.0 !

 ! D92 D(13,14,15,18) 178.6986 -DE/DX = 0.0 !

 ! D93 D(29,14,15,16) -179.893 -DE/DX = 0.0 !

 ! D94 D(29,14,15,18) -0.8406 -DE/DX = 0.0 !

 ! D95 D(13,14,29,28) 0.2931 -DE/DX = 0.0 !

 ! D96 D(13,14,29,43) -179.7958 -DE/DX = 0.0 !

 ! D97 D(15,14,29,28) 179.7813 -DE/DX = 0.0 !

 ! D98 D(15,14,29,43) -0.3077 -DE/DX = 0.0 !

 ! D99 D(14,15,16,17) 0.5537 -DE/DX = 0.0 !

 ! D100 D(14,15,16,25) -170.2647 -DE/DX = 0.0 !

 ! D101 D(18,15,16,17) -178.4686 -DE/DX = 0.0 !

 ! D102 D(18,15,16,25) 10.7131 -DE/DX = 0.0 !

 ! D103 D(14,15,18,20) -178.1842 -DE/DX = 0.0 !

 ! D104 D(16,15,18,20) 0.6826 -DE/DX = 0.0 !

 ! D105 D(15,16,17,12) 178.8274 -DE/DX = 0.0 !

 ! D106 D(15,16,17,13) -0.5252 -DE/DX = 0.0 !

 ! D107 D(25,16,17,12) -10.4569 -DE/DX = 0.0 !

 ! D108 D(25,16,17,13) 170.1905 -DE/DX = 0.0 !

 ! D109 D(15,16,25,2) -175.2712 -DE/DX = 0.0 !

 ! D110 D(15,16,25,8) -95.1637 -DE/DX = 0.0 !

 ! D111 D(15,16,25,19) -15.2636 -DE/DX = 0.0 !

 ! D112 D(17,16,25,2) 15.2177 -DE/DX = 0.0 !

 ! D113 D(17,16,25,8) 95.3251 -DE/DX = 0.0 !

 ! D114 D(17,16,25,19) 175.2252 -DE/DX = 0.0 !

 ! D115 D(15,18,20,19) -0.6826 -DE/DX = 0.0 !

 ! D116 D(15,18,20,21) 178.1842 -DE/DX = 0.0 !

 ! D117 D(23,19,20,18) 178.4686 -DE/DX = 0.0 !

 ! D118 D(23,19,20,21) -0.5537 -DE/DX = 0.0 !

 ! D119 D(25,19,20,18) -10.7131 -DE/DX = 0.0 !

 ! D120 D(25,19,20,21) 170.2647 -DE/DX = 0.0 !

 ! D121 D(20,19,23,22) 0.5252 -DE/DX = 0.0 !

 ! D122 D(20,19,23,24) -178.8274 -DE/DX = 0.0 !

 ! D123 D(25,19,23,22) -170.1905 -DE/DX = 0.0 !

 ! D124 D(25,19,23,24) 10.4569 -DE/DX = 0.0 !

 ! D125 D(20,19,25,2) 95.1637 -DE/DX = 0.0 !

 ! D126 D(20,19,25,8) 175.2712 -DE/DX = 0.0 !

 ! D127 D(20,19,25,16) 15.2636 -DE/DX = 0.0 !

 ! D128 D(23,19,25,2) -95.3251 -DE/DX = 0.0 !

 ! D129 D(23,19,25,8) -15.2177 -DE/DX = 0.0 !

 ! D130 D(23,19,25,16) -175.2252 -DE/DX = 0.0 !

 ! D131 D(18,20,21,22) -178.6986 -DE/DX = 0.0 !

 ! D132 D(18,20,21,33) 0.8406 -DE/DX = 0.0 !

 ! D133 D(19,20,21,22) 0.3538 -DE/DX = 0.0 !

 ! D134 D(19,20,21,33) 179.893 -DE/DX = 0.0 !

 ! D135 D(20,21,22,23) -0.0443 -DE/DX = 0.0 !

 ! D136 D(20,21,22,30) 179.6842 -DE/DX = 0.0 !

 ! D137 D(33,21,22,23) -179.6537 -DE/DX = 0.0 !

 ! D138 D(33,21,22,30) 0.0748 -DE/DX = 0.0 !

 ! D139 D(20,21,33,32) -179.7813 -DE/DX = 0.0 !

 ! D140 D(20,21,33,45) 0.3077 -DE/DX = 0.0 !

 ! D141 D(22,21,33,32) -0.2931 -DE/DX = 0.0 !

 ! D142 D(22,21,33,45) 179.7958 -DE/DX = 0.0 !

 ! D143 D(21,22,23,19) -0.2876 -DE/DX = 0.0 !

 ! D144 D(21,22,23,24) 179.1022 -DE/DX = 0.0 !

 ! D145 D(30,22,23,19) -179.9721 -DE/DX = 0.0 !

 ! D146 D(30,22,23,24) -0.5823 -DE/DX = 0.0 !

 ! D147 D(21,22,30,31) 0.1952 -DE/DX = 0.0 !

 ! D148 D(21,22,30,44) -179.8703 -DE/DX = 0.0 !

 ! D149 D(23,22,30,31) 179.8429 -DE/DX = 0.0 !

 ! D150 D(23,22,30,44) -0.2226 -DE/DX = 0.0 !

 ! D151 D(19,23,24,9) 1.3309 -DE/DX = 0.0 !

 ! D152 D(22,23,24,9) -177.9318 -DE/DX = 0.0 !

 ! D153 D(13,26,27,28) 0.2442 -DE/DX = 0.0 !

 ! D154 D(13,26,27,54) -179.8206 -DE/DX = 0.0 !

 ! D155 D(42,26,27,28) -179.8215 -DE/DX = 0.0 !

 ! D156 D(42,26,27,54) 0.1137 -DE/DX = 0.0 !

 ! D157 D(26,27,28,29) -0.0238 -DE/DX = 0.0 !

 ! D158 D(26,27,28,55) 179.9383 -DE/DX = 0.0 !

 ! D159 D(54,27,28,29) -179.9593 -DE/DX = 0.0 !

 ! D160 D(54,27,28,55) 0.0029 -DE/DX = 0.0 !

 ! D161 D(27,28,29,14) -0.2463 -DE/DX = 0.0 !

 ! D162 D(27,28,29,43) 179.8428 -DE/DX = 0.0 !

 ! D163 D(55,28,29,14) 179.7917 -DE/DX = 0.0 !

 ! D164 D(55,28,29,43) -0.1192 -DE/DX = 0.0 !

 ! D165 D(22,30,31,32) -0.2442 -DE/DX = 0.0 !

 ! D166 D(22,30,31,57) 179.8206 -DE/DX = 0.0 !

 ! D167 D(44,30,31,32) 179.8215 -DE/DX = 0.0 !

 ! D168 D(44,30,31,57) -0.1137 -DE/DX = 0.0 !

 ! D169 D(30,31,32,33) 0.0238 -DE/DX = 0.0 !

 ! D170 D(30,31,32,56) -179.9383 -DE/DX = 0.0 !

 ! D171 D(57,31,32,33) 179.9593 -DE/DX = 0.0 !

 ! D172 D(57,31,32,56) -0.0029 -DE/DX = 0.0 !

 ! D173 D(31,32,33,21) 0.2463 -DE/DX = 0.0 !

 ! D174 D(31,32,33,45) -179.8428 -DE/DX = 0.0 !

 ! D175 D(56,32,33,21) -179.7917 -DE/DX = 0.0 !

 ! D176 D(56,32,33,45) 0.1192 -DE/DX = 0.0 !

 ! D177 D(11,34,35,36) -0.2463 -DE/DX = 0.0 !

 ! D178 D(11,34,35,50) 179.7917 -DE/DX = 0.0 !

 ! D179 D(46,34,35,36) 179.8428 -DE/DX = 0.0 !

 ! D180 D(46,34,35,50) -0.1192 -DE/DX = 0.0 !

 ! D181 D(34,35,36,37) -0.0238 -DE/DX = 0.0 !

 ! D182 D(34,35,36,51) -179.9593 -DE/DX = 0.0 !

 ! D183 D(50,35,36,37) 179.9383 -DE/DX = 0.0 !

 ! D184 D(50,35,36,51) 0.0029 -DE/DX = 0.0 !

 ! D185 D(35,36,37,10) 0.2442 -DE/DX = 0.0 !

 ! D186 D(35,36,37,47) -179.8215 -DE/DX = 0.0 !

 ! D187 D(51,36,37,10) -179.8206 -DE/DX = 0.0 !

 ! D188 D(51,36,37,47) 0.1137 -DE/DX = 0.0 !

 ! D189 D(5,38,39,40) -0.2442 -DE/DX = 0.0 !

 ! D190 D(5,38,39,53) 179.8206 -DE/DX = 0.0 !

 ! D191 D(48,38,39,40) 179.8215 -DE/DX = 0.0 !

 ! D192 D(48,38,39,53) -0.1137 -DE/DX = 0.0 !

 ! D193 D(38,39,40,41) 0.0238 -DE/DX = 0.0 !

 ! D194 D(38,39,40,52) -179.9383 -DE/DX = 0.0 !

 ! D195 D(53,39,40,41) 179.9593 -DE/DX = 0.0 !

 ! D196 D(53,39,40,52) -0.0029 -DE/DX = 0.0 !

 ! D197 D(39,40,41,4) 0.2463 -DE/DX = 0.0 !

 ! D198 D(39,40,41,49) -179.8428 -DE/DX = 0.0 !

 ! D199 D(52,40,41,4) -179.7917 -DE/DX = 0.0 !

 ! D200 D(52,40,41,49) 0.1192 -DE/DX = 0.0 !

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 Lowest energy point so far. Saving SCF results.

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Largest change from initial coordinates is atom 51 0.031 Angstoms.

 Leave Link 103 at Sat Jun 15 12:23:02 2019, MaxMem= 1342177280 cpu: 11.0

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

 Stoichiometry C32H16N8Zn(1-,2)

 Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C32H16N4)]

 Deg. of freedom 43

 Full point group C2V NOp 4

 RotChk: IX=0 Diff= 5.47D-17

 Largest Abelian subgroup C2V NOp 4

 Largest concise Abelian subgroup C2V NOp 4

 Standard orientation:

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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

 1 6 0 2.772273 1.184599 0.011272

 2 7 0 1.438273 1.423126 0.046118

 3 6 0 1.186644 2.785828 0.011707

 4 6 0 2.465490 3.475468 -0.036881

 5 6 0 3.467672 2.471738 -0.038040

 6 7 0 0.000000 3.385559 0.002346

 7 6 0 -1.186644 2.785828 0.011707

 8 7 0 -1.438273 1.423126 0.046118

 9 6 0 -2.772273 1.184599 0.011272

 10 6 0 -3.467672 2.471738 -0.038040

 11 6 0 -2.465490 3.475468 -0.036881

 12 7 0 3.404078 0.000000 0.006486

 13 6 0 3.467672 -2.471738 -0.038040

 14 6 0 2.465490 -3.475468 -0.036881

 15 6 0 1.186644 -2.785828 0.011707

 16 7 0 1.438273 -1.423126 0.046118

 17 6 0 2.772273 -1.184599 0.011272

 18 7 0 0.000000 -3.385559 0.002346

 19 7 0 -1.438273 -1.423126 0.046118

 20 6 0 -1.186644 -2.785828 0.011707

 21 6 0 -2.465490 -3.475468 -0.036881

 22 6 0 -3.467672 -2.471738 -0.038040

 23 6 0 -2.772273 -1.184599 0.011272

 24 7 0 -3.404078 0.000000 0.006486

 25 30 0 0.000000 0.000000 0.408403

 26 6 0 4.819867 -2.808971 -0.086640

 27 6 0 5.163187 -4.157451 -0.129918

 28 6 0 4.169683 -5.154917 -0.129873

 29 6 0 2.818508 -4.826834 -0.086274

 30 6 0 -4.819867 -2.808971 -0.086640

 31 6 0 -5.163187 -4.157451 -0.129918

 32 6 0 -4.169683 -5.154917 -0.129873

 33 6 0 -2.818508 -4.826834 -0.086274

 34 6 0 -2.818508 4.826834 -0.086274

 35 6 0 -4.169683 5.154917 -0.129873

 36 6 0 -5.163187 4.157451 -0.129918

 37 6 0 -4.819867 2.808971 -0.086640

 38 6 0 4.819867 2.808971 -0.086640

 39 6 0 5.163187 4.157451 -0.129918

 40 6 0 4.169683 5.154917 -0.129873

 41 6 0 2.818508 4.826834 -0.086274

 42 1 0 5.583123 -2.037692 -0.089448

 43 1 0 2.056911 -5.599739 -0.089010

 44 1 0 -5.583123 -2.037692 -0.089448

 45 1 0 -2.056911 -5.599739 -0.089010

 46 1 0 -2.056911 5.599739 -0.089010

 47 1 0 -5.583123 2.037692 -0.089448

 48 1 0 5.583123 2.037692 -0.089448

 49 1 0 2.056911 5.599739 -0.089010

 50 1 0 -4.466568 6.198153 -0.165178

 51 1 0 -6.208147 4.447087 -0.165237

 52 1 0 4.466568 6.198153 -0.165178

 53 1 0 6.208147 4.447087 -0.165237

 54 1 0 6.208147 -4.447087 -0.165237

 55 1 0 4.466568 -6.198153 -0.165178

 56 1 0 -4.466568 -6.198153 -0.165178

 57 1 0 -6.208147 -4.447087 -0.165237

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 Rotational constants (GHZ): 0.0880319 0.0879157 0.0440907

 Leave Link 202 at Sat Jun 15 12:23:03 2019, MaxMem= 1342177280 cpu: 3.1

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

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

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

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

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

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

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

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

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 The electronic state is 2-B1.

 Alpha occ. eigenvalues -- -14.30461 -14.30461 -14.29732 -14.29732 -14.29732

 Alpha occ. eigenvalues -- -14.29732 -14.29148 -14.29147 -10.23122 -10.23122

 Alpha occ. eigenvalues -- -10.23122 -10.23122 -10.22296 -10.22296 -10.22296

 Alpha occ. eigenvalues -- -10.22296 -10.17267 -10.17267 -10.17267 -10.17267

 Alpha occ. eigenvalues -- -10.17202 -10.17201 -10.17201 -10.17201 -10.17140

 Alpha occ. eigenvalues -- -10.17139 -10.17139 -10.17139 -10.17011 -10.17011

 Alpha occ. eigenvalues -- -10.17011 -10.17011 -10.17002 -10.17002 -10.17002

 Alpha occ. eigenvalues -- -10.17001 -10.16850 -10.16850 -10.16850 -10.16850

 Alpha occ. eigenvalues -- -0.98706 -0.97352 -0.97337 -0.94680 -0.92521

 Alpha occ. eigenvalues -- -0.88821 -0.88259 -0.85726 -0.84614 -0.84610

 Alpha occ. eigenvalues -- -0.84573 -0.84257 -0.76486 -0.75246 -0.75158

 Alpha occ. eigenvalues -- -0.74993 -0.74756 -0.74698 -0.74645 -0.74497

 Alpha occ. eigenvalues -- -0.70964 -0.68423 -0.67777 -0.62853 -0.62470

 Alpha occ. eigenvalues -- -0.61925 -0.61901 -0.61611 -0.60902 -0.58665

 Alpha occ. eigenvalues -- -0.58546 -0.58110 -0.57725 -0.56773 -0.55772

 Alpha occ. eigenvalues -- -0.55279 -0.55246 -0.54143 -0.53866 -0.53811

 Alpha occ. eigenvalues -- -0.53659 -0.51859 -0.51553 -0.51418 -0.48647

 Alpha occ. eigenvalues -- -0.48399 -0.47106 -0.47083 -0.46273 -0.45671

 Alpha occ. eigenvalues -- -0.45669 -0.45272 -0.45230 -0.44888 -0.43400

 Alpha occ. eigenvalues -- -0.43352 -0.43341 -0.43241 -0.43234 -0.43198

 Alpha occ. eigenvalues -- -0.42118 -0.41613 -0.41468 -0.40898 -0.40826

 Alpha occ. eigenvalues -- -0.37366 -0.37309 -0.36378 -0.36073 -0.36007

 Alpha occ. eigenvalues -- -0.35943 -0.35915 -0.35795 -0.35280 -0.34535

 Alpha occ. eigenvalues -- -0.34018 -0.33918 -0.33872 -0.33307 -0.31661

 Alpha occ. eigenvalues -- -0.31620 -0.31083 -0.30984 -0.29510 -0.27496

 Alpha occ. eigenvalues -- -0.26774 -0.26601 -0.25583 -0.25478 -0.25373

 Alpha occ. eigenvalues -- -0.25010 -0.24981 -0.24861 -0.24239 -0.24184

 Alpha occ. eigenvalues -- -0.24170 -0.23976 -0.18115 -0.12791

 Alpha virt. eigenvalues -- -0.09006 -0.04265 -0.02618 -0.02158 -0.01921

 Alpha virt. eigenvalues -- -0.01847 0.02694 0.02822 0.03140 0.03142

 Alpha virt. eigenvalues -- 0.05261 0.05269 0.05862 0.05871 0.06207

 Alpha virt. eigenvalues -- 0.07099 0.07101 0.07152 0.07281 0.07710

 Alpha virt. eigenvalues -- 0.09095 0.09108 0.10054 0.10783 0.11761

 Alpha virt. eigenvalues -- 0.11826 0.12102 0.12109 0.12730 0.13098

 Alpha virt. eigenvalues -- 0.14689 0.15358 0.15495 0.16279 0.17663

 Alpha virt. eigenvalues -- 0.18239 0.18311 0.18375 0.19642 0.20751

 Alpha virt. eigenvalues -- 0.20906 0.21678 0.22170 0.22300 0.23126

 Alpha virt. eigenvalues -- 0.24247 0.24256 0.24428 0.24721 0.25284

 Alpha virt. eigenvalues -- 0.25560 0.25955 0.27116 0.27177 0.27686

 Alpha virt. eigenvalues -- 0.27759 0.28084 0.28251 0.28942 0.28954

 Alpha virt. eigenvalues -- 0.29011 0.29070 0.29512 0.30494 0.30747

 Alpha virt. eigenvalues -- 0.31093 0.31118 0.32423 0.33356 0.33580

 Alpha virt. eigenvalues -- 0.34309 0.34821 0.35724 0.35745 0.36386

 Alpha virt. eigenvalues -- 0.36619 0.37092 0.37369 0.38134 0.38207

 Alpha virt. eigenvalues -- 0.38774 0.39263 0.39273 0.39918 0.39928

 Alpha virt. eigenvalues -- 0.40216 0.40929 0.41035 0.41052 0.41115

 Alpha virt. eigenvalues -- 0.41338 0.41761 0.42048 0.42297 0.42606

 Alpha virt. eigenvalues -- 0.42747 0.42992 0.43068 0.43110 0.43601

 Alpha virt. eigenvalues -- 0.43603 0.43648 0.43649 0.43735 0.43757

 Alpha virt. eigenvalues -- 0.43839 0.43964 0.44261 0.44392 0.45905

 Alpha virt. eigenvalues -- 0.46040 0.47062 0.47201 0.47424 0.47494

 Alpha virt. eigenvalues -- 0.47922 0.47958 0.48267 0.48490 0.48957

 Alpha virt. eigenvalues -- 0.50349 0.50473 0.50771 0.51216 0.51599

 Alpha virt. eigenvalues -- 0.51695 0.51990 0.52050 0.52326 0.52418

 Alpha virt. eigenvalues -- 0.52538 0.53826 0.54483 0.54542 0.54738

 Alpha virt. eigenvalues -- 0.55206 0.56274 0.56297 0.57270 0.59028

 Alpha virt. eigenvalues -- 0.60314 0.60514 0.60871 0.60880 0.60933

 Alpha virt. eigenvalues -- 0.61051 0.61058 0.61450 0.61508 0.61525

 Alpha virt. eigenvalues -- 0.61978 0.62370 0.62456 0.63383 0.63508

 Alpha virt. eigenvalues -- 0.63519 0.63639 0.64193 0.64985 0.65133

 Alpha virt. eigenvalues -- 0.65314 0.65379 0.65436 0.66665 0.67307

 Alpha virt. eigenvalues -- 0.67491 0.67603 0.68148 0.68200 0.69982

 Alpha virt. eigenvalues -- 0.70423 0.70464 0.70762 0.71079 0.71245

 Alpha virt. eigenvalues -- 0.71471 0.72382 0.72673 0.73843 0.74087

 Alpha virt. eigenvalues -- 0.74421 0.74722 0.75168 0.75474 0.76760

 Alpha virt. eigenvalues -- 0.77624 0.77953 0.77957 0.78118 0.78251

 Alpha virt. eigenvalues -- 0.78743 0.78877 0.79768 0.80395 0.80449

 Alpha virt. eigenvalues -- 0.80521 0.80563 0.80876 0.82014 0.82498

 Alpha virt. eigenvalues -- 0.82551 0.82573 0.83549 0.83913 0.84709

 Alpha virt. eigenvalues -- 0.84852 0.86814 0.87070 0.87329 0.87442

 Alpha virt. eigenvalues -- 0.87579 0.88851 0.89382 0.89499 0.90168

 Alpha virt. eigenvalues -- 0.90727 0.91278 0.91554 0.91789 0.92011

 Alpha virt. eigenvalues -- 0.92762 0.92942 0.93259 0.94589 0.95204

 Alpha virt. eigenvalues -- 0.96660 0.98142 0.99726 0.99808 0.99862

 Alpha virt. eigenvalues -- 1.00286 1.00513 1.00566 1.00662 1.01210

 Alpha virt. eigenvalues -- 1.02748 1.02779 1.02967 1.03740 1.03813

 Alpha virt. eigenvalues -- 1.06295 1.06405 1.06563 1.07613 1.10875

 Alpha virt. eigenvalues -- 1.11275 1.11394 1.11500 1.11671 1.12133

 Alpha virt. eigenvalues -- 1.12572 1.12677 1.12950 1.14316 1.14521

 Alpha virt. eigenvalues -- 1.14982 1.15035 1.15306 1.15531 1.16267

 Alpha virt. eigenvalues -- 1.17294 1.19187 1.19955 1.21191 1.21357

 Alpha virt. eigenvalues -- 1.21374 1.21564 1.21666 1.21742 1.21756

 Alpha virt. eigenvalues -- 1.21780 1.23643 1.23807 1.26013 1.26202

 Alpha virt. eigenvalues -- 1.26336 1.26801 1.27566 1.27611 1.27762

 Alpha virt. eigenvalues -- 1.28753 1.29295 1.29794 1.30251 1.32717

 Alpha virt. eigenvalues -- 1.34700 1.34766 1.34928 1.35343 1.35610

 Alpha virt. eigenvalues -- 1.36268 1.39195 1.39797 1.42310 1.42339

 Alpha virt. eigenvalues -- 1.42837 1.43316 1.43596 1.43606 1.45705

 Alpha virt. eigenvalues -- 1.46013 1.46066 1.46080 1.46148 1.46204

 Alpha virt. eigenvalues -- 1.49078 1.50450 1.51785 1.51883 1.52444

 Alpha virt. eigenvalues -- 1.53432 1.53550 1.53631 1.53842 1.53844

 Alpha virt. eigenvalues -- 1.54287 1.54389 1.55654 1.56382 1.58509

 Alpha virt. eigenvalues -- 1.58529 1.60377 1.62859 1.62896 1.63327

 Alpha virt. eigenvalues -- 1.63614 1.64248 1.65427 1.66421 1.66636

 Alpha virt. eigenvalues -- 1.67162 1.68225 1.69094 1.69356 1.72778

 Alpha virt. eigenvalues -- 1.72882 1.73159 1.74766 1.74892 1.74973

 Alpha virt. eigenvalues -- 1.75115 1.75479 1.76236 1.76272 1.76345

 Alpha virt. eigenvalues -- 1.81712 1.81829 1.81909 1.81960 1.82501

 Alpha virt. eigenvalues -- 1.83021 1.83251 1.83690 1.83717 1.84172

 Alpha virt. eigenvalues -- 1.85009 1.85191 1.85480 1.87243 1.87422

 Alpha virt. eigenvalues -- 1.87779 1.89699 1.90560 1.91374 1.91510

 Alpha virt. eigenvalues -- 1.91539 1.91648 1.91663 1.91883 1.91904

 Alpha virt. eigenvalues -- 1.91921 1.92145 1.92661 1.92989 1.93088

 Alpha virt. eigenvalues -- 1.93507 1.93705 1.94621 1.95530 1.95908

 Alpha virt. eigenvalues -- 1.96247 1.97244 1.99539 1.99912 2.00109

 Alpha virt. eigenvalues -- 2.00690 2.01993 2.03421 2.03447 2.03956

 Alpha virt. eigenvalues -- 2.04557 2.05660 2.06309 2.06410 2.08852

 Alpha virt. eigenvalues -- 2.12258 2.14289 2.14330 2.16755 2.16775

 Alpha virt. eigenvalues -- 2.18861 2.20006 2.22451 2.23635 2.24083

 Alpha virt. eigenvalues -- 2.24372 2.24763 2.25479 2.25944 2.26328

 Alpha virt. eigenvalues -- 2.27172 2.27740 2.28200 2.28284 2.28628

 Alpha virt. eigenvalues -- 2.28812 2.28880 2.29335 2.29649 2.30769

 Alpha virt. eigenvalues -- 2.31113 2.31194 2.31318 2.33408 2.33704

 Alpha virt. eigenvalues -- 2.33728 2.34388 2.37952 2.39307 2.39591

 Alpha virt. eigenvalues -- 2.40253 2.40399 2.40571 2.41534 2.42479

 Alpha virt. eigenvalues -- 2.44243 2.44394 2.44919 2.46218 2.47022

 Alpha virt. eigenvalues -- 2.49880 2.49982 2.52844 2.53248 2.54084

 Alpha virt. eigenvalues -- 2.54226 2.55441 2.56061 2.56998 2.57396

 Alpha virt. eigenvalues -- 2.58422 2.58684 2.59055 2.59173 2.60223

 Alpha virt. eigenvalues -- 2.62106 2.65059 2.65471 2.65846 2.66277

 Alpha virt. eigenvalues -- 2.66526 2.66946 2.68971 2.69391 2.69515

 Alpha virt. eigenvalues -- 2.69585 2.70840 2.74078 2.75037 2.75063

 Alpha virt. eigenvalues -- 2.75253 2.75704 2.75792 2.75826 2.76720

 Alpha virt. eigenvalues -- 2.78277 2.78411 2.78497 2.79380 2.79816

 Alpha virt. eigenvalues -- 2.80176 2.80270 2.82675 2.82974 2.83226

 Alpha virt. eigenvalues -- 2.83275 2.83347 2.85094 2.85861 2.86258

 Alpha virt. eigenvalues -- 2.87220 2.88851 2.89069 2.89337 2.89891

 Alpha virt. eigenvalues -- 2.92600 2.92815 2.92992 2.93143 2.93205

 Alpha virt. eigenvalues -- 2.98020 2.98337 3.00864 3.04601 3.05604

 Alpha virt. eigenvalues -- 3.05618 3.06233 3.08310 3.09462 3.10575

 Alpha virt. eigenvalues -- 3.16786 3.17590 3.17645 3.17847 3.18670

 Alpha virt. eigenvalues -- 3.19758 3.20586 3.20681 3.21006 3.22365

 Alpha virt. eigenvalues -- 3.23519 3.23818 3.24441 3.27009 3.27168

 Alpha virt. eigenvalues -- 3.27502 3.27564 3.28267 3.28362 3.28616

 Alpha virt. eigenvalues -- 3.29407 3.31091 3.31513 3.31781 3.31782

 Alpha virt. eigenvalues -- 3.31973 3.33966 3.34105 3.37117 3.38695

 Alpha virt. eigenvalues -- 3.40806 3.40860 3.42306 3.46788 3.47674

 Alpha virt. eigenvalues -- 3.47760 3.48278 3.48538 3.48880 3.48982

 Alpha virt. eigenvalues -- 3.50448 3.57058 3.62077 3.62531 3.65642

 Alpha virt. eigenvalues -- 3.65669 3.65741 3.66280 3.73211 3.73407

 Alpha virt. eigenvalues -- 3.73939 3.75127 3.76364 3.77393 3.77840

 Alpha virt. eigenvalues -- 3.78005 3.83466 3.84611 3.84861 3.85325

 Alpha virt. eigenvalues -- 3.88285 3.89338 3.90642 3.90980 3.91930

 Alpha virt. eigenvalues -- 3.96259 3.97001 3.97029 3.97935 4.11638

 Alpha virt. eigenvalues -- 4.12647 4.13290 4.19042 4.19368 4.19465

 Alpha virt. eigenvalues -- 4.21522 4.24360 4.35380 4.40889 4.41761

 Alpha virt. eigenvalues -- 4.41894 4.47717 4.53485 4.55589 4.55595

 Alpha virt. eigenvalues -- 4.79521 4.79688 4.79691 4.80018 5.13444

 Alpha virt. eigenvalues -- 5.14239 5.14852 5.17859 5.22018 5.35829

 Alpha virt. eigenvalues -- 5.38089 5.53143 7.85768 7.85902 7.86462

 Alpha virt. eigenvalues -- 7.92559 8.16141 11.13864 23.28579 23.31646

 Alpha virt. eigenvalues -- 23.31661 23.33433 23.77727 23.79384 23.79596

 Alpha virt. eigenvalues -- 23.79613 23.79843 23.80068 23.80285 23.81984

 Alpha virt. eigenvalues -- 23.89513 23.89797 23.90642 23.90764 23.92006

 Alpha virt. eigenvalues -- 23.92078 23.92160 23.92575 24.03811 24.04089

 Alpha virt. eigenvalues -- 24.04144 24.04718 24.06515 24.06523 24.06569

 Alpha virt. eigenvalues -- 24.06645 24.14429 24.14568 24.14589 24.14919

 Alpha virt. eigenvalues -- 35.58212 35.61556 35.62057 35.62804 35.70159

 Alpha virt. eigenvalues -- 35.70850 35.70899 35.71032

 Beta occ. eigenvalues -- -14.30579 -14.30579 -14.29677 -14.29677 -14.29677

 Beta occ. eigenvalues -- -14.29676 -14.28815 -14.28815 -10.23158 -10.23158

 Beta occ. eigenvalues -- -10.23158 -10.23157 -10.22063 -10.22063 -10.22063

 Beta occ. eigenvalues -- -10.22063 -10.17297 -10.17297 -10.17297 -10.17297

 Beta occ. eigenvalues -- -10.17195 -10.17195 -10.17195 -10.17195 -10.17134

 Beta occ. eigenvalues -- -10.17134 -10.17134 -10.17134 -10.17031 -10.17031

 Beta occ. eigenvalues -- -10.17031 -10.17031 -10.16932 -10.16932 -10.16932

 Beta occ. eigenvalues -- -10.16932 -10.16791 -10.16791 -10.16791 -10.16791

 Beta occ. eigenvalues -- -0.98482 -0.97158 -0.97086 -0.94491 -0.92261

 Beta occ. eigenvalues -- -0.88799 -0.87807 -0.85573 -0.84557 -0.84553

 Beta occ. eigenvalues -- -0.84488 -0.84087 -0.76341 -0.75124 -0.75112

 Beta occ. eigenvalues -- -0.74905 -0.74702 -0.74610 -0.74560 -0.74405

 Beta occ. eigenvalues -- -0.70750 -0.67994 -0.67741 -0.62729 -0.62403

 Beta occ. eigenvalues -- -0.61866 -0.61849 -0.61461 -0.60820 -0.58593

 Beta occ. eigenvalues -- -0.58471 -0.58003 -0.57654 -0.56760 -0.55757

 Beta occ. eigenvalues -- -0.55239 -0.55237 -0.54091 -0.53778 -0.53770

 Beta occ. eigenvalues -- -0.53582 -0.51735 -0.51474 -0.51381 -0.48559

 Beta occ. eigenvalues -- -0.48294 -0.47055 -0.46964 -0.46238 -0.45632

 Beta occ. eigenvalues -- -0.45631 -0.45223 -0.45174 -0.44338 -0.43319

 Beta occ. eigenvalues -- -0.43225 -0.43216 -0.43185 -0.42856 -0.42799

 Beta occ. eigenvalues -- -0.42076 -0.41560 -0.41437 -0.40856 -0.40419

 Beta occ. eigenvalues -- -0.37250 -0.36603 -0.36338 -0.36027 -0.35971

 Beta occ. eigenvalues -- -0.35697 -0.35602 -0.35596 -0.35227 -0.34513

 Beta occ. eigenvalues -- -0.33883 -0.33850 -0.33720 -0.33279 -0.31518

 Beta occ. eigenvalues -- -0.31468 -0.30889 -0.29994 -0.29350 -0.27156

 Beta occ. eigenvalues -- -0.26650 -0.26425 -0.25409 -0.25287 -0.25042

 Beta occ. eigenvalues -- -0.24881 -0.24861 -0.24623 -0.23951 -0.23767

 Beta occ. eigenvalues -- -0.23727 -0.23254 -0.16894

 Beta virt. eigenvalues -- -0.09118 -0.08667 -0.03365 -0.02279 -0.01975

 Beta virt. eigenvalues -- -0.01688 -0.01629 0.03045 0.03193 0.03323

 Beta virt. eigenvalues -- 0.03429 0.05298 0.05299 0.05890 0.06547

 Beta virt. eigenvalues -- 0.06833 0.07114 0.07117 0.07159 0.07319

 Beta virt. eigenvalues -- 0.07717 0.09099 0.09120 0.10070 0.10790

 Beta virt. eigenvalues -- 0.12097 0.12112 0.12513 0.12526 0.12747

 Beta virt. eigenvalues -- 0.13618 0.14698 0.15382 0.15498 0.16288

 Beta virt. eigenvalues -- 0.17925 0.18551 0.18674 0.18698 0.19780

 Beta virt. eigenvalues -- 0.20982 0.20998 0.21690 0.22291 0.22555

 Beta virt. eigenvalues -- 0.23370 0.24286 0.24334 0.24692 0.24864

 Beta virt. eigenvalues -- 0.25338 0.25636 0.25997 0.27203 0.27292

 Beta virt. eigenvalues -- 0.27745 0.27811 0.28119 0.28377 0.29005

 Beta virt. eigenvalues -- 0.29008 0.29071 0.29125 0.29552 0.30666

 Beta virt. eigenvalues -- 0.30817 0.31141 0.31179 0.32641 0.33428

 Beta virt. eigenvalues -- 0.33712 0.34397 0.34844 0.35799 0.35845

 Beta virt. eigenvalues -- 0.36534 0.36746 0.37358 0.37436 0.38203

 Beta virt. eigenvalues -- 0.38283 0.38848 0.39333 0.39401 0.39997

 Beta virt. eigenvalues -- 0.40078 0.40277 0.41040 0.41053 0.41139

 Beta virt. eigenvalues -- 0.41176 0.41554 0.41849 0.42162 0.42435

 Beta virt. eigenvalues -- 0.42697 0.42806 0.43080 0.43156 0.43165

 Beta virt. eigenvalues -- 0.43662 0.43673 0.43712 0.43785 0.43786

 Beta virt. eigenvalues -- 0.43926 0.43969 0.44148 0.44300 0.44476

 Beta virt. eigenvalues -- 0.45974 0.46094 0.47220 0.47374 0.47452

 Beta virt. eigenvalues -- 0.47566 0.47992 0.48054 0.48324 0.48571

 Beta virt. eigenvalues -- 0.49018 0.50538 0.50585 0.50883 0.51370

 Beta virt. eigenvalues -- 0.51628 0.51788 0.52068 0.52229 0.52457

 Beta virt. eigenvalues -- 0.52540 0.52669 0.53896 0.54588 0.54607

 Beta virt. eigenvalues -- 0.54861 0.55300 0.56363 0.56418 0.57385

 Beta virt. eigenvalues -- 0.59176 0.60410 0.60610 0.60889 0.60930

 Beta virt. eigenvalues -- 0.60988 0.61095 0.61102 0.61476 0.61538

 Beta virt. eigenvalues -- 0.61783 0.62157 0.62428 0.62520 0.63432

 Beta virt. eigenvalues -- 0.63583 0.63632 0.63702 0.64266 0.65042

 Beta virt. eigenvalues -- 0.65172 0.65374 0.65459 0.65496 0.66729

 Beta virt. eigenvalues -- 0.67398 0.67639 0.67667 0.68252 0.68263

 Beta virt. eigenvalues -- 0.70082 0.70515 0.70561 0.70824 0.71306

 Beta virt. eigenvalues -- 0.71324 0.71691 0.72528 0.72732 0.73912

 Beta virt. eigenvalues -- 0.74131 0.74523 0.74763 0.75302 0.75507

 Beta virt. eigenvalues -- 0.76941 0.77648 0.77972 0.78018 0.78188

 Beta virt. eigenvalues -- 0.78331 0.78857 0.79220 0.79903 0.80405

 Beta virt. eigenvalues -- 0.80566 0.80646 0.80755 0.81041 0.82245

 Beta virt. eigenvalues -- 0.82587 0.82619 0.82625 0.83601 0.83940

 Beta virt. eigenvalues -- 0.84760 0.84884 0.86897 0.87253 0.87421

 Beta virt. eigenvalues -- 0.87571 0.87594 0.88888 0.89457 0.89543

 Beta virt. eigenvalues -- 0.90220 0.90779 0.91336 0.91574 0.91876

 Beta virt. eigenvalues -- 0.92049 0.92824 0.93095 0.93345 0.94632

 Beta virt. eigenvalues -- 0.95279 0.96712 0.98292 0.99792 0.99866

 Beta virt. eigenvalues -- 0.99973 1.00405 1.00600 1.00633 1.00715

 Beta virt. eigenvalues -- 1.01295 1.02810 1.02819 1.02988 1.03860

 Beta virt. eigenvalues -- 1.03875 1.06454 1.06565 1.06733 1.07684

 Beta virt. eigenvalues -- 1.10991 1.11312 1.11549 1.11691 1.11906

 Beta virt. eigenvalues -- 1.12358 1.12704 1.12835 1.13012 1.14435

 Beta virt. eigenvalues -- 1.14648 1.15145 1.15160 1.15408 1.15705

 Beta virt. eigenvalues -- 1.16428 1.17398 1.19558 1.20028 1.21301

 Beta virt. eigenvalues -- 1.21434 1.21509 1.21698 1.21702 1.21815

 Beta virt. eigenvalues -- 1.21833 1.21870 1.23699 1.23904 1.26057

 Beta virt. eigenvalues -- 1.26352 1.26627 1.26870 1.27609 1.27666

 Beta virt. eigenvalues -- 1.27829 1.28820 1.29332 1.29873 1.30458

 Beta virt. eigenvalues -- 1.32802 1.34830 1.34925 1.35102 1.35473

 Beta virt. eigenvalues -- 1.35737 1.36390 1.39483 1.39998 1.42519

 Beta virt. eigenvalues -- 1.42575 1.43144 1.43345 1.43604 1.43760

 Beta virt. eigenvalues -- 1.45698 1.46090 1.46097 1.46163 1.46233

 Beta virt. eigenvalues -- 1.46235 1.49157 1.50497 1.51802 1.51917

 Beta virt. eigenvalues -- 1.52508 1.53533 1.53773 1.53805 1.54024

 Beta virt. eigenvalues -- 1.54075 1.54352 1.54508 1.55736 1.56516

 Beta virt. eigenvalues -- 1.58607 1.58697 1.60539 1.63030 1.63152

 Beta virt. eigenvalues -- 1.63461 1.63809 1.64369 1.65502 1.66504

 Beta virt. eigenvalues -- 1.66768 1.67254 1.68379 1.69243 1.69443

 Beta virt. eigenvalues -- 1.72895 1.73048 1.73241 1.74828 1.74957

 Beta virt. eigenvalues -- 1.75059 1.75123 1.75572 1.76288 1.76339

 Beta virt. eigenvalues -- 1.76428 1.81829 1.81956 1.81999 1.82016

 Beta virt. eigenvalues -- 1.82609 1.83155 1.83409 1.83739 1.83761

 Beta virt. eigenvalues -- 1.84232 1.85086 1.85283 1.85681 1.87310

 Beta virt. eigenvalues -- 1.87553 1.87914 1.89758 1.90718 1.91487

 Beta virt. eigenvalues -- 1.91592 1.91643 1.91729 1.91789 1.91987

 Beta virt. eigenvalues -- 1.91988 1.92045 1.92285 1.92698 1.93103

 Beta virt. eigenvalues -- 1.93119 1.93645 1.93756 1.94665 1.95579

 Beta virt. eigenvalues -- 1.95956 1.96320 1.97295 1.99723 1.99992

 Beta virt. eigenvalues -- 2.00309 2.00883 2.02144 2.03591 2.03685

 Beta virt. eigenvalues -- 2.04166 2.04888 2.05886 2.06576 2.06736

 Beta virt. eigenvalues -- 2.09055 2.12359 2.14634 2.14653 2.16766

 Beta virt. eigenvalues -- 2.16943 2.18978 2.20121 2.22766 2.23818

 Beta virt. eigenvalues -- 2.24185 2.24513 2.24812 2.25607 2.25988

 Beta virt. eigenvalues -- 2.26356 2.27193 2.27792 2.28251 2.28339

 Beta virt. eigenvalues -- 2.28730 2.28905 2.29151 2.29399 2.29841

 Beta virt. eigenvalues -- 2.30798 2.31137 2.31224 2.31358 2.33439

 Beta virt. eigenvalues -- 2.33722 2.33801 2.34436 2.38161 2.39343

 Beta virt. eigenvalues -- 2.39621 2.40427 2.40621 2.40683 2.41707

 Beta virt. eigenvalues -- 2.42705 2.44394 2.44758 2.45234 2.46363

 Beta virt. eigenvalues -- 2.47317 2.49990 2.50158 2.53144 2.53380

 Beta virt. eigenvalues -- 2.54253 2.54339 2.55583 2.56209 2.57240

 Beta virt. eigenvalues -- 2.57442 2.58463 2.58786 2.59081 2.59391

 Beta virt. eigenvalues -- 2.60284 2.62336 2.65323 2.65764 2.65946

 Beta virt. eigenvalues -- 2.66451 2.66842 2.67029 2.69211 2.69499

 Beta virt. eigenvalues -- 2.69665 2.69847 2.70999 2.74229 2.75369

 Beta virt. eigenvalues -- 2.75374 2.75378 2.75860 2.75928 2.76040

 Beta virt. eigenvalues -- 2.76770 2.78431 2.78447 2.78545 2.79581

 Beta virt. eigenvalues -- 2.80131 2.80315 2.80488 2.82955 2.83097

 Beta virt. eigenvalues -- 2.83330 2.83543 2.83563 2.85140 2.85924

 Beta virt. eigenvalues -- 2.86422 2.87266 2.89056 2.89342 2.89401

 Beta virt. eigenvalues -- 2.89966 2.92844 2.93065 2.93161 2.93203

 Beta virt. eigenvalues -- 2.93256 2.98184 2.98813 3.01114 3.04706

 Beta virt. eigenvalues -- 3.05748 3.05755 3.06306 3.08554 3.09536

 Beta virt. eigenvalues -- 3.10635 3.16807 3.17614 3.17669 3.17871

 Beta virt. eigenvalues -- 3.18730 3.19874 3.20705 3.20733 3.21059

 Beta virt. eigenvalues -- 3.22415 3.23551 3.23861 3.24482 3.27071

 Beta virt. eigenvalues -- 3.27195 3.27517 3.27634 3.28291 3.28384

 Beta virt. eigenvalues -- 3.28659 3.29463 3.31114 3.31541 3.31815

 Beta virt. eigenvalues -- 3.31816 3.32009 3.33988 3.34143 3.37153

 Beta virt. eigenvalues -- 3.38725 3.40837 3.40887 3.42330 3.46820

 Beta virt. eigenvalues -- 3.47707 3.47792 3.48307 3.48566 3.48911

 Beta virt. eigenvalues -- 3.49013 3.50480 3.57157 3.62167 3.62623

 Beta virt. eigenvalues -- 3.65673 3.65696 3.65767 3.66308 3.73284

 Beta virt. eigenvalues -- 3.73469 3.74004 3.75211 3.76419 3.77477

 Beta virt. eigenvalues -- 3.77955 3.78096 3.83882 3.84772 3.85406

 Beta virt. eigenvalues -- 3.85512 3.88580 3.89903 3.90986 3.91450

 Beta virt. eigenvalues -- 3.92287 3.96302 3.97049 3.97071 3.97980

 Beta virt. eigenvalues -- 4.11703 4.12646 4.13448 4.19124 4.19445

 Beta virt. eigenvalues -- 4.19559 4.21616 4.24447 4.35500 4.41066

 Beta virt. eigenvalues -- 4.41923 4.42028 4.47844 4.53572 4.55673

 Beta virt. eigenvalues -- 4.55710 4.79568 4.79738 4.79741 4.80069

 Beta virt. eigenvalues -- 5.13620 5.14368 5.15000 5.18001 5.22206

 Beta virt. eigenvalues -- 5.36021 5.38251 5.53323 7.85772 7.85932

 Beta virt. eigenvalues -- 7.86460 7.92563 8.16145 11.13874 23.28601

 Beta virt. eigenvalues -- 23.31667 23.31683 23.33454 23.77814 23.79399

 Beta virt. eigenvalues -- 23.79610 23.79631 23.79857 23.80128 23.80388

 Beta virt. eigenvalues -- 23.82064 23.89547 23.89847 23.90746 23.90794

 Beta virt. eigenvalues -- 23.92111 23.92130 23.92275 23.92723 24.03838

 Beta virt. eigenvalues -- 24.04114 24.04171 24.04742 24.06530 24.06538

 Beta virt. eigenvalues -- 24.06586 24.06661 24.14446 24.14586 24.14606

 Beta virt. eigenvalues -- 24.14937 35.58294 35.61658 35.62094 35.62863

 Beta virt. eigenvalues -- 35.70247 35.70933 35.71017 35.71158

 Condensed to atoms (all electrons):

 Atomic-Atomic Spin Densities.

 Mulliken charges and spin densities:

 1 2

 1 C 0.363101 -0.018571

 2 N -0.669265 0.022956

 3 C 0.319666 0.142611

 4 C -0.053399 -0.022438

 5 C -0.079973 0.047921

 6 N -0.394542 -0.063372

 7 C 0.319666 0.142611

 8 N -0.669265 0.022956

 9 C 0.363101 -0.018571

 10 C -0.079973 0.047921

 11 C -0.053399 -0.022438

 12 N -0.443653 0.150787

 13 C -0.079973 0.047921

 14 C -0.053399 -0.022438

 15 C 0.319666 0.142611

 16 N -0.669265 0.022956

 17 C 0.363101 -0.018571

 18 N -0.394542 -0.063372

 19 N -0.669265 0.022956

 20 C 0.319666 0.142611

 21 C -0.053399 -0.022438

 22 C -0.079973 0.047921

 23 C 0.363101 -0.018571

 24 N -0.443653 0.150787

 25 Zn 1.364098 -0.002679

 26 C -0.223104 -0.023512

 27 C -0.241192 0.044379

 28 C -0.233055 -0.018658

 29 C -0.230505 0.034780

 30 C -0.223104 -0.023512

 31 C -0.241192 0.044379

 32 C -0.233055 -0.018658

 33 C -0.230505 0.034780

 34 C -0.230505 0.034780

 35 C -0.233055 -0.018658

 36 C -0.241192 0.044379

 37 C -0.223104 -0.023512

 38 C -0.223104 -0.023512

 39 C -0.241192 0.044379

 40 C -0.233055 -0.018658

 41 C -0.230505 0.034780

 42 H 0.215635 0.000776

 43 H 0.215694 -0.001577

 44 H 0.215635 0.000776

 45 H 0.215694 -0.001577

 46 H 0.215694 -0.001577

 47 H 0.215635 0.000776

 48 H 0.215635 0.000776

 49 H 0.215694 -0.001577

 50 H 0.222561 0.000780

 51 H 0.221907 -0.002485

 52 H 0.222561 0.000780

 53 H 0.221907 -0.002485

 54 H 0.221907 -0.002485

 55 H 0.222561 0.000780

 56 H 0.222561 0.000780

 57 H 0.221907 -0.002485

 Sum of Mulliken charges = -1.00000 1.00000

 Mulliken charges and spin densities with hydrogens summed into heavy atoms:

 1 2

 1 C 0.363101 -0.018571

 2 N -0.669265 0.022956

 3 C 0.319666 0.142611

 4 C -0.053399 -0.022438

 5 C -0.079973 0.047921

 6 N -0.394542 -0.063372

 7 C 0.319666 0.142611

 8 N -0.669265 0.022956

 9 C 0.363101 -0.018571

 10 C -0.079973 0.047921

 11 C -0.053399 -0.022438

 12 N -0.443653 0.150787

 13 C -0.079973 0.047921

 14 C -0.053399 -0.022438

 15 C 0.319666 0.142611

 16 N -0.669265 0.022956

 17 C 0.363101 -0.018571

 18 N -0.394542 -0.063372

 19 N -0.669265 0.022956

 20 C 0.319666 0.142611

 21 C -0.053399 -0.022438

 22 C -0.079973 0.047921

 23 C 0.363101 -0.018571

 24 N -0.443653 0.150787

 25 Zn 1.364098 -0.002679

 26 C -0.007469 -0.022736

 27 C -0.019284 0.041893

 28 C -0.010494 -0.017878

 29 C -0.014810 0.033204

 30 C -0.007469 -0.022736

 31 C -0.019284 0.041893

 32 C -0.010494 -0.017878

 33 C -0.014810 0.033204

 34 C -0.014810 0.033204

 35 C -0.010494 -0.017878

 36 C -0.019284 0.041893

 37 C -0.007469 -0.022736

 38 C -0.007469 -0.022736

 39 C -0.019284 0.041893

 40 C -0.010494 -0.017878

 41 C -0.014810 0.033204

 Electronic spatial extent (au): <R\*\*2>= 22378.4174

 Charge= -1.0000 electrons

 Dipole moment (field-independent basis, Debye):

 X= 0.0000 Y= 0.0000 Z= 2.1157 Tot= 2.1157

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

 XX= -261.0807 YY= -258.1328 ZZ= -247.9716

 XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

 XX= -5.3523 YY= -2.4044 ZZ= 7.7568

 XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

 XXX= 0.0000 YYY= 0.0000 ZZZ= 28.1810 XYY= 0.0000

 XXY= 0.0000 XXZ= -2.6723 XZZ= 0.0000 YZZ= 0.0000

 YYZ= -2.5590 XYZ= 0.0000

 Hexadecapole moment (field-independent basis, Debye-Ang\*\*3):

 XXXX= -14796.8646 YYYY= -14680.5860 ZZZZ= -288.5005 XXXY= 0.0000

 XXXZ= 0.0000 YYYX= 0.0000 YYYZ= 0.0000 ZZZX= 0.0000

 ZZZY= 0.0000 XXYY= -4716.7449 XXZZ= -2963.2199 YYZZ= -2958.8498

 XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

 N-N= 4.373820765202D+03 E-N=-1.289479184448D+04 KE= 1.776674872624D+03

 Symmetry A1 KE= 5.098465934376D+02

 Symmetry A2 KE= 3.906850566463D+02

 Symmetry B1 KE= 4.388338743691D+02

 Symmetry B2 KE= 4.373093481709D+02

 Isotropic Fermi Contact Couplings

 Atom a.u. MegaHertz Gauss 10(-4) cm-1

 1 C(13) -0.00730 -8.20194 -2.92665 -2.73587

 2 N(14) 0.00055 0.17859 0.06373 0.05957

 3 C(13) 0.01057 11.87773 4.23827 3.96199

 4 C(13) -0.00692 -7.77795 -2.77537 -2.59444

 5 C(13) 0.00321 3.61211 1.28889 1.20487

 6 N(14) -0.01147 -3.70517 -1.32210 -1.23591

 7 C(13) 0.01057 11.87773 4.23827 3.96199

 8 N(14) 0.00055 0.17859 0.06373 0.05957

 9 C(13) -0.00730 -8.20194 -2.92665 -2.73587

 10 C(13) 0.00321 3.61211 1.28889 1.20487

 11 C(13) -0.00692 -7.77795 -2.77537 -2.59444

 12 N(14) 0.01772 5.72565 2.04305 1.90987

 13 C(13) 0.00321 3.61211 1.28889 1.20487

 14 C(13) -0.00692 -7.77795 -2.77537 -2.59444

 15 C(13) 0.01057 11.87773 4.23827 3.96199

 16 N(14) 0.00055 0.17859 0.06373 0.05957

 17 C(13) -0.00730 -8.20194 -2.92665 -2.73587

 18 N(14) -0.01147 -3.70517 -1.32210 -1.23591

 19 N(14) 0.00055 0.17859 0.06373 0.05957

 20 C(13) 0.01057 11.87773 4.23827 3.96199

 21 C(13) -0.00692 -7.77795 -2.77537 -2.59444

 22 C(13) 0.00321 3.61211 1.28889 1.20487

 23 C(13) -0.00730 -8.20194 -2.92665 -2.73587

 24 N(14) 0.01772 5.72565 2.04305 1.90987

 25 Zn(67) 0.00000 0.00000 0.00000 0.00000

 26 C(13) -0.00343 -3.85534 -1.37568 -1.28600

 27 C(13) 0.00305 3.43241 1.22477 1.14493

 28 C(13) -0.00275 -3.08805 -1.10189 -1.03006

 29 C(13) 0.00222 2.49477 0.89020 0.83217

 30 C(13) -0.00343 -3.85534 -1.37568 -1.28600

 31 C(13) 0.00305 3.43241 1.22477 1.14493

 32 C(13) -0.00275 -3.08805 -1.10189 -1.03006

 33 C(13) 0.00222 2.49477 0.89020 0.83217

 34 C(13) 0.00222 2.49477 0.89020 0.83217

 35 C(13) -0.00275 -3.08805 -1.10189 -1.03006

 36 C(13) 0.00305 3.43241 1.22477 1.14493

 37 C(13) -0.00343 -3.85534 -1.37568 -1.28600

 38 C(13) -0.00343 -3.85534 -1.37568 -1.28600

 39 C(13) 0.00305 3.43241 1.22477 1.14493

 40 C(13) -0.00275 -3.08805 -1.10189 -1.03006

 41 C(13) 0.00222 2.49477 0.89020 0.83217

 42 H(1) 0.00027 1.20466 0.42985 0.40183

 43 H(1) -0.00049 -2.19544 -0.78339 -0.73232

 44 H(1) 0.00027 1.20466 0.42985 0.40183

 45 H(1) -0.00049 -2.19544 -0.78339 -0.73232

 46 H(1) -0.00049 -2.19544 -0.78339 -0.73232

 47 H(1) 0.00027 1.20466 0.42985 0.40183

 48 H(1) 0.00027 1.20466 0.42985 0.40183

 49 H(1) -0.00049 -2.19544 -0.78339 -0.73232

 50 H(1) 0.00020 0.88508 0.31582 0.29523

 51 H(1) -0.00064 -2.85058 -1.01716 -0.95085

 52 H(1) 0.00020 0.88508 0.31582 0.29523

 53 H(1) -0.00064 -2.85058 -1.01716 -0.95085

 54 H(1) -0.00064 -2.85058 -1.01716 -0.95085

 55 H(1) 0.00020 0.88508 0.31582 0.29523

 56 H(1) 0.00020 0.88508 0.31582 0.29523

 57 H(1) -0.00064 -2.85058 -1.01716 -0.95085

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 Center ---- Spin Dipole Couplings ----

 3XX-RR 3YY-RR 3ZZ-RR

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 1 Atom 0.008494 0.012752 -0.021245

 2 Atom -0.034987 -0.036052 0.071038

 3 Atom -0.094652 -0.094545 0.189197

 4 Atom 0.006783 0.007583 -0.014366

 5 Atom -0.027419 -0.027500 0.054919

 6 Atom 0.061678 0.046884 -0.108561

 7 Atom -0.094652 -0.094545 0.189197

 8 Atom -0.034987 -0.036052 0.071038

 9 Atom 0.008494 0.012752 -0.021245

 10 Atom -0.027419 -0.027500 0.054919

 11 Atom 0.006783 0.007583 -0.014366

 12 Atom -0.187197 -0.188825 0.376022

 13 Atom -0.027419 -0.027500 0.054919

 14 Atom 0.006783 0.007583 -0.014366

 15 Atom -0.094652 -0.094545 0.189197

 16 Atom -0.034987 -0.036052 0.071038

 17 Atom 0.008494 0.012752 -0.021245

 18 Atom 0.061678 0.046884 -0.108561

 19 Atom -0.034987 -0.036052 0.071038

 20 Atom -0.094652 -0.094545 0.189197

 21 Atom 0.006783 0.007583 -0.014366

 22 Atom -0.027419 -0.027500 0.054919

 23 Atom 0.008494 0.012752 -0.021245

 24 Atom -0.187197 -0.188825 0.376022

 25 Atom 0.005698 -0.006920 0.001222

 26 Atom 0.011304 0.011071 -0.022375

 27 Atom -0.022516 -0.024259 0.046775

 28 Atom 0.008949 0.007663 -0.016612

 29 Atom -0.017469 -0.016635 0.034103

 30 Atom 0.011304 0.011071 -0.022375

 31 Atom -0.022516 -0.024259 0.046775

 32 Atom 0.008949 0.007663 -0.016612

 33 Atom -0.017469 -0.016635 0.034103

 34 Atom -0.017469 -0.016635 0.034103

 35 Atom 0.008949 0.007663 -0.016612

 36 Atom -0.022516 -0.024259 0.046775

 37 Atom 0.011304 0.011071 -0.022375

 38 Atom 0.011304 0.011071 -0.022375

 39 Atom -0.022516 -0.024259 0.046775

 40 Atom 0.008949 0.007663 -0.016612

 41 Atom -0.017469 -0.016635 0.034103

 42 Atom 0.001123 0.000401 -0.001524

 43 Atom -0.000146 0.001351 -0.001205

 44 Atom 0.001123 0.000401 -0.001524

 45 Atom -0.000146 0.001351 -0.001205

 46 Atom -0.000146 0.001351 -0.001205

 47 Atom 0.001123 0.000401 -0.001524

 48 Atom 0.001123 0.000401 -0.001524

 49 Atom -0.000146 0.001351 -0.001205

 50 Atom 0.000960 -0.000168 -0.000791

 51 Atom 0.002883 -0.002387 -0.000497

 52 Atom 0.000960 -0.000168 -0.000791

 53 Atom 0.002883 -0.002387 -0.000497

 54 Atom 0.002883 -0.002387 -0.000497

 55 Atom 0.000960 -0.000168 -0.000791

 56 Atom 0.000960 -0.000168 -0.000791

 57 Atom 0.002883 -0.002387 -0.000497

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 XY XZ YZ

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 1 Atom -0.007021 -0.000752 -0.000640

 2 Atom -0.001278 0.006532 0.007996

 3 Atom 0.002556 0.004323 0.009922

 4 Atom 0.002757 -0.001134 -0.000752

 5 Atom 0.000626 0.003101 0.003544

 6 Atom 0.000000 0.000000 -0.003594

 7 Atom -0.002556 -0.004323 0.009922

 8 Atom 0.001278 -0.006532 0.007996

 9 Atom 0.007021 0.000752 -0.000640

 10 Atom -0.000626 -0.003101 0.003544

 11 Atom -0.002757 0.001134 -0.000752

 12 Atom 0.000000 0.017095 0.000000

 13 Atom -0.000626 0.003101 -0.003544

 14 Atom -0.002757 -0.001134 0.000752

 15 Atom -0.002556 0.004323 -0.009922

 16 Atom 0.001278 0.006532 -0.007996

 17 Atom 0.007021 -0.000752 0.000640

 18 Atom 0.000000 0.000000 0.003594

 19 Atom -0.001278 -0.006532 -0.007996

 20 Atom 0.002556 -0.004323 -0.009922

 21 Atom 0.002757 0.001134 0.000752

 22 Atom 0.000626 -0.003101 -0.003544

 23 Atom -0.007021 0.000752 0.000640

 24 Atom 0.000000 -0.017095 0.000000

 25 Atom 0.000000 0.000000 0.000000

 26 Atom -0.002150 -0.000957 0.000869

 27 Atom -0.001102 0.001746 -0.001561

 28 Atom -0.000040 -0.000576 0.000617

 29 Atom -0.000851 0.001187 -0.001313

 30 Atom 0.002150 0.000957 0.000869

 31 Atom 0.001102 -0.001746 -0.001561

 32 Atom 0.000040 0.000576 0.000617

 33 Atom 0.000851 -0.001187 -0.001313

 34 Atom -0.000851 -0.001187 0.001313

 35 Atom -0.000040 0.000576 -0.000617

 36 Atom -0.001102 -0.001746 0.001561

 37 Atom -0.002150 0.000957 -0.000869

 38 Atom 0.002150 -0.000957 -0.000869

 39 Atom 0.001102 0.001746 0.001561

 40 Atom 0.000040 -0.000576 -0.000617

 41 Atom 0.000851 0.001187 0.001313

 42 Atom -0.002085 -0.000103 0.000092

 43 Atom 0.001529 0.000036 0.000038

 44 Atom 0.002085 0.000103 0.000092

 45 Atom -0.001529 -0.000036 0.000038

 46 Atom 0.001529 -0.000036 -0.000038

 47 Atom -0.002085 0.000103 -0.000092

 48 Atom 0.002085 -0.000103 -0.000092

 49 Atom -0.001529 0.000036 -0.000038

 50 Atom -0.000211 0.000045 -0.000015

 51 Atom -0.002217 0.000140 -0.000015

 52 Atom 0.000211 -0.000045 -0.000015

 53 Atom 0.002217 -0.000140 -0.000015

 54 Atom -0.002217 -0.000140 0.000015

 55 Atom -0.000211 -0.000045 0.000015

 56 Atom 0.000211 0.000045 0.000015

 57 Atom 0.002217 0.000140 0.000015

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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 -0.0213 -2.856 -1.019 -0.953 0.0312 0.0252 0.9992

 1 C(13) Bbb 0.0033 0.446 0.159 0.149 0.8026 0.5951 -0.0401

 Bcc 0.0180 2.410 0.860 0.804 -0.5957 0.8032 -0.0017

 Baa -0.0379 -1.461 -0.521 -0.487 0.5730 0.8141 -0.0941

 2 N(14) Bbb -0.0341 -1.317 -0.470 -0.439 0.8174 -0.5761 -0.0070

 Bcc 0.0720 2.778 0.991 0.926 0.0599 0.0730 0.9955

 Baa -0.0972 -13.045 -4.655 -4.351 -0.6943 0.7195 -0.0144

 3 C(13) Bbb -0.0924 -12.399 -4.424 -4.136 0.7195 0.6936 -0.0355

 Bcc 0.1896 25.444 9.079 8.487 0.0155 0.0350 0.9993

 Baa -0.0144 -1.938 -0.692 -0.646 0.0497 0.0279 0.9984

 4 C(13) Bbb 0.0044 0.591 0.211 0.197 0.7531 -0.6577 -0.0191

 Bcc 0.0100 1.347 0.481 0.449 0.6561 0.7528 -0.0537

 Baa -0.0281 -3.769 -1.345 -1.257 -0.6646 0.7472 -0.0071

 5 C(13) Bbb -0.0271 -3.636 -1.298 -1.213 0.7462 0.6632 -0.0569

 Bcc 0.0552 7.406 2.643 2.470 0.0378 0.0431 0.9984

 Baa -0.1086 -4.190 -1.495 -1.398 0.0000 0.0231 0.9997

 6 N(14) Bbb 0.0470 1.811 0.646 0.604 0.0000 0.9997 -0.0231

 Bcc 0.0617 2.379 0.849 0.793 1.0000 0.0000 0.0000

 Baa -0.0972 -13.045 -4.655 -4.351 0.6943 0.7195 -0.0144

 7 C(13) Bbb -0.0924 -12.399 -4.424 -4.136 0.7195 -0.6936 0.0355

 Bcc 0.1896 25.444 9.079 8.487 -0.0155 0.0350 0.9993

 Baa -0.0379 -1.461 -0.521 -0.487 -0.5730 0.8141 -0.0941

 8 N(14) Bbb -0.0341 -1.317 -0.470 -0.439 0.8174 0.5761 0.0070

 Bcc 0.0720 2.778 0.991 0.926 -0.0599 0.0730 0.9955

 Baa -0.0213 -2.856 -1.019 -0.953 -0.0312 0.0252 0.9992

 9 C(13) Bbb 0.0033 0.446 0.159 0.149 0.8026 -0.5951 0.0401

 Bcc 0.0180 2.410 0.860 0.804 0.5957 0.8032 -0.0017

 Baa -0.0281 -3.769 -1.345 -1.257 0.6646 0.7472 -0.0071

 10 C(13) Bbb -0.0271 -3.636 -1.298 -1.213 0.7462 -0.6632 0.0569

 Bcc 0.0552 7.406 2.643 2.470 -0.0378 0.0431 0.9984

 Baa -0.0144 -1.938 -0.692 -0.646 -0.0497 0.0279 0.9984

 11 C(13) Bbb 0.0044 0.591 0.211 0.197 0.7531 0.6577 0.0191

 Bcc 0.0100 1.347 0.481 0.449 -0.6561 0.7528 -0.0537

 Baa -0.1888 -7.283 -2.599 -2.429 0.0000 1.0000 0.0000

 12 N(14) Bbb -0.1877 -7.240 -2.583 -2.415 0.9995 0.0000 -0.0303

 Bcc 0.3765 14.522 5.182 4.844 0.0303 0.0000 0.9995

 Baa -0.0281 -3.769 -1.345 -1.257 0.6646 0.7472 0.0071

 13 C(13) Bbb -0.0271 -3.636 -1.298 -1.213 0.7462 -0.6632 -0.0569

 Bcc 0.0552 7.406 2.643 2.470 0.0378 -0.0431 0.9984

 Baa -0.0144 -1.938 -0.692 -0.646 0.0497 -0.0279 0.9984

 14 C(13) Bbb 0.0044 0.591 0.211 0.197 0.7531 0.6577 -0.0191

 Bcc 0.0100 1.347 0.481 0.449 -0.6561 0.7528 0.0537

 Baa -0.0972 -13.045 -4.655 -4.351 0.6943 0.7195 0.0144

 15 C(13) Bbb -0.0924 -12.399 -4.424 -4.136 0.7195 -0.6936 -0.0355

 Bcc 0.1896 25.444 9.079 8.487 0.0155 -0.0350 0.9993

 Baa -0.0379 -1.461 -0.521 -0.487 -0.5730 0.8141 0.0941

 16 N(14) Bbb -0.0341 -1.317 -0.470 -0.439 0.8174 0.5761 -0.0070

 Bcc 0.0720 2.778 0.991 0.926 0.0599 -0.0730 0.9955

 Baa -0.0213 -2.856 -1.019 -0.953 0.0312 -0.0252 0.9992

 17 C(13) Bbb 0.0033 0.446 0.159 0.149 0.8026 -0.5951 -0.0401

 Bcc 0.0180 2.410 0.860 0.804 0.5957 0.8032 0.0017

 Baa -0.1086 -4.190 -1.495 -1.398 0.0000 -0.0231 0.9997

 18 N(14) Bbb 0.0470 1.811 0.646 0.604 0.0000 0.9997 0.0231

 Bcc 0.0617 2.379 0.849 0.793 1.0000 0.0000 0.0000

 Baa -0.0379 -1.461 -0.521 -0.487 0.5730 0.8141 0.0941

 19 N(14) Bbb -0.0341 -1.317 -0.470 -0.439 0.8174 -0.5761 0.0070

 Bcc 0.0720 2.778 0.991 0.926 -0.0599 -0.0730 0.9955

 Baa -0.0972 -13.045 -4.655 -4.351 -0.6943 0.7195 0.0144

 20 C(13) Bbb -0.0924 -12.399 -4.424 -4.136 0.7195 0.6936 0.0355

 Bcc 0.1896 25.444 9.079 8.487 -0.0155 -0.0350 0.9993

 Baa -0.0144 -1.938 -0.692 -0.646 -0.0497 -0.0279 0.9984

 21 C(13) Bbb 0.0044 0.591 0.211 0.197 0.7531 -0.6577 0.0191

 Bcc 0.0100 1.347 0.481 0.449 0.6561 0.7528 0.0537

 Baa -0.0281 -3.769 -1.345 -1.257 -0.6646 0.7472 0.0071

 22 C(13) Bbb -0.0271 -3.636 -1.298 -1.213 0.7462 0.6632 0.0569

 Bcc 0.0552 7.406 2.643 2.470 -0.0378 -0.0431 0.9984

 Baa -0.0213 -2.856 -1.019 -0.953 -0.0312 -0.0252 0.9992

 23 C(13) Bbb 0.0033 0.446 0.159 0.149 0.8026 0.5951 0.0401

 Bcc 0.0180 2.410 0.860 0.804 -0.5957 0.8032 0.0017

 Baa -0.1888 -7.283 -2.599 -2.429 0.0000 1.0000 0.0000

 24 N(14) Bbb -0.1877 -7.240 -2.583 -2.415 0.9995 0.0000 0.0303

 Bcc 0.3765 14.522 5.182 4.844 -0.0303 0.0000 0.9995

 Baa -0.0069 -0.231 -0.083 -0.077 0.0000 1.0000 0.0000

 25 Zn(67) Bbb 0.0012 0.041 0.015 0.014 0.0000 0.0000 1.0000

 Bcc 0.0057 0.191 0.068 0.064 1.0000 0.0000 0.0000

 Baa -0.0224 -3.009 -1.074 -1.004 0.0268 -0.0242 0.9993

 26 C(13) Bbb 0.0090 1.212 0.433 0.404 0.6875 0.7261 -0.0009

 Bcc 0.0134 1.796 0.641 0.599 0.7256 -0.6871 -0.0361

 Baa -0.0248 -3.328 -1.187 -1.110 0.4291 0.9032 0.0092

 27 C(13) Bbb -0.0221 -2.960 -1.056 -0.987 0.9029 -0.4286 -0.0326

 Bcc 0.0469 6.287 2.244 2.097 0.0255 -0.0223 0.9994

 Baa -0.0166 -2.233 -0.797 -0.745 0.0225 -0.0253 0.9994

 28 C(13) Bbb 0.0077 1.030 0.368 0.344 0.0424 0.9988 0.0244

 Bcc 0.0090 1.203 0.429 0.401 0.9988 -0.0418 -0.0235

 Baa -0.0180 -2.416 -0.862 -0.806 0.8515 0.5243 -0.0062

 29 C(13) Bbb -0.0162 -2.169 -0.774 -0.724 -0.5238 0.8511 0.0346

 Bcc 0.0342 4.585 1.636 1.529 0.0234 -0.0262 0.9994

 Baa -0.0224 -3.009 -1.074 -1.004 -0.0268 -0.0242 0.9993

 30 C(13) Bbb 0.0090 1.212 0.433 0.404 -0.6875 0.7261 -0.0009

 Bcc 0.0134 1.796 0.641 0.599 0.7256 0.6871 0.0361

 Baa -0.0248 -3.328 -1.187 -1.110 -0.4291 0.9032 0.0092

 31 C(13) Bbb -0.0221 -2.960 -1.056 -0.987 0.9029 0.4286 0.0326

 Bcc 0.0469 6.287 2.244 2.097 -0.0255 -0.0223 0.9994

 Baa -0.0166 -2.233 -0.797 -0.745 -0.0225 -0.0253 0.9994

 32 C(13) Bbb 0.0077 1.030 0.368 0.344 -0.0424 0.9988 0.0244

 Bcc 0.0090 1.203 0.429 0.401 0.9988 0.0418 0.0235

 Baa -0.0180 -2.416 -0.862 -0.806 0.8515 -0.5243 0.0062

 33 C(13) Bbb -0.0162 -2.169 -0.774 -0.724 0.5238 0.8511 0.0346

 Bcc 0.0342 4.585 1.636 1.529 -0.0234 -0.0262 0.9994

 Baa -0.0180 -2.416 -0.862 -0.806 0.8515 0.5243 0.0062

 34 C(13) Bbb -0.0162 -2.169 -0.774 -0.724 -0.5238 0.8511 -0.0346

 Bcc 0.0342 4.585 1.636 1.529 -0.0234 0.0262 0.9994

 Baa -0.0166 -2.233 -0.797 -0.745 -0.0225 0.0253 0.9994

 35 C(13) Bbb 0.0077 1.030 0.368 0.344 0.0424 0.9988 -0.0244

 Bcc 0.0090 1.203 0.429 0.401 0.9988 -0.0418 0.0235

 Baa -0.0248 -3.328 -1.187 -1.110 0.4291 0.9032 -0.0092

 36 C(13) Bbb -0.0221 -2.960 -1.056 -0.987 0.9029 -0.4286 0.0326

 Bcc 0.0469 6.287 2.244 2.097 -0.0255 0.0223 0.9994

 Baa -0.0224 -3.009 -1.074 -1.004 -0.0268 0.0242 0.9993

 37 C(13) Bbb 0.0090 1.212 0.433 0.404 0.6875 0.7261 0.0009

 Bcc 0.0134 1.796 0.641 0.599 0.7256 -0.6871 0.0361

 Baa -0.0224 -3.009 -1.074 -1.004 0.0268 0.0242 0.9993

 38 C(13) Bbb 0.0090 1.212 0.433 0.404 -0.6875 0.7261 0.0009

 Bcc 0.0134 1.796 0.641 0.599 0.7256 0.6871 -0.0361

 Baa -0.0248 -3.328 -1.187 -1.110 -0.4291 0.9032 -0.0092

 39 C(13) Bbb -0.0221 -2.960 -1.056 -0.987 0.9029 0.4286 -0.0326

 Bcc 0.0469 6.287 2.244 2.097 0.0255 0.0223 0.9994

 Baa -0.0166 -2.233 -0.797 -0.745 0.0225 0.0253 0.9994

 40 C(13) Bbb 0.0077 1.030 0.368 0.344 -0.0424 0.9988 -0.0244

 Bcc 0.0090 1.203 0.429 0.401 0.9988 0.0418 -0.0235

 Baa -0.0180 -2.416 -0.862 -0.806 0.8515 -0.5243 -0.0062

 41 C(13) Bbb -0.0162 -2.169 -0.774 -0.724 0.5238 0.8511 -0.0346

 Bcc 0.0342 4.585 1.636 1.529 0.0234 0.0262 0.9994

 Baa -0.0015 -0.815 -0.291 -0.272 0.0104 -0.0362 0.9993

 42 H(1) Bbb -0.0014 -0.723 -0.258 -0.241 0.6444 0.7644 0.0210

 Bcc 0.0029 1.538 0.549 0.513 0.7646 -0.6437 -0.0313

 Baa -0.0012 -0.644 -0.230 -0.215 -0.0918 0.0403 0.9950

 43 H(1) Bbb -0.0011 -0.586 -0.209 -0.196 0.8435 -0.5279 0.0992

 Bcc 0.0023 1.230 0.439 0.410 0.5293 0.8483 0.0145

 Baa -0.0015 -0.815 -0.291 -0.272 -0.0104 -0.0362 0.9993

 44 H(1) Bbb -0.0014 -0.723 -0.258 -0.241 -0.6444 0.7644 0.0210

 Bcc 0.0029 1.538 0.549 0.513 0.7646 0.6437 0.0313

 Baa -0.0012 -0.644 -0.230 -0.215 0.0918 0.0403 0.9950

 45 H(1) Bbb -0.0011 -0.586 -0.209 -0.196 0.8435 0.5279 -0.0992

 Bcc 0.0023 1.230 0.439 0.410 -0.5293 0.8483 0.0145

 Baa -0.0012 -0.644 -0.230 -0.215 0.0918 -0.0403 0.9950

 46 H(1) Bbb -0.0011 -0.586 -0.209 -0.196 0.8435 -0.5279 -0.0992

 Bcc 0.0023 1.230 0.439 0.410 0.5293 0.8483 -0.0145

 Baa -0.0015 -0.815 -0.291 -0.272 -0.0104 0.0362 0.9993

 47 H(1) Bbb -0.0014 -0.723 -0.258 -0.241 0.6444 0.7644 -0.0210

 Bcc 0.0029 1.538 0.549 0.513 0.7646 -0.6437 0.0313

 Baa -0.0015 -0.815 -0.291 -0.272 0.0104 0.0362 0.9993

 48 H(1) Bbb -0.0014 -0.723 -0.258 -0.241 -0.6444 0.7644 -0.0210

 Bcc 0.0029 1.538 0.549 0.513 0.7646 0.6437 -0.0313

 Baa -0.0012 -0.644 -0.230 -0.215 -0.0918 -0.0403 0.9950

 49 H(1) Bbb -0.0011 -0.586 -0.209 -0.196 0.8435 0.5279 0.0992

 Bcc 0.0023 1.230 0.439 0.410 -0.5293 0.8483 -0.0145

 Baa -0.0008 -0.423 -0.151 -0.141 -0.0238 0.0158 0.9996

 50 H(1) Bbb -0.0002 -0.110 -0.039 -0.037 0.1785 0.9839 -0.0113

 Bcc 0.0010 0.533 0.190 0.178 0.9837 -0.1781 0.0262

 Baa -0.0032 -1.705 -0.608 -0.569 0.3429 0.9393 -0.0126

 51 H(1) Bbb -0.0005 -0.267 -0.095 -0.089 -0.0262 0.0230 0.9994

 Bcc 0.0037 1.972 0.704 0.658 0.9390 -0.3423 0.0325

 Baa -0.0008 -0.423 -0.151 -0.141 0.0238 0.0158 0.9996

 52 H(1) Bbb -0.0002 -0.110 -0.039 -0.037 -0.1785 0.9839 -0.0113

 Bcc 0.0010 0.533 0.190 0.178 0.9837 0.1781 -0.0262

 Baa -0.0032 -1.705 -0.608 -0.569 -0.3429 0.9393 -0.0126

 53 H(1) Bbb -0.0005 -0.267 -0.095 -0.089 0.0262 0.0230 0.9994

 Bcc 0.0037 1.972 0.704 0.658 0.9390 0.3423 -0.0325

 Baa -0.0032 -1.705 -0.608 -0.569 0.3429 0.9393 0.0126

 54 H(1) Bbb -0.0005 -0.267 -0.095 -0.089 0.0262 -0.0230 0.9994

 Bcc 0.0037 1.972 0.704 0.658 0.9390 -0.3423 -0.0325

 Baa -0.0008 -0.423 -0.151 -0.141 0.0238 -0.0158 0.9996

 55 H(1) Bbb -0.0002 -0.110 -0.039 -0.037 0.1785 0.9839 0.0113

 Bcc 0.0010 0.533 0.190 0.178 0.9837 -0.1781 -0.0262

 Baa -0.0008 -0.423 -0.151 -0.141 -0.0238 -0.0158 0.9996

 56 H(1) Bbb -0.0002 -0.110 -0.039 -0.037 -0.1785 0.9839 0.0113

 Bcc 0.0010 0.533 0.190 0.178 0.9837 0.1781 0.0262

 Baa -0.0032 -1.705 -0.608 -0.569 -0.3429 0.9393 0.0126

 57 H(1) Bbb -0.0005 -0.267 -0.095 -0.089 -0.0262 -0.0230 0.9994

 Bcc 0.0037 1.972 0.704 0.658 0.9390 0.3423 0.0325

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 No NMR shielding tensors so no spin-rotation constants.

 Leave Link 601 at Sat Jun 15 12:23:07 2019, MaxMem= 1342177280 cpu: 42.0

 (Enter /apps/gaussian/g09d01/g09/l9999.exe)

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 668666,-2.8089711611,-0.080976616\C,-5.1631867793,-4.1574510341,-0.124

 2541901\C,-4.1696829056,-5.1549166378,-0.1242096179\C,-2.8185079821,-4

 .8268339125,-0.0806103493\C,-2.8185079821,4.8268339125,-0.0806103493\C

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 3601,-0.0833458549\H,-5.5831231335,2.037691608,-0.0837838532\H,5.58312

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 471853,4.4470873137,-0.1595734526\H,6.2081471853,-4.4470873137,-0.1595

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 ),SGV'(N2),X(C32H16N4)]\\@

 Experience is what you get when you don't get what you want.

 -- Dan Stanford

 Job cpu time: 0 days 3 hours 23 minutes 2.9 seconds.

 File lengths (MBytes): RWF= 1379 Int= 0 D2E= 0 Chk= 62 Scr= 2

 Normal termination of Gaussian 09 at Sat Jun 15 12:23:08 2019.