Entering Gaussian System, Link 0=g09

 Initial command:

 /apps/gaussian/g09d01/g09/l1.exe "/srv/scratch/z5105842/Gau-68446.inp" -scrdir="/srv/scratch/z5105842/"

 Entering Link 1 = /apps/gaussian/g09d01/g09/l1.exe PID= 68465.

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 Cite this work as:

 Gaussian 09, Revision D.01,

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

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

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

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

 5-Jul-2019

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

 %nprocshared=12

 Will use up to 12 processors via shared memory.

 %mem=10GB

 %chk=ZntAzPcation.chk

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

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

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

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

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

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

 4//1;

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

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

 7//1,2,3,16;

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

 2/9=110/2;

 99//99;

 2/9=110/2;

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

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

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

 7//1,2,3,16;

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

 2/9=110/2;

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

 99/9=1/99;

 Leave Link 1 at Fri Jul 5 21:06:56 2019, MaxMem= 1342177280 cpu: 1.5

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

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

 ZntAzPcation

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

 Symbolic Z-matrix:

 Charge = 1 Multiplicity = 2

 C -2.06677 -2.19041 0.

 N -0.7423 -1.86521 0.

 C 0. -3.00728 0.

 C -0.9161 -4.16652 0.

 C -2.18334 -3.64784 0.

 N 1.33695 -3.10409 0.

 C 2.19041 -2.06677 0.

 N 1.86521 -0.7423 0.

 C 3.00728 0. 0.

 C 4.16652 -0.9161 0.

 C 3.64784 -2.18334 0.

 N -3.10409 -1.33695 0.

 C -4.16652 0.9161 0.

 C -3.64784 2.18334 0.

 C -2.19041 2.06677 0.

 N -1.86521 0.7423 0.

 C -3.00728 0. 0.

 N -1.33695 3.10409 0.

 N 0.7423 1.86521 0.

 C 0. 3.00728 0.

 C 0.9161 4.16652 0.

 C 2.18334 3.64784 0.

 C 2.06677 2.19041 0.

 N 3.10409 1.33695 0.

 Zn 0. 0. 0.

 C -0.48237 -5.59359 0.

 H -3.11869 -4.19296 0.

 C 5.59359 -0.48237 0.

 H 4.19296 -3.11869 0.

 C -5.59359 0.48237 0.

 H -4.19296 3.11869 0.

 C 0.48237 5.59359 0.

 H 3.11869 4.19296 0.

 H -1.34628 -6.26359 0.

 H 0.1302 -5.81848 0.88508

 H 0.1302 -5.81848 -0.88508

 H 5.81848 0.1302 0.88508

 H 5.81848 0.1302 -0.88508

 H 6.26359 -1.34628 0.

 H -5.81848 -0.1302 0.88508

 H -5.81848 -0.1302 -0.88508

 H -6.26359 1.34628 0.

 H -0.1302 5.81848 0.88508

 H -0.1302 5.81848 -0.88508

 H 1.34628 6.26359 0.

 NAtoms= 45 NQM= 45 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 1 12 1 12

 AtmWgt= 12.0000000 12.0000000 12.0000000 14.0030740 63.9291454 12.0000000 1.0078250 12.0000000 1.0078250 12.0000000

 NucSpn= 0 0 0 2 0 0 1 0 1 0

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

 NQMom= 0.0000000 0.0000000 0.0000000 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 2.7928460 0.0000000 2.7928460 0.0000000

 AtZNuc= 6.0000000 6.0000000 6.0000000 7.0000000 30.0000000 6.0000000 1.0000000 6.0000000 1.0000000 6.0000000

 Atom 31 32 33 34 35 36 37 38 39 40

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

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

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

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

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

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

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

 Atom 41 42 43 44 45

 IAtWgt= 1 1 1 1 1

 AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

 NucSpn= 1 1 1 1 1

 AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

 NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

 NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

 AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

 Leave Link 101 at Fri Jul 5 21:06:57 2019, MaxMem= 1342177280 cpu: 2.7

 (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) 1.3638 estimate D2E/DX2 !

 ! R2 R(1,5) 1.4621 estimate D2E/DX2 !

 ! R3 R(1,12) 1.3433 estimate D2E/DX2 !

 ! R4 R(2,3) 1.3621 estimate D2E/DX2 !

 ! R5 R(2,25) 2.0075 estimate D2E/DX2 !

 ! R6 R(3,4) 1.4775 estimate D2E/DX2 !

 ! R7 R(3,6) 1.3404 estimate D2E/DX2 !

 ! R8 R(4,5) 1.3693 estimate D2E/DX2 !

 ! R9 R(4,26) 1.4915 estimate D2E/DX2 !

 ! R10 R(5,27) 1.0826 estimate D2E/DX2 !

 ! R11 R(6,7) 1.3433 estimate D2E/DX2 !

 ! R12 R(7,8) 1.3638 estimate D2E/DX2 !

 ! R13 R(7,11) 1.4621 estimate D2E/DX2 !

 ! R14 R(8,9) 1.3621 estimate D2E/DX2 !

 ! R15 R(8,25) 2.0075 estimate D2E/DX2 !

 ! R16 R(9,10) 1.4775 estimate D2E/DX2 !

 ! R17 R(9,24) 1.3404 estimate D2E/DX2 !

 ! R18 R(10,11) 1.3693 estimate D2E/DX2 !

 ! R19 R(10,28) 1.4915 estimate D2E/DX2 !

 ! R20 R(11,29) 1.0826 estimate D2E/DX2 !

 ! R21 R(12,17) 1.3404 estimate D2E/DX2 !

 ! R22 R(13,14) 1.3693 estimate D2E/DX2 !

 ! R23 R(13,17) 1.4775 estimate D2E/DX2 !

 ! R24 R(13,30) 1.4915 estimate D2E/DX2 !

 ! R25 R(14,15) 1.4621 estimate D2E/DX2 !

 ! R26 R(14,31) 1.0826 estimate D2E/DX2 !

 ! R27 R(15,16) 1.3638 estimate D2E/DX2 !

 ! R28 R(15,18) 1.3433 estimate D2E/DX2 !

 ! R29 R(16,17) 1.3621 estimate D2E/DX2 !

 ! R30 R(16,25) 2.0075 estimate D2E/DX2 !

 ! R31 R(18,20) 1.3404 estimate D2E/DX2 !

 ! R32 R(19,20) 1.3621 estimate D2E/DX2 !

 ! R33 R(19,23) 1.3638 estimate D2E/DX2 !

 ! R34 R(19,25) 2.0075 estimate D2E/DX2 !

 ! R35 R(20,21) 1.4775 estimate D2E/DX2 !

 ! R36 R(21,22) 1.3693 estimate D2E/DX2 !

 ! R37 R(21,32) 1.4915 estimate D2E/DX2 !

 ! R38 R(22,23) 1.4621 estimate D2E/DX2 !

 ! R39 R(22,33) 1.0826 estimate D2E/DX2 !

 ! R40 R(23,24) 1.3433 estimate D2E/DX2 !

 ! R41 R(26,34) 1.0933 estimate D2E/DX2 !

 ! R42 R(26,35) 1.0996 estimate D2E/DX2 !

 ! R43 R(26,36) 1.0996 estimate D2E/DX2 !

 ! R44 R(28,37) 1.0996 estimate D2E/DX2 !

 ! R45 R(28,38) 1.0996 estimate D2E/DX2 !

 ! R46 R(28,39) 1.0933 estimate D2E/DX2 !

 ! R47 R(30,40) 1.0996 estimate D2E/DX2 !

 ! R48 R(30,41) 1.0996 estimate D2E/DX2 !

 ! R49 R(30,42) 1.0933 estimate D2E/DX2 !

 ! R50 R(32,43) 1.0996 estimate D2E/DX2 !

 ! R51 R(32,44) 1.0996 estimate D2E/DX2 !

 ! R52 R(32,45) 1.0933 estimate D2E/DX2 !

 ! A1 A(2,1,5) 108.3677 estimate D2E/DX2 !

 ! A2 A(2,1,12) 126.7588 estimate D2E/DX2 !

 ! A3 A(5,1,12) 124.8735 estimate D2E/DX2 !

 ! A4 A(1,2,3) 109.2275 estimate D2E/DX2 !

 ! A5 A(1,2,25) 125.496 estimate D2E/DX2 !

 ! A6 A(3,2,25) 125.2764 estimate D2E/DX2 !

 ! A7 A(2,3,4) 108.6597 estimate D2E/DX2 !

 ! A8 A(2,3,6) 127.1639 estimate D2E/DX2 !

 ! A9 A(4,3,6) 124.1764 estimate D2E/DX2 !

 ! A10 A(3,4,5) 106.0588 estimate D2E/DX2 !

 ! A11 A(3,4,26) 124.7765 estimate D2E/DX2 !

 ! A12 A(5,4,26) 129.1647 estimate D2E/DX2 !

 ! A13 A(1,5,4) 107.6862 estimate D2E/DX2 !

 ! A14 A(1,5,27) 124.8063 estimate D2E/DX2 !

 ! A15 A(4,5,27) 127.5074 estimate D2E/DX2 !

 ! A16 A(3,6,7) 125.3048 estimate D2E/DX2 !

 ! A17 A(6,7,8) 126.7588 estimate D2E/DX2 !

 ! A18 A(6,7,11) 124.8735 estimate D2E/DX2 !

 ! A19 A(8,7,11) 108.3677 estimate D2E/DX2 !

 ! A20 A(7,8,9) 109.2275 estimate D2E/DX2 !

 ! A21 A(7,8,25) 125.496 estimate D2E/DX2 !

 ! A22 A(9,8,25) 125.2764 estimate D2E/DX2 !

 ! A23 A(8,9,10) 108.6597 estimate D2E/DX2 !

 ! A24 A(8,9,24) 127.1639 estimate D2E/DX2 !

 ! A25 A(10,9,24) 124.1764 estimate D2E/DX2 !

 ! A26 A(9,10,11) 106.0588 estimate D2E/DX2 !

 ! A27 A(9,10,28) 124.7765 estimate D2E/DX2 !

 ! A28 A(11,10,28) 129.1647 estimate D2E/DX2 !

 ! A29 A(7,11,10) 107.6862 estimate D2E/DX2 !

 ! A30 A(7,11,29) 124.8063 estimate D2E/DX2 !

 ! A31 A(10,11,29) 127.5074 estimate D2E/DX2 !

 ! A32 A(1,12,17) 125.3048 estimate D2E/DX2 !

 ! A33 A(14,13,17) 106.0588 estimate D2E/DX2 !

 ! A34 A(14,13,30) 129.1647 estimate D2E/DX2 !

 ! A35 A(17,13,30) 124.7765 estimate D2E/DX2 !

 ! A36 A(13,14,15) 107.6862 estimate D2E/DX2 !

 ! A37 A(13,14,31) 127.5074 estimate D2E/DX2 !

 ! A38 A(15,14,31) 124.8063 estimate D2E/DX2 !

 ! A39 A(14,15,16) 108.3677 estimate D2E/DX2 !

 ! A40 A(14,15,18) 124.8735 estimate D2E/DX2 !

 ! A41 A(16,15,18) 126.7588 estimate D2E/DX2 !

 ! A42 A(15,16,17) 109.2275 estimate D2E/DX2 !

 ! A43 A(15,16,25) 125.496 estimate D2E/DX2 !

 ! A44 A(17,16,25) 125.2764 estimate D2E/DX2 !

 ! A45 A(12,17,13) 124.1764 estimate D2E/DX2 !

 ! A46 A(12,17,16) 127.1639 estimate D2E/DX2 !

 ! A47 A(13,17,16) 108.6597 estimate D2E/DX2 !

 ! A48 A(15,18,20) 125.3048 estimate D2E/DX2 !

 ! A49 A(20,19,23) 109.2275 estimate D2E/DX2 !

 ! A50 A(20,19,25) 125.2764 estimate D2E/DX2 !

 ! A51 A(23,19,25) 125.496 estimate D2E/DX2 !

 ! A52 A(18,20,19) 127.1639 estimate D2E/DX2 !

 ! A53 A(18,20,21) 124.1764 estimate D2E/DX2 !

 ! A54 A(19,20,21) 108.6597 estimate D2E/DX2 !

 ! A55 A(20,21,22) 106.0588 estimate D2E/DX2 !

 ! A56 A(20,21,32) 124.7765 estimate D2E/DX2 !

 ! A57 A(22,21,32) 129.1647 estimate D2E/DX2 !

 ! A58 A(21,22,23) 107.6862 estimate D2E/DX2 !

 ! A59 A(21,22,33) 127.5074 estimate D2E/DX2 !

 ! A60 A(23,22,33) 124.8063 estimate D2E/DX2 !

 ! A61 A(19,23,22) 108.3677 estimate D2E/DX2 !

 ! A62 A(19,23,24) 126.7588 estimate D2E/DX2 !

 ! A63 A(22,23,24) 124.8735 estimate D2E/DX2 !

 ! A64 A(9,24,23) 125.3048 estimate D2E/DX2 !

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

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

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

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

 ! A69 A(4,26,34) 110.889 estimate D2E/DX2 !

 ! A70 A(4,26,35) 110.9568 estimate D2E/DX2 !

 ! A71 A(4,26,36) 110.9568 estimate D2E/DX2 !

 ! A72 A(34,26,35) 108.353 estimate D2E/DX2 !

 ! A73 A(34,26,36) 108.353 estimate D2E/DX2 !

 ! A74 A(35,26,36) 107.1998 estimate D2E/DX2 !

 ! A75 A(10,28,37) 110.9568 estimate D2E/DX2 !

 ! A76 A(10,28,38) 110.9568 estimate D2E/DX2 !

 ! A77 A(10,28,39) 110.889 estimate D2E/DX2 !

 ! A78 A(37,28,38) 107.1998 estimate D2E/DX2 !

 ! A79 A(37,28,39) 108.353 estimate D2E/DX2 !

 ! A80 A(38,28,39) 108.353 estimate D2E/DX2 !

 ! A81 A(13,30,40) 110.9568 estimate D2E/DX2 !

 ! A82 A(13,30,41) 110.9568 estimate D2E/DX2 !

 ! A83 A(13,30,42) 110.889 estimate D2E/DX2 !

 ! A84 A(40,30,41) 107.1998 estimate D2E/DX2 !

 ! A85 A(40,30,42) 108.353 estimate D2E/DX2 !

 ! A86 A(41,30,42) 108.353 estimate D2E/DX2 !

 ! A87 A(21,32,43) 110.9568 estimate D2E/DX2 !

 ! A88 A(21,32,44) 110.9568 estimate D2E/DX2 !

 ! A89 A(21,32,45) 110.889 estimate D2E/DX2 !

 ! A90 A(43,32,44) 107.1998 estimate D2E/DX2 !

 ! A91 A(43,32,45) 108.353 estimate D2E/DX2 !

 ! A92 A(44,32,45) 108.353 estimate D2E/DX2 !

 ! A93 L(2,25,19,16,-1) 180.0 estimate D2E/DX2 !

 ! A94 L(8,25,16,19,-1) 180.0 estimate D2E/DX2 !

 ! A95 L(2,25,19,16,-2) 180.0 estimate D2E/DX2 !

 ! A96 L(8,25,16,19,-2) 180.0 estimate D2E/DX2 !

 ! D1 D(5,1,2,3) 0.0 estimate D2E/DX2 !

 ! D2 D(5,1,2,25) 180.0 estimate D2E/DX2 !

 ! D3 D(12,1,2,3) 180.0 estimate D2E/DX2 !

 ! D4 D(12,1,2,25) 0.0 estimate D2E/DX2 !

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

 ! D6 D(2,1,5,27) 180.0 estimate D2E/DX2 !

 ! D7 D(12,1,5,4) 180.0 estimate D2E/DX2 !

 ! D8 D(12,1,5,27) 0.0 estimate D2E/DX2 !

 ! D9 D(2,1,12,17) 0.0 estimate D2E/DX2 !

 ! D10 D(5,1,12,17) 180.0 estimate D2E/DX2 !

 ! D11 D(1,2,3,4) 0.0 estimate D2E/DX2 !

 ! D12 D(1,2,3,6) 180.0 estimate D2E/DX2 !

 ! D13 D(25,2,3,4) 180.0 estimate D2E/DX2 !

 ! D14 D(25,2,3,6) 0.0 estimate D2E/DX2 !

 ! D15 D(1,2,25,8) 180.0 estimate D2E/DX2 !

 ! D16 D(1,2,25,16) 0.0 estimate D2E/DX2 !

 ! D17 D(3,2,25,8) 0.0 estimate D2E/DX2 !

 ! D18 D(3,2,25,16) 180.0 estimate D2E/DX2 !

 ! D19 D(2,3,4,5) 0.0 estimate D2E/DX2 !

 ! D20 D(2,3,4,26) 180.0 estimate D2E/DX2 !

 ! D21 D(6,3,4,5) 180.0 estimate D2E/DX2 !

 ! D22 D(6,3,4,26) 0.0 estimate D2E/DX2 !

 ! D23 D(2,3,6,7) 0.0 estimate D2E/DX2 !

 ! D24 D(4,3,6,7) 180.0 estimate D2E/DX2 !

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

 ! D26 D(3,4,5,27) 180.0 estimate D2E/DX2 !

 ! D27 D(26,4,5,1) 180.0 estimate D2E/DX2 !

 ! D28 D(26,4,5,27) 0.0 estimate D2E/DX2 !

 ! D29 D(3,4,26,34) 180.0 estimate D2E/DX2 !

 ! D30 D(3,4,26,35) 59.5315 estimate D2E/DX2 !

 ! D31 D(3,4,26,36) -59.5315 estimate D2E/DX2 !

 ! D32 D(5,4,26,34) 0.0 estimate D2E/DX2 !

 ! D33 D(5,4,26,35) -120.4685 estimate D2E/DX2 !

 ! D34 D(5,4,26,36) 120.4685 estimate D2E/DX2 !

 ! D35 D(3,6,7,8) 0.0 estimate D2E/DX2 !

 ! D36 D(3,6,7,11) 180.0 estimate D2E/DX2 !

 ! D37 D(6,7,8,9) 180.0 estimate D2E/DX2 !

 ! D38 D(6,7,8,25) 0.0 estimate D2E/DX2 !

 ! D39 D(11,7,8,9) 0.0 estimate D2E/DX2 !

 ! D40 D(11,7,8,25) 180.0 estimate D2E/DX2 !

 ! D41 D(6,7,11,10) 180.0 estimate D2E/DX2 !

 ! D42 D(6,7,11,29) 0.0 estimate D2E/DX2 !

 ! D43 D(8,7,11,10) 0.0 estimate D2E/DX2 !

 ! D44 D(8,7,11,29) 180.0 estimate D2E/DX2 !

 ! D45 D(7,8,9,10) 0.0 estimate D2E/DX2 !

 ! D46 D(7,8,9,24) 180.0 estimate D2E/DX2 !

 ! D47 D(25,8,9,10) 180.0 estimate D2E/DX2 !

 ! D48 D(25,8,9,24) 0.0 estimate D2E/DX2 !

 ! D49 D(7,8,25,2) 0.0 estimate D2E/DX2 !

 ! D50 D(7,8,25,19) 180.0 estimate D2E/DX2 !

 ! D51 D(9,8,25,2) 180.0 estimate D2E/DX2 !

 ! D52 D(9,8,25,19) 0.0 estimate D2E/DX2 !

 ! D53 D(8,9,10,11) 0.0 estimate D2E/DX2 !

 ! D54 D(8,9,10,28) 180.0 estimate D2E/DX2 !

 ! D55 D(24,9,10,11) 180.0 estimate D2E/DX2 !

 ! D56 D(24,9,10,28) 0.0 estimate D2E/DX2 !

 ! D57 D(8,9,24,23) 0.0 estimate D2E/DX2 !

 ! D58 D(10,9,24,23) 180.0 estimate D2E/DX2 !

 ! D59 D(9,10,11,7) 0.0 estimate D2E/DX2 !

 ! D60 D(9,10,11,29) 180.0 estimate D2E/DX2 !

 ! D61 D(28,10,11,7) 180.0 estimate D2E/DX2 !

 ! D62 D(28,10,11,29) 0.0 estimate D2E/DX2 !

 ! D63 D(9,10,28,37) 59.5315 estimate D2E/DX2 !

 ! D64 D(9,10,28,38) -59.5315 estimate D2E/DX2 !

 ! D65 D(9,10,28,39) 180.0 estimate D2E/DX2 !

 ! D66 D(11,10,28,37) -120.4685 estimate D2E/DX2 !

 ! D67 D(11,10,28,38) 120.4685 estimate D2E/DX2 !

 ! D68 D(11,10,28,39) 0.0 estimate D2E/DX2 !

 ! D69 D(1,12,17,13) 180.0 estimate D2E/DX2 !

 ! D70 D(1,12,17,16) 0.0 estimate D2E/DX2 !

 ! D71 D(17,13,14,15) 0.0 estimate D2E/DX2 !

 ! D72 D(17,13,14,31) 180.0 estimate D2E/DX2 !

 ! D73 D(30,13,14,15) 180.0 estimate D2E/DX2 !

 ! D74 D(30,13,14,31) 0.0 estimate D2E/DX2 !

 ! D75 D(14,13,17,12) 180.0 estimate D2E/DX2 !

 ! D76 D(14,13,17,16) 0.0 estimate D2E/DX2 !

 ! D77 D(30,13,17,12) 0.0 estimate D2E/DX2 !

 ! D78 D(30,13,17,16) 180.0 estimate D2E/DX2 !

 ! D79 D(14,13,30,40) -120.4685 estimate D2E/DX2 !

 ! D80 D(14,13,30,41) 120.4685 estimate D2E/DX2 !

 ! D81 D(14,13,30,42) 0.0 estimate D2E/DX2 !

 ! D82 D(17,13,30,40) 59.5315 estimate D2E/DX2 !

 ! D83 D(17,13,30,41) -59.5315 estimate D2E/DX2 !

 ! D84 D(17,13,30,42) 180.0 estimate D2E/DX2 !

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

 ! D86 D(13,14,15,18) 180.0 estimate D2E/DX2 !

 ! D87 D(31,14,15,16) 180.0 estimate D2E/DX2 !

 ! D88 D(31,14,15,18) 0.0 estimate D2E/DX2 !

 ! D89 D(14,15,16,17) 0.0 estimate D2E/DX2 !

 ! D90 D(14,15,16,25) 180.0 estimate D2E/DX2 !

 ! D91 D(18,15,16,17) 180.0 estimate D2E/DX2 !

 ! D92 D(18,15,16,25) 0.0 estimate D2E/DX2 !

 ! D93 D(14,15,18,20) 180.0 estimate D2E/DX2 !

 ! D94 D(16,15,18,20) 0.0 estimate D2E/DX2 !

 ! D95 D(15,16,17,12) 180.0 estimate D2E/DX2 !

 ! D96 D(15,16,17,13) 0.0 estimate D2E/DX2 !

 ! D97 D(25,16,17,12) 0.0 estimate D2E/DX2 !

 ! D98 D(25,16,17,13) 180.0 estimate D2E/DX2 !

 ! D99 D(15,16,25,2) 180.0 estimate D2E/DX2 !

 ! D100 D(15,16,25,19) 0.0 estimate D2E/DX2 !

 ! D101 D(17,16,25,2) 0.0 estimate D2E/DX2 !

 ! D102 D(17,16,25,19) 180.0 estimate D2E/DX2 !

 ! D103 D(15,18,20,19) 0.0 estimate D2E/DX2 !

 ! D104 D(15,18,20,21) 180.0 estimate D2E/DX2 !

 ! D105 D(23,19,20,18) 180.0 estimate D2E/DX2 !

 ! D106 D(23,19,20,21) 0.0 estimate D2E/DX2 !

 ! D107 D(25,19,20,18) 0.0 estimate D2E/DX2 !

 ! D108 D(25,19,20,21) 180.0 estimate D2E/DX2 !

 ! D109 D(20,19,23,22) 0.0 estimate D2E/DX2 !

 ! D110 D(20,19,23,24) 180.0 estimate D2E/DX2 !

 ! D111 D(25,19,23,22) 180.0 estimate D2E/DX2 !

 ! D112 D(25,19,23,24) 0.0 estimate D2E/DX2 !

 ! D113 D(20,19,25,8) 180.0 estimate D2E/DX2 !

 ! D114 D(20,19,25,16) 0.0 estimate D2E/DX2 !

 ! D115 D(23,19,25,8) 0.0 estimate D2E/DX2 !

 ! D116 D(23,19,25,16) 180.0 estimate D2E/DX2 !

 ! D117 D(18,20,21,22) 180.0 estimate D2E/DX2 !

 ! D118 D(18,20,21,32) 0.0 estimate D2E/DX2 !

 ! D119 D(19,20,21,22) 0.0 estimate D2E/DX2 !

 ! D120 D(19,20,21,32) 180.0 estimate D2E/DX2 !

 ! D121 D(20,21,22,23) 0.0 estimate D2E/DX2 !

 ! D122 D(20,21,22,33) 180.0 estimate D2E/DX2 !

 ! D123 D(32,21,22,23) 180.0 estimate D2E/DX2 !

 ! D124 D(32,21,22,33) 0.0 estimate D2E/DX2 !

 ! D125 D(20,21,32,43) 59.5315 estimate D2E/DX2 !

 ! D126 D(20,21,32,44) -59.5315 estimate D2E/DX2 !

 ! D127 D(20,21,32,45) 180.0 estimate D2E/DX2 !

 ! D128 D(22,21,32,43) -120.4685 estimate D2E/DX2 !

 ! D129 D(22,21,32,44) 120.4685 estimate D2E/DX2 !

 ! D130 D(22,21,32,45) 0.0 estimate D2E/DX2 !

 ! D131 D(21,22,23,19) 0.0 estimate D2E/DX2 !

 ! D132 D(21,22,23,24) 180.0 estimate D2E/DX2 !

 ! D133 D(33,22,23,19) 180.0 estimate D2E/DX2 !

 ! D134 D(33,22,23,24) 0.0 estimate D2E/DX2 !

 ! D135 D(19,23,24,9) 0.0 estimate D2E/DX2 !

 ! D136 D(22,23,24,9) 180.0 estimate D2E/DX2 !

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

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

 Number of steps in this run= 270 maximum allowed number of steps= 270.

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link 103 at Fri Jul 5 21:06:57 2019, MaxMem= 1342177280 cpu: 0.2

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

 Input orientation:

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

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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

 1 6 0 -2.066774 -2.190409 0.000000

 2 7 0 -0.742302 -1.865213 0.000000

 3 6 0 0.000000 -3.007280 0.000000

 4 6 0 -0.916097 -4.166516 0.000000

 5 6 0 -2.183341 -3.647838 0.000000

 6 7 0 1.336945 -3.104087 0.000000

 7 6 0 2.190409 -2.066774 0.000000

 8 7 0 1.865213 -0.742302 0.000000

 9 6 0 3.007280 0.000000 0.000000

 10 6 0 4.166516 -0.916097 0.000000

 11 6 0 3.647838 -2.183341 0.000000

 12 7 0 -3.104087 -1.336945 0.000000

 13 6 0 -4.166516 0.916097 0.000000

 14 6 0 -3.647838 2.183341 0.000000

 15 6 0 -2.190409 2.066774 0.000000

 16 7 0 -1.865213 0.742302 0.000000

 17 6 0 -3.007280 0.000000 0.000000

 18 7 0 -1.336945 3.104087 0.000000

 19 7 0 0.742302 1.865213 0.000000

 20 6 0 0.000000 3.007280 0.000000

 21 6 0 0.916097 4.166516 0.000000

 22 6 0 2.183341 3.647838 0.000000

 23 6 0 2.066774 2.190409 0.000000

 24 7 0 3.104087 1.336945 0.000000

 25 30 0 0.000000 0.000000 0.000000

 26 6 0 -0.482366 -5.593592 0.000000

 27 1 0 -3.118690 -4.192956 0.000000

 28 6 0 5.593592 -0.482366 0.000000

 29 1 0 4.192956 -3.118690 0.000000

 30 6 0 -5.593592 0.482366 0.000000

 31 1 0 -4.192956 3.118690 0.000000

 32 6 0 0.482366 5.593592 0.000000

 33 1 0 3.118690 4.192956 0.000000

 34 1 0 -1.346284 -6.263586 0.000000

 35 1 0 0.130195 -5.818475 0.885075

 36 1 0 0.130195 -5.818475 -0.885075

 37 1 0 5.818475 0.130195 0.885075

 38 1 0 5.818475 0.130195 -0.885075

 39 1 0 6.263586 -1.346284 0.000000

 40 1 0 -5.818475 -0.130195 0.885075

 41 1 0 -5.818475 -0.130195 -0.885075

 42 1 0 -6.263586 1.346284 0.000000

 43 1 0 -0.130195 5.818475 0.885075

 44 1 0 -0.130195 5.818475 -0.885075

 45 1 0 1.346284 6.263586 0.000000

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

 Distance matrix (angstroms):

 1 2 3 4 5

 1 C 0.000000

 2 N 1.363810 0.000000

 3 C 2.222349 1.362105 0.000000

 4 C 2.286713 2.307856 1.477519 0.000000

 5 C 1.462083 2.292236 2.275366 1.369282 0.000000

 6 N 3.524218 2.420346 1.340445 2.490974 3.562033

 7 C 4.258978 2.939629 2.383788 3.749573 4.650748

 8 N 4.190171 2.839025 2.934134 4.411454 4.983265

 9 C 5.526655 4.187885 4.252936 5.723001 6.344231

 10 C 6.362215 4.999732 4.661856 6.033090 6.912532

 11 C 5.714616 4.401651 3.739732 4.976192 6.012271

 12 N 1.343287 2.420144 3.524965 3.576838 2.487569

 13 C 3.749573 4.411454 5.723001 6.033090 4.976192

 14 C 4.650748 4.983265 6.344231 6.912532 6.012271

 15 C 4.258978 4.190171 5.526655 6.362215 5.714616

 16 N 2.939629 2.839025 4.187885 4.999732 4.401651

 17 C 2.383788 2.934134 4.252936 4.661856 3.739732

 18 N 5.344562 5.004752 6.255896 7.282773 6.804769

 19 N 4.933455 4.014988 4.928712 6.255561 6.241243

 20 C 5.593525 4.928712 6.014560 7.232052 7.004111

 21 C 7.021967 6.255561 7.232052 8.532078 8.406583

 22 C 7.221399 6.241243 7.004111 8.406583 8.502635

 23 C 6.023104 4.933455 5.593525 7.021967 7.221399

 24 N 6.259395 5.004850 5.339255 6.815421 7.266702

 25 Zn 3.011552 2.007494 3.007280 4.266039 4.251317

 26 C 3.753932 3.737429 2.630910 1.491532 2.584429

 27 H 2.262017 3.326501 3.336473 2.202752 1.082604

 28 C 7.848479 6.485046 6.137056 7.479907 8.396481

 29 H 6.328185 5.091952 4.194436 5.215397 6.398215

 30 C 4.425175 5.389447 6.592867 6.594775 5.356155

 31 H 5.719019 6.061873 7.423502 7.988243 7.058644

 32 C 8.190774 7.558676 8.614388 9.859787 9.618213

 33 H 8.224134 7.183918 7.846631 9.282256 9.465177

 34 H 4.136409 4.439649 3.523636 2.140739 2.746416

 35 H 4.332770 4.144018 2.950106 2.146405 3.293550

 36 H 4.332770 4.144018 2.950106 2.146405 3.293550

 37 H 8.267147 6.914391 6.669465 8.037384 8.893028

 38 H 8.267147 6.914391 6.669465 8.037384 8.893028

 39 H 8.373019 7.025080 6.480078 7.713725 8.754869

 40 H 4.370709 5.437019 6.551002 6.411595 5.135306

 41 H 4.370709 5.437019 6.551002 6.411595 5.135306

 42 H 5.488299 6.387354 7.627977 7.680274 6.449004

 43 H 8.287094 7.758679 8.870979 10.054902 9.726759

 44 H 8.287094 7.758679 8.870979 10.054902 9.726759

 45 H 9.116962 8.392828 9.368107 10.672647 10.521149

 6 7 8 9 10

 6 N 0.000000

 7 C 1.343287 0.000000

 8 N 2.420144 1.363810 0.000000

 9 C 3.524965 2.222349 1.362105 0.000000

 10 C 3.576838 2.286713 2.307856 1.477519 0.000000

 11 C 2.487569 1.462083 2.292236 2.275366 1.369282

 12 N 4.779703 5.344562 5.004752 6.255896 7.282773

 13 C 6.815421 7.021967 6.255561 7.232052 8.532078

 14 C 7.266702 7.221399 6.241243 7.004111 8.406583

 15 C 6.259395 6.023104 4.933455 5.593525 7.021967

 16 N 5.004850 4.933455 4.014988 4.928712 6.255561

 17 C 5.339255 5.593525 4.928712 6.014560 7.232052

 18 N 6.759520 6.259395 5.004850 5.339255 6.815421

 19 N 5.004752 4.190171 2.839025 2.934134 4.411454

 20 C 6.255896 5.526655 4.187885 4.252936 5.723001

 21 C 7.282773 6.362215 4.999732 4.661856 6.033090

 22 C 6.804769 5.714616 4.401651 3.739732 4.976192

 23 C 5.344562 4.258978 2.939629 2.383788 3.749573

 24 N 4.779703 3.524218 2.420346 1.340445 2.490974

 25 Zn 3.379760 3.011552 2.007494 3.007280 4.266039

 26 C 3.083428 4.425175 5.389447 6.592867 6.594775

 27 H 4.586755 5.719019 6.061873 7.423502 7.988243

 28 C 4.999246 3.753932 3.737429 2.630910 1.491532

 29 H 2.856048 2.262017 3.326501 3.336473 2.202752

 30 C 7.803524 8.190774 7.558676 8.614388 9.859787

 31 H 8.324828 8.224134 7.183918 7.846631 9.282256

 32 C 8.739561 7.848479 6.485046 6.137056 7.479907

 33 H 7.511421 6.328185 5.091952 4.194436 5.215397

 34 H 4.145136 5.488299 6.387354 7.627977 7.680274

 35 H 3.099598 4.370709 5.437019 6.551002 6.411595

 36 H 3.099598 4.370709 5.437019 6.551002 6.411595

 37 H 5.597147 4.332770 4.144018 2.950106 2.146405

 38 H 5.597147 4.332770 4.144018 2.950106 2.146405

 39 H 5.230838 4.136409 4.439649 3.523636 2.140739

 40 H 7.799194 8.287094 7.758679 8.870979 10.054902

 41 H 7.799194 8.287094 7.758679 8.870979 10.054902

 42 H 8.807603 9.116962 8.392828 9.368107 10.672647

 43 H 9.085591 8.267147 6.914391 6.669465 8.037384

 44 H 9.085591 8.267147 6.914391 6.669465 8.037384

 45 H 9.367678 8.373019 7.025080 6.480078 7.713725

 11 12 13 14 15

 11 C 0.000000

 12 N 6.804769 0.000000

 13 C 8.406583 2.490974 0.000000

 14 C 8.502635 3.562033 1.369282 0.000000

 15 C 7.221399 3.524218 2.286713 1.462083 0.000000

 16 N 6.241243 2.420346 2.307856 2.292236 1.363810

 17 C 7.004111 1.340445 1.477519 2.275366 2.222349

 18 N 7.266702 4.779703 3.576838 2.487569 1.343287

 19 N 4.983265 5.004850 4.999732 4.401651 2.939629

 20 C 6.344231 5.339255 4.661856 3.739732 2.383788

 21 C 6.912532 6.815421 6.033090 4.976192 3.749573

 22 C 6.012271 7.266702 6.912532 6.012271 4.650748

 23 C 4.650748 6.259395 6.362215 5.714616 4.258978

 24 N 3.562033 6.759520 7.282773 6.804769 5.344562

 25 Zn 4.251317 3.379760 4.266039 4.251317 3.011552

 26 C 5.356155 4.999246 7.479907 8.396481 7.848479

 27 H 7.058644 2.856048 5.215397 6.398215 6.328185

 28 C 2.584429 8.739561 9.859787 9.618213 8.190774

 29 H 1.082604 7.511421 9.282256 9.465177 8.224134

 30 C 9.618213 3.083428 1.491532 2.584429 3.753932

 31 H 9.465177 4.586755 2.202752 1.082604 2.262017

 32 C 8.396481 7.803524 6.594775 5.356155 4.425175

 33 H 6.398215 8.324828 7.988243 7.058644 5.719019

 34 H 6.449004 5.230838 7.713725 8.754869 8.373019

 35 H 5.135306 5.597147 8.037384 8.893028 8.267147

 36 H 5.135306 5.597147 8.037384 8.893028 8.267147

 37 H 3.293550 9.085591 10.054902 9.726759 8.287094

 38 H 3.293550 9.085591 10.054902 9.726759 8.287094

 39 H 2.746416 9.367678 10.672647 10.521149 9.116962

 40 H 9.726759 3.099598 2.146405 3.293550 4.332770

 41 H 9.726759 3.099598 2.146405 3.293550 4.332770

 42 H 10.521149 4.145136 2.140739 2.746416 4.136409

 43 H 8.893028 7.799194 6.411595 5.135306 4.370709

 44 H 8.893028 7.799194 6.411595 5.135306 4.370709

 45 H 8.754869 8.807603 7.680274 6.449004 5.488299

 16 17 18 19 20

 16 N 0.000000

 17 C 1.362105 0.000000

 18 N 2.420144 3.524965 0.000000

 19 N 2.839025 4.187885 2.420346 0.000000

 20 C 2.934134 4.252936 1.340445 1.362105 0.000000

 21 C 4.411454 5.723001 2.490974 2.307856 1.477519

 22 C 4.983265 6.344231 3.562033 2.292236 2.275366

 23 C 4.190171 5.526655 3.524218 1.363810 2.222349

 24 N 5.004752 6.255896 4.779703 2.420144 3.524965

 25 Zn 2.007494 3.007280 3.379760 2.007494 3.007280

 26 C 6.485046 6.137056 8.739561 7.558676 8.614388

 27 H 5.091952 4.194436 7.511421 7.183918 7.846631

 28 C 7.558676 8.614388 7.803524 5.389447 6.592867

 29 H 7.183918 7.846631 8.324828 6.061873 7.423502

 30 C 3.737429 2.630910 4.999246 6.485046 6.137056

 31 H 3.326501 3.336473 2.856048 5.091952 4.194436

 32 C 5.389447 6.592867 3.083428 3.737429 2.630910

 33 H 6.061873 7.423502 4.586755 3.326501 3.336473

 34 H 7.025080 6.480078 9.367678 8.392828 9.368107

 35 H 6.914391 6.669465 9.085591 7.758679 8.870979

 36 H 6.914391 6.669465 9.085591 7.758679 8.870979

 37 H 7.758679 8.870979 7.799194 5.437019 6.551002

 38 H 7.758679 8.870979 7.799194 5.437019 6.551002

 39 H 8.392828 9.368107 8.807603 6.387354 7.627977

 40 H 4.144018 2.950106 5.597147 6.914391 6.669465

 41 H 4.144018 2.950106 5.597147 6.914391 6.669465

 42 H 4.439649 3.523636 5.230838 7.025080 6.480078

 43 H 5.437019 6.551002 3.099598 4.144018 2.950106

 44 H 5.437019 6.551002 3.099598 4.144018 2.950106

 45 H 6.387354 7.627977 4.145136 4.439649 3.523636

 21 22 23 24 25

 21 C 0.000000

 22 C 1.369282 0.000000

 23 C 2.286713 1.462083 0.000000

 24 N 3.576838 2.487569 1.343287 0.000000

 25 Zn 4.266039 4.251317 3.011552 3.379760 0.000000

 26 C 9.859787 9.618213 8.190774 7.803524 5.614352

 27 H 9.282256 9.465177 8.224134 8.324828 5.225620

 28 C 6.594775 5.356155 4.425175 3.083428 5.614352

 29 H 7.988243 7.058644 5.719019 4.586755 5.225620

 30 C 7.479907 8.396481 7.848479 8.739561 5.614352

 31 H 5.215397 6.398215 6.328185 7.511421 5.225620

 32 C 1.491532 2.584429 3.753932 4.999246 5.614352

 33 H 2.202752 1.082604 2.262017 2.856048 5.225620

 34 H 10.672647 10.521149 9.116962 8.807603 6.406636

 35 H 10.054902 9.726759 8.287094 7.799194 5.886846

 36 H 10.054902 9.726759 8.287094 7.799194 5.886846

 37 H 6.411595 5.135306 4.370709 3.099598 5.886846

 38 H 6.411595 5.135306 4.370709 3.099598 5.886846

 39 H 7.680274 6.449004 5.488299 4.145136 6.406636

 40 H 8.037384 8.893028 8.267147 9.085591 5.886846

 41 H 8.037384 8.893028 8.267147 9.085591 5.886846

 42 H 7.713725 8.754869 8.373019 9.367678 6.406636

 43 H 2.146405 3.293550 4.332770 5.597147 5.886846

 44 H 2.146405 3.293550 4.332770 5.597147 5.886846

 45 H 2.140739 2.746416 4.136409 5.230838 6.406636

 26 27 28 29 30

 26 C 0.000000

 27 H 2.985295 0.000000

 28 C 7.939893 9.469548 0.000000

 29 H 5.289969 7.390143 2.985295 0.000000

 30 C 7.939893 5.289969 11.228704 10.428045 0.000000

 31 H 9.469548 7.390143 10.428045 10.451241 2.985295

 32 C 11.228704 10.428045 7.939893 9.469548 7.939893

 33 H 10.428045 10.451241 5.289969 7.390143 9.469548

 34 H 1.093273 2.725607 9.032407 6.369737 7.971668

 35 H 1.099619 3.739107 7.688051 4.957643 8.558370

 36 H 1.099619 3.739107 7.688051 4.957643 8.558370

 37 H 8.558370 9.967242 1.099619 3.739107 11.451753

 38 H 8.558370 9.967242 1.099619 3.739107 11.451753

 39 H 7.971668 9.804624 1.093273 2.725607 11.997359

 40 H 7.688051 4.957643 11.451753 10.485381 1.099619

 41 H 7.688051 4.957643 11.451753 10.485381 1.099619

 42 H 9.032407 6.369737 11.997359 11.369928 1.093273

 43 H 11.451753 10.485381 8.558370 9.967242 7.688051

 44 H 11.451753 10.485381 8.558370 9.967242 7.688051

 45 H 11.997359 11.369928 7.971668 9.804624 9.032407

 31 32 33 34 35

 31 H 0.000000

 32 C 5.289969 0.000000

 33 H 7.390143 2.985295 0.000000

 34 H 9.804624 11.997359 11.369928 0.000000

 35 H 9.967242 11.451753 10.485381 1.778053 0.000000

 36 H 9.967242 11.451753 10.485381 1.778053 1.770150

 37 H 10.485381 7.688051 4.957643 9.643524 8.230626

 38 H 10.485381 7.688051 4.957643 9.643524 8.418826

 39 H 11.369928 9.032407 6.369737 9.060352 7.642142

 40 H 3.739107 8.558370 9.967242 7.642142 8.230626

 41 H 3.739107 8.558370 9.967242 7.642142 8.418826

 42 H 2.725607 7.971668 9.804624 9.060352 9.643524

 43 H 4.957643 1.099619 3.739107 12.175320 11.639863

 44 H 4.957643 1.099619 3.739107 12.175320 11.773693

 45 H 6.369737 1.093273 2.725607 12.813273 12.175320

 36 37 38 39 40

 36 H 0.000000

 37 H 8.418826 0.000000

 38 H 8.230626 1.770150 0.000000

 39 H 7.642142 1.778053 1.778053 0.000000

 40 H 8.418826 11.639863 11.773693 12.175320 0.000000

 41 H 8.230626 11.773693 11.639863 12.175320 1.770150

 42 H 9.643524 12.175320 12.175320 12.813273 1.778053

 43 H 11.773693 8.230626 8.418826 9.643524 8.230626

 44 H 11.639863 8.418826 8.230626 9.643524 8.418826

 45 H 12.175320 7.642142 7.642142 9.060352 9.643524

 41 42 43 44 45

 41 H 0.000000

 42 H 1.778053 0.000000

 43 H 8.418826 7.642142 0.000000

 44 H 8.230626 7.642142 1.770150 0.000000

 45 H 9.643524 9.060352 1.778053 1.778053 0.000000

 Stoichiometry C20H16N8Zn(1+,2)

 Framework group C4H[O(Zn),SGH(C20H8N8),X(H8)]

 Deg. of freedom 20

 Full point group C4H NOp 8

 Largest Abelian subgroup C2H NOp 4

 Largest concise Abelian subgroup C2H NOp 4

 Standard orientation:

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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

 1 6 0 -2.190409 2.066774 0.000000

 2 7 0 -1.865213 0.742302 0.000000

 3 6 0 -3.007280 0.000000 0.000000

 4 6 0 -4.166516 0.916097 0.000000

 5 6 0 -3.647838 2.183341 0.000000

 6 7 0 -3.104087 -1.336945 0.000000

 7 6 0 -2.066774 -2.190409 0.000000

 8 7 0 -0.742302 -1.865213 0.000000

 9 6 0 0.000000 -3.007280 0.000000

 10 6 0 -0.916097 -4.166516 0.000000

 11 6 0 -2.183341 -3.647838 0.000000

 12 7 0 -1.336945 3.104087 0.000000

 13 6 0 0.916097 4.166516 0.000000

 14 6 0 2.183341 3.647838 0.000000

 15 6 0 2.066774 2.190409 0.000000

 16 7 0 0.742302 1.865213 0.000000

 17 6 0 0.000000 3.007280 0.000000

 18 7 0 3.104087 1.336945 0.000000

 19 7 0 1.865213 -0.742302 0.000000

 20 6 0 3.007280 0.000000 0.000000

 21 6 0 4.166516 -0.916097 0.000000

 22 6 0 3.647838 -2.183341 0.000000

 23 6 0 2.190409 -2.066774 0.000000

 24 7 0 1.336945 -3.104087 0.000000

 25 30 0 0.000000 0.000000 0.000000

 26 6 0 -5.593592 0.482366 0.000000

 27 1 0 -4.192956 3.118690 0.000000

 28 6 0 -0.482366 -5.593592 0.000000

 29 1 0 -3.118690 -4.192956 0.000000

 30 6 0 0.482366 5.593592 0.000000

 31 1 0 3.118690 4.192956 0.000000

 32 6 0 5.593592 -0.482366 0.000000

 33 1 0 4.192956 -3.118690 0.000000

 34 1 0 -6.263586 1.346284 0.000000

 35 1 0 -5.818475 -0.130195 0.885075

 36 1 0 -5.818475 -0.130195 -0.885075

 37 1 0 0.130195 -5.818475 0.885075

 38 1 0 0.130195 -5.818475 -0.885075

 39 1 0 -1.346284 -6.263586 0.000000

 40 1 0 -0.130195 5.818475 0.885075

 41 1 0 -0.130195 5.818475 -0.885075

 42 1 0 1.346284 6.263586 0.000000

 43 1 0 5.818475 0.130195 0.885075

 44 1 0 5.818475 0.130195 -0.885075

 45 1 0 6.263586 -1.346284 0.000000

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 Rotational constants (GHZ): 0.1821070 0.1821070 0.0912612

 Leave Link 202 at Fri Jul 5 21:06:57 2019, MaxMem= 1342177280 cpu: 0.2

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

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

 Centers: 25

 S 1 1.00

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

 S 1 1.00

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

 S 1 1.00

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

 P 1 1.00

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

 P 1 1.00

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

 D 3 1.00

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

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

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

 D 1 1.00

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

 D 1 1.00

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

 \*\*\*\*

 Centers: 27 29 31 33 34 35 36 37 38 39

 Centers: 40 41 42 43 44 45 1 3 4 5

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

 Centers: 22 23 26 28 30 32 2 6 8 12

 Centers: 16 18 19 24

 6-311G\*

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

 Pseudopotential Parameters

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 Center Atomic Valence Angular Power

 Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

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 1 6

 No pseudopotential on this center.

 2 7

 No pseudopotential on this center.

 3 6

 No pseudopotential on this center.

 4 6

 No pseudopotential on this center.

 5 6

 No pseudopotential on this center.

 6 7

 No pseudopotential on this center.

 7 6

 No pseudopotential on this center.

 8 7

 No pseudopotential on this center.

 9 6

 No pseudopotential on this center.

 10 6

 No pseudopotential on this center.

 11 6

 No pseudopotential on this center.

 12 7

 No pseudopotential on this center.

 13 6

 No pseudopotential on this center.

 14 6

 No pseudopotential on this center.

 15 6

 No pseudopotential on this center.

 16 7

 No pseudopotential on this center.

 17 6

 No pseudopotential on this center.

 18 7

 No pseudopotential on this center.

 19 7

 No pseudopotential on this center.

 20 6

 No pseudopotential on this center.

 21 6

 No pseudopotential on this center.

 22 6

 No pseudopotential on this center.

 23 6

 No pseudopotential on this center.

 24 7

 No pseudopotential on this center.

 25 30 12

 F and up

 1 386.7379660 -18.00000000 0.00000000

 2 72.8587359 -124.35274030 0.00000000

 2 15.9066170 -30.66018220 0.00000000

 2 4.3502340 -10.63589890 0.00000000

 2 1.2842199 -0.76836230 0.00000000

 S - F

 0 19.0867858 3.00000000 0.00000000

 1 5.0231080 22.52342250 0.00000000

 2 1.2701744 48.44659420 0.00000000

 2 1.0671287 -44.55601190 0.00000000

 2 0.9264190 12.99839580 0.00000000

 P - F

 0 43.4927750 5.00000000 0.00000000

 1 20.8692669 20.74355890 0.00000000

 2 21.7118378 90.30271580 0.00000000

 2 6.3616915 74.66103160 0.00000000

 2 1.2291195 9.88944240 0.00000000

 D - F

 2 13.5851800 -4.84903590 0.00000000

 2 9.8373050 3.69133790 0.00000000

 2 0.8373113 -0.50373190 0.00000000

 26 6

 No pseudopotential on this center.

 27 1

 No pseudopotential on this center.

 28 6

 No pseudopotential on this center.

 29 1

 No pseudopotential on this center.

 30 6

 No pseudopotential on this center.

 31 1

 No pseudopotential on this center.

 32 6

 No pseudopotential on this center.

 33 1

 No pseudopotential on this center.

 34 1

 No pseudopotential on this center.

 35 1

 No pseudopotential on this center.

 36 1

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 37 1

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 38 1

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 39 1

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 40 1

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 41 1

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 42 1

 No pseudopotential on this center.

 43 1

 No pseudopotential on this center.

 44 1

 No pseudopotential on this center.

 45 1

 No pseudopotential on this center.

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

 There are 229 symmetry adapted cartesian basis functions of AG symmetry.

 There are 82 symmetry adapted cartesian basis functions of BG symmetry.

 There are 78 symmetry adapted cartesian basis functions of AU symmetry.

 There are 218 symmetry adapted cartesian basis functions of BU symmetry.

 There are 212 symmetry adapted basis functions of AG symmetry.

 There are 82 symmetry adapted basis functions of BG symmetry.

 There are 78 symmetry adapted basis functions of AU symmetry.

 There are 204 symmetry adapted basis functions of BU symmetry.

 576 basis functions, 1015 primitive gaussians, 607 cartesian basis functions

 102 alpha electrons 101 beta electrons

 nuclear repulsion energy 2759.9985592461 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= 45 NActive= 45 NUniq= 11 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= -0.1140368129 Hartrees.

 Nuclear repulsion after empirical dispersion term = 2759.8845224332 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= 45.

 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 = 45

 GePol: Total number of spheres = 45

 GePol: Number of exposed spheres = 45 (100.00%)

 GePol: Number of points = 3558

 GePol: Average weight of points = 0.11

 GePol: Minimum weight of points = 0.58D-09

 GePol: Maximum weight of points = 0.18390

 GePol: Number of points with low weight = 180

 GePol: Fraction of low-weight points (<1% of avg) = 5.06%

 GePol: Cavity surface area = 383.317 Ang\*\*2

 GePol: Cavity volume = 379.762 Ang\*\*3

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

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 PCM non-electrostatic energy = -0.0109045791 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 2759.8736178541 Hartrees.

 Leave Link 301 at Fri Jul 5 21:06:57 2019, MaxMem= 1342177280 cpu: 1.4

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

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

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

 One-electron integrals computed using PRISM.

 One-electron integral symmetry used in STVInt

 8 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15315 LenP2D= 41224.

 LDataN: DoStor=T MaxTD1= 5 Len= 102

 GSVD: received Info= 1 from GESDD.

 NBasis= 576 RedAO= T EigKep= 1.84D-04 NBF= 212 82 78 204

 NBsUse= 576 1.00D-06 EigRej= -1.00D+00 NBFU= 212 82 78 204

 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= 594 594 594 594 594 MxSgAt= 45 MxSgA2= 45.

 Leave Link 302 at Fri Jul 5 21:06:58 2019, MaxMem= 1342177280 cpu: 8.1

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

 DipDrv: MaxL=1.

 Leave Link 303 at Fri Jul 5 21:06:58 2019, MaxMem= 1342177280 cpu: 1.0

 (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= -1275.92411446635

 JPrj=0 DoOrth=F DoCkMO=F.

 Initial guess orbital symmetries:

 Alpha Orbitals:

 Occupied (EU) (EU) (BG) (AG) (BG) (EU) (EU) (AG) (BG) (EU)

 (EU) (AG) (EU) (EU) (AG) (BG) (EU) (EU) (AG) (BG)

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

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

 Leave Link 401 at Fri Jul 5 21:07:00 2019, MaxMem= 1342177280 cpu: 16.4

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

 UHF open shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 1138797 IEndB= 1138797 NGot= 1342177280 MDV= 1341424180

 LenX= 1341424180 LenY= 1341055124

 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= 670000000 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= 37978092.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 8.22D-15 for 3557.

 Iteration 1 A\*A^-1 deviation from orthogonality is 4.66D-15 for 3205 2074.

 Iteration 1 A^-1\*A deviation from unit magnitude is 8.44D-15 for 3557.

 Iteration 1 A^-1\*A deviation from orthogonality is 2.47D-12 for 1595 1524.

 E= -1275.03904728182

 DIIS: error= 9.30D-02 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -1275.03904728182 IErMin= 1 ErrMin= 9.30D-02

 ErrMax= 9.30D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.85D+00 BMatP= 3.85D+00

 IDIUse=3 WtCom= 7.05D-02 WtEn= 9.30D-01

 Coeff-Com: 0.100D+01

 Coeff-En: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.103 Goal= None Shift= 0.000

 Gap= 0.017 Goal= None Shift= 0.000

 GapD= 0.017 DampG=0.250 DampE=0.250 DampFc=0.1250 IDamp=-1.

 Damping current iteration by 1.25D-01

 RMSDP=2.64D-03 MaxDP=1.27D-01 OVMax= 2.36D-01

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 3.28D-04 CP: 9.96D-01

 E= -1275.17953494205 Delta-E= -0.140487660222 Rises=F Damp=T

 DIIS: error= 6.15D-02 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -1275.17953494205 IErMin= 2 ErrMin= 6.15D-02

 ErrMax= 6.15D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.06D+00 BMatP= 3.85D+00

 IDIUse=3 WtCom= 3.85D-01 WtEn= 6.15D-01

 Coeff-Com: -0.243D+01 0.343D+01

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

 Coeff: -0.937D+00 0.194D+01

 Gap= 0.117 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 21319 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

 Gap= 0.041 Goal= None Shift= 0.000

 RMSDP=1.45D-03 MaxDP=8.05D-02 DE=-1.40D-01 OVMax= 1.31D-01

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 1.01D-03 CP: 9.83D-01 3.00D+00

 E= -1275.55572764664 Delta-E= -0.376192704595 Rises=F Damp=F

 DIIS: error= 2.70D-02 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 3 EnMin= -1275.55572764664 IErMin= 3 ErrMin= 2.70D-02

 ErrMax= 2.70D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.50D-01 BMatP= 2.06D+00

 IDIUse=3 WtCom= 7.30D-01 WtEn= 2.70D-01

 EnCoef did 100 forward-backward iterations

 Coeff-Com: -0.949D-01 0.470D+00 0.625D+00

 Coeff-En: 0.117D+00 0.275D-03 0.883D+00

 Coeff: -0.377D-01 0.343D+00 0.695D+00

 Gap= 0.098 Goal= None Shift= 0.000

 Gap= 0.080 Goal= None Shift= 0.000

 RMSDP=7.33D-04 MaxDP=4.36D-02 DE=-3.76D-01 OVMax= 6.44D-02

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 4.23D-04 CP: 9.89D-01 2.81D+00 4.67D-01

 E= -1275.67723827422 Delta-E= -0.121510627578 Rises=F Damp=F

 DIIS: error= 7.31D-03 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -1275.67723827422 IErMin= 4 ErrMin= 7.31D-03

 ErrMax= 7.31D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.50D-02 BMatP= 6.50D-01

 IDIUse=3 WtCom= 9.27D-01 WtEn= 7.31D-02

 Coeff-Com: 0.151D+00-0.880D-01 0.371D+00 0.566D+00

 Coeff-En: 0.000D+00 0.000D+00 0.447D-01 0.955D+00

 Coeff: 0.140D+00-0.816D-01 0.347D+00 0.595D+00

 Gap= 0.103 Goal= None Shift= 0.000

 Gap= 0.074 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 31774 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

 RMSDP=2.17D-04 MaxDP=1.16D-02 DE=-1.22D-01 OVMax= 3.04D-02

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 1.29D-04 CP: 9.88D-01 3.00D+00 5.61D-01 7.65D-01

 E= -1275.69472607475 Delta-E= -0.017487800534 Rises=F Damp=F

 DIIS: error= 3.15D-03 at cycle 5 NSaved= 5.

 NSaved= 5 IEnMin= 5 EnMin= -1275.69472607475 IErMin= 5 ErrMin= 3.15D-03

 ErrMax= 3.15D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.84D-03 BMatP= 8.50D-02

 IDIUse=3 WtCom= 9.69D-01 WtEn= 3.15D-02

 Coeff-Com: 0.103D+00-0.105D+00 0.152D+00 0.349D+00 0.500D+00

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

 Coeff: 0.100D+00-0.101D+00 0.147D+00 0.338D+00 0.516D+00

 Gap= 0.102 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 31774 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

 Gap= 0.075 Goal= None Shift= 0.000

 RMSDP=6.92D-05 MaxDP=3.14D-03 DE=-1.75D-02 OVMax= 1.30D-02

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 4.41D-05 CP: 9.88D-01 3.00D+00 5.52D-01 8.18D-01 6.31D-01

 E= -1275.69664644001 Delta-E= -0.001920365252 Rises=F Damp=F

 DIIS: error= 1.18D-03 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -1275.69664644001 IErMin= 6 ErrMin= 1.18D-03

 ErrMax= 1.18D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-03 BMatP= 9.84D-03

 IDIUse=3 WtCom= 9.88D-01 WtEn= 1.18D-02

 Coeff-Com: 0.626D-01-0.733D-01 0.484D-01 0.119D+00 0.293D+00 0.550D+00

 Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.214D-01 0.979D+00

 Coeff: 0.619D-01-0.725D-01 0.478D-01 0.118D+00 0.290D+00 0.555D+00

 Gap= 0.103 Goal= None Shift= 0.000

 Gap= 0.076 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

 RMSDP=2.61D-05 MaxDP=1.31D-03 DE=-1.92D-03 OVMax= 4.69D-03

 Cycle 7 Pass 1 IDiag 1:

 RMSU= 2.11D-05 CP: 9.88D-01 3.00D+00 5.59D-01 8.10D-01 6.88D-01

 CP: 7.56D-01

 E= -1275.69690169596 Delta-E= -0.000255255955 Rises=F Damp=F

 DIIS: error= 5.01D-04 at cycle 7 NSaved= 7.

 NSaved= 7 IEnMin= 7 EnMin= -1275.69690169596 IErMin= 7 ErrMin= 5.01D-04

 ErrMax= 5.01D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.69D-05 BMatP= 1.05D-03

 IDIUse=3 WtCom= 9.95D-01 WtEn= 5.01D-03

 Coeff-Com: 0.148D-01-0.185D-01-0.528D-02-0.251D-01 0.557D-04 0.164D+00

 Coeff-Com: 0.869D+00

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

 Coeff-En: 0.100D+01

 Coeff: 0.148D-01-0.184D-01-0.525D-02-0.250D-01 0.554D-04 0.164D+00

 Coeff: 0.870D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.076 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 31774 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

 RMSDP=1.17D-05 MaxDP=6.78D-04 DE=-2.55D-04 OVMax= 3.21D-03

 Cycle 8 Pass 1 IDiag 1:

 RMSU= 8.38D-06 CP: 9.88D-01 3.00D+00 5.60D-01 8.10D-01 7.18D-01

 CP: 9.09D-01 1.12D+00

 E= -1275.69694911512 Delta-E= -0.000047419157 Rises=F Damp=F

 DIIS: error= 1.47D-04 at cycle 8 NSaved= 8.

 NSaved= 8 IEnMin= 8 EnMin= -1275.69694911512 IErMin= 8 ErrMin= 1.47D-04

 ErrMax= 1.47D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.29D-05 BMatP= 7.69D-05

 IDIUse=3 WtCom= 9.99D-01 WtEn= 1.47D-03

 Coeff-Com: -0.136D-01 0.159D-01-0.126D-01-0.333D-01-0.850D-01-0.148D+00

 Coeff-Com: 0.799D-01 0.120D+01

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

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

 Coeff: -0.136D-01 0.159D-01-0.126D-01-0.332D-01-0.849D-01-0.147D+00

 Coeff: 0.798D-01 0.120D+01

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=9.18D-06 MaxDP=5.47D-04 DE=-4.74D-05 OVMax= 2.92D-03

 Cycle 9 Pass 1 IDiag 1:

 RMSU= 4.43D-06 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.27D-01

 CP: 9.85D-01 1.40D+00 1.49D+00

 E= -1275.69696601495 Delta-E= -0.000016899835 Rises=F Damp=F

 DIIS: error= 1.02D-04 at cycle 9 NSaved= 9.

 NSaved= 9 IEnMin= 9 EnMin= -1275.69696601495 IErMin= 9 ErrMin= 1.02D-04

 ErrMax= 1.02D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.59D-06 BMatP= 1.29D-05

 IDIUse=3 WtCom= 9.99D-01 WtEn= 1.02D-03

 Coeff-Com: -0.113D-01 0.133D-01-0.655D-02-0.138D-01-0.476D-01-0.111D+00

 Coeff-Com: -0.846D-01 0.699D+00 0.563D+00

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

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

 Coeff: -0.113D-01 0.133D-01-0.654D-02-0.138D-01-0.475D-01-0.111D+00

 Coeff: -0.845D-01 0.698D+00 0.563D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=2.64D-06 MaxDP=1.46D-04 DE=-1.69D-05 OVMax= 7.27D-04

 Cycle 10 Pass 1 IDiag 1:

 RMSU= 1.90D-06 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.30D-01

 CP: 1.01D+00 1.44D+00 1.63D+00 1.04D+00

 E= -1275.69696834906 Delta-E= -0.000002334111 Rises=F Damp=F

 DIIS: error= 3.26D-05 at cycle 10 NSaved= 10.

 NSaved=10 IEnMin=10 EnMin= -1275.69696834906 IErMin=10 ErrMin= 3.26D-05

 ErrMax= 3.26D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.32D-07 BMatP= 6.59D-06

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

 Coeff-Com: -0.456D-02 0.525D-02-0.117D-02 0.713D-03-0.257D-02-0.162D-01

 Coeff-Com: -0.505D-01 0.184D-01 0.218D+00 0.833D+00

 Coeff: -0.456D-02 0.525D-02-0.117D-02 0.713D-03-0.257D-02-0.162D-01

 Coeff: -0.505D-01 0.184D-01 0.218D+00 0.833D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=1.43D-06 MaxDP=7.15D-05 DE=-2.33D-06 OVMax= 4.57D-04

 Cycle 11 Pass 1 IDiag 1:

 RMSU= 7.23D-07 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.30D-01

 CP: 1.01D+00 1.47D+00 1.70D+00 1.23D+00 1.07D+00

 E= -1275.69696875272 Delta-E= -0.000000403659 Rises=F Damp=F

 DIIS: error= 2.47D-05 at cycle 11 NSaved= 11.

 NSaved=11 IEnMin=11 EnMin= -1275.69696875272 IErMin=11 ErrMin= 2.47D-05

 ErrMax= 2.47D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.15D-07 BMatP= 9.32D-07

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

 Coeff-Com: -0.212D-02 0.241D-02-0.188D-03 0.196D-02 0.380D-02 0.279D-02

 Coeff-Com: -0.201D-01-0.708D-01 0.588D-01 0.509D+00 0.514D+00

 Coeff: -0.212D-02 0.241D-02-0.188D-03 0.196D-02 0.380D-02 0.279D-02

 Coeff: -0.201D-01-0.708D-01 0.588D-01 0.509D+00 0.514D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=4.69D-07 MaxDP=2.49D-05 DE=-4.04D-07 OVMax= 1.75D-04

 Cycle 12 Pass 1 IDiag 1:

 RMSU= 3.04D-07 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.30D-01

 CP: 1.01D+00 1.47D+00 1.72D+00 1.27D+00 1.18D+00

 CP: 8.17D-01

 E= -1275.69696884611 Delta-E= -0.000000093384 Rises=F Damp=F

 DIIS: error= 1.16D-05 at cycle 12 NSaved= 12.

 NSaved=12 IEnMin=12 EnMin= -1275.69696884611 IErMin=12 ErrMin= 1.16D-05

 ErrMax= 1.16D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.43D-08 BMatP= 3.15D-07

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

 Coeff-Com: -0.507D-03 0.579D-03-0.107D-03 0.249D-03 0.798D-03 0.207D-02

 Coeff-Com: 0.227D-02-0.143D-01-0.175D-01-0.158D-01 0.112D+00 0.931D+00

 Coeff: -0.507D-03 0.579D-03-0.107D-03 0.249D-03 0.798D-03 0.207D-02

 Coeff: 0.227D-02-0.143D-01-0.175D-01-0.158D-01 0.112D+00 0.931D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=2.94D-07 MaxDP=1.74D-05 DE=-9.34D-08 OVMax= 1.49D-04

 Cycle 13 Pass 1 IDiag 1:

 RMSU= 1.47D-07 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.31D-01

 CP: 1.01D+00 1.47D+00 1.72D+00 1.29D+00 1.23D+00

 CP: 1.02D+00 1.43D+00

 E= -1275.69696886903 Delta-E= -0.000000022923 Rises=F Damp=F

 DIIS: error= 3.90D-06 at cycle 13 NSaved= 13.

 NSaved=13 IEnMin=13 EnMin= -1275.69696886903 IErMin=13 ErrMin= 3.90D-06

 ErrMax= 3.90D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.08D-08 BMatP= 3.43D-08

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

 Coeff-Com: 0.979D-04-0.106D-03-0.856D-04-0.457D-03-0.810D-03-0.120D-03

 Coeff-Com: 0.687D-02 0.134D-01-0.235D-01-0.154D+00-0.750D-01 0.507D+00

 Coeff-Com: 0.726D+00

 Coeff: 0.979D-04-0.106D-03-0.856D-04-0.457D-03-0.810D-03-0.120D-03

 Coeff: 0.687D-02 0.134D-01-0.235D-01-0.154D+00-0.750D-01 0.507D+00

 Coeff: 0.726D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=2.00D-07 MaxDP=1.24D-05 DE=-2.29D-08 OVMax= 1.11D-04

 Cycle 14 Pass 1 IDiag 1:

 RMSU= 7.80D-08 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.31D-01

 CP: 1.01D+00 1.47D+00 1.73D+00 1.31D+00 1.27D+00

 CP: 1.13D+00 1.85D+00 1.33D+00

 E= -1275.69696887968 Delta-E= -0.000000010655 Rises=F Damp=F

 DIIS: error= 2.47D-06 at cycle 14 NSaved= 14.

 NSaved=14 IEnMin=14 EnMin= -1275.69696887968 IErMin=14 ErrMin= 2.47D-06

 ErrMax= 2.47D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.40D-09 BMatP= 1.08D-08

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

 Coeff-Com: 0.373D-03-0.427D-03 0.867D-04-0.152D-03-0.400D-03-0.724D-03

 Coeff-Com: 0.151D-02 0.653D-02 0.436D-02-0.346D-01-0.651D-01-0.370D+00

 Coeff-Com: 0.182D+00 0.128D+01

 Coeff: 0.373D-03-0.427D-03 0.867D-04-0.152D-03-0.400D-03-0.724D-03

 Coeff: 0.151D-02 0.653D-02 0.436D-02-0.346D-01-0.651D-01-0.370D+00

 Coeff: 0.182D+00 0.128D+01

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=2.30D-07 MaxDP=1.37D-05 DE=-1.07D-08 OVMax= 1.26D-04

 Cycle 15 Pass 1 IDiag 1:

 RMSU= 4.09D-08 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.31D-01

 CP: 1.01D+00 1.47D+00 1.73D+00 1.32D+00 1.30D+00

 CP: 1.26D+00 2.31D+00 2.11D+00 1.62D+00

 E= -1275.69696888545 Delta-E= -0.000000005770 Rises=F Damp=F

 DIIS: error= 3.03D-06 at cycle 15 NSaved= 15.

 NSaved=15 IEnMin=15 EnMin= -1275.69696888545 IErMin=14 ErrMin= 2.47D-06

 ErrMax= 3.03D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D-09 BMatP= 2.40D-09

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

 Coeff-Com: 0.212D-03-0.243D-03 0.705D-04 0.482D-05-0.273D-04-0.228D-03

 Coeff-Com: -0.760D-03-0.657D-05 0.799D-02 0.139D-01-0.851D-02-0.233D+00

 Coeff-Com: -0.689D-01 0.552D+00 0.737D+00

 Coeff: 0.212D-03-0.243D-03 0.705D-04 0.482D-05-0.273D-04-0.228D-03

 Coeff: -0.760D-03-0.657D-05 0.799D-02 0.139D-01-0.851D-02-0.233D+00

 Coeff: -0.689D-01 0.552D+00 0.737D+00

 Gap= 0.104 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 21319 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=5.76D-08 MaxDP=3.93D-06 DE=-5.77D-09 OVMax= 3.00D-05

 Cycle 16 Pass 1 IDiag 1:

 RMSU= 1.83D-08 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.31D-01

 CP: 1.01D+00 1.47D+00 1.73D+00 1.32D+00 1.30D+00

 CP: 1.29D+00 2.42D+00 2.33D+00 1.91D+00 1.10D+00

 E= -1275.69696888598 Delta-E= -0.000000000529 Rises=F Damp=F

 DIIS: error= 1.30D-06 at cycle 16 NSaved= 16.

 NSaved=16 IEnMin=16 EnMin= -1275.69696888598 IErMin=16 ErrMin= 1.30D-06

 ErrMax= 1.30D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.08D-10 BMatP= 1.37D-09

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

 Coeff-Com: 0.697D-04-0.809D-04 0.389D-04 0.763D-04 0.189D-03 0.296D-03

 Coeff-Com: -0.107D-02-0.316D-02 0.392D-02 0.217D-01 0.203D-01-0.706D-02

 Coeff-Com: -0.129D+00-0.134D+00 0.390D+00 0.838D+00

 Coeff: 0.697D-04-0.809D-04 0.389D-04 0.763D-04 0.189D-03 0.296D-03

 Coeff: -0.107D-02-0.316D-02 0.392D-02 0.217D-01 0.203D-01-0.706D-02

 Coeff: -0.129D+00-0.134D+00 0.390D+00 0.838D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=4.16D-08 MaxDP=2.68D-06 DE=-5.29D-10 OVMax= 1.81D-05

 Cycle 17 Pass 1 IDiag 1:

 RMSU= 8.50D-09 CP: 9.88D-01 3.00D+00 5.60D-01 8.12D-01 7.31D-01

 CP: 1.01D+00 1.47D+00 1.73D+00 1.32D+00 1.30D+00

 CP: 1.30D+00 2.49D+00 2.49D+00 2.12D+00 1.42D+00

 CP: 1.02D+00

 E= -1275.69696888627 Delta-E= -0.000000000290 Rises=F Damp=F

 DIIS: error= 5.29D-07 at cycle 17 NSaved= 17.

 NSaved=17 IEnMin=17 EnMin= -1275.69696888627 IErMin=17 ErrMin= 5.29D-07

 ErrMax= 5.29D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.46D-11 BMatP= 5.08D-10

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

 Coeff-Com: 0.498D-05-0.573D-05 0.371D-05 0.115D-04 0.302D-04 0.868D-04

 Coeff-Com: -0.492D-04-0.384D-03-0.354D-03 0.469D-03 0.327D-02 0.275D-01

 Coeff-Com: -0.857D-02-0.646D-01-0.866D-01 0.113D+00 0.102D+01

 Coeff: 0.498D-05-0.573D-05 0.371D-05 0.115D-04 0.302D-04 0.868D-04

 Coeff: -0.492D-04-0.384D-03-0.354D-03 0.469D-03 0.327D-02 0.275D-01

 Coeff: -0.857D-02-0.646D-01-0.866D-01 0.113D+00 0.102D+01

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.077 Goal= None Shift= 0.000

 RMSDP=8.93D-09 MaxDP=6.21D-07 DE=-2.90D-10 OVMax= 2.43D-06

 Error on total polarization charges = 0.06047

 SCF Done: E(UB3LYP) = -1275.69696889 A.U. after 17 cycles

 NFock= 17 Conv=0.89D-08 -V/T= 1.9662

 <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7830 S= 0.5163

 <L.S>= 0.000000000000E+00

 KE= 1.320283431434D+03 PE=-8.543513833603D+03 EE= 3.187659815428D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.84

 (included in total energy above)

 Annihilation of the first spin contaminant:

 S\*\*2 before annihilation 0.7830, after 0.7509

 Leave Link 502 at Fri Jul 5 21:08:40 2019, MaxMem= 1342177280 cpu: 1163.5

 (Enter /apps/gaussian/g09d01/g09/l601.exe)

 Copying SCF densities to generalized density rwf, IOpCl= 1 IROHF=0.

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 Population analysis using the SCF density.

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 Orbital symmetries:

 Alpha Orbitals:

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 The electronic state is 2-AU.

 Alpha occ. eigenvalues -- -14.34377 -14.34377 -14.34377 -14.34377 -14.32908

 Alpha occ. eigenvalues -- -14.32908 -14.32908 -14.32908 -10.28532 -10.28532

 Alpha occ. eigenvalues -- -10.28532 -10.28532 -10.28465 -10.28465 -10.28465

 Alpha occ. eigenvalues -- -10.28464 -10.21460 -10.21460 -10.21460 -10.21460

 Alpha occ. eigenvalues -- -10.19491 -10.19491 -10.19491 -10.19491 -10.17347

 Alpha occ. eigenvalues -- -10.17347 -10.17347 -10.17347 -1.03087 -1.01677

 Alpha occ. eigenvalues -- -1.01677 -0.98939 -0.96701 -0.92500 -0.92500

 Alpha occ. eigenvalues -- -0.89115 -0.81830 -0.81283 -0.81283 -0.81020

 Alpha occ. eigenvalues -- -0.77823 -0.74039 -0.74039 -0.71814 -0.70638

 Alpha occ. eigenvalues -- -0.69914 -0.69914 -0.65837 -0.63385 -0.60995

 Alpha occ. eigenvalues -- -0.59651 -0.59237 -0.58967 -0.58967 -0.57246

 Alpha occ. eigenvalues -- -0.57246 -0.56589 -0.56373 -0.56373 -0.56070

 Alpha occ. eigenvalues -- -0.53700 -0.52495 -0.52495 -0.51657 -0.50524

 Alpha occ. eigenvalues -- -0.48544 -0.46883 -0.46883 -0.45886 -0.44911

 Alpha occ. eigenvalues -- -0.44911 -0.44540 -0.44283 -0.41754 -0.41648

 Alpha occ. eigenvalues -- -0.41648 -0.41638 -0.41245 -0.41184 -0.40828

 Alpha occ. eigenvalues -- -0.40828 -0.39708 -0.39588 -0.39069 -0.39069

 Alpha occ. eigenvalues -- -0.38366 -0.38225 -0.34962 -0.34962 -0.34318

 Alpha occ. eigenvalues -- -0.34318 -0.32934 -0.30163 -0.30163 -0.28408

 Alpha occ. eigenvalues -- -0.27963 -0.27944 -0.26908 -0.26908 -0.26767

 Alpha occ. eigenvalues -- -0.26644 -0.23988

 Alpha virt. eigenvalues -- -0.13559 -0.13559 -0.07014 0.00088 0.02359

 Alpha virt. eigenvalues -- 0.02359 0.02725 0.03823 0.04049 0.04049

 Alpha virt. eigenvalues -- 0.04879 0.06466 0.06634 0.07391 0.07784

 Alpha virt. eigenvalues -- 0.07784 0.08501 0.08852 0.08885 0.08885

 Alpha virt. eigenvalues -- 0.09527 0.09527 0.09585 0.12426 0.13025

 Alpha virt. eigenvalues -- 0.13057 0.13057 0.13123 0.13216 0.13216

 Alpha virt. eigenvalues -- 0.13613 0.16627 0.18773 0.19065 0.19386

 Alpha virt. eigenvalues -- 0.19386 0.19469 0.19921 0.19921 0.21002

 Alpha virt. eigenvalues -- 0.21032 0.21172 0.21468 0.21468 0.24237

 Alpha virt. eigenvalues -- 0.25505 0.26359 0.26359 0.27130 0.27304

 Alpha virt. eigenvalues -- 0.27787 0.27787 0.28120 0.30523 0.30523

 Alpha virt. eigenvalues -- 0.30585 0.30798 0.30974 0.30974 0.31411

 Alpha virt. eigenvalues -- 0.31481 0.33581 0.33979 0.33979 0.34608

 Alpha virt. eigenvalues -- 0.35980 0.35980 0.36192 0.37172 0.37550

 Alpha virt. eigenvalues -- 0.37550 0.38456 0.38765 0.38765 0.39350

 Alpha virt. eigenvalues -- 0.40416 0.41975 0.41975 0.42168 0.42241

 Alpha virt. eigenvalues -- 0.42805 0.43988 0.45197 0.45197 0.45330

 Alpha virt. eigenvalues -- 0.46484 0.47467 0.47467 0.47798 0.47907

 Alpha virt. eigenvalues -- 0.47907 0.48176 0.49542 0.50326 0.50530

 Alpha virt. eigenvalues -- 0.50530 0.51881 0.52143 0.52775 0.52775

 Alpha virt. eigenvalues -- 0.53357 0.54837 0.54837 0.55167 0.55242

 Alpha virt. eigenvalues -- 0.56244 0.56244 0.56595 0.57555 0.57624

 Alpha virt. eigenvalues -- 0.57624 0.57727 0.58470 0.58470 0.58851

 Alpha virt. eigenvalues -- 0.59780 0.59799 0.61316 0.61454 0.61454

 Alpha virt. eigenvalues -- 0.62266 0.62294 0.62294 0.63359 0.63838

 Alpha virt. eigenvalues -- 0.63838 0.66775 0.66888 0.67551 0.67622

 Alpha virt. eigenvalues -- 0.67622 0.68084 0.68084 0.68352 0.69389

 Alpha virt. eigenvalues -- 0.70318 0.71895 0.71988 0.71988 0.73123

 Alpha virt. eigenvalues -- 0.73888 0.74532 0.74532 0.76442 0.76442

 Alpha virt. eigenvalues -- 0.77838 0.78306 0.78619 0.79541 0.79541

 Alpha virt. eigenvalues -- 0.79893 0.80090 0.80090 0.80933 0.81330

 Alpha virt. eigenvalues -- 0.83973 0.84208 0.84208 0.86051 0.87242

 Alpha virt. eigenvalues -- 0.87667 0.87667 0.88560 0.93122 0.95498

 Alpha virt. eigenvalues -- 0.95498 0.96375 0.96415 0.98659 0.98659

 Alpha virt. eigenvalues -- 0.98683 1.01550 1.01550 1.02890 1.03680

 Alpha virt. eigenvalues -- 1.03680 1.05126 1.06637 1.06637 1.06722

 Alpha virt. eigenvalues -- 1.08623 1.09007 1.11602 1.11602 1.11803

 Alpha virt. eigenvalues -- 1.11804 1.11881 1.12272 1.12272 1.12378

 Alpha virt. eigenvalues -- 1.12986 1.16360 1.16612 1.17604 1.17604

 Alpha virt. eigenvalues -- 1.19005 1.19005 1.19301 1.21863 1.22349

 Alpha virt. eigenvalues -- 1.25914 1.26453 1.27723 1.27723 1.28775

 Alpha virt. eigenvalues -- 1.34262 1.34262 1.35571 1.36205 1.37567

 Alpha virt. eigenvalues -- 1.38415 1.39295 1.39295 1.40480 1.40480

 Alpha virt. eigenvalues -- 1.42429 1.43470 1.47881 1.48396 1.48396

 Alpha virt. eigenvalues -- 1.50276 1.50303 1.50303 1.50498 1.50559

 Alpha virt. eigenvalues -- 1.50614 1.50614 1.51602 1.51976 1.53457

 Alpha virt. eigenvalues -- 1.53457 1.54177 1.54578 1.54578 1.55609

 Alpha virt. eigenvalues -- 1.56793 1.58928 1.59281 1.59281 1.60606

 Alpha virt. eigenvalues -- 1.61360 1.61360 1.61539 1.65664 1.66509

 Alpha virt. eigenvalues -- 1.66614 1.66614 1.67468 1.67468 1.67798

 Alpha virt. eigenvalues -- 1.69103 1.69888 1.69888 1.72086 1.73839

 Alpha virt. eigenvalues -- 1.73839 1.73884 1.78096 1.78203 1.78203

 Alpha virt. eigenvalues -- 1.78309 1.83124 1.84562 1.84562 1.85273

 Alpha virt. eigenvalues -- 1.86812 1.88363 1.88363 1.88741 1.89652

 Alpha virt. eigenvalues -- 1.92088 1.93428 1.94668 1.94668 1.94908

 Alpha virt. eigenvalues -- 1.98963 1.99083 1.99083 1.99151 1.99738

 Alpha virt. eigenvalues -- 1.99919 2.00089 2.00089 2.03412 2.04312

 Alpha virt. eigenvalues -- 2.05938 2.06833 2.06833 2.10564 2.10564

 Alpha virt. eigenvalues -- 2.13244 2.13788 2.13788 2.15034 2.15449

 Alpha virt. eigenvalues -- 2.18074 2.25799 2.26795 2.27309 2.27602

 Alpha virt. eigenvalues -- 2.27602 2.28197 2.31073 2.31073 2.33928

 Alpha virt. eigenvalues -- 2.34173 2.34173 2.35344 2.35344 2.35380

 Alpha virt. eigenvalues -- 2.36249 2.37004 2.37677 2.37677 2.37859

 Alpha virt. eigenvalues -- 2.42057 2.45972 2.46177 2.46177 2.46230

 Alpha virt. eigenvalues -- 2.46329 2.46329 2.47225 2.47423 2.53431

 Alpha virt. eigenvalues -- 2.53533 2.53533 2.54113 2.55831 2.55831

 Alpha virt. eigenvalues -- 2.57206 2.58208 2.58208 2.60992 2.61397

 Alpha virt. eigenvalues -- 2.62415 2.63956 2.65092 2.68148 2.68148

 Alpha virt. eigenvalues -- 2.69426 2.70128 2.70255 2.70255 2.73227

 Alpha virt. eigenvalues -- 2.73227 2.74036 2.77047 2.80668 2.81527

 Alpha virt. eigenvalues -- 2.81527 2.81813 2.81895 2.82483 2.82483

 Alpha virt. eigenvalues -- 2.82649 2.89295 2.89295 2.90535 2.91567

 Alpha virt. eigenvalues -- 2.93648 2.94775 2.94775 2.99077 3.01204

 Alpha virt. eigenvalues -- 3.02412 3.02412 3.03677 3.10292 3.10778

 Alpha virt. eigenvalues -- 3.11702 3.12036 3.12036 3.12214 3.12214

 Alpha virt. eigenvalues -- 3.12532 3.13590 3.15004 3.15004 3.16576

 Alpha virt. eigenvalues -- 3.18485 3.18485 3.18843 3.19960 3.22231

 Alpha virt. eigenvalues -- 3.24717 3.25998 3.25998 3.26337 3.28451

 Alpha virt. eigenvalues -- 3.28451 3.34185 3.35659 3.36902 3.36902

 Alpha virt. eigenvalues -- 3.37400 3.50865 3.55032 3.55032 3.67530

 Alpha virt. eigenvalues -- 3.69824 3.69971 3.69971 3.73889 3.75448

 Alpha virt. eigenvalues -- 3.75948 3.75948 3.76552 3.78866 3.79684

 Alpha virt. eigenvalues -- 3.79684 3.84990 3.85672 3.85807 3.85807

 Alpha virt. eigenvalues -- 3.89007 4.02773 4.02773 4.03385 4.03449

 Alpha virt. eigenvalues -- 4.09202 4.10238 4.10238 4.16380 4.25941

 Alpha virt. eigenvalues -- 4.32919 4.32919 4.35320 4.43637 4.49194

 Alpha virt. eigenvalues -- 4.59142 4.59142 4.97083 5.00327 5.00327

 Alpha virt. eigenvalues -- 5.08892 5.12385 5.30431 5.30431 5.47645

 Alpha virt. eigenvalues -- 7.76867 7.76867 7.88056 7.93529 8.21149

 Alpha virt. eigenvalues -- 11.17965 23.41511 23.44044 23.44044 23.45459

 Alpha virt. eigenvalues -- 23.65108 23.65687 23.65687 23.65802 23.78269

 Alpha virt. eigenvalues -- 23.79126 23.79126 23.80222 23.82697 23.83841

 Alpha virt. eigenvalues -- 23.83841 23.84026 24.07298 24.07784 24.07784

 Alpha virt. eigenvalues -- 24.08486 35.53841 35.58427 35.58427 35.59601

 Alpha virt. eigenvalues -- 35.64821 35.66068 35.66068 35.66385

 Beta occ. eigenvalues -- -14.34525 -14.34525 -14.34525 -14.34524 -14.33007

 Beta occ. eigenvalues -- -14.33007 -14.33007 -14.33007 -10.28263 -10.28262

 Beta occ. eigenvalues -- -10.28262 -10.28262 -10.28194 -10.28194 -10.28194

 Beta occ. eigenvalues -- -10.28194 -10.21392 -10.21392 -10.21392 -10.21392

 Beta occ. eigenvalues -- -10.19511 -10.19511 -10.19511 -10.19510 -10.17348

 Beta occ. eigenvalues -- -10.17348 -10.17348 -10.17348 -1.02885 -1.01475

 Beta occ. eigenvalues -- -1.01475 -0.98722 -0.96616 -0.92480 -0.92480

 Beta occ. eigenvalues -- -0.89295 -0.81713 -0.81203 -0.81203 -0.80949

 Beta occ. eigenvalues -- -0.77249 -0.73749 -0.73749 -0.71769 -0.70506

 Beta occ. eigenvalues -- -0.69704 -0.69704 -0.65554 -0.63123 -0.60939

 Beta occ. eigenvalues -- -0.59580 -0.59195 -0.58802 -0.58802 -0.57267

 Beta occ. eigenvalues -- -0.57267 -0.56480 -0.56220 -0.56220 -0.56037

 Beta occ. eigenvalues -- -0.53577 -0.52403 -0.52403 -0.51553 -0.50450

 Beta occ. eigenvalues -- -0.47803 -0.46126 -0.46126 -0.45852 -0.44874

 Beta occ. eigenvalues -- -0.44874 -0.44232 -0.43899 -0.41600 -0.41525

 Beta occ. eigenvalues -- -0.41445 -0.41445 -0.41245 -0.40717 -0.40717

 Beta occ. eigenvalues -- -0.40516 -0.39586 -0.39105 -0.39032 -0.39032

 Beta occ. eigenvalues -- -0.38318 -0.38162 -0.34965 -0.34965 -0.33555

 Beta occ. eigenvalues -- -0.33555 -0.33023 -0.30261 -0.30261 -0.28526

 Beta occ. eigenvalues -- -0.27994 -0.27891 -0.27627 -0.26894 -0.26894

 Beta occ. eigenvalues -- -0.26630

 Beta virt. eigenvalues -- -0.18906 -0.12186 -0.12186 -0.06360 0.01283

 Beta virt. eigenvalues -- 0.02967 0.03232 0.03232 0.04101 0.04101

 Beta virt. eigenvalues -- 0.04635 0.04886 0.06468 0.06649 0.07815

 Beta virt. eigenvalues -- 0.07815 0.08161 0.08869 0.08891 0.09541

 Beta virt. eigenvalues -- 0.09541 0.09634 0.09634 0.09635 0.12433

 Beta virt. eigenvalues -- 0.13073 0.13073 0.13132 0.13137 0.13390

 Beta virt. eigenvalues -- 0.13390 0.13786 0.16848 0.19002 0.19291

 Beta virt. eigenvalues -- 0.19539 0.19539 0.19717 0.20203 0.20203

 Beta virt. eigenvalues -- 0.21111 0.21114 0.21394 0.21747 0.21747

 Beta virt. eigenvalues -- 0.24522 0.25794 0.26473 0.26473 0.27216

 Beta virt. eigenvalues -- 0.27780 0.28019 0.28019 0.28274 0.30662

 Beta virt. eigenvalues -- 0.30684 0.30684 0.30867 0.31039 0.31039

 Beta virt. eigenvalues -- 0.31509 0.31571 0.33640 0.34185 0.34185

 Beta virt. eigenvalues -- 0.34779 0.36114 0.36114 0.36399 0.37456

 Beta virt. eigenvalues -- 0.38214 0.38214 0.38605 0.38916 0.38916

 Beta virt. eigenvalues -- 0.39512 0.40869 0.42115 0.42115 0.42355

 Beta virt. eigenvalues -- 0.42924 0.43314 0.44142 0.45428 0.45428

 Beta virt. eigenvalues -- 0.45517 0.46617 0.47634 0.47634 0.48049

 Beta virt. eigenvalues -- 0.48049 0.48084 0.48304 0.49683 0.50611

 Beta virt. eigenvalues -- 0.50881 0.50881 0.52273 0.52322 0.52843

 Beta virt. eigenvalues -- 0.52843 0.53414 0.54907 0.54907 0.55243

 Beta virt. eigenvalues -- 0.55335 0.56331 0.56331 0.56905 0.57598

 Beta virt. eigenvalues -- 0.57750 0.57750 0.57782 0.58546 0.58546

 Beta virt. eigenvalues -- 0.58898 0.59870 0.59880 0.61452 0.61632

 Beta virt. eigenvalues -- 0.61632 0.62311 0.62656 0.62656 0.63446

 Beta virt. eigenvalues -- 0.63893 0.63893 0.67031 0.67075 0.67622

 Beta virt. eigenvalues -- 0.67753 0.67753 0.67928 0.67928 0.68506

 Beta virt. eigenvalues -- 0.69525 0.70333 0.72019 0.72141 0.72141

 Beta virt. eigenvalues -- 0.73210 0.74082 0.74621 0.74621 0.76577

 Beta virt. eigenvalues -- 0.76577 0.77821 0.78196 0.78822 0.79448

 Beta virt. eigenvalues -- 0.79448 0.79699 0.80199 0.80199 0.81011

 Beta virt. eigenvalues -- 0.81400 0.84048 0.84311 0.84311 0.86129

 Beta virt. eigenvalues -- 0.87297 0.87738 0.87738 0.88660 0.93273

 Beta virt. eigenvalues -- 0.95552 0.95552 0.96453 0.96616 0.98766

 Beta virt. eigenvalues -- 0.98766 0.99097 1.01872 1.01872 1.02953

 Beta virt. eigenvalues -- 1.03846 1.03846 1.05308 1.06826 1.07074

 Beta virt. eigenvalues -- 1.07074 1.08979 1.09018 1.11856 1.11858

 Beta virt. eigenvalues -- 1.12245 1.12245 1.12379 1.12379 1.12392

 Beta virt. eigenvalues -- 1.12910 1.13481 1.16823 1.16974 1.17638

 Beta virt. eigenvalues -- 1.17638 1.19464 1.19464 1.19486 1.21897

 Beta virt. eigenvalues -- 1.22396 1.25997 1.26894 1.27861 1.27861

 Beta virt. eigenvalues -- 1.28820 1.34752 1.34752 1.35737 1.36801

 Beta virt. eigenvalues -- 1.37646 1.38872 1.39368 1.39368 1.40600

 Beta virt. eigenvalues -- 1.40600 1.42662 1.43611 1.47878 1.48443

 Beta virt. eigenvalues -- 1.48443 1.50343 1.50367 1.50367 1.50516

 Beta virt. eigenvalues -- 1.50546 1.50598 1.50598 1.51690 1.52420

 Beta virt. eigenvalues -- 1.53565 1.53565 1.54245 1.54742 1.54742

 Beta virt. eigenvalues -- 1.55836 1.57035 1.59027 1.59574 1.59574

 Beta virt. eigenvalues -- 1.60685 1.61484 1.61484 1.61752 1.65731

 Beta virt. eigenvalues -- 1.66786 1.66786 1.66882 1.67561 1.67561

 Beta virt. eigenvalues -- 1.67993 1.69212 1.70390 1.70390 1.72230

 Beta virt. eigenvalues -- 1.74000 1.74000 1.74531 1.78400 1.78428

 Beta virt. eigenvalues -- 1.78428 1.78493 1.83244 1.84714 1.84714

 Beta virt. eigenvalues -- 1.85528 1.86936 1.88718 1.88718 1.88886

 Beta virt. eigenvalues -- 1.90008 1.92428 1.93738 1.95006 1.95006

 Beta virt. eigenvalues -- 1.95013 1.99141 1.99253 1.99253 1.99311

 Beta virt. eigenvalues -- 2.00090 2.00160 2.00614 2.00614 2.03481

 Beta virt. eigenvalues -- 2.04721 2.05943 2.06868 2.06868 2.10613

 Beta virt. eigenvalues -- 2.10613 2.13368 2.14100 2.14100 2.15149

 Beta virt. eigenvalues -- 2.15894 2.18220 2.25851 2.27065 2.27355

 Beta virt. eigenvalues -- 2.27636 2.27636 2.28229 2.31157 2.31157

 Beta virt. eigenvalues -- 2.33973 2.34231 2.34231 2.35428 2.35683

 Beta virt. eigenvalues -- 2.35683 2.36286 2.37074 2.37709 2.37709

 Beta virt. eigenvalues -- 2.38248 2.42104 2.45893 2.46348 2.46348

 Beta virt. eigenvalues -- 2.46358 2.46358 2.46364 2.47480 2.47510

 Beta virt. eigenvalues -- 2.53355 2.53422 2.53422 2.54111 2.55816

 Beta virt. eigenvalues -- 2.55816 2.57651 2.58628 2.58628 2.61301

 Beta virt. eigenvalues -- 2.61312 2.62292 2.64286 2.65088 2.68359

 Beta virt. eigenvalues -- 2.68359 2.69590 2.70087 2.70191 2.70191

 Beta virt. eigenvalues -- 2.74010 2.74010 2.74778 2.77950 2.81223

 Beta virt. eigenvalues -- 2.81856 2.82199 2.82199 2.82553 2.82553

 Beta virt. eigenvalues -- 2.82677 2.82716 2.89375 2.89375 2.90647

 Beta virt. eigenvalues -- 2.92023 2.93709 2.95383 2.95383 2.99808

 Beta virt. eigenvalues -- 3.01293 3.02491 3.02491 3.03759 3.10337

 Beta virt. eigenvalues -- 3.10834 3.11778 3.12106 3.12106 3.12308

 Beta virt. eigenvalues -- 3.12308 3.12630 3.13724 3.15062 3.15062

 Beta virt. eigenvalues -- 3.16614 3.18551 3.18551 3.18903 3.19977

 Beta virt. eigenvalues -- 3.22299 3.24774 3.26059 3.26059 3.26423

 Beta virt. eigenvalues -- 3.28532 3.28532 3.34270 3.35689 3.36942

 Beta virt. eigenvalues -- 3.36942 3.37454 3.51013 3.55165 3.55165

 Beta virt. eigenvalues -- 3.67641 3.69951 3.70117 3.70117 3.73995

 Beta virt. eigenvalues -- 3.75621 3.76082 3.76082 3.76693 3.78376

 Beta virt. eigenvalues -- 3.79292 3.79292 3.84676 3.85205 3.85414

 Beta virt. eigenvalues -- 3.85414 3.88685 4.02884 4.02884 4.03491

 Beta virt. eigenvalues -- 4.03568 4.09199 4.10283 4.10283 4.16492

 Beta virt. eigenvalues -- 4.26002 4.33087 4.33087 4.35562 4.43693

 Beta virt. eigenvalues -- 4.49204 4.59167 4.59167 4.97258 5.00504

 Beta virt. eigenvalues -- 5.00504 5.09087 5.12541 5.30612 5.30612

 Beta virt. eigenvalues -- 5.47827 7.76849 7.76849 7.88056 7.93524

 Beta virt. eigenvalues -- 8.21145 11.17955 23.41569 23.44093 23.44093

 Beta virt. eigenvalues -- 23.45503 23.65136 23.65709 23.65709 23.65821

 Beta virt. eigenvalues -- 23.78523 23.79401 23.79401 23.80504 23.83010

 Beta virt. eigenvalues -- 23.84150 23.84150 23.84337 24.07330 24.07816

 Beta virt. eigenvalues -- 24.07816 24.08517 35.53715 35.58313 35.58313

 Beta virt. eigenvalues -- 35.59500 35.64668 35.65927 35.65927 35.66255

 Condensed to atoms (all electrons):

 1 2 3 4 5 6

 1 C 4.563057 0.401781 -0.125072 -0.046360 0.403509 -0.001839

 2 N 0.401781 7.123694 0.386031 -0.063158 -0.093413 -0.077438

 3 C -0.125072 0.386031 4.599754 0.378724 -0.065400 0.553895

 4 C -0.046360 -0.063158 0.378724 5.030078 0.628331 -0.069071

 5 C 0.403509 -0.093413 -0.065400 0.628331 5.085094 0.004185

 6 N -0.001839 -0.077438 0.553895 -0.069071 0.004185 6.574328

 7 C -0.001037 -0.004590 -0.088060 0.004303 -0.000302 0.511057

 8 N 0.000675 -0.018506 -0.005334 -0.000123 -0.000192 -0.070768

 9 C -0.000005 0.000578 -0.000855 0.000022 -0.000003 0.000087

 10 C -0.000003 -0.000101 0.000041 0.000014 0.000000 0.003239

 11 C 0.000022 0.000213 0.004004 -0.000253 0.000010 -0.040211

 12 N 0.511057 -0.070768 0.000087 0.003239 -0.040211 -0.000146

 13 C 0.004303 -0.000123 0.000022 0.000014 -0.000253 0.000000

 14 C -0.000302 -0.000192 -0.000003 0.000000 0.000010 0.000000

 15 C -0.001037 0.000675 -0.000005 -0.000003 0.000022 -0.000001

 16 N -0.004590 -0.018506 0.000578 -0.000101 0.000213 -0.000005

 17 C -0.088060 -0.005334 -0.000855 0.000041 0.004004 -0.000024

 18 N -0.000018 -0.000004 -0.000001 0.000000 0.000000 0.000000

 19 N 0.000153 -0.003445 0.000205 0.000002 0.000003 -0.000004

 20 C -0.000048 0.000205 -0.000010 0.000000 0.000000 -0.000001

 21 C 0.000000 0.000002 0.000000 0.000000 0.000000 0.000000

 22 C 0.000000 0.000003 0.000000 0.000000 0.000000 0.000000

 23 C -0.000004 0.000153 -0.000048 0.000000 0.000000 -0.000018

 24 N -0.000001 -0.000005 -0.000024 0.000000 0.000000 -0.000146

 25 Zn -0.015245 0.106371 -0.016060 -0.001148 -0.001056 -0.004692

 26 C 0.008714 0.008230 -0.067873 0.271487 -0.052204 0.012814

 27 H -0.045762 0.005683 0.008982 -0.039659 0.394018 -0.000010

 28 C 0.000000 0.000000 0.000002 0.000000 0.000000 -0.000019

 29 H 0.000001 0.000065 -0.000206 -0.000126 -0.000003 0.005429

 30 C -0.000458 0.000054 0.000000 0.000000 -0.000045 0.000000

 31 H 0.000010 0.000001 0.000000 0.000000 0.000000 0.000000

 32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 33 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 34 H 0.000274 -0.000225 0.006143 -0.040049 -0.005591 0.000052

 35 H -0.000200 0.000371 -0.005175 -0.041871 -0.000130 0.003338

 36 H -0.000200 0.000371 -0.005175 -0.041871 -0.000130 0.003338

 37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000007

 38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000007

 39 H 0.000000 0.000000 0.000001 0.000000 0.000000 -0.000011

 40 H -0.000035 0.000011 0.000000 0.000000 -0.000018 0.000000

 41 H -0.000035 0.000011 0.000000 0.000000 -0.000018 0.000000

 42 H 0.000034 0.000000 0.000000 0.000000 -0.000001 0.000000

 43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 7 8 9 10 11 12

 1 C -0.001037 0.000675 -0.000005 -0.000003 0.000022 0.511057

 2 N -0.004590 -0.018506 0.000578 -0.000101 0.000213 -0.070768

 3 C -0.088060 -0.005334 -0.000855 0.000041 0.004004 0.000087

 4 C 0.004303 -0.000123 0.000022 0.000014 -0.000253 0.003239

 5 C -0.000302 -0.000192 -0.000003 0.000000 0.000010 -0.040211

 6 N 0.511057 -0.070768 0.000087 0.003239 -0.040211 -0.000146

 7 C 4.563057 0.401781 -0.125072 -0.046360 0.403509 -0.000018

 8 N 0.401781 7.123694 0.386031 -0.063158 -0.093413 -0.000004

 9 C -0.125072 0.386031 4.599754 0.378724 -0.065400 -0.000001

 10 C -0.046360 -0.063158 0.378724 5.030078 0.628331 0.000000

 11 C 0.403509 -0.093413 -0.065400 0.628331 5.085094 0.000000

 12 N -0.000018 -0.000004 -0.000001 0.000000 0.000000 6.574328

 13 C 0.000000 0.000002 0.000000 0.000000 0.000000 -0.069071

 14 C 0.000000 0.000003 0.000000 0.000000 0.000000 0.004185

 15 C -0.000004 0.000153 -0.000048 0.000000 0.000000 -0.001839

 16 N 0.000153 -0.003445 0.000205 0.000002 0.000003 -0.077438

 17 C -0.000048 0.000205 -0.000010 0.000000 0.000000 0.553895

 18 N -0.000001 -0.000005 -0.000024 0.000000 0.000000 -0.000146

 19 N 0.000675 -0.018506 -0.005334 -0.000123 -0.000192 -0.000005

 20 C -0.000005 0.000578 -0.000855 0.000022 -0.000003 -0.000024

 21 C -0.000003 -0.000101 0.000041 0.000014 0.000000 0.000000

 22 C 0.000022 0.000213 0.004004 -0.000253 0.000010 0.000000

 23 C -0.001037 -0.004590 -0.088060 0.004303 -0.000302 -0.000001

 24 N -0.001839 -0.077438 0.553895 -0.069071 0.004185 0.000000

 25 Zn -0.015245 0.106371 -0.016060 -0.001148 -0.001056 -0.004692

 26 C -0.000458 0.000054 0.000000 0.000000 -0.000045 -0.000019

 27 H 0.000010 0.000001 0.000000 0.000000 0.000000 0.005429

 28 C 0.008714 0.008230 -0.067873 0.271487 -0.052204 0.000000

 29 H -0.045762 0.005683 0.008982 -0.039659 0.394018 0.000000

 30 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.012814

 31 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000010

 32 C 0.000000 0.000000 0.000002 0.000000 0.000000 0.000000

 33 H 0.000001 0.000065 -0.000206 -0.000126 -0.000003 0.000000

 34 H 0.000034 0.000000 0.000000 0.000000 -0.000001 -0.000011

 35 H -0.000035 0.000011 0.000000 0.000000 -0.000018 0.000007

 36 H -0.000035 0.000011 0.000000 0.000000 -0.000018 0.000007

 37 H -0.000200 0.000371 -0.005175 -0.041871 -0.000130 0.000000

 38 H -0.000200 0.000371 -0.005175 -0.041871 -0.000130 0.000000

 39 H 0.000274 -0.000225 0.006143 -0.040049 -0.005591 0.000000

 40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.003338

 41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.003338

 42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000052

 43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 45 H 0.000000 0.000000 0.000001 0.000000 0.000000 0.000000

 13 14 15 16 17 18

 1 C 0.004303 -0.000302 -0.001037 -0.004590 -0.088060 -0.000018

 2 N -0.000123 -0.000192 0.000675 -0.018506 -0.005334 -0.000004

 3 C 0.000022 -0.000003 -0.000005 0.000578 -0.000855 -0.000001

 4 C 0.000014 0.000000 -0.000003 -0.000101 0.000041 0.000000

 5 C -0.000253 0.000010 0.000022 0.000213 0.004004 0.000000

 6 N 0.000000 0.000000 -0.000001 -0.000005 -0.000024 0.000000

 7 C 0.000000 0.000000 -0.000004 0.000153 -0.000048 -0.000001

 8 N 0.000002 0.000003 0.000153 -0.003445 0.000205 -0.000005

 9 C 0.000000 0.000000 -0.000048 0.000205 -0.000010 -0.000024

 10 C 0.000000 0.000000 0.000000 0.000002 0.000000 0.000000

 11 C 0.000000 0.000000 0.000000 0.000003 0.000000 0.000000

 12 N -0.069071 0.004185 -0.001839 -0.077438 0.553895 -0.000146

 13 C 5.030078 0.628331 -0.046360 -0.063158 0.378724 0.003239

 14 C 0.628331 5.085094 0.403509 -0.093413 -0.065400 -0.040211

 15 C -0.046360 0.403509 4.563057 0.401781 -0.125072 0.511057

 16 N -0.063158 -0.093413 0.401781 7.123694 0.386031 -0.070768

 17 C 0.378724 -0.065400 -0.125072 0.386031 4.599754 0.000087

 18 N 0.003239 -0.040211 0.511057 -0.070768 0.000087 6.574328

 19 N -0.000101 0.000213 -0.004590 -0.018506 0.000578 -0.077438

 20 C 0.000041 0.004004 -0.088060 -0.005334 -0.000855 0.553895

 21 C 0.000014 -0.000253 0.004303 -0.000123 0.000022 -0.069071

 22 C 0.000000 0.000010 -0.000302 -0.000192 -0.000003 0.004185

 23 C -0.000003 0.000022 -0.001037 0.000675 -0.000005 -0.001839

 24 N 0.000000 0.000000 -0.000018 -0.000004 -0.000001 -0.000146

 25 Zn -0.001148 -0.001056 -0.015245 0.106371 -0.016060 -0.004692

 26 C 0.000000 0.000000 0.000000 0.000000 0.000002 0.000000

 27 H -0.000126 -0.000003 0.000001 0.000065 -0.000206 0.000000

 28 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 29 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 30 C 0.271487 -0.052204 0.008714 0.008230 -0.067873 -0.000019

 31 H -0.039659 0.394018 -0.045762 0.005683 0.008982 0.005429

 32 C 0.000000 -0.000045 -0.000458 0.000054 0.000000 0.012814

 33 H 0.000000 0.000000 0.000010 0.000001 0.000000 -0.000010

 34 H 0.000000 0.000000 0.000000 0.000000 0.000001 0.000000

 35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 40 H -0.041871 -0.000130 -0.000200 0.000371 -0.005175 0.000007

 41 H -0.041871 -0.000130 -0.000200 0.000371 -0.005175 0.000007

 42 H -0.040049 -0.005591 0.000274 -0.000225 0.006143 -0.000011

 43 H 0.000000 -0.000018 -0.000035 0.000011 0.000000 0.003338

 44 H 0.000000 -0.000018 -0.000035 0.000011 0.000000 0.003338

 45 H 0.000000 -0.000001 0.000034 0.000000 0.000000 0.000052

 19 20 21 22 23 24

 1 C 0.000153 -0.000048 0.000000 0.000000 -0.000004 -0.000001

 2 N -0.003445 0.000205 0.000002 0.000003 0.000153 -0.000005

 3 C 0.000205 -0.000010 0.000000 0.000000 -0.000048 -0.000024

 4 C 0.000002 0.000000 0.000000 0.000000 0.000000 0.000000

 5 C 0.000003 0.000000 0.000000 0.000000 0.000000 0.000000

 6 N -0.000004 -0.000001 0.000000 0.000000 -0.000018 -0.000146

 7 C 0.000675 -0.000005 -0.000003 0.000022 -0.001037 -0.001839

 8 N -0.018506 0.000578 -0.000101 0.000213 -0.004590 -0.077438

 9 C -0.005334 -0.000855 0.000041 0.004004 -0.088060 0.553895

 10 C -0.000123 0.000022 0.000014 -0.000253 0.004303 -0.069071

 11 C -0.000192 -0.000003 0.000000 0.000010 -0.000302 0.004185

 12 N -0.000005 -0.000024 0.000000 0.000000 -0.000001 0.000000

 13 C -0.000101 0.000041 0.000014 0.000000 -0.000003 0.000000

 14 C 0.000213 0.004004 -0.000253 0.000010 0.000022 0.000000

 15 C -0.004590 -0.088060 0.004303 -0.000302 -0.001037 -0.000018

 16 N -0.018506 -0.005334 -0.000123 -0.000192 0.000675 -0.000004

 17 C 0.000578 -0.000855 0.000022 -0.000003 -0.000005 -0.000001

 18 N -0.077438 0.553895 -0.069071 0.004185 -0.001839 -0.000146

 19 N 7.123694 0.386031 -0.063158 -0.093413 0.401781 -0.070768

 20 C 0.386031 4.599754 0.378724 -0.065400 -0.125072 0.000087

 21 C -0.063158 0.378724 5.030078 0.628331 -0.046360 0.003239

 22 C -0.093413 -0.065400 0.628331 5.085094 0.403509 -0.040211

 23 C 0.401781 -0.125072 -0.046360 0.403509 4.563057 0.511057

 24 N -0.070768 0.000087 0.003239 -0.040211 0.511057 6.574328

 25 Zn 0.106371 -0.016060 -0.001148 -0.001056 -0.015245 -0.004692

 26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 28 C 0.000054 0.000000 0.000000 -0.000045 -0.000458 0.012814

 29 H 0.000001 0.000000 0.000000 0.000000 0.000010 -0.000010

 30 C 0.000000 0.000002 0.000000 0.000000 0.000000 0.000000

 31 H 0.000065 -0.000206 -0.000126 -0.000003 0.000001 0.000000

 32 C 0.008230 -0.067873 0.271487 -0.052204 0.008714 -0.000019

 33 H 0.005683 0.008982 -0.039659 0.394018 -0.045762 0.005429

 34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 37 H 0.000011 0.000000 0.000000 -0.000018 -0.000035 0.003338

 38 H 0.000011 0.000000 0.000000 -0.000018 -0.000035 0.003338

 39 H 0.000000 0.000000 0.000000 -0.000001 0.000034 0.000052

 40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 42 H 0.000000 0.000001 0.000000 0.000000 0.000000 0.000000

 43 H 0.000371 -0.005175 -0.041871 -0.000130 -0.000200 0.000007

 44 H 0.000371 -0.005175 -0.041871 -0.000130 -0.000200 0.000007

 45 H -0.000225 0.006143 -0.040049 -0.005591 0.000274 -0.000011

 25 26 27 28 29 30

 1 C -0.015245 0.008714 -0.045762 0.000000 0.000001 -0.000458

 2 N 0.106371 0.008230 0.005683 0.000000 0.000065 0.000054

 3 C -0.016060 -0.067873 0.008982 0.000002 -0.000206 0.000000

 4 C -0.001148 0.271487 -0.039659 0.000000 -0.000126 0.000000

 5 C -0.001056 -0.052204 0.394018 0.000000 -0.000003 -0.000045

 6 N -0.004692 0.012814 -0.000010 -0.000019 0.005429 0.000000

 7 C -0.015245 -0.000458 0.000010 0.008714 -0.045762 0.000000

 8 N 0.106371 0.000054 0.000001 0.008230 0.005683 0.000000

 9 C -0.016060 0.000000 0.000000 -0.067873 0.008982 0.000000

 10 C -0.001148 0.000000 0.000000 0.271487 -0.039659 0.000000

 11 C -0.001056 -0.000045 0.000000 -0.052204 0.394018 0.000000

 12 N -0.004692 -0.000019 0.005429 0.000000 0.000000 0.012814

 13 C -0.001148 0.000000 -0.000126 0.000000 0.000000 0.271487

 14 C -0.001056 0.000000 -0.000003 0.000000 0.000000 -0.052204

 15 C -0.015245 0.000000 0.000001 0.000000 0.000000 0.008714

 16 N 0.106371 0.000000 0.000065 0.000000 0.000000 0.008230

 17 C -0.016060 0.000002 -0.000206 0.000000 0.000000 -0.067873

 18 N -0.004692 0.000000 0.000000 0.000000 0.000000 -0.000019

 19 N 0.106371 0.000000 0.000000 0.000054 0.000001 0.000000

 20 C -0.016060 0.000000 0.000000 0.000000 0.000000 0.000002

 21 C -0.001148 0.000000 0.000000 0.000000 0.000000 0.000000

 22 C -0.001056 0.000000 0.000000 -0.000045 0.000000 0.000000

 23 C -0.015245 0.000000 0.000000 -0.000458 0.000010 0.000000

 24 N -0.004692 0.000000 0.000000 0.012814 -0.000010 0.000000

 25 Zn 10.187981 0.000379 0.000005 0.000379 0.000005 0.000379

 26 C 0.000379 5.357363 -0.004195 0.000000 0.000055 0.000000

 27 H 0.000005 -0.004195 0.425541 0.000000 0.000000 0.000055

 28 C 0.000379 0.000000 0.000000 5.357363 -0.004195 0.000000

 29 H 0.000005 0.000055 0.000000 -0.004195 0.425541 0.000000

 30 C 0.000379 0.000000 0.000055 0.000000 0.000000 5.357363

 31 H 0.000005 0.000000 0.000000 0.000000 0.000000 -0.004195

 32 C 0.000379 0.000000 0.000000 0.000000 0.000000 0.000000

 33 H 0.000005 0.000000 0.000000 0.000055 0.000000 0.000000

 34 H 0.000046 0.388258 0.001216 0.000000 0.000000 0.000000

 35 H 0.000074 0.385664 -0.000087 0.000000 0.000028 0.000000

 36 H 0.000074 0.385664 -0.000087 0.000000 0.000028 0.000000

 37 H 0.000074 0.000000 0.000000 0.385664 -0.000087 0.000000

 38 H 0.000074 0.000000 0.000000 0.385664 -0.000087 0.000000

 39 H 0.000046 0.000000 0.000000 0.388258 0.001216 0.000000

 40 H 0.000074 0.000000 0.000028 0.000000 0.000000 0.385664

 41 H 0.000074 0.000000 0.000028 0.000000 0.000000 0.385664

 42 H 0.000046 0.000000 0.000000 0.000000 0.000000 0.388258

 43 H 0.000074 0.000000 0.000000 0.000000 0.000000 0.000000

 44 H 0.000074 0.000000 0.000000 0.000000 0.000000 0.000000

 45 H 0.000046 0.000000 0.000000 0.000000 0.000000 0.000000

 31 32 33 34 35 36

 1 C 0.000010 0.000000 0.000000 0.000274 -0.000200 -0.000200

 2 N 0.000001 0.000000 0.000000 -0.000225 0.000371 0.000371

 3 C 0.000000 0.000000 0.000000 0.006143 -0.005175 -0.005175

 4 C 0.000000 0.000000 0.000000 -0.040049 -0.041871 -0.041871

 5 C 0.000000 0.000000 0.000000 -0.005591 -0.000130 -0.000130

 6 N 0.000000 0.000000 0.000000 0.000052 0.003338 0.003338

 7 C 0.000000 0.000000 0.000001 0.000034 -0.000035 -0.000035

 8 N 0.000000 0.000000 0.000065 0.000000 0.000011 0.000011

 9 C 0.000000 0.000002 -0.000206 0.000000 0.000000 0.000000

 10 C 0.000000 0.000000 -0.000126 0.000000 0.000000 0.000000

 11 C 0.000000 0.000000 -0.000003 -0.000001 -0.000018 -0.000018

 12 N -0.000010 0.000000 0.000000 -0.000011 0.000007 0.000007

 13 C -0.039659 0.000000 0.000000 0.000000 0.000000 0.000000

 14 C 0.394018 -0.000045 0.000000 0.000000 0.000000 0.000000

 15 C -0.045762 -0.000458 0.000010 0.000000 0.000000 0.000000

 16 N 0.005683 0.000054 0.000001 0.000000 0.000000 0.000000

 17 C 0.008982 0.000000 0.000000 0.000001 0.000000 0.000000

 18 N 0.005429 0.012814 -0.000010 0.000000 0.000000 0.000000

 19 N 0.000065 0.008230 0.005683 0.000000 0.000000 0.000000

 20 C -0.000206 -0.067873 0.008982 0.000000 0.000000 0.000000

 21 C -0.000126 0.271487 -0.039659 0.000000 0.000000 0.000000

 22 C -0.000003 -0.052204 0.394018 0.000000 0.000000 0.000000

 23 C 0.000001 0.008714 -0.045762 0.000000 0.000000 0.000000

 24 N 0.000000 -0.000019 0.005429 0.000000 0.000000 0.000000

 25 Zn 0.000005 0.000379 0.000005 0.000046 0.000074 0.000074

 26 C 0.000000 0.000000 0.000000 0.388258 0.385664 0.385664

 27 H 0.000000 0.000000 0.000000 0.001216 -0.000087 -0.000087

 28 C 0.000000 0.000000 0.000055 0.000000 0.000000 0.000000

 29 H 0.000000 0.000000 0.000000 0.000000 0.000028 0.000028

 30 C -0.004195 0.000000 0.000000 0.000000 0.000000 0.000000

 31 H 0.425541 0.000055 0.000000 0.000000 0.000000 0.000000

 32 C 0.000055 5.357363 -0.004195 0.000000 0.000000 0.000000

 33 H 0.000000 -0.004195 0.425541 0.000000 0.000000 0.000000

 34 H 0.000000 0.000000 0.000000 0.448379 -0.024293 -0.024293

 35 H 0.000000 0.000000 0.000000 -0.024293 0.458233 -0.026445

 36 H 0.000000 0.000000 0.000000 -0.024293 -0.026445 0.458233

 37 H 0.000000 0.000000 0.000028 0.000000 0.000000 0.000000

 38 H 0.000000 0.000000 0.000028 0.000000 0.000000 0.000000

 39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 40 H -0.000087 0.000000 0.000000 0.000000 0.000000 0.000000

 41 H -0.000087 0.000000 0.000000 0.000000 0.000000 0.000000

 42 H 0.001216 0.000000 0.000000 0.000000 0.000000 0.000000

 43 H 0.000028 0.385664 -0.000087 0.000000 0.000000 0.000000

 44 H 0.000028 0.385664 -0.000087 0.000000 0.000000 0.000000

 45 H 0.000000 0.388258 0.001216 0.000000 0.000000 0.000000

 37 38 39 40 41 42

 1 C 0.000000 0.000000 0.000000 -0.000035 -0.000035 0.000034

 2 N 0.000000 0.000000 0.000000 0.000011 0.000011 0.000000

 3 C 0.000000 0.000000 0.000001 0.000000 0.000000 0.000000

 4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 5 C 0.000000 0.000000 0.000000 -0.000018 -0.000018 -0.000001

 6 N 0.000007 0.000007 -0.000011 0.000000 0.000000 0.000000

 7 C -0.000200 -0.000200 0.000274 0.000000 0.000000 0.000000

 8 N 0.000371 0.000371 -0.000225 0.000000 0.000000 0.000000

 9 C -0.005175 -0.005175 0.006143 0.000000 0.000000 0.000000

 10 C -0.041871 -0.041871 -0.040049 0.000000 0.000000 0.000000

 11 C -0.000130 -0.000130 -0.005591 0.000000 0.000000 0.000000

 12 N 0.000000 0.000000 0.000000 0.003338 0.003338 0.000052

 13 C 0.000000 0.000000 0.000000 -0.041871 -0.041871 -0.040049

 14 C 0.000000 0.000000 0.000000 -0.000130 -0.000130 -0.005591

 15 C 0.000000 0.000000 0.000000 -0.000200 -0.000200 0.000274

 16 N 0.000000 0.000000 0.000000 0.000371 0.000371 -0.000225

 17 C 0.000000 0.000000 0.000000 -0.005175 -0.005175 0.006143

 18 N 0.000000 0.000000 0.000000 0.000007 0.000007 -0.000011

 19 N 0.000011 0.000011 0.000000 0.000000 0.000000 0.000000

 20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000001

 21 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 22 C -0.000018 -0.000018 -0.000001 0.000000 0.000000 0.000000

 23 C -0.000035 -0.000035 0.000034 0.000000 0.000000 0.000000

 24 N 0.003338 0.003338 0.000052 0.000000 0.000000 0.000000

 25 Zn 0.000074 0.000074 0.000046 0.000074 0.000074 0.000046

 26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 27 H 0.000000 0.000000 0.000000 0.000028 0.000028 0.000000

 28 C 0.385664 0.385664 0.388258 0.000000 0.000000 0.000000

 29 H -0.000087 -0.000087 0.001216 0.000000 0.000000 0.000000

 30 C 0.000000 0.000000 0.000000 0.385664 0.385664 0.388258

 31 H 0.000000 0.000000 0.000000 -0.000087 -0.000087 0.001216

 32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 33 H 0.000028 0.000028 0.000000 0.000000 0.000000 0.000000

 34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 37 H 0.458233 -0.026445 -0.024293 0.000000 0.000000 0.000000

 38 H -0.026445 0.458233 -0.024293 0.000000 0.000000 0.000000

 39 H -0.024293 -0.024293 0.448379 0.000000 0.000000 0.000000

 40 H 0.000000 0.000000 0.000000 0.458233 -0.026445 -0.024293

 41 H 0.000000 0.000000 0.000000 -0.026445 0.458233 -0.024293

 42 H 0.000000 0.000000 0.000000 -0.024293 -0.024293 0.448379

 43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 43 44 45

 1 C 0.000000 0.000000 0.000000

 2 N 0.000000 0.000000 0.000000

 3 C 0.000000 0.000000 0.000000

 4 C 0.000000 0.000000 0.000000

 5 C 0.000000 0.000000 0.000000

 6 N 0.000000 0.000000 0.000000

 7 C 0.000000 0.000000 0.000000

 8 N 0.000000 0.000000 0.000000

 9 C 0.000000 0.000000 0.000001

 10 C 0.000000 0.000000 0.000000

 11 C 0.000000 0.000000 0.000000

 12 N 0.000000 0.000000 0.000000

 13 C 0.000000 0.000000 0.000000

 14 C -0.000018 -0.000018 -0.000001

 15 C -0.000035 -0.000035 0.000034

 16 N 0.000011 0.000011 0.000000

 17 C 0.000000 0.000000 0.000000

 18 N 0.003338 0.003338 0.000052

 19 N 0.000371 0.000371 -0.000225

 20 C -0.005175 -0.005175 0.006143

 21 C -0.041871 -0.041871 -0.040049

 22 C -0.000130 -0.000130 -0.005591

 23 C -0.000200 -0.000200 0.000274

 24 N 0.000007 0.000007 -0.000011

 25 Zn 0.000074 0.000074 0.000046

 26 C 0.000000 0.000000 0.000000

 27 H 0.000000 0.000000 0.000000

 28 C 0.000000 0.000000 0.000000

 29 H 0.000000 0.000000 0.000000

 30 C 0.000000 0.000000 0.000000

 31 H 0.000028 0.000028 0.000000

 32 C 0.385664 0.385664 0.388258

 33 H -0.000087 -0.000087 0.001216

 34 H 0.000000 0.000000 0.000000

 35 H 0.000000 0.000000 0.000000

 36 H 0.000000 0.000000 0.000000

 37 H 0.000000 0.000000 0.000000

 38 H 0.000000 0.000000 0.000000

 39 H 0.000000 0.000000 0.000000

 40 H 0.000000 0.000000 0.000000

 41 H 0.000000 0.000000 0.000000

 42 H 0.000000 0.000000 0.000000

 43 H 0.458233 -0.026445 -0.024293

 44 H -0.026445 0.458233 -0.024293

 45 H -0.024293 -0.024293 0.448379

 Atomic-Atomic Spin Densities.

 1 2 3 4 5 6

 1 C 0.183879 0.003437 -0.011952 -0.008579 0.013738 0.000170

 2 N 0.003437 -0.058671 -0.001081 -0.001522 0.000311 0.001058

 3 C -0.011952 -0.001081 0.186096 0.021388 -0.006149 -0.000491

 4 C -0.008579 -0.001522 0.021388 0.051698 -0.008656 -0.000676

 5 C 0.013738 0.000311 -0.006149 -0.008656 -0.016380 -0.000071

 6 N 0.000170 0.001058 -0.000491 -0.000676 -0.000071 -0.083734

 7 C 0.000174 0.000009 -0.010915 -0.000416 0.000034 0.002644

 8 N 0.000030 0.000207 -0.000270 -0.000012 0.000000 0.000690

 9 C -0.000007 0.000022 0.000182 0.000002 0.000000 0.000071

 10 C 0.000000 -0.000002 0.000054 0.000000 0.000000 0.000015

 11 C 0.000001 -0.000004 -0.000292 0.000009 0.000000 0.000241

 12 N 0.002644 0.000690 0.000071 0.000015 0.000241 0.000001

 13 C -0.000416 -0.000012 0.000002 0.000000 0.000009 0.000000

 14 C 0.000034 0.000000 0.000000 0.000000 0.000000 0.000000

 15 C 0.000174 0.000030 -0.000007 0.000000 0.000001 0.000000

 16 N 0.000009 0.000207 0.000022 -0.000002 -0.000004 0.000000

 17 C -0.010915 -0.000270 0.000182 0.000054 -0.000292 0.000000

 18 N 0.000000 -0.000001 0.000000 0.000000 0.000000 0.000000

 19 N 0.000001 0.000013 0.000000 0.000000 0.000000 -0.000001

 20 C -0.000007 0.000000 0.000002 0.000000 0.000000 0.000000

 21 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 22 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 23 C 0.000001 0.000001 -0.000007 0.000000 0.000000 0.000000

 24 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000001

 25 Zn 0.000198 0.001147 -0.000427 -0.000047 0.000011 -0.000109

 26 C -0.000002 0.000003 -0.001189 -0.003477 0.001229 0.000297

 27 H 0.000037 -0.000020 -0.000087 0.000299 0.000341 -0.000002

 28 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000001

 29 H 0.000000 0.000001 -0.000005 0.000000 0.000000 0.000082

 30 C 0.000032 0.000000 0.000000 0.000000 0.000001 0.000000

 31 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 33 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 34 H 0.000011 0.000000 0.000032 -0.000178 0.000014 -0.000001

 35 H 0.000024 0.000007 -0.000439 -0.001119 0.000078 0.000023

 36 H 0.000024 0.000007 -0.000439 -0.001119 0.000078 0.000023

 37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 40 H 0.000025 0.000000 0.000000 0.000000 0.000002 0.000000

 41 H 0.000025 0.000000 0.000000 0.000000 0.000002 0.000000

 42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 7 8 9 10 11 12

 1 C 0.000174 0.000030 -0.000007 0.000000 0.000001 0.002644

 2 N 0.000009 0.000207 0.000022 -0.000002 -0.000004 0.000690

 3 C -0.010915 -0.000270 0.000182 0.000054 -0.000292 0.000071

 4 C -0.000416 -0.000012 0.000002 0.000000 0.000009 0.000015

 5 C 0.000034 0.000000 0.000000 0.000000 0.000000 0.000241

 6 N 0.002644 0.000690 0.000071 0.000015 0.000241 0.000001

 7 C 0.183879 0.003437 -0.011952 -0.008579 0.013738 0.000000

 8 N 0.003437 -0.058671 -0.001081 -0.001522 0.000311 -0.000001

 9 C -0.011952 -0.001081 0.186096 0.021388 -0.006149 0.000000

 10 C -0.008579 -0.001522 0.021388 0.051698 -0.008656 0.000000

 11 C 0.013738 0.000311 -0.006149 -0.008656 -0.016380 0.000000

 12 N 0.000000 -0.000001 0.000000 0.000000 0.000000 -0.083734

 13 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000676

 14 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000071

 15 C 0.000001 0.000001 -0.000007 0.000000 0.000000 0.000170

 16 N 0.000001 0.000013 0.000000 0.000000 0.000000 0.001058

 17 C -0.000007 0.000000 0.000002 0.000000 0.000000 -0.000491

 18 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000001

 19 N 0.000030 0.000207 -0.000270 -0.000012 0.000000 0.000000

 20 C -0.000007 0.000022 0.000182 0.000002 0.000000 0.000000

 21 C 0.000000 -0.000002 0.000054 0.000000 0.000000 0.000000

 22 C 0.000001 -0.000004 -0.000292 0.000009 0.000000 0.000000

 23 C 0.000174 0.000009 -0.010915 -0.000416 0.000034 0.000000

 24 N 0.000170 0.001058 -0.000491 -0.000676 -0.000071 0.000000

 25 Zn 0.000198 0.001147 -0.000427 -0.000047 0.000011 -0.000109

 26 C 0.000032 0.000000 0.000000 0.000000 0.000001 0.000001

 27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000082

 28 C -0.000002 0.000003 -0.001189 -0.003477 0.001229 0.000000

 29 H 0.000037 -0.000020 -0.000087 0.000299 0.000341 0.000000

 30 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000297

 31 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

 32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 33 H 0.000000 0.000001 -0.000005 0.000000 0.000000 0.000000

 34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 35 H 0.000025 0.000000 0.000000 0.000000 0.000002 0.000000

 36 H 0.000025 0.000000 0.000000 0.000000 0.000002 0.000000

 37 H 0.000024 0.000007 -0.000439 -0.001119 0.000078 0.000000

 38 H 0.000024 0.000007 -0.000439 -0.001119 0.000078 0.000000

 39 H 0.000011 0.000000 0.000032 -0.000178 0.000014 0.000000

 40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000023

 41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000023

 42 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000001

 43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 13 14 15 16 17 18

 1 C -0.000416 0.000034 0.000174 0.000009 -0.010915 0.000000

 2 N -0.000012 0.000000 0.000030 0.000207 -0.000270 -0.000001

 3 C 0.000002 0.000000 -0.000007 0.000022 0.000182 0.000000

 4 C 0.000000 0.000000 0.000000 -0.000002 0.000054 0.000000

 5 C 0.000009 0.000000 0.000001 -0.000004 -0.000292 0.000000

 6 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 7 C 0.000000 0.000000 0.000001 0.000001 -0.000007 0.000000

 8 N 0.000000 0.000000 0.000001 0.000013 0.000000 0.000000

 9 C 0.000000 0.000000 -0.000007 0.000000 0.000002 0.000000

 10 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 11 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 12 N -0.000676 -0.000071 0.000170 0.001058 -0.000491 0.000001

 13 C 0.051698 -0.008656 -0.008579 -0.001522 0.021388 0.000015

 14 C -0.008656 -0.016380 0.013738 0.000311 -0.006149 0.000241

 15 C -0.008579 0.013738 0.183879 0.003437 -0.011952 0.002644

 16 N -0.001522 0.000311 0.003437 -0.058671 -0.001081 0.000690

 17 C 0.021388 -0.006149 -0.011952 -0.001081 0.186096 0.000071

 18 N 0.000015 0.000241 0.002644 0.000690 0.000071 -0.083734

 19 N -0.000002 -0.000004 0.000009 0.000207 0.000022 0.001058

 20 C 0.000054 -0.000292 -0.010915 -0.000270 0.000182 -0.000491

 21 C 0.000000 0.000009 -0.000416 -0.000012 0.000002 -0.000676

 22 C 0.000000 0.000000 0.000034 0.000000 0.000000 -0.000071

 23 C 0.000000 0.000001 0.000174 0.000030 -0.000007 0.000170

 24 N 0.000000 0.000000 0.000000 -0.000001 0.000000 0.000001

 25 Zn -0.000047 0.000011 0.000198 0.001147 -0.000427 -0.000109

 26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 27 H 0.000000 0.000000 0.000000 0.000001 -0.000005 0.000000

 28 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 29 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 30 C -0.003477 0.001229 -0.000002 0.000003 -0.001189 0.000001

 31 H 0.000299 0.000341 0.000037 -0.000020 -0.000087 0.000082

 32 C 0.000000 0.000001 0.000032 0.000000 0.000000 0.000297

 33 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

 34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 40 H -0.001119 0.000078 0.000024 0.000007 -0.000439 0.000000

 41 H -0.001119 0.000078 0.000024 0.000007 -0.000439 0.000000

 42 H -0.000178 0.000014 0.000011 0.000000 0.000032 0.000000

 43 H 0.000000 0.000002 0.000025 0.000000 0.000000 0.000023

 44 H 0.000000 0.000002 0.000025 0.000000 0.000000 0.000023

 45 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000001

 19 20 21 22 23 24

 1 C 0.000001 -0.000007 0.000000 0.000000 0.000001 0.000000

 2 N 0.000013 0.000000 0.000000 0.000000 0.000001 0.000000

 3 C 0.000000 0.000002 0.000000 0.000000 -0.000007 0.000000

 4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 5 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 6 N -0.000001 0.000000 0.000000 0.000000 0.000000 0.000001

 7 C 0.000030 -0.000007 0.000000 0.000001 0.000174 0.000170

 8 N 0.000207 0.000022 -0.000002 -0.000004 0.000009 0.001058

 9 C -0.000270 0.000182 0.000054 -0.000292 -0.010915 -0.000491

 10 C -0.000012 0.000002 0.000000 0.000009 -0.000416 -0.000676

 11 C 0.000000 0.000000 0.000000 0.000000 0.000034 -0.000071

 12 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 13 C -0.000002 0.000054 0.000000 0.000000 0.000000 0.000000

 14 C -0.000004 -0.000292 0.000009 0.000000 0.000001 0.000000

 15 C 0.000009 -0.010915 -0.000416 0.000034 0.000174 0.000000

 16 N 0.000207 -0.000270 -0.000012 0.000000 0.000030 -0.000001

 17 C 0.000022 0.000182 0.000002 0.000000 -0.000007 0.000000

 18 N 0.001058 -0.000491 -0.000676 -0.000071 0.000170 0.000001

 19 N -0.058671 -0.001081 -0.001522 0.000311 0.003437 0.000690

 20 C -0.001081 0.186096 0.021388 -0.006149 -0.011952 0.000071

 21 C -0.001522 0.021388 0.051698 -0.008656 -0.008579 0.000015

 22 C 0.000311 -0.006149 -0.008656 -0.016380 0.013738 0.000241

 23 C 0.003437 -0.011952 -0.008579 0.013738 0.183879 0.002644

 24 N 0.000690 0.000071 0.000015 0.000241 0.002644 -0.083734

 25 Zn 0.001147 -0.000427 -0.000047 0.000011 0.000198 -0.000109

 26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 28 C 0.000000 0.000000 0.000000 0.000001 0.000032 0.000297

 29 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

 30 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 31 H 0.000001 -0.000005 0.000000 0.000000 0.000000 0.000000

 32 C 0.000003 -0.001189 -0.003477 0.001229 -0.000002 0.000001

 33 H -0.000020 -0.000087 0.000299 0.000341 0.000037 0.000082

 34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 37 H 0.000000 0.000000 0.000000 0.000002 0.000025 0.000023

 38 H 0.000000 0.000000 0.000000 0.000002 0.000025 0.000023

 39 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000001

 40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 43 H 0.000007 -0.000439 -0.001119 0.000078 0.000024 0.000000

 44 H 0.000007 -0.000439 -0.001119 0.000078 0.000024 0.000000

 45 H 0.000000 0.000032 -0.000178 0.000014 0.000011 0.000000

 25 26 27 28 29 30

 1 C 0.000198 -0.000002 0.000037 0.000000 0.000000 0.000032

 2 N 0.001147 0.000003 -0.000020 0.000000 0.000001 0.000000

 3 C -0.000427 -0.001189 -0.000087 0.000000 -0.000005 0.000000

 4 C -0.000047 -0.003477 0.000299 0.000000 0.000000 0.000000

 5 C 0.000011 0.001229 0.000341 0.000000 0.000000 0.000001

 6 N -0.000109 0.000297 -0.000002 0.000001 0.000082 0.000000

 7 C 0.000198 0.000032 0.000000 -0.000002 0.000037 0.000000

 8 N 0.001147 0.000000 0.000000 0.000003 -0.000020 0.000000

 9 C -0.000427 0.000000 0.000000 -0.001189 -0.000087 0.000000

 10 C -0.000047 0.000000 0.000000 -0.003477 0.000299 0.000000

 11 C 0.000011 0.000001 0.000000 0.001229 0.000341 0.000000

 12 N -0.000109 0.000001 0.000082 0.000000 0.000000 0.000297

 13 C -0.000047 0.000000 0.000000 0.000000 0.000000 -0.003477

 14 C 0.000011 0.000000 0.000000 0.000000 0.000000 0.001229

 15 C 0.000198 0.000000 0.000000 0.000000 0.000000 -0.000002

 16 N 0.001147 0.000000 0.000001 0.000000 0.000000 0.000003

 17 C -0.000427 0.000000 -0.000005 0.000000 0.000000 -0.001189

 18 N -0.000109 0.000000 0.000000 0.000000 0.000000 0.000001

 19 N 0.001147 0.000000 0.000000 0.000000 0.000000 0.000000

 20 C -0.000427 0.000000 0.000000 0.000000 0.000000 0.000000

 21 C -0.000047 0.000000 0.000000 0.000000 0.000000 0.000000

 22 C 0.000011 0.000000 0.000000 0.000001 0.000000 0.000000

 23 C 0.000198 0.000000 0.000000 0.000032 0.000000 0.000000

 24 N -0.000109 0.000000 0.000000 0.000297 -0.000002 0.000000

 25 Zn -0.000445 0.000000 0.000000 0.000000 0.000000 0.000000

 26 C 0.000000 -0.002708 0.000124 0.000000 0.000000 0.000000

 27 H 0.000000 0.000124 -0.000667 0.000000 0.000000 0.000000

 28 C 0.000000 0.000000 0.000000 -0.002708 0.000124 0.000000

 29 H 0.000000 0.000000 0.000000 0.000124 -0.000667 0.000000

 30 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.002708

 31 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000124

 32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 33 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 34 H 0.000002 0.000264 -0.000036 0.000000 0.000000 0.000000

 35 H 0.000000 0.001627 0.000001 0.000000 0.000000 0.000000

 36 H 0.000000 0.001627 0.000001 0.000000 0.000000 0.000000

 37 H 0.000000 0.000000 0.000000 0.001627 0.000001 0.000000

 38 H 0.000000 0.000000 0.000000 0.001627 0.000001 0.000000

 39 H 0.000002 0.000000 0.000000 0.000264 -0.000036 0.000000

 40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.001627

 41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.001627

 42 H 0.000002 0.000000 0.000000 0.000000 0.000000 0.000264

 43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 45 H 0.000002 0.000000 0.000000 0.000000 0.000000 0.000000

 31 32 33 34 35 36

 1 C 0.000000 0.000000 0.000000 0.000011 0.000024 0.000024

 2 N 0.000000 0.000000 0.000000 0.000000 0.000007 0.000007

 3 C 0.000000 0.000000 0.000000 0.000032 -0.000439 -0.000439

 4 C 0.000000 0.000000 0.000000 -0.000178 -0.001119 -0.001119

 5 C 0.000000 0.000000 0.000000 0.000014 0.000078 0.000078

 6 N 0.000000 0.000000 0.000000 -0.000001 0.000023 0.000023

 7 C 0.000000 0.000000 0.000000 0.000000 0.000025 0.000025

 8 N 0.000000 0.000000 0.000001 0.000000 0.000000 0.000000

 9 C 0.000000 0.000000 -0.000005 0.000000 0.000000 0.000000

 10 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 11 C 0.000000 0.000000 0.000000 0.000000 0.000002 0.000002

 12 N -0.000002 0.000000 0.000000 0.000000 0.000000 0.000000

 13 C 0.000299 0.000000 0.000000 0.000000 0.000000 0.000000

 14 C 0.000341 0.000001 0.000000 0.000000 0.000000 0.000000

 15 C 0.000037 0.000032 0.000000 0.000000 0.000000 0.000000

 16 N -0.000020 0.000000 0.000000 0.000000 0.000000 0.000000

 17 C -0.000087 0.000000 0.000000 0.000000 0.000000 0.000000

 18 N 0.000082 0.000297 -0.000002 0.000000 0.000000 0.000000

 19 N 0.000001 0.000003 -0.000020 0.000000 0.000000 0.000000

 20 C -0.000005 -0.001189 -0.000087 0.000000 0.000000 0.000000

 21 C 0.000000 -0.003477 0.000299 0.000000 0.000000 0.000000

 22 C 0.000000 0.001229 0.000341 0.000000 0.000000 0.000000

 23 C 0.000000 -0.000002 0.000037 0.000000 0.000000 0.000000

 24 N 0.000000 0.000001 0.000082 0.000000 0.000000 0.000000

 25 Zn 0.000000 0.000000 0.000000 0.000002 0.000000 0.000000

 26 C 0.000000 0.000000 0.000000 0.000264 0.001627 0.001627

 27 H 0.000000 0.000000 0.000000 -0.000036 0.000001 0.000001

 28 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 29 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 30 C 0.000124 0.000000 0.000000 0.000000 0.000000 0.000000

 31 H -0.000667 0.000000 0.000000 0.000000 0.000000 0.000000

 32 C 0.000000 -0.002708 0.000124 0.000000 0.000000 0.000000

 33 H 0.000000 0.000124 -0.000667 0.000000 0.000000 0.000000

 34 H 0.000000 0.000000 0.000000 -0.000376 -0.000004 -0.000004

 35 H 0.000000 0.000000 0.000000 -0.000004 0.003885 -0.000788

 36 H 0.000000 0.000000 0.000000 -0.000004 -0.000788 0.003885

 37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 40 H 0.000001 0.000000 0.000000 0.000000 0.000000 0.000000

 41 H 0.000001 0.000000 0.000000 0.000000 0.000000 0.000000

 42 H -0.000036 0.000000 0.000000 0.000000 0.000000 0.000000

 43 H 0.000000 0.001627 0.000001 0.000000 0.000000 0.000000

 44 H 0.000000 0.001627 0.000001 0.000000 0.000000 0.000000

 45 H 0.000000 0.000264 -0.000036 0.000000 0.000000 0.000000

 37 38 39 40 41 42

 1 C 0.000000 0.000000 0.000000 0.000025 0.000025 0.000000

 2 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 3 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 5 C 0.000000 0.000000 0.000000 0.000002 0.000002 0.000000

 6 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 7 C 0.000024 0.000024 0.000011 0.000000 0.000000 0.000000

 8 N 0.000007 0.000007 0.000000 0.000000 0.000000 0.000000

 9 C -0.000439 -0.000439 0.000032 0.000000 0.000000 0.000000

 10 C -0.001119 -0.001119 -0.000178 0.000000 0.000000 0.000000

 11 C 0.000078 0.000078 0.000014 0.000000 0.000000 0.000000

 12 N 0.000000 0.000000 0.000000 0.000023 0.000023 -0.000001

 13 C 0.000000 0.000000 0.000000 -0.001119 -0.001119 -0.000178

 14 C 0.000000 0.000000 0.000000 0.000078 0.000078 0.000014

 15 C 0.000000 0.000000 0.000000 0.000024 0.000024 0.000011

 16 N 0.000000 0.000000 0.000000 0.000007 0.000007 0.000000

 17 C 0.000000 0.000000 0.000000 -0.000439 -0.000439 0.000032

 18 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 19 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 21 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 22 C 0.000002 0.000002 0.000000 0.000000 0.000000 0.000000

 23 C 0.000025 0.000025 0.000000 0.000000 0.000000 0.000000

 24 N 0.000023 0.000023 -0.000001 0.000000 0.000000 0.000000

 25 Zn 0.000000 0.000000 0.000002 0.000000 0.000000 0.000002

 26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 28 C 0.001627 0.001627 0.000264 0.000000 0.000000 0.000000

 29 H 0.000001 0.000001 -0.000036 0.000000 0.000000 0.000000

 30 C 0.000000 0.000000 0.000000 0.001627 0.001627 0.000264

 31 H 0.000000 0.000000 0.000000 0.000001 0.000001 -0.000036

 32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 33 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 37 H 0.003885 -0.000788 -0.000004 0.000000 0.000000 0.000000

 38 H -0.000788 0.003885 -0.000004 0.000000 0.000000 0.000000

 39 H -0.000004 -0.000004 -0.000376 0.000000 0.000000 0.000000

 40 H 0.000000 0.000000 0.000000 0.003885 -0.000788 -0.000004

 41 H 0.000000 0.000000 0.000000 -0.000788 0.003885 -0.000004

 42 H 0.000000 0.000000 0.000000 -0.000004 -0.000004 -0.000376

 43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 43 44 45

 1 C 0.000000 0.000000 0.000000

 2 N 0.000000 0.000000 0.000000

 3 C 0.000000 0.000000 0.000000

 4 C 0.000000 0.000000 0.000000

 5 C 0.000000 0.000000 0.000000

 6 N 0.000000 0.000000 0.000000

 7 C 0.000000 0.000000 0.000000

 8 N 0.000000 0.000000 0.000000

 9 C 0.000000 0.000000 0.000000

 10 C 0.000000 0.000000 0.000000

 11 C 0.000000 0.000000 0.000000

 12 N 0.000000 0.000000 0.000000

 13 C 0.000000 0.000000 0.000000

 14 C 0.000002 0.000002 0.000000

 15 C 0.000025 0.000025 0.000000

 16 N 0.000000 0.000000 0.000000

 17 C 0.000000 0.000000 0.000000

 18 N 0.000023 0.000023 -0.000001

 19 N 0.000007 0.000007 0.000000

 20 C -0.000439 -0.000439 0.000032

 21 C -0.001119 -0.001119 -0.000178

 22 C 0.000078 0.000078 0.000014

 23 C 0.000024 0.000024 0.000011

 24 N 0.000000 0.000000 0.000000

 25 Zn 0.000000 0.000000 0.000002

 26 C 0.000000 0.000000 0.000000

 27 H 0.000000 0.000000 0.000000

 28 C 0.000000 0.000000 0.000000

 29 H 0.000000 0.000000 0.000000

 30 C 0.000000 0.000000 0.000000

 31 H 0.000000 0.000000 0.000000

 32 C 0.001627 0.001627 0.000264

 33 H 0.000001 0.000001 -0.000036

 34 H 0.000000 0.000000 0.000000

 35 H 0.000000 0.000000 0.000000

 36 H 0.000000 0.000000 0.000000

 37 H 0.000000 0.000000 0.000000

 38 H 0.000000 0.000000 0.000000

 39 H 0.000000 0.000000 0.000000

 40 H 0.000000 0.000000 0.000000

 41 H 0.000000 0.000000 0.000000

 42 H 0.000000 0.000000 0.000000

 43 H 0.003885 -0.000788 -0.000004

 44 H -0.000788 0.003885 -0.000004

 45 H -0.000004 -0.000004 -0.000376

 Mulliken charges and spin densities:

 1 2

 1 C 0.436720 0.172790

 2 N -0.678698 -0.054430

 3 C 0.441688 0.174281

 4 C 0.027539 0.047662

 5 C -0.260428 -0.015462

 6 N -0.407373 -0.079767

 7 C 0.436720 0.172790

 8 N -0.678698 -0.054430

 9 C 0.441688 0.174281

 10 C 0.027539 0.047662

 11 C -0.260428 -0.015462

 12 N -0.407373 -0.079767

 13 C 0.027539 0.047662

 14 C -0.260428 -0.015462

 15 C 0.436720 0.172790

 16 N -0.678698 -0.054430

 17 C 0.441688 0.174281

 18 N -0.407373 -0.079767

 19 N -0.678698 -0.054430

 20 C 0.441688 0.174281

 21 C 0.027539 0.047662

 22 C -0.260428 -0.015462

 23 C 0.436720 0.172790

 24 N -0.407373 -0.079767

 25 Zn 1.537029 0.002655

 26 C -0.693889 -0.002172

 27 H 0.249072 0.000070

 28 C -0.693889 -0.002172

 29 H 0.249072 0.000070

 30 C -0.693889 -0.002172

 31 H 0.249072 0.000070

 32 C -0.693889 -0.002172

 33 H 0.249072 0.000070

 34 H 0.250059 -0.000277

 35 H 0.250526 0.003320

 36 H 0.250526 0.003320

 37 H 0.250526 0.003320

 38 H 0.250526 0.003320

 39 H 0.250059 -0.000277

 40 H 0.250526 0.003320

 41 H 0.250526 0.003320

 42 H 0.250059 -0.000277

 43 H 0.250526 0.003320

 44 H 0.250526 0.003320

 45 H 0.250059 -0.000277

 Sum of Mulliken charges = 1.00000 1.00000

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

 1 2

 1 C 0.436720 0.172790

 2 N -0.678698 -0.054430

 3 C 0.441688 0.174281

 4 C 0.027539 0.047662

 5 C -0.011356 -0.015392

 6 N -0.407373 -0.079767

 7 C 0.436720 0.172790

 8 N -0.678698 -0.054430

 9 C 0.441688 0.174281

 10 C 0.027539 0.047662

 11 C -0.011356 -0.015392

 12 N -0.407373 -0.079767

 13 C 0.027539 0.047662

 14 C -0.011356 -0.015392

 15 C 0.436720 0.172790

 16 N -0.678698 -0.054430

 17 C 0.441688 0.174281

 18 N -0.407373 -0.079767

 19 N -0.678698 -0.054430

 20 C 0.441688 0.174281

 21 C 0.027539 0.047662

 22 C -0.011356 -0.015392

 23 C 0.436720 0.172790

 24 N -0.407373 -0.079767

 25 Zn 1.537029 0.002655

 26 C 0.057223 0.004192

 28 C 0.057223 0.004192

 30 C 0.057223 0.004192

 32 C 0.057223 0.004192

 Electronic spatial extent (au): <R\*\*2>= 11176.5599

 Charge= 1.0000 electrons

 Dipole moment (field-independent basis, Debye):

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

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

 XX= -119.6138 YY= -119.6138 ZZ= -167.4250

 XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

 XX= 15.9371 YY= 15.9371 ZZ= -31.8741

 XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

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

 XXY= 0.0000 XXZ= 0.0000 XZZ= 0.0000 YZZ= 0.0000

 YYZ= 0.0000 XYZ= 0.0000

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

 XXXX= -6213.2124 YYYY= -6213.2124 ZZZZ= -198.2630 XXXY= -323.0018

 XXXZ= 0.0000 YYYX= 323.0018 YYYZ= 0.0000 ZZZX= 0.0000

 ZZZY= 0.0000 XXYY= -2267.1181 XXZZ= -1323.6280 YYZZ= -1323.6280

 XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

 N-N= 2.759873617854D+03 E-N=-8.543513847690D+03 KE= 1.320283431434D+03

 Symmetry AG KE= 6.512722584995D+02

 Symmetry BG KE= 6.558854295226D+01

 Symmetry AU KE= 2.126547440389D+01

 Symmetry BU KE= 5.821571555787D+02

 Isotropic Fermi Contact Couplings

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

 1 C(13) 0.01407 15.81600 5.64354 5.27565

 2 N(14) -0.00842 -2.71954 -0.97040 -0.90714

 3 C(13) 0.01283 14.42151 5.14595 4.81050

 4 C(13) -0.00079 -0.89029 -0.31768 -0.29697

 5 C(13) -0.00576 -6.47782 -2.31145 -2.16077

 6 N(14) -0.01208 -3.90455 -1.39324 -1.30242

 7 C(13) 0.01407 15.81600 5.64354 5.27565

 8 N(14) -0.00842 -2.71954 -0.97040 -0.90714

 9 C(13) 0.01283 14.42151 5.14595 4.81050

 10 C(13) -0.00079 -0.89029 -0.31768 -0.29697

 11 C(13) -0.00576 -6.47782 -2.31145 -2.16077

 12 N(14) -0.01208 -3.90455 -1.39324 -1.30242

 13 C(13) -0.00079 -0.89029 -0.31768 -0.29697

 14 C(13) -0.00576 -6.47782 -2.31145 -2.16077

 15 C(13) 0.01407 15.81600 5.64354 5.27565

 16 N(14) -0.00842 -2.71954 -0.97040 -0.90714

 17 C(13) 0.01283 14.42151 5.14595 4.81050

 18 N(14) -0.01208 -3.90455 -1.39324 -1.30242

 19 N(14) -0.00842 -2.71954 -0.97040 -0.90714

 20 C(13) 0.01283 14.42151 5.14595 4.81050

 21 C(13) -0.00079 -0.89029 -0.31768 -0.29697

 22 C(13) -0.00576 -6.47782 -2.31145 -2.16077

 23 C(13) 0.01407 15.81600 5.64354 5.27565

 24 N(14) -0.01208 -3.90455 -1.39324 -1.30242

 25 Zn(67) 0.00000 0.00000 0.00000 0.00000

 26 C(13) -0.00200 -2.24679 -0.80171 -0.74945

 27 H(1) -0.00009 -0.38395 -0.13700 -0.12807

 28 C(13) -0.00200 -2.24679 -0.80171 -0.74945

 29 H(1) -0.00009 -0.38395 -0.13700 -0.12807

 30 C(13) -0.00200 -2.24679 -0.80171 -0.74945

 31 H(1) -0.00009 -0.38395 -0.13700 -0.12807

 32 C(13) -0.00200 -2.24679 -0.80171 -0.74945

 33 H(1) -0.00009 -0.38395 -0.13700 -0.12807

 34 H(1) -0.00009 -0.41764 -0.14903 -0.13931

 35 H(1) 0.00208 9.30324 3.31963 3.10323

 36 H(1) 0.00208 9.30324 3.31963 3.10323

 37 H(1) 0.00208 9.30324 3.31963 3.10323

 38 H(1) 0.00208 9.30324 3.31963 3.10323

 39 H(1) -0.00009 -0.41764 -0.14903 -0.13931

 40 H(1) 0.00208 9.30324 3.31963 3.10323

 41 H(1) 0.00208 9.30324 3.31963 3.10323

 42 H(1) -0.00009 -0.41764 -0.14903 -0.13931

 43 H(1) 0.00208 9.30324 3.31963 3.10323

 44 H(1) 0.00208 9.30324 3.31963 3.10323

 45 H(1) -0.00009 -0.41764 -0.14903 -0.13931

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

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

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 1 Atom -0.103334 -0.108220 0.211554

 2 Atom 0.045221 0.046859 -0.092080

 3 Atom -0.107158 -0.109045 0.216203

 4 Atom -0.029869 -0.035414 0.065284

 5 Atom 0.002165 0.003315 -0.005480

 6 Atom 0.065585 0.076684 -0.142269

 7 Atom -0.108220 -0.103334 0.211554

 8 Atom 0.046859 0.045221 -0.092080

 9 Atom -0.109045 -0.107158 0.216203

 10 Atom -0.035414 -0.029869 0.065284

 11 Atom 0.003315 0.002165 -0.005480

 12 Atom 0.076684 0.065585 -0.142269

 13 Atom -0.035414 -0.029869 0.065284

 14 Atom 0.003315 0.002165 -0.005480

 15 Atom -0.108220 -0.103334 0.211554

 16 Atom 0.046859 0.045221 -0.092080

 17 Atom -0.109045 -0.107158 0.216203

 18 Atom 0.065585 0.076684 -0.142269

 19 Atom 0.045221 0.046859 -0.092080

 20 Atom -0.107158 -0.109045 0.216203

 21 Atom -0.029869 -0.035414 0.065284

 22 Atom 0.002165 0.003315 -0.005480

 23 Atom -0.103334 -0.108220 0.211554

 24 Atom 0.076684 0.065585 -0.142269

 25 Atom 0.003474 0.003474 -0.006948

 26 Atom 0.000722 -0.004147 0.003425

 27 Atom 0.001858 0.000114 -0.001972

 28 Atom -0.004147 0.000722 0.003425

 29 Atom 0.000114 0.001858 -0.001972

 30 Atom -0.004147 0.000722 0.003425

 31 Atom 0.000114 0.001858 -0.001972

 32 Atom 0.000722 -0.004147 0.003425

 33 Atom 0.001858 0.000114 -0.001972

 34 Atom 0.001806 -0.000700 -0.001106

 35 Atom 0.001949 -0.000864 -0.001084

 36 Atom 0.001949 -0.000864 -0.001084

 37 Atom -0.000864 0.001949 -0.001084

 38 Atom -0.000864 0.001949 -0.001084

 39 Atom -0.000700 0.001806 -0.001106

 40 Atom -0.000864 0.001949 -0.001084

 41 Atom -0.000864 0.001949 -0.001084

 42 Atom -0.000700 0.001806 -0.001106

 43 Atom 0.001949 -0.000864 -0.001084

 44 Atom 0.001949 -0.000864 -0.001084

 45 Atom 0.001806 -0.000700 -0.001106

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 XY XZ YZ

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 1 Atom -0.000159 0.000000 0.000000

 2 Atom 0.001301 0.000000 0.000000

 3 Atom -0.003886 0.000000 0.000000

 4 Atom -0.000804 0.000000 0.000000

 5 Atom -0.001411 0.000000 0.000000

 6 Atom -0.005870 0.000000 0.000000

 7 Atom 0.000159 0.000000 0.000000

 8 Atom -0.001301 0.000000 0.000000

 9 Atom 0.003886 0.000000 0.000000

 10 Atom 0.000804 0.000000 0.000000

 11 Atom 0.001411 0.000000 0.000000

 12 Atom 0.005870 0.000000 0.000000

 13 Atom 0.000804 0.000000 0.000000

 14 Atom 0.001411 0.000000 0.000000

 15 Atom 0.000159 0.000000 0.000000

 16 Atom -0.001301 0.000000 0.000000

 17 Atom 0.003886 0.000000 0.000000

 18 Atom -0.005870 0.000000 0.000000

 19 Atom 0.001301 0.000000 0.000000

 20 Atom -0.003886 0.000000 0.000000

 21 Atom -0.000804 0.000000 0.000000

 22 Atom -0.001411 0.000000 0.000000

 23 Atom -0.000159 0.000000 0.000000

 24 Atom 0.005870 0.000000 0.000000

 25 Atom 0.000000 0.000000 0.000000

 26 Atom -0.000305 0.000000 0.000000

 27 Atom -0.002300 0.000000 0.000000

 28 Atom 0.000305 0.000000 0.000000

 29 Atom 0.002300 0.000000 0.000000

 30 Atom 0.000305 0.000000 0.000000

 31 Atom 0.002300 0.000000 0.000000

 32 Atom -0.000305 0.000000 0.000000

 33 Atom -0.002300 0.000000 0.000000

 34 Atom -0.000969 0.000000 0.000000

 35 Atom 0.000814 -0.001059 -0.000844

 36 Atom 0.000814 0.001059 0.000844

 37 Atom -0.000814 0.000844 -0.001059

 38 Atom -0.000814 -0.000844 0.001059

 39 Atom 0.000969 0.000000 0.000000

 40 Atom -0.000814 -0.000844 0.001059

 41 Atom -0.000814 0.000844 -0.001059

 42 Atom 0.000969 0.000000 0.000000

 43 Atom 0.000814 0.001059 0.000844

 44 Atom 0.000814 -0.001059 -0.000844

 45 Atom -0.000969 0.000000 0.000000

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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 -0.1082 -14.523 -5.182 -4.844 0.0325 0.9995 0.0000

 1 C(13) Bbb -0.1033 -13.866 -4.948 -4.625 0.9995 -0.0325 0.0000

 Bcc 0.2116 28.389 10.130 9.469 0.0000 0.0000 1.0000

 Baa -0.0921 -3.551 -1.267 -1.185 0.0000 0.0000 1.0000

 2 N(14) Bbb 0.0445 1.716 0.612 0.573 0.8754 -0.4834 0.0000

 Bcc 0.0476 1.835 0.655 0.612 0.4834 0.8754 0.0000

 Baa -0.1121 -15.043 -5.368 -5.018 0.6181 0.7861 0.0000

 3 C(13) Bbb -0.1041 -13.970 -4.985 -4.660 0.7861 -0.6181 0.0000

 Bcc 0.2162 29.012 10.352 9.678 0.0000 0.0000 1.0000

 Baa -0.0355 -4.768 -1.701 -1.590 0.1407 0.9900 0.0000

 4 C(13) Bbb -0.0298 -3.993 -1.425 -1.332 0.9900 -0.1407 0.0000

 Bcc 0.0653 8.760 3.126 2.922 0.0000 0.0000 1.0000

 Baa -0.0055 -0.735 -0.262 -0.245 0.0000 0.0000 1.0000

 5 C(13) Bbb 0.0012 0.163 0.058 0.054 0.8298 0.5580 0.0000

 Bcc 0.0043 0.572 0.204 0.191 -0.5580 0.8298 0.0000

 Baa -0.1423 -5.487 -1.958 -1.830 0.0000 0.0000 1.0000

 6 N(14) Bbb 0.0631 2.432 0.868 0.811 0.9184 0.3956 0.0000

 Bcc 0.0792 3.055 1.090 1.019 -0.3956 0.9184 0.0000

 Baa -0.1082 -14.523 -5.182 -4.844 0.9995 -0.0325 0.0000

 7 C(13) Bbb -0.1033 -13.866 -4.948 -4.625 0.0325 0.9995 0.0000

 Bcc 0.2116 28.389 10.130 9.469 0.0000 0.0000 1.0000

 Baa -0.0921 -3.551 -1.267 -1.185 0.0000 0.0000 1.0000

 8 N(14) Bbb 0.0445 1.716 0.612 0.573 0.4834 0.8754 0.0000

 Bcc 0.0476 1.835 0.655 0.612 0.8754 -0.4834 0.0000

 Baa -0.1121 -15.043 -5.368 -5.018 0.7861 -0.6181 0.0000

 9 C(13) Bbb -0.1041 -13.970 -4.985 -4.660 0.6181 0.7861 0.0000

 Bcc 0.2162 29.012 10.352 9.678 0.0000 0.0000 1.0000

 Baa -0.0355 -4.768 -1.701 -1.590 0.9900 -0.1407 0.0000

 10 C(13) Bbb -0.0298 -3.993 -1.425 -1.332 0.1407 0.9900 0.0000

 Bcc 0.0653 8.760 3.126 2.922 0.0000 0.0000 1.0000

 Baa -0.0055 -0.735 -0.262 -0.245 0.0000 0.0000 1.0000

 11 C(13) Bbb 0.0012 0.163 0.058 0.054 -0.5580 0.8298 0.0000

 Bcc 0.0043 0.572 0.204 0.191 0.8298 0.5580 0.0000

 Baa -0.1423 -5.487 -1.958 -1.830 0.0000 0.0000 1.0000

 12 N(14) Bbb 0.0631 2.432 0.868 0.811 -0.3956 0.9184 0.0000

 Bcc 0.0792 3.055 1.090 1.019 0.9184 0.3956 0.0000

 Baa -0.0355 -4.768 -1.701 -1.590 0.9900 -0.1407 0.0000

 13 C(13) Bbb -0.0298 -3.993 -1.425 -1.332 0.1407 0.9900 0.0000

 Bcc 0.0653 8.760 3.126 2.922 0.0000 0.0000 1.0000

 Baa -0.0055 -0.735 -0.262 -0.245 0.0000 0.0000 1.0000

 14 C(13) Bbb 0.0012 0.163 0.058 0.054 -0.5580 0.8298 0.0000

 Bcc 0.0043 0.572 0.204 0.191 0.8298 0.5580 0.0000

 Baa -0.1082 -14.523 -5.182 -4.844 0.9995 -0.0325 0.0000

 15 C(13) Bbb -0.1033 -13.866 -4.948 -4.625 0.0325 0.9995 0.0000

 Bcc 0.2116 28.389 10.130 9.469 0.0000 0.0000 1.0000

 Baa -0.0921 -3.551 -1.267 -1.185 0.0000 0.0000 1.0000

 16 N(14) Bbb 0.0445 1.716 0.612 0.573 0.4834 0.8754 0.0000

 Bcc 0.0476 1.835 0.655 0.612 0.8754 -0.4834 0.0000

 Baa -0.1121 -15.043 -5.368 -5.018 0.7861 -0.6181 0.0000

 17 C(13) Bbb -0.1041 -13.970 -4.985 -4.660 0.6181 0.7861 0.0000

 Bcc 0.2162 29.012 10.352 9.678 0.0000 0.0000 1.0000

 Baa -0.1423 -5.487 -1.958 -1.830 0.0000 0.0000 1.0000

 18 N(14) Bbb 0.0631 2.432 0.868 0.811 0.9184 0.3956 0.0000

 Bcc 0.0792 3.055 1.090 1.019 -0.3956 0.9184 0.0000

 Baa -0.0921 -3.551 -1.267 -1.185 0.0000 0.0000 1.0000

 19 N(14) Bbb 0.0445 1.716 0.612 0.573 0.8754 -0.4834 0.0000

 Bcc 0.0476 1.835 0.655 0.612 0.4834 0.8754 0.0000

 Baa -0.1121 -15.043 -5.368 -5.018 0.6181 0.7861 0.0000

 20 C(13) Bbb -0.1041 -13.970 -4.985 -4.660 0.7861 -0.6181 0.0000

 Bcc 0.2162 29.012 10.352 9.678 0.0000 0.0000 1.0000

 Baa -0.0355 -4.768 -1.701 -1.590 0.1407 0.9900 0.0000

 21 C(13) Bbb -0.0298 -3.993 -1.425 -1.332 0.9900 -0.1407 0.0000

 Bcc 0.0653 8.760 3.126 2.922 0.0000 0.0000 1.0000

 Baa -0.0055 -0.735 -0.262 -0.245 0.0000 0.0000 1.0000

 22 C(13) Bbb 0.0012 0.163 0.058 0.054 0.8298 0.5580 0.0000

 Bcc 0.0043 0.572 0.204 0.191 -0.5580 0.8298 0.0000

 Baa -0.1082 -14.523 -5.182 -4.844 0.0325 0.9995 0.0000

 23 C(13) Bbb -0.1033 -13.866 -4.948 -4.625 0.9995 -0.0325 0.0000

 Bcc 0.2116 28.389 10.130 9.469 0.0000 0.0000 1.0000

 Baa -0.1423 -5.487 -1.958 -1.830 0.0000 0.0000 1.0000

 24 N(14) Bbb 0.0631 2.432 0.868 0.811 -0.3956 0.9184 0.0000

 Bcc 0.0792 3.055 1.090 1.019 0.9184 0.3956 0.0000

 Baa -0.0069 -0.232 -0.083 -0.078 0.0000 0.0000 1.0000

 25 Zn(67) Bbb 0.0035 0.116 0.041 0.039 -0.0039 1.0000 0.0000

 Bcc 0.0035 0.116 0.041 0.039 1.0000 0.0039 0.0000

 Baa -0.0042 -0.559 -0.199 -0.186 0.0623 0.9981 0.0000

 26 C(13) Bbb 0.0007 0.099 0.035 0.033 0.9981 -0.0623 0.0000

 Bcc 0.0034 0.460 0.164 0.153 0.0000 0.0000 1.0000

 Baa -0.0020 -1.052 -0.375 -0.351 0.0000 0.0000 1.0000

 27 H(1) Bbb -0.0015 -0.786 -0.281 -0.262 0.5681 0.8230 0.0000

 Bcc 0.0034 1.838 0.656 0.613 0.8230 -0.5681 0.0000

 Baa -0.0042 -0.559 -0.199 -0.186 0.9981 -0.0623 0.0000

 28 C(13) Bbb 0.0007 0.099 0.035 0.033 0.0623 0.9981 0.0000

 Bcc 0.0034 0.460 0.164 0.153 0.0000 0.0000 1.0000

 Baa -0.0020 -1.052 -0.375 -0.351 0.0000 0.0000 1.0000

 29 H(1) Bbb -0.0015 -0.786 -0.281 -0.262 0.8230 -0.5681 0.0000

 Bcc 0.0034 1.838 0.656 0.613 0.5681 0.8230 0.0000

 Baa -0.0042 -0.559 -0.199 -0.186 0.9981 -0.0623 0.0000

 30 C(13) Bbb 0.0007 0.099 0.035 0.033 0.0623 0.9981 0.0000

 Bcc 0.0034 0.460 0.164 0.153 0.0000 0.0000 1.0000

 Baa -0.0020 -1.052 -0.375 -0.351 0.0000 0.0000 1.0000

 31 H(1) Bbb -0.0015 -0.786 -0.281 -0.262 0.8230 -0.5681 0.0000

 Bcc 0.0034 1.838 0.656 0.613 0.5681 0.8230 0.0000

 Baa -0.0042 -0.559 -0.199 -0.186 0.0623 0.9981 0.0000

 32 C(13) Bbb 0.0007 0.099 0.035 0.033 0.9981 -0.0623 0.0000

 Bcc 0.0034 0.460 0.164 0.153 0.0000 0.0000 1.0000

 Baa -0.0020 -1.052 -0.375 -0.351 0.0000 0.0000 1.0000

 33 H(1) Bbb -0.0015 -0.786 -0.281 -0.262 0.5681 0.8230 0.0000

 Bcc 0.0034 1.838 0.656 0.613 0.8230 -0.5681 0.0000

 Baa -0.0011 -0.590 -0.211 -0.197 0.0000 0.0000 1.0000

 34 H(1) Bbb -0.0010 -0.550 -0.196 -0.183 0.3233 0.9463 0.0000

 Bcc 0.0021 1.140 0.407 0.380 0.9463 -0.3233 0.0000

 Baa -0.0018 -0.987 -0.352 -0.329 0.0916 0.6032 0.7923

 35 H(1) Bbb -0.0007 -0.398 -0.142 -0.133 -0.4270 0.7426 -0.5160

 Bcc 0.0026 1.385 0.494 0.462 0.8996 0.2910 -0.3256

 Baa -0.0018 -0.987 -0.352 -0.329 -0.0916 -0.6032 0.7923

 36 H(1) Bbb -0.0007 -0.398 -0.142 -0.133 -0.4270 0.7426 0.5160

 Bcc 0.0026 1.385 0.494 0.462 0.8996 0.2910 0.3256

 Baa -0.0018 -0.987 -0.352 -0.329 -0.6032 0.0916 0.7923

 37 H(1) Bbb -0.0007 -0.398 -0.142 -0.133 0.7426 0.4270 0.5160

 Bcc 0.0026 1.385 0.494 0.462 -0.2910 0.8996 -0.3256

 Baa -0.0018 -0.987 -0.352 -0.329 0.6032 -0.0916 0.7923

 38 H(1) Bbb -0.0007 -0.398 -0.142 -0.133 0.7426 0.4270 -0.5160

 Bcc 0.0026 1.385 0.494 0.462 -0.2910 0.8996 0.3256

 Baa -0.0011 -0.590 -0.211 -0.197 0.0000 0.0000 1.0000

 39 H(1) Bbb -0.0010 -0.550 -0.196 -0.183 0.9463 -0.3233 0.0000

 Bcc 0.0021 1.140 0.407 0.380 0.3233 0.9463 0.0000

 Baa -0.0018 -0.987 -0.352 -0.329 0.6032 -0.0916 0.7923

 40 H(1) Bbb -0.0007 -0.398 -0.142 -0.133 0.7426 0.4270 -0.5160

 Bcc 0.0026 1.385 0.494 0.462 -0.2910 0.8996 0.3256

 Baa -0.0018 -0.987 -0.352 -0.329 -0.6032 0.0916 0.7923

 41 H(1) Bbb -0.0007 -0.398 -0.142 -0.133 0.7426 0.4270 0.5160

 Bcc 0.0026 1.385 0.494 0.462 -0.2910 0.8996 -0.3256

 Baa -0.0011 -0.590 -0.211 -0.197 0.0000 0.0000 1.0000

 42 H(1) Bbb -0.0010 -0.550 -0.196 -0.183 0.9463 -0.3233 0.0000

 Bcc 0.0021 1.140 0.407 0.380 0.3233 0.9463 0.0000

 Baa -0.0018 -0.987 -0.352 -0.329 -0.0916 -0.6032 0.7923

 43 H(1) Bbb -0.0007 -0.398 -0.142 -0.133 -0.4270 0.7426 0.5160

 Bcc 0.0026 1.385 0.494 0.462 0.8996 0.2910 0.3256

 Baa -0.0018 -0.987 -0.352 -0.329 0.0916 0.6032 0.7923

 44 H(1) Bbb -0.0007 -0.398 -0.142 -0.133 -0.4270 0.7426 -0.5160

 Bcc 0.0026 1.385 0.494 0.462 0.8996 0.2910 -0.3256

 Baa -0.0011 -0.590 -0.211 -0.197 0.0000 0.0000 1.0000

 45 H(1) Bbb -0.0010 -0.550 -0.196 -0.183 0.3233 0.9463 0.0000

 Bcc 0.0021 1.140 0.407 0.380 0.9463 -0.3233 0.0000

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 No NMR shielding tensors so no spin-rotation constants.

 Leave Link 601 at Fri Jul 5 21:08:41 2019, MaxMem= 1342177280 cpu: 16.6

 (Enter /apps/gaussian/g09d01/g09/l701.exe)

 Compute integral first derivatives.

 ... and contract with generalized density number 0.

 R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

 8 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15315 LenP2D= 41224.

 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 = 254

 Leave Link 701 at Fri Jul 5 21:08:46 2019, MaxMem= 1342177280 cpu: 54.2

 (Enter /apps/gaussian/g09d01/g09/l702.exe)

 L702 exits ... SP integral derivatives will be done elsewhere.

 Leave Link 702 at Fri Jul 5 21:08:46 2019, MaxMem= 1342177280 cpu: 0.2

 (Enter /apps/gaussian/g09d01/g09/l703.exe)

 Compute integral first derivatives, UseDBF=F ICtDFT= 0.

 Integral derivatives from FoFJK, PRISM(SPDF).

 Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

 FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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 Fri Jul 5 21:08:54 2019, MaxMem= 1342177280 cpu: 91.6

 (Enter /apps/gaussian/g09d01/g09/l716.exe)

 Dipole =-1.40332190D-13 1.33226763D-15-4.44089210D-16

 \*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

 Center Atomic Forces (Hartrees/Bohr)

 Number Number X Y Z

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

 1 6 0.002910864 0.007310752 0.000000000

 2 7 0.000680794 -0.003050920 0.000000000

 3 6 0.007020202 0.014221933 0.000000000

 4 6 -0.015410626 -0.006780355 0.000000000

 5 6 0.007985139 -0.009773662 0.000000000

 6 7 -0.002170522 0.000597974 0.000000000

 7 6 -0.007310752 0.002910864 0.000000000

 8 7 0.003050920 0.000680794 0.000000000

 9 6 -0.014221933 0.007020202 0.000000000

 10 6 0.006780355 -0.015410626 0.000000000

 11 6 0.009773662 0.007985139 0.000000000

 12 7 0.000597974 0.002170522 0.000000000

 13 6 -0.006780355 0.015410626 0.000000000

 14 6 -0.009773662 -0.007985139 0.000000000

 15 6 0.007310752 -0.002910864 0.000000000

 16 7 -0.003050920 -0.000680794 0.000000000

 17 6 0.014221933 -0.007020202 0.000000000

 18 7 0.002170522 -0.000597974 0.000000000

 19 7 -0.000680794 0.003050920 0.000000000

 20 6 -0.007020202 -0.014221933 0.000000000

 21 6 0.015410626 0.006780355 0.000000000

 22 6 -0.007985139 0.009773662 0.000000000

 23 6 -0.002910864 -0.007310752 0.000000000

 24 7 -0.000597974 -0.002170522 0.000000000

 25 30 0.000000000 0.000000000 0.000000000

 26 6 0.000208115 0.001267614 0.000000000

 27 1 0.001315226 0.001055427 0.000000000

 28 6 -0.001267614 0.000208115 0.000000000

 29 1 -0.001055427 0.001315226 0.000000000

 30 6 0.001267614 -0.000208115 0.000000000

 31 1 0.001055427 -0.001315226 0.000000000

 32 6 -0.000208115 -0.001267614 0.000000000

 33 1 -0.001315226 -0.001055427 0.000000000

 34 1 0.001411382 0.001182284 0.000000000

 35 1 -0.001205848 0.001010923 -0.003187130

 36 1 -0.001205848 0.001010923 0.003187130

 37 1 -0.001010923 -0.001205848 -0.003187130

 38 1 -0.001010923 -0.001205848 0.003187130

 39 1 -0.001182284 0.001411382 0.000000000

 40 1 0.001010923 0.001205848 -0.003187130

 41 1 0.001010923 0.001205848 0.003187130

 42 1 0.001182284 -0.001411382 0.000000000

 43 1 0.001205848 -0.001010923 -0.003187130

 44 1 0.001205848 -0.001010923 0.003187130

 45 1 -0.001411382 -0.001182284 0.000000000

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

 Cartesian Forces: Max 0.015410626 RMS 0.004881427

 Leave Link 716 at Fri Jul 5 21:08:54 2019, MaxMem= 1342177280 cpu: 0.4

 (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 0.010999812 RMS 0.002346279

 Search for a local minimum.

 Step number 1 out of a maximum of 270

 All quantities printed in internal units (Hartrees-Bohrs-Radians)

 RMS Force = .23463D-02 SwitMx=.10000D-02 MixMth= 1

 Mixed Optimization -- RFO/linear search

 Second derivative matrix not updated -- first step.

 ITU= 0

 Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01333

 Eigenvalues --- 0.01336 0.01336 0.01336 0.01604 0.01623

 Eigenvalues --- 0.01636 0.01636 0.01772 0.01788 0.01811

 Eigenvalues --- 0.01811 0.01885 0.01901 0.01940 0.01940

 Eigenvalues --- 0.01997 0.01998 0.02045 0.02045 0.02070

 Eigenvalues --- 0.02086 0.02100 0.02111 0.02111 0.02205

 Eigenvalues --- 0.02317 0.02317 0.02353 0.02374 0.07287

 Eigenvalues --- 0.07287 0.07287 0.07287 0.07341 0.07341

 Eigenvalues --- 0.07341 0.07341 0.14497 0.14497 0.16000

 Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

 Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

 Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

 Eigenvalues --- 0.16499 0.18264 0.22088 0.22088 0.23816

 Eigenvalues --- 0.23854 0.23854 0.23879 0.25000 0.25000

 Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

 Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

 Eigenvalues --- 0.25000 0.33191 0.33191 0.33222 0.33234

 Eigenvalues --- 0.33282 0.33282 0.33282 0.33282 0.33724

 Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

 Eigenvalues --- 0.33724 0.33724 0.34437 0.34437 0.34437

 Eigenvalues --- 0.34437 0.35364 0.35417 0.35563 0.35563

 Eigenvalues --- 0.35682 0.35682 0.35682 0.35682 0.39288

 Eigenvalues --- 0.41735 0.41735 0.42785 0.47883 0.48973

 Eigenvalues --- 0.48973 0.49843 0.50268 0.50571 0.51360

 Eigenvalues --- 0.51360 0.51797 0.53989 0.53989 0.54934

 Eigenvalues --- 0.56287 0.56340 0.56340 0.56414

 RFO step: Lambda=-3.99587473D-03 EMin= 8.77959372D-03

 Linear search not attempted -- first point.

 Iteration 1 RMS(Cart)= 0.01151218 RMS(Int)= 0.00003262

 Iteration 2 RMS(Cart)= 0.00004150 RMS(Int)= 0.00000525

 Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000525

 ITry= 1 IFail=0 DXMaxC= 4.83D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

 ClnCor: largest displacement from symmetrization is 2.10D-10 for atom 37.

 Variable Old X -DE/DX Delta X Delta X Delta X New X

 (Linear) (Quad) (Total)

 R1 2.57723 -0.00384 0.00000 -0.00659 -0.00660 2.57063

 R2 2.76294 0.00473 0.00000 0.01239 0.01239 2.77533

 R3 2.53844 -0.00244 0.00000 -0.00624 -0.00624 2.53220

 R4 2.57400 -0.00713 0.00000 -0.01321 -0.01321 2.56079

 R5 3.79361 -0.00485 0.00000 -0.02108 -0.02109 3.77253

 R6 2.79211 0.00863 0.00000 0.02391 0.02391 2.81601

 R7 2.53307 -0.00383 0.00000 -0.00875 -0.00875 2.52433

 R8 2.58757 -0.01100 0.00000 -0.02248 -0.02248 2.56509

 R9 2.81859 -0.00446 0.00000 -0.01325 -0.01325 2.80534

 R10 2.04583 -0.00168 0.00000 -0.00465 -0.00465 2.04117

 R11 2.53844 -0.00244 0.00000 -0.00624 -0.00624 2.53220

 R12 2.57723 -0.00384 0.00000 -0.00659 -0.00660 2.57063

 R13 2.76294 0.00473 0.00000 0.01239 0.01239 2.77533

 R14 2.57400 -0.00713 0.00000 -0.01321 -0.01321 2.56079

 R15 3.79361 -0.00485 0.00000 -0.02108 -0.02109 3.77253

 R16 2.79211 0.00863 0.00000 0.02391 0.02391 2.81601

 R17 2.53307 -0.00383 0.00000 -0.00875 -0.00875 2.52433

 R18 2.58757 -0.01100 0.00000 -0.02248 -0.02248 2.56509

 R19 2.81859 -0.00446 0.00000 -0.01325 -0.01325 2.80534

 R20 2.04583 -0.00168 0.00000 -0.00465 -0.00465 2.04117

 R21 2.53307 -0.00383 0.00000 -0.00875 -0.00875 2.52433

 R22 2.58757 -0.01100 0.00000 -0.02248 -0.02248 2.56509

 R23 2.79211 0.00863 0.00000 0.02391 0.02391 2.81601

 R24 2.81859 -0.00446 0.00000 -0.01325 -0.01325 2.80534

 R25 2.76294 0.00473 0.00000 0.01239 0.01239 2.77533

 R26 2.04583 -0.00168 0.00000 -0.00465 -0.00465 2.04117

 R27 2.57723 -0.00384 0.00000 -0.00659 -0.00660 2.57063

 R28 2.53844 -0.00244 0.00000 -0.00624 -0.00624 2.53220

 R29 2.57400 -0.00713 0.00000 -0.01321 -0.01321 2.56079

 R30 3.79361 -0.00485 0.00000 -0.02108 -0.02109 3.77253

 R31 2.53307 -0.00383 0.00000 -0.00875 -0.00875 2.52433

 R32 2.57400 -0.00713 0.00000 -0.01321 -0.01321 2.56079

 R33 2.57723 -0.00384 0.00000 -0.00659 -0.00660 2.57063

 R34 3.79361 -0.00485 0.00000 -0.02108 -0.02109 3.77253

 R35 2.79211 0.00863 0.00000 0.02391 0.02391 2.81601

 R36 2.58757 -0.01100 0.00000 -0.02248 -0.02248 2.56509

 R37 2.81859 -0.00446 0.00000 -0.01325 -0.01325 2.80534

 R38 2.76294 0.00473 0.00000 0.01239 0.01239 2.77533

 R39 2.04583 -0.00168 0.00000 -0.00465 -0.00465 2.04117

 R40 2.53844 -0.00244 0.00000 -0.00624 -0.00624 2.53220

 R41 2.06599 -0.00186 0.00000 -0.00535 -0.00535 2.06064

 R42 2.07798 -0.00343 0.00000 -0.01004 -0.01004 2.06794

 R43 2.07798 -0.00343 0.00000 -0.01004 -0.01004 2.06794

 R44 2.07798 -0.00343 0.00000 -0.01004 -0.01004 2.06794

 R45 2.07798 -0.00343 0.00000 -0.01004 -0.01004 2.06794

 R46 2.06599 -0.00186 0.00000 -0.00535 -0.00535 2.06064

 R47 2.07798 -0.00343 0.00000 -0.01004 -0.01004 2.06794

 R48 2.07798 -0.00343 0.00000 -0.01004 -0.01004 2.06794

 R49 2.06599 -0.00186 0.00000 -0.00535 -0.00535 2.06064

 R50 2.07798 -0.00343 0.00000 -0.01004 -0.01004 2.06794

 R51 2.07798 -0.00343 0.00000 -0.01004 -0.01004 2.06794

 R52 2.06599 -0.00186 0.00000 -0.00535 -0.00535 2.06064

 A1 1.89137 0.00057 0.00000 0.00500 0.00500 1.89637

 A2 2.21236 -0.00033 0.00000 -0.00114 -0.00114 2.21121

 A3 2.17945 -0.00024 0.00000 -0.00386 -0.00385 2.17560

 A4 1.90638 0.00059 0.00000 -0.00200 -0.00200 1.90438

 A5 2.19032 -0.00015 0.00000 0.00260 0.00259 2.19291

 A6 2.18649 -0.00044 0.00000 -0.00060 -0.00060 2.18589

 A7 1.89647 -0.00081 0.00000 -0.00029 -0.00030 1.89617

 A8 2.21943 0.00174 0.00000 0.00609 0.00610 2.22553

 A9 2.16729 -0.00093 0.00000 -0.00580 -0.00580 2.16149

 A10 1.85108 0.00018 0.00000 0.00006 0.00006 1.85113

 A11 2.17776 -0.00165 0.00000 -0.00618 -0.00618 2.17158

 A12 2.25435 0.00147 0.00000 0.00612 0.00612 2.26047

 A13 1.87948 -0.00053 0.00000 -0.00276 -0.00276 1.87672

 A14 2.17828 0.00004 0.00000 -0.00001 -0.00001 2.17827

 A15 2.22542 0.00050 0.00000 0.00277 0.00277 2.22820

 A16 2.18698 -0.00082 0.00000 -0.00695 -0.00695 2.18003

 A17 2.21236 -0.00033 0.00000 -0.00114 -0.00114 2.21121

 A18 2.17945 -0.00024 0.00000 -0.00386 -0.00385 2.17560

 A19 1.89137 0.00057 0.00000 0.00500 0.00500 1.89637

 A20 1.90638 0.00059 0.00000 -0.00200 -0.00200 1.90438

 A21 2.19032 -0.00015 0.00000 0.00260 0.00259 2.19291

 A22 2.18649 -0.00044 0.00000 -0.00060 -0.00060 2.18589

 A23 1.89647 -0.00081 0.00000 -0.00029 -0.00030 1.89617

 A24 2.21943 0.00174 0.00000 0.00609 0.00610 2.22553

 A25 2.16729 -0.00093 0.00000 -0.00580 -0.00580 2.16149

 A26 1.85108 0.00018 0.00000 0.00006 0.00006 1.85113

 A27 2.17776 -0.00165 0.00000 -0.00618 -0.00618 2.17158

 A28 2.25435 0.00147 0.00000 0.00612 0.00612 2.26047

 A29 1.87948 -0.00053 0.00000 -0.00276 -0.00276 1.87672

 A30 2.17828 0.00004 0.00000 -0.00001 -0.00001 2.17827

 A31 2.22542 0.00050 0.00000 0.00277 0.00277 2.22820

 A32 2.18698 -0.00082 0.00000 -0.00695 -0.00695 2.18003

 A33 1.85108 0.00018 0.00000 0.00006 0.00006 1.85113

 A34 2.25435 0.00147 0.00000 0.00612 0.00612 2.26047

 A35 2.17776 -0.00165 0.00000 -0.00618 -0.00618 2.17158

 A36 1.87948 -0.00053 0.00000 -0.00276 -0.00276 1.87672

 A37 2.22542 0.00050 0.00000 0.00277 0.00277 2.22820

 A38 2.17828 0.00004 0.00000 -0.00001 -0.00001 2.17827

 A39 1.89137 0.00057 0.00000 0.00500 0.00500 1.89637

 A40 2.17945 -0.00024 0.00000 -0.00386 -0.00385 2.17560

 A41 2.21236 -0.00033 0.00000 -0.00114 -0.00114 2.21121

 A42 1.90638 0.00059 0.00000 -0.00200 -0.00200 1.90438

 A43 2.19032 -0.00015 0.00000 0.00260 0.00259 2.19291

 A44 2.18649 -0.00044 0.00000 -0.00060 -0.00060 2.18589

 A45 2.16729 -0.00093 0.00000 -0.00580 -0.00580 2.16149

 A46 2.21943 0.00174 0.00000 0.00609 0.00610 2.22553

 A47 1.89647 -0.00081 0.00000 -0.00029 -0.00030 1.89617

 A48 2.18698 -0.00082 0.00000 -0.00695 -0.00695 2.18003

 A49 1.90638 0.00059 0.00000 -0.00200 -0.00200 1.90438

 A50 2.18649 -0.00044 0.00000 -0.00060 -0.00060 2.18589

 A51 2.19032 -0.00015 0.00000 0.00260 0.00259 2.19291

 A52 2.21943 0.00174 0.00000 0.00609 0.00610 2.22553

 A53 2.16729 -0.00093 0.00000 -0.00580 -0.00580 2.16149

 A54 1.89647 -0.00081 0.00000 -0.00029 -0.00030 1.89617

 A55 1.85108 0.00018 0.00000 0.00006 0.00006 1.85113

 A56 2.17776 -0.00165 0.00000 -0.00618 -0.00618 2.17158

 A57 2.25435 0.00147 0.00000 0.00612 0.00612 2.26047

 A58 1.87948 -0.00053 0.00000 -0.00276 -0.00276 1.87672

 A59 2.22542 0.00050 0.00000 0.00277 0.00277 2.22820

 A60 2.17828 0.00004 0.00000 -0.00001 -0.00001 2.17827

 A61 1.89137 0.00057 0.00000 0.00500 0.00500 1.89637

 A62 2.21236 -0.00033 0.00000 -0.00114 -0.00114 2.21121

 A63 2.17945 -0.00024 0.00000 -0.00386 -0.00385 2.17560

 A64 2.18698 -0.00082 0.00000 -0.00695 -0.00695 2.18003

 A65 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

 A66 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

 A67 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

 A68 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

 A69 1.93538 0.00031 0.00000 0.00419 0.00419 1.93957

 A70 1.93656 -0.00027 0.00000 -0.00275 -0.00277 1.93379

 A71 1.93656 -0.00027 0.00000 -0.00275 -0.00277 1.93379

 A72 1.89112 0.00038 0.00000 0.00446 0.00446 1.89557

 A73 1.89112 0.00038 0.00000 0.00446 0.00446 1.89557

 A74 1.87099 -0.00054 0.00000 -0.00765 -0.00768 1.86331

 A75 1.93656 -0.00027 0.00000 -0.00275 -0.00277 1.93379

 A76 1.93656 -0.00027 0.00000 -0.00275 -0.00277 1.93379

 A77 1.93538 0.00031 0.00000 0.00419 0.00419 1.93957

 A78 1.87099 -0.00054 0.00000 -0.00765 -0.00768 1.86331

 A79 1.89112 0.00038 0.00000 0.00446 0.00446 1.89557

 A80 1.89112 0.00038 0.00000 0.00446 0.00446 1.89557

 A81 1.93656 -0.00027 0.00000 -0.00275 -0.00277 1.93379

 A82 1.93656 -0.00027 0.00000 -0.00275 -0.00277 1.93379

 A83 1.93538 0.00031 0.00000 0.00419 0.00419 1.93957

 A84 1.87099 -0.00054 0.00000 -0.00765 -0.00768 1.86331

 A85 1.89112 0.00038 0.00000 0.00446 0.00446 1.89557

 A86 1.89112 0.00038 0.00000 0.00446 0.00446 1.89557

 A87 1.93656 -0.00027 0.00000 -0.00275 -0.00277 1.93379

 A88 1.93656 -0.00027 0.00000 -0.00275 -0.00277 1.93379

 A89 1.93538 0.00031 0.00000 0.00419 0.00419 1.93957

 A90 1.87099 -0.00054 0.00000 -0.00765 -0.00768 1.86331

 A91 1.89112 0.00038 0.00000 0.00446 0.00446 1.89557

 A92 1.89112 0.00038 0.00000 0.00446 0.00446 1.89557

 A93 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 A94 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 A95 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 A96 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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 D29 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D30 1.03902 -0.00051 0.00000 -0.00659 -0.00658 1.03244

 D31 -1.03902 0.00051 0.00000 0.00659 0.00658 -1.03244

 D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D33 -2.10257 -0.00051 0.00000 -0.00659 -0.00658 -2.10915

 D34 2.10257 0.00051 0.00000 0.00659 0.00658 2.10915

 D35 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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 D61 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D62 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D63 1.03902 -0.00051 0.00000 -0.00659 -0.00658 1.03244

 D64 -1.03902 0.00051 0.00000 0.00659 0.00658 -1.03244

 D65 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D66 -2.10257 -0.00051 0.00000 -0.00659 -0.00658 -2.10915

 D67 2.10257 0.00051 0.00000 0.00659 0.00658 2.10915

 D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D69 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D70 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D71 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D72 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D73 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D74 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D75 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D76 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D77 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D78 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D79 -2.10257 -0.00051 0.00000 -0.00659 -0.00658 -2.10915

 D80 2.10257 0.00051 0.00000 0.00659 0.00658 2.10915

 D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D82 1.03902 -0.00051 0.00000 -0.00659 -0.00658 1.03244

 D83 -1.03902 0.00051 0.00000 0.00659 0.00658 -1.03244

 D84 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D85 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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 D98 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D99 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D100 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D101 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D102 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D103 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D104 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D105 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D106 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D107 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D108 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D109 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D110 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D111 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D112 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D113 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D114 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D116 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D117 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D119 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D120 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D121 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D122 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D123 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D124 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D125 1.03902 -0.00051 0.00000 -0.00659 -0.00658 1.03244

 D126 -1.03902 0.00051 0.00000 0.00659 0.00658 -1.03244

 D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D128 -2.10257 -0.00051 0.00000 -0.00659 -0.00658 -2.10915

 D129 2.10257 0.00051 0.00000 0.00659 0.00658 2.10915

 D130 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D131 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D132 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D133 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D134 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D136 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 Item Value Threshold Converged?

 Maximum Force 0.011000 0.000450 NO

 RMS Force 0.002346 0.000300 NO

 Maximum Displacement 0.048338 0.001800 NO

 RMS Displacement 0.011520 0.001200 NO

 Predicted change in Energy=-2.021879D-03

 Lowest energy point so far. Saving SCF results.

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link 103 at Fri Jul 5 21:08:54 2019, MaxMem= 1342177280 cpu: 1.6

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

 Input orientation:

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -2.059287 -2.181809 0.000000

 2 7 0 -0.738920 -1.854548 0.000000

 3 6 0 -0.000206 -2.990610 0.000000

 4 6 0 -0.924270 -4.159674 0.000000

 5 6 0 -2.180482 -3.645442 0.000000

 6 7 0 1.331529 -3.094943 0.000000

 7 6 0 2.181809 -2.059287 0.000000

 8 7 0 1.854548 -0.738920 0.000000

 9 6 0 2.990610 -0.000206 0.000000

 10 6 0 4.159674 -0.924270 0.000000

 11 6 0 3.645442 -2.180482 0.000000

 12 7 0 -3.094943 -1.331529 0.000000

 13 6 0 -4.159674 0.924270 0.000000

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 15 6 0 -2.181809 2.059287 0.000000

 16 7 0 -1.854548 0.738920 0.000000

 17 6 0 -2.990610 0.000206 0.000000

 18 7 0 -1.331529 3.094943 0.000000

 19 7 0 0.738920 1.854548 0.000000

 20 6 0 0.000206 2.990610 0.000000

 21 6 0 0.924270 4.159674 0.000000

 22 6 0 2.180482 3.645442 0.000000

 23 6 0 2.059287 2.181809 0.000000

 24 7 0 3.094943 1.331529 0.000000

 25 30 0 0.000000 0.000000 0.000000

 26 6 0 -0.483956 -5.577392 0.000000

 27 1 0 -3.115233 -4.186688 0.000000

 28 6 0 5.577392 -0.483956 0.000000

 29 1 0 4.186688 -3.115233 0.000000

 30 6 0 -5.577392 0.483956 0.000000

 31 1 0 -4.186688 3.115233 0.000000

 32 6 0 0.483956 5.577392 0.000000

 33 1 0 3.115233 4.186688 0.000000

 34 1 0 -1.338734 -6.254460 0.000000

 35 1 0 0.132206 -5.792895 0.878298

 36 1 0 0.132206 -5.792895 -0.878298

 37 1 0 5.792895 0.132206 0.878298

 38 1 0 5.792895 0.132206 -0.878298

 39 1 0 6.254460 -1.338734 0.000000

 40 1 0 -5.792895 -0.132206 0.878298

 41 1 0 -5.792895 -0.132206 -0.878298

 42 1 0 -6.254460 1.338734 0.000000

 43 1 0 -0.132206 5.792895 0.878298

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 45 1 0 1.338734 6.254460 0.000000

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 Distance matrix (angstroms):

 1 2 3 4 5

 1 C 0.000000

 2 N 1.360320 0.000000

 3 C 2.212233 1.355114 0.000000

 4 C 2.280398 2.312565 1.490169 0.000000

 5 C 1.468642 2.299001 2.276491 1.357389 0.000000

 6 N 3.511616 2.413574 1.335816 2.494450 3.554894

 7 C 4.242866 2.927896 2.372457 3.749580 4.641711

 8 N 4.171336 2.823244 2.917229 4.407197 4.972861

 9 C 5.500987 4.165090 4.229361 5.712045 6.326764

 10 C 6.344831 4.986145 4.644821 6.026137 6.899447

 11 C 5.704730 4.396460 3.734576 4.979906 6.007288

 12 N 1.339985 2.413379 3.511402 3.565141 2.488058

 13 C 3.749580 4.407197 5.712045 6.026137 4.979906

 14 C 4.641711 4.972861 6.326764 6.899447 6.007288

 15 C 4.242866 4.171336 5.500987 6.344831 5.704730

 16 N 2.927896 2.823244 4.165090 4.986145 4.396460

 17 C 2.372457 2.917229 4.229361 4.644821 3.734576

 18 N 5.326702 4.984843 6.229477 7.266040 6.793638

 19 N 4.911430 3.992670 4.901211 6.239958 6.226782

 20 C 5.567354 4.901211 5.981220 7.209800 6.985169

 21 C 7.008282 6.239958 7.209800 8.522244 8.399960

 22 C 7.206421 6.226782 6.985169 8.399960 8.495588

 23 C 6.000319 4.911430 5.567354 7.008282 7.206421

 24 N 6.237759 4.984937 5.316092 6.804953 7.252611

 25 Zn 3.000159 1.996335 2.990610 4.261122 4.247794

 26 C 3.743213 3.731564 2.631626 1.484520 2.571115

 27 H 2.265957 3.329525 3.336764 2.191130 1.080142

 28 C 7.823143 6.463305 6.114974 7.468768 8.377327

 29 H 6.315337 5.084382 4.188748 5.216583 6.389208

 30 C 4.413996 5.373957 6.570967 6.573800 5.347048

 31 H 5.708283 6.048622 7.403239 7.972932 7.052063

 32 C 8.165371 7.531876 8.581670 9.838371 9.599995

 33 H 8.205694 7.165963 7.824293 9.272504 9.454463

 34 H 4.135902 4.440608 3.527659 2.135395 2.741444

 35 H 4.314394 4.128056 2.939684 2.134235 3.275895

 36 H 4.314394 4.128056 2.939684 2.134235 3.275895

 37 H 8.233034 6.883546 6.639534 8.019473 8.866611

 38 H 8.233034 6.883546 6.639534 8.019473 8.866611

 39 H 8.356385 7.012377 6.469122 7.713097 8.744665

 40 H 4.348806 5.411149 6.518982 6.379296 5.115053

 41 H 4.348806 5.411149 6.518982 6.379296 5.115053

 42 H 5.476651 6.373244 7.606505 7.657900 6.437338

 43 H 8.251119 7.721587 8.828295 10.022595 9.697889

 44 H 8.251119 7.721587 8.828295 10.022595 9.697889

 45 H 9.094900 8.370942 9.341525 10.657175 10.506805

 6 7 8 9 10

 6 N 0.000000

 7 C 1.339985 0.000000

 8 N 2.413379 1.360320 0.000000

 9 C 3.511402 2.212233 1.355114 0.000000

 10 C 3.565141 2.280398 2.312565 1.490169 0.000000

 11 C 2.488058 1.468642 2.299001 2.276491 1.357389

 12 N 4.764797 5.326702 4.984843 6.229477 7.266040

 13 C 6.804953 7.008282 6.239958 7.209800 8.522244

 14 C 7.252611 7.206421 6.226782 6.985169 8.399960

 15 C 6.237759 6.000319 4.911430 5.567354 7.008282

 16 N 4.984937 4.911430 3.992670 4.901211 6.239958

 17 C 5.316092 5.567354 4.901211 5.981220 7.209800

 18 N 6.738440 6.237759 4.984937 5.316092 6.804953

 19 N 4.984843 4.171336 2.823244 2.917229 4.407197

 20 C 6.229477 5.500987 4.165090 4.229361 5.712045

 21 C 7.266040 6.344831 4.986145 4.644821 6.026137

 22 C 6.793638 5.704730 4.396460 3.734576 4.979906

 23 C 5.326702 4.242866 2.927896 2.372457 3.749580

 24 N 4.764797 3.511616 2.413574 1.335816 2.494450

 25 Zn 3.369220 3.000159 1.996335 2.990610 4.261122

 26 C 3.075473 4.413996 5.373957 6.570967 6.573800

 27 H 4.578821 5.708283 6.048622 7.403239 7.972932

 28 C 4.984436 3.743213 3.731564 2.631626 1.484520

 29 H 2.855231 2.265957 3.329525 3.336764 2.191130

 30 C 7.780855 8.165371 7.531876 8.581670 9.838371

 31 H 8.307648 8.205694 7.165963 7.824293 9.272504

 32 C 8.713655 7.823143 6.463305 6.114974 7.468768

 33 H 7.496916 6.315337 5.084382 4.188748 5.216583

 34 H 4.136769 5.476651 6.373244 7.606505 7.657900

 35 H 3.080378 4.348806 5.411149 6.518982 6.379296

 36 H 3.080378 4.348806 5.411149 6.518982 6.379296

 37 H 5.575813 4.314394 4.128056 2.939684 2.134235

 38 H 5.575813 4.314394 4.128056 2.939684 2.134235

 39 H 5.226808 4.135902 4.440608 3.527659 2.135395

 40 H 7.765735 8.251119 7.721587 8.828295 10.022595

 41 H 7.765735 8.251119 7.721587 8.828295 10.022595

 42 H 8.786623 9.094900 8.370942 9.341525 10.657175

 43 H 9.050282 8.233034 6.883546 6.639534 8.019473

 44 H 9.050282 8.233034 6.883546 6.639534 8.019473

 45 H 9.349407 8.356385 7.012377 6.469122 7.713097

 11 12 13 14 15

 11 C 0.000000

 12 N 6.793638 0.000000

 13 C 8.399960 2.494450 0.000000

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 17 C 6.985169 1.335816 1.490169 2.276491 2.212233

 18 N 7.252611 4.764797 3.565141 2.488058 1.339985

 19 N 4.972861 4.984937 4.986145 4.396460 2.927896

 20 C 6.326764 5.316092 4.644821 3.734576 2.372457

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 22 C 6.007288 7.252611 6.899447 6.007288 4.641711

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 24 N 3.554894 6.738440 7.266040 6.793638 5.326702

 25 Zn 4.247794 3.369220 4.261122 4.247794 3.000159

 26 C 5.347048 4.984436 7.468768 8.377327 7.823143

 27 H 7.052063 2.855231 5.216583 6.389208 6.315337

 28 C 2.571115 8.713655 9.838371 9.599995 8.165371

 29 H 1.080142 7.496916 9.272504 9.454463 8.205694

 30 C 9.599995 3.075473 1.484520 2.571115 3.743213

 31 H 9.454463 4.578821 2.191130 1.080142 2.265957

 32 C 8.377327 7.780855 6.573800 5.347048 4.413996

 33 H 6.389208 8.307648 7.972932 7.052063 5.708283

 34 H 6.437338 5.226808 7.713097 8.744665 8.356385

 35 H 5.115053 5.575813 8.019473 8.866611 8.233034

 36 H 5.115053 5.575813 8.019473 8.866611 8.233034

 37 H 3.275895 9.050282 10.022595 9.697889 8.251119

 38 H 3.275895 9.050282 10.022595 9.697889 8.251119

 39 H 2.741444 9.349407 10.657175 10.506805 9.094900

 40 H 9.697889 3.080378 2.134235 3.275895 4.314394

 41 H 9.697889 3.080378 2.134235 3.275895 4.314394

 42 H 10.506805 4.136769 2.135395 2.741444 4.135902

 43 H 8.866611 7.765735 6.379296 5.115053 4.348806

 44 H 8.866611 7.765735 6.379296 5.115053 4.348806

 45 H 8.744665 8.786623 7.657900 6.437338 5.476651

 16 17 18 19 20

 16 N 0.000000

 17 C 1.355114 0.000000

 18 N 2.413379 3.511402 0.000000

 19 N 2.823244 4.165090 2.413574 0.000000

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 22 C 4.972861 6.326764 3.554894 2.299001 2.276491

 23 C 4.171336 5.500987 3.511616 1.360320 2.212233

 24 N 4.984843 6.229477 4.764797 2.413379 3.511402

 25 Zn 1.996335 2.990610 3.369220 1.996335 2.990610

 26 C 6.463305 6.114974 8.713655 7.531876 8.581670

 27 H 5.084382 4.188748 7.496916 7.165963 7.824293

 28 C 7.531876 8.581670 7.780855 5.373957 6.570967

 29 H 7.165963 7.824293 8.307648 6.048622 7.403239

 30 C 3.731564 2.631626 4.984436 6.463305 6.114974

 31 H 3.329525 3.336764 2.855231 5.084382 4.188748

 32 C 5.373957 6.570967 3.075473 3.731564 2.631626

 33 H 6.048622 7.403239 4.578821 3.329525 3.336764

 34 H 7.012377 6.469122 9.349407 8.370942 9.341525

 35 H 6.883546 6.639534 9.050282 7.721587 8.828295

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 38 H 7.721587 8.828295 7.765735 5.411149 6.518982

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 40 H 4.128056 2.939684 5.575813 6.883546 6.639534

 41 H 4.128056 2.939684 5.575813 6.883546 6.639534

 42 H 4.440608 3.527659 5.226808 7.012377 6.469122

 43 H 5.411149 6.518982 3.080378 4.128056 2.939684

 44 H 5.411149 6.518982 3.080378 4.128056 2.939684

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 35 H 10.022595 9.697889 8.251119 7.765735 5.860591

 36 H 10.022595 9.697889 8.251119 7.765735 5.860591

 37 H 6.379296 5.115053 4.348806 3.080378 5.860591

 38 H 6.379296 5.115053 4.348806 3.080378 5.860591

 39 H 7.657900 6.437338 5.476651 4.136769 6.396130

 40 H 8.019473 8.866611 8.233034 9.050282 5.860591

 41 H 8.019473 8.866611 8.233034 9.050282 5.860591

 42 H 7.713097 8.744665 8.356385 9.349407 6.396130

 43 H 2.134235 3.275895 4.314394 5.575813 5.860591

 44 H 2.134235 3.275895 4.314394 5.575813 5.860591

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 26 27 28 29 30

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 32 C 11.196698 10.406316 7.917261 9.448383 7.917261

 33 H 10.406316 10.437056 5.279881 7.380113 9.448383

 34 H 1.090444 2.726102 9.007304 6.354923 7.960683

 35 H 1.094305 3.727891 7.655474 4.937621 8.530520

 36 H 1.094305 3.727891 7.655474 4.937621 8.530520

 37 H 8.530520 9.938763 1.094305 3.727891 11.409582

 38 H 8.530520 9.938763 1.094305 3.727891 11.409582

 39 H 7.960683 9.792956 1.090444 2.726102 11.971421

 40 H 7.655474 4.937621 11.409582 10.452844 1.094305

 41 H 7.655474 4.937621 11.409582 10.452844 1.094305

 42 H 9.007304 6.354923 11.971421 11.351449 1.090444

 43 H 11.409582 10.452844 8.530520 9.938763 7.655474

 44 H 11.409582 10.452844 8.530520 9.938763 7.655474

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 32 C 5.279881 0.000000

 33 H 7.380113 2.976185 0.000000

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 35 H 9.938763 11.409582 10.452844 1.774293 0.000000

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 37 H 10.452844 7.655474 4.937621 9.613587 8.194524

 38 H 10.452844 7.655474 4.937621 9.613587 8.380684

 39 H 11.351449 9.007304 6.354923 9.045494 7.621873

 40 H 3.727891 8.530520 9.938763 7.621873 8.194524

 41 H 3.727891 8.530520 9.938763 7.621873 8.380684

 42 H 2.726102 7.960683 9.792956 9.045494 9.613587

 43 H 4.937621 1.094305 3.727891 12.139436 11.588808

 44 H 4.937621 1.094305 3.727891 12.139436 11.721181

 45 H 6.354923 1.090444 2.726102 12.792261 12.139436

 36 37 38 39 40

 36 H 0.000000

 37 H 8.380684 0.000000

 38 H 8.194524 1.756595 0.000000

 39 H 7.621873 1.774293 1.774293 0.000000

 40 H 8.380684 11.588808 11.721181 12.139436 0.000000

 41 H 8.194524 11.721181 11.588808 12.139436 1.756595

 42 H 9.613587 12.139436 12.139436 12.792261 1.774293

 43 H 11.721181 8.194524 8.380684 9.613587 8.194524

 44 H 11.588808 8.380684 8.194524 9.613587 8.380684

 45 H 12.139436 7.621873 7.621873 9.045494 9.613587

 41 42 43 44 45

 41 H 0.000000

 42 H 1.774293 0.000000

 43 H 8.380684 7.621873 0.000000

 44 H 8.194524 7.621873 1.756595 0.000000

 45 H 9.613587 9.045494 1.774293 1.774293 0.000000

 Stoichiometry C20H16N8Zn(1+,2)

 Framework group C4H[O(Zn),SGH(C20H8N8),X(H8)]

 Deg. of freedom 20

 Full point group C4H NOp 8

 RotChk: IX=0 Diff= 9.74D-05

 Largest Abelian subgroup C2H NOp 4

 Largest concise Abelian subgroup C2H NOp 4

 Standard orientation:

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 5 6 0 -3.645593 2.180231 0.000000

 6 7 0 -3.094852 -1.331743 0.000000

 7 6 0 -2.059137 -2.181951 0.000000

 8 7 0 -0.738792 -1.854599 0.000000

 9 6 0 0.000000 -2.990610 0.000000

 10 6 0 -0.923983 -4.159738 0.000000

 11 6 0 -2.180231 -3.645593 0.000000

 12 7 0 -1.331743 3.094852 0.000000

 13 6 0 0.923983 4.159738 0.000000

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 17 6 0 0.000000 2.990610 0.000000

 18 7 0 3.094852 1.331743 0.000000

 19 7 0 1.854599 -0.738792 0.000000

 20 6 0 2.990610 0.000000 0.000000

 21 6 0 4.159738 -0.923983 0.000000

 22 6 0 3.645593 -2.180231 0.000000

 23 6 0 2.181951 -2.059137 0.000000

 24 7 0 1.331743 -3.094852 0.000000

 25 30 0 0.000000 0.000000 0.000000

 26 6 0 -5.577425 0.483572 0.000000

 27 1 0 -4.186903 3.114945 0.000000

 28 6 0 -0.483572 -5.577425 0.000000

 29 1 0 -3.114945 -4.186903 0.000000

 30 6 0 0.483572 5.577425 0.000000

 31 1 0 3.114945 4.186903 0.000000

 32 6 0 5.577425 -0.483572 0.000000

 33 1 0 4.186903 -3.114945 0.000000

 34 1 0 -6.254553 1.338304 0.000000

 35 1 0 -5.792886 -0.132605 0.878298

 36 1 0 -5.792886 -0.132605 -0.878298

 37 1 0 0.132605 -5.792886 0.878298

 38 1 0 0.132605 -5.792886 -0.878298

 39 1 0 -1.338304 -6.254553 0.000000

 40 1 0 -0.132605 5.792886 0.878298

 41 1 0 -0.132605 5.792886 -0.878298

 42 1 0 1.338304 6.254553 0.000000

 43 1 0 5.792886 0.132605 0.878298

 44 1 0 5.792886 0.132605 -0.878298

 45 1 0 6.254553 -1.338304 0.000000

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

 Rotational constants (GHZ): 0.1830987 0.1830987 0.0917561

 Leave Link 202 at Fri Jul 5 21:08:54 2019, MaxMem= 1342177280 cpu: 0.2

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

 Basis read from rwf: (5D, 7F)

 Pseudo-potential data read from rwf file.

 There are 229 symmetry adapted cartesian basis functions of AG symmetry.

 There are 82 symmetry adapted cartesian basis functions of BG symmetry.

 There are 78 symmetry adapted cartesian basis functions of AU symmetry.

 There are 218 symmetry adapted cartesian basis functions of BU symmetry.

 There are 212 symmetry adapted basis functions of AG symmetry.

 There are 82 symmetry adapted basis functions of BG symmetry.

 There are 78 symmetry adapted basis functions of AU symmetry.

 There are 204 symmetry adapted basis functions of BU symmetry.

 576 basis functions, 1015 primitive gaussians, 607 cartesian basis functions

 102 alpha electrons 101 beta electrons

 nuclear repulsion energy 2767.4139286336 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= 45 NActive= 45 NUniq= 11 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= -0.1141878158 Hartrees.

 Nuclear repulsion after empirical dispersion term = 2767.2997408178 Hartrees.

 No density basis found on file 724.

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

 Polarizable Continuum Model (PCM)

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

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

 Atomic radii : SMD-Coulomb.

 Polarization charges : Total charges.

 Charge compensation : None.

 Solution method : On-the-fly selection.

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

 Cavity algorithm : GePol (No added spheres)

 Default sphere list used, NSphG= 45.

 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 = 45

 GePol: Total number of spheres = 45

 GePol: Number of exposed spheres = 45 (100.00%)

 GePol: Number of points = 3534

 GePol: Average weight of points = 0.11

 GePol: Minimum weight of points = 0.55D-07

 GePol: Maximum weight of points = 0.18390

 GePol: Number of points with low weight = 156

 GePol: Fraction of low-weight points (<1% of avg) = 4.41%

 GePol: Cavity surface area = 381.790 Ang\*\*2

 GePol: Cavity volume = 378.632 Ang\*\*3

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

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 PCM non-electrostatic energy = -0.0110224291 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 2767.2887183886 Hartrees.

 Leave Link 301 at Fri Jul 5 21:08:54 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

 One-electron integrals computed using PRISM.

 One-electron integral symmetry used in STVInt

 8 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15363 LenP2D= 41360.

 LDataN: DoStor=T MaxTD1= 5 Len= 102

 NBasis= 576 RedAO= T EigKep= 1.83D-04 NBF= 212 82 78 204

 NBsUse= 576 1.00D-06 EigRej= -1.00D+00 NBFU= 212 82 78 204

 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= 594 594 594 594 594 MxSgAt= 45 MxSgA2= 45.

 Leave Link 302 at Fri Jul 5 21:08:55 2019, MaxMem= 1342177280 cpu: 7.8

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

 DipDrv: MaxL=1.

 Leave Link 303 at Fri Jul 5 21:08:55 2019, MaxMem= 1342177280 cpu: 0.8

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

 Initial guess from the checkpoint file: "ZntAzPcation.chk"

 B after Tr= 0.000000 0.000000 0.000000

 Rot= 1.000000 0.000000 0.000000 0.000168 Ang= 0.02 deg.

 Guess basis will be translated and rotated to current coordinates.

 JPrj=2 DoOrth=T DoCkMO=T.

 Initial guess orbital symmetries:

 Alpha Orbitals:

 Occupied (BG) (EU) (EU) (AG) (EU) (EU) (BG) (AG) (BG) (EU)

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

 Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7828 S= 0.5163

 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= -1275.93768598349

 Leave Link 401 at Fri Jul 5 21:08:58 2019, MaxMem= 1342177280 cpu: 32.8

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

 UHF open shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 1138797 IEndB= 1138797 NGot= 1342177280 MDV= 1341424180

 LenX= 1341424180 LenY= 1341055124

 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= 670000000 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= 37467468.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 7.55D-15 for 272.

 Iteration 1 A\*A^-1 deviation from orthogonality is 6.37D-15 for 3515 2677.

 Iteration 1 A^-1\*A deviation from unit magnitude is 7.99D-15 for 3529.

 Iteration 1 A^-1\*A deviation from orthogonality is 3.89D-12 for 1538 1510.

 E= -1275.69829803588

 DIIS: error= 1.34D-03 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -1275.69829803588 IErMin= 1 ErrMin= 1.34D-03

 ErrMax= 1.34D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.45D-03 BMatP= 3.45D-03

 IDIUse=3 WtCom= 9.87D-01 WtEn= 1.34D-02

 Coeff-Com: 0.100D+01

 Coeff-En: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.373 Goal= None Shift= 0.000

 Gap= 0.407 Goal= None Shift= 0.000

 GapD= 0.373 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

 RMSDP=7.41D-05 MaxDP=1.82D-03 OVMax= 6.94D-03

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 7.41D-05 CP: 1.00D+00

 E= -1275.69910529858 Delta-E= -0.000807262702 Rises=F Damp=F

 DIIS: error= 4.97D-04 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -1275.69910529858 IErMin= 2 ErrMin= 4.97D-04

 ErrMax= 4.97D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.61D-04 BMatP= 3.45D-03

 IDIUse=3 WtCom= 9.95D-01 WtEn= 4.97D-03

 Coeff-Com: 0.185D+00 0.815D+00

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

 Coeff: 0.184D+00 0.816D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.081 Goal= None Shift= 0.000

 RMSDP=2.47D-05 MaxDP=1.47D-03 DE=-8.07D-04 OVMax= 3.13D-03

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 2.42D-05 CP: 1.00D+00 9.34D-01

 E= -1275.69912140926 Delta-E= -0.000016110675 Rises=F Damp=F

 DIIS: error= 5.15D-04 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 3 EnMin= -1275.69912140926 IErMin= 2 ErrMin= 4.97D-04

 ErrMax= 5.15D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.18D-04 BMatP= 5.61D-04

 IDIUse=3 WtCom= 9.95D-01 WtEn= 5.15D-03

 Coeff-Com: -0.423D-02 0.490D+00 0.514D+00

 Coeff-En: 0.000D+00 0.466D+00 0.534D+00

 Coeff: -0.421D-02 0.490D+00 0.514D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.082 Goal= None Shift= 0.000

 RMSDP=1.34D-05 MaxDP=8.10D-04 DE=-1.61D-05 OVMax= 2.18D-03

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 6.87D-06 CP: 1.00D+00 9.89D-01 5.58D-01

 E= -1275.69921748463 Delta-E= -0.000096075374 Rises=F Damp=F

 DIIS: error= 1.46D-04 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -1275.69921748463 IErMin= 4 ErrMin= 1.46D-04

 ErrMax= 1.46D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.09D-05 BMatP= 5.18D-04

 IDIUse=3 WtCom= 9.99D-01 WtEn= 1.46D-03

 Coeff-Com: -0.855D-02 0.219D+00 0.270D+00 0.519D+00

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

 Coeff: -0.854D-02 0.219D+00 0.270D+00 0.520D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.082 Goal= None Shift= 0.000

 RMSDP=3.92D-06 MaxDP=1.44D-04 DE=-9.61D-05 OVMax= 7.58D-04

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 2.14D-06 CP: 1.00D+00 9.91D-01 5.83D-01 5.31D-01

 E= -1275.69922197889 Delta-E= -0.000004494257 Rises=F Damp=F

 DIIS: error= 3.51D-05 at cycle 5 NSaved= 5.

 NSaved= 5 IEnMin= 5 EnMin= -1275.69922197889 IErMin= 5 ErrMin= 3.51D-05

 ErrMax= 3.51D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.92D-06 BMatP= 2.09D-05

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

 Coeff-Com: -0.397D-02 0.597D-01 0.822D-01 0.276D+00 0.586D+00

 Coeff: -0.397D-02 0.597D-01 0.822D-01 0.276D+00 0.586D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.082 Goal= None Shift= 0.000

 RMSDP=1.10D-06 MaxDP=3.86D-05 DE=-4.49D-06 OVMax= 1.86D-04

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 7.25D-07 CP: 1.00D+00 9.93D-01 5.80D-01 6.24D-01 7.74D-01

 E= -1275.69922238436 Delta-E= -0.000000405477 Rises=F Damp=F

 DIIS: error= 1.36D-05 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -1275.69922238436 IErMin= 6 ErrMin= 1.36D-05

 ErrMax= 1.36D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.47D-07 BMatP= 1.92D-06

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

 Coeff-Com: -0.116D-02 0.120D-01 0.192D-01 0.101D+00 0.289D+00 0.580D+00

 Coeff: -0.116D-02 0.120D-01 0.192D-01 0.101D+00 0.289D+00 0.580D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.082 Goal= None Shift= 0.000

 RMSDP=3.31D-07 MaxDP=1.41D-05 DE=-4.05D-07 OVMax= 1.05D-04

 Cycle 7 Pass 1 IDiag 1:

 RMSU= 2.71D-07 CP: 1.00D+00 9.94D-01 5.82D-01 6.31D-01 8.31D-01

 CP: 8.25D-01

 E= -1275.69922241599 Delta-E= -0.000000031623 Rises=F Damp=F

 DIIS: error= 7.00D-06 at cycle 7 NSaved= 7.

 NSaved= 7 IEnMin= 7 EnMin= -1275.69922241599 IErMin= 7 ErrMin= 7.00D-06

 ErrMax= 7.00D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.07D-08 BMatP= 1.47D-07

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

 Coeff-Com: -0.101D-03-0.251D-02-0.162D-02 0.188D-01 0.764D-01 0.341D+00

 Coeff-Com: 0.568D+00

 Coeff: -0.101D-03-0.251D-02-0.162D-02 0.188D-01 0.764D-01 0.341D+00

 Coeff: 0.568D+00

 Gap= 0.104 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

 Gap= 0.082 Goal= None Shift= 0.000

 RMSDP=1.65D-07 MaxDP=8.65D-06 DE=-3.16D-08 OVMax= 6.78D-05

 Cycle 8 Pass 1 IDiag 1:

 RMSU= 1.23D-07 CP: 1.00D+00 9.94D-01 5.83D-01 6.36D-01 8.57D-01

 CP: 9.11D-01 8.23D-01

 E= -1275.69922242469 Delta-E= -0.000000008709 Rises=F Damp=F

 DIIS: error= 1.98D-06 at cycle 8 NSaved= 8.

 NSaved= 8 IEnMin= 8 EnMin= -1275.69922242469 IErMin= 8 ErrMin= 1.98D-06

 ErrMax= 1.98D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.34D-09 BMatP= 3.07D-08

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

 Coeff-Com: 0.132D-03-0.299D-02-0.377D-02-0.714D-02-0.155D-01 0.582D-01

 Coeff-Com: 0.231D+00 0.741D+00

 Coeff: 0.132D-03-0.299D-02-0.377D-02-0.714D-02-0.155D-01 0.582D-01

 Coeff: 0.231D+00 0.741D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.082 Goal= None Shift= 0.000

 RMSDP=8.26D-08 MaxDP=2.97D-06 DE=-8.71D-09 OVMax= 5.13D-05

 Cycle 9 Pass 1 IDiag 1:

 RMSU= 4.89D-08 CP: 1.00D+00 9.94D-01 5.83D-01 6.38D-01 8.66D-01

 CP: 9.59D-01 1.00D+00 1.12D+00

 E= -1275.69922242630 Delta-E= -0.000000001603 Rises=F Damp=F

 DIIS: error= 8.48D-07 at cycle 9 NSaved= 9.

 NSaved= 9 IEnMin= 9 EnMin= -1275.69922242630 IErMin= 9 ErrMin= 8.48D-07

 ErrMax= 8.48D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.22D-10 BMatP= 2.34D-09

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

 Coeff-Com: 0.422D-04-0.108D-03-0.425D-03-0.443D-02-0.165D-01-0.511D-01

 Coeff-Com: -0.566D-01 0.158D+00 0.971D+00

 Coeff: 0.422D-04-0.108D-03-0.425D-03-0.443D-02-0.165D-01-0.511D-01

 Coeff: -0.566D-01 0.158D+00 0.971D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.082 Goal= None Shift= 0.000

 RMSDP=5.78D-08 MaxDP=2.33D-06 DE=-1.60D-09 OVMax= 3.51D-05

 Cycle 10 Pass 1 IDiag 1:

 RMSU= 2.36D-08 CP: 1.00D+00 9.94D-01 5.83D-01 6.39D-01 8.73D-01

 CP: 9.92D-01 1.08D+00 1.38D+00 1.45D+00

 E= -1275.69922242711 Delta-E= -0.000000000810 Rises=F Damp=F

 DIIS: error= 5.30D-07 at cycle 10 NSaved= 10.

 NSaved=10 IEnMin=10 EnMin= -1275.69922242711 IErMin=10 ErrMin= 5.30D-07

 ErrMax= 5.30D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.77D-10 BMatP= 4.22D-10

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

 Coeff-Com: -0.230D-04 0.900D-03 0.998D-03 0.486D-03-0.110D-02-0.366D-01

 Coeff-Com: -0.810D-01-0.131D+00 0.459D+00 0.788D+00

 Coeff: -0.230D-04 0.900D-03 0.998D-03 0.486D-03-0.110D-02-0.366D-01

 Coeff: -0.810D-01-0.131D+00 0.459D+00 0.788D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.082 Goal= None Shift= 0.000

 RMSDP=3.16D-08 MaxDP=1.92D-06 DE=-8.10D-10 OVMax= 1.59D-05

 Cycle 11 Pass 1 IDiag 1:

 RMSU= 1.27D-08 CP: 1.00D+00 9.94D-01 5.83D-01 6.39D-01 8.76D-01

 CP: 1.00D+00 1.12D+00 1.52D+00 1.76D+00 1.34D+00

 E= -1275.69922242724 Delta-E= -0.000000000137 Rises=F Damp=F

 DIIS: error= 3.70D-07 at cycle 11 NSaved= 11.

 NSaved=11 IEnMin=11 EnMin= -1275.69922242724 IErMin=11 ErrMin= 3.70D-07

 ErrMax= 3.70D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.61D-11 BMatP= 1.77D-10

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

 Coeff-Com: -0.186D-04 0.273D-03 0.387D-03 0.112D-02 0.427D-02 0.738D-03

 Coeff-Com: -0.109D-01-0.101D+00-0.165D+00 0.246D+00 0.102D+01

 Coeff: -0.186D-04 0.273D-03 0.387D-03 0.112D-02 0.427D-02 0.738D-03

 Coeff: -0.109D-01-0.101D+00-0.165D+00 0.246D+00 0.102D+01

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.082 Goal= None Shift= 0.000

 RMSDP=2.40D-08 MaxDP=1.50D-06 DE=-1.37D-10 OVMax= 1.04D-05

 Cycle 12 Pass 1 IDiag 1:

 RMSU= 8.14D-09 CP: 1.00D+00 9.94D-01 5.83D-01 6.39D-01 8.78D-01

 CP: 1.01D+00 1.15D+00 1.60D+00 2.01D+00 1.85D+00

 CP: 1.46D+00

 E= -1275.69922242749 Delta-E= -0.000000000243 Rises=F Damp=F

 DIIS: error= 2.57D-07 at cycle 12 NSaved= 12.

 NSaved=12 IEnMin=12 EnMin= -1275.69922242749 IErMin=12 ErrMin= 2.57D-07

 ErrMax= 2.57D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.39D-11 BMatP= 4.61D-11

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

 Coeff-Com: -0.591D-05-0.866D-04-0.287D-04 0.800D-03 0.363D-02 0.144D-01

 Coeff-Com: 0.222D-01-0.134D-01-0.224D+00-0.839D-01 0.617D+00 0.663D+00

 Coeff: -0.591D-05-0.866D-04-0.287D-04 0.800D-03 0.363D-02 0.144D-01

 Coeff: 0.222D-01-0.134D-01-0.224D+00-0.839D-01 0.617D+00 0.663D+00

 Gap= 0.104 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

 Gap= 0.082 Goal= None Shift= 0.000

 RMSDP=8.45D-09 MaxDP=6.04D-07 DE=-2.43D-10 OVMax= 4.04D-06

 Error on total polarization charges = 0.06020

 SCF Done: E(UB3LYP) = -1275.69922243 A.U. after 12 cycles

 NFock= 12 Conv=0.84D-08 -V/T= 1.9660

 <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7820 S= 0.5159

 <L.S>= 0.000000000000E+00

 KE= 1.320615687339D+03 PE=-8.558478107178D+03 EE= 3.194874479023D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.92

 (included in total energy above)

 Annihilation of the first spin contaminant:

 S\*\*2 before annihilation 0.7820, after 0.7509

 Leave Link 502 at Fri Jul 5 21:10:12 2019, MaxMem= 1342177280 cpu: 852.8

 (Enter /apps/gaussian/g09d01/g09/l701.exe)

 Compute integral first derivatives.

 ... and contract with generalized density number 0.

 R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

 8 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15363 LenP2D= 41360.

 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 = 252

 Leave Link 701 at Fri Jul 5 21:10:17 2019, MaxMem= 1342177280 cpu: 53.4

 (Enter /apps/gaussian/g09d01/g09/l702.exe)

 L702 exits ... SP integral derivatives will be done elsewhere.

 Leave Link 702 at Fri Jul 5 21:10:17 2019, MaxMem= 1342177280 cpu: 0.2

 (Enter /apps/gaussian/g09d01/g09/l703.exe)

 Compute integral first derivatives, UseDBF=F ICtDFT= 0.

 Integral derivatives from FoFJK, PRISM(SPDF).

 Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

 FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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 Fri Jul 5 21:10:24 2019, MaxMem= 1342177280 cpu: 92.4

 (Enter /apps/gaussian/g09d01/g09/l716.exe)

 Dipole =-4.97379915D-14 1.62092562D-13 0.00000000D+00

 \*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

 Center Atomic Forces (Hartrees/Bohr)

 Number Number X Y Z

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

 1 6 -0.001190550 0.002342220 0.000000000

 2 7 -0.001003503 -0.003661979 0.000000000

 3 6 0.003363733 0.004087129 0.000000000

 4 6 -0.004271749 -0.002580000 0.000000000

 5 6 0.002264445 -0.001197823 0.000000000

 6 7 -0.000481261 -0.000444642 0.000000000

 7 6 -0.002342220 -0.001190550 0.000000000

 8 7 0.003661979 -0.001003503 0.000000000

 9 6 -0.004087129 0.003363733 0.000000000

 10 6 0.002580000 -0.004271749 0.000000000

 11 6 0.001197823 0.002264445 0.000000000

 12 7 -0.000444642 0.000481261 0.000000000

 13 6 -0.002580000 0.004271749 0.000000000

 14 6 -0.001197823 -0.002264445 0.000000000

 15 6 0.002342220 0.001190550 0.000000000

 16 7 -0.003661979 0.001003503 0.000000000

 17 6 0.004087129 -0.003363733 0.000000000

 18 7 0.000481261 0.000444642 0.000000000

 19 7 0.001003503 0.003661979 0.000000000

 20 6 -0.003363733 -0.004087129 0.000000000

 21 6 0.004271749 0.002580000 0.000000000

 22 6 -0.002264445 0.001197823 0.000000000

 23 6 0.001190550 -0.002342220 0.000000000

 24 7 0.000444642 -0.000481261 0.000000000

 25 30 0.000000000 0.000000000 0.000000000

 26 6 0.000261417 0.000650376 0.000000000

 27 1 -0.000340192 0.000524067 0.000000000

 28 6 -0.000650376 0.000261417 0.000000000

 29 1 -0.000524067 -0.000340192 0.000000000

 30 6 0.000650376 -0.000261417 0.000000000

 31 1 0.000524067 0.000340192 0.000000000

 32 6 -0.000261417 -0.000650376 0.000000000

 33 1 0.000340192 -0.000524067 0.000000000

 34 1 0.000063217 -0.000023112 0.000000000

 35 1 0.000285590 -0.000084597 -0.000098269

 36 1 0.000285590 -0.000084597 0.000098269

 37 1 0.000084597 0.000285590 -0.000098269

 38 1 0.000084597 0.000285590 0.000098269

 39 1 0.000023112 0.000063217 0.000000000

 40 1 -0.000084597 -0.000285590 -0.000098269

 41 1 -0.000084597 -0.000285590 0.000098269

 42 1 -0.000023112 -0.000063217 0.000000000

 43 1 -0.000285590 0.000084597 -0.000098269

 44 1 -0.000285590 0.000084597 0.000098269

 45 1 -0.000063217 0.000023112 0.000000000

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

 Cartesian Forces: Max 0.004271749 RMS 0.001561755

 Leave Link 716 at Fri Jul 5 21:10:24 2019, MaxMem= 1342177280 cpu: 0.3

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

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Berny optimization.

 Using GEDIIS/GDIIS optimizer.

 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

 GSVD: received Info= 1 from GESDD.

 Internal Forces: Max 0.002610598 RMS 0.000577776

 Search for a local minimum.

 Step number 2 out of a maximum of 270

 All quantities printed in internal units (Hartrees-Bohrs-Radians)

 RMS Force = .57778D-03 SwitMx=.10000D-02 MixMth= 2

 Mixed Optimization -- En-DIIS/RFO-DIIS

 Update second derivatives using D2CorX and points 1 2

 DE= -2.25D-03 DEPred=-2.02D-03 R= 1.11D+00

 TightC=F SS= 1.41D+00 RLast= 1.10D-01 DXNew= 5.0454D-01 3.2880D-01

 Trust test= 1.11D+00 RLast= 1.10D-01 DXMaxT set to 3.29D-01

 ITU= 1 0

 Use linear search instead of GDIIS.

 Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01336

 Eigenvalues --- 0.01339 0.01339 0.01339 0.01600 0.01618

 Eigenvalues --- 0.01631 0.01631 0.01774 0.01789 0.01814

 Eigenvalues --- 0.01814 0.01887 0.01903 0.01941 0.01941

 Eigenvalues --- 0.01997 0.01997 0.02044 0.02044 0.02070

 Eigenvalues --- 0.02085 0.02100 0.02111 0.02111 0.02204

 Eigenvalues --- 0.02316 0.02316 0.02352 0.02374 0.07248

 Eigenvalues --- 0.07248 0.07248 0.07248 0.07284 0.07387

 Eigenvalues --- 0.07387 0.07387 0.14502 0.14502 0.15827

 Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

 Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

 Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16005

 Eigenvalues --- 0.16516 0.19896 0.21732 0.22078 0.22078

 Eigenvalues --- 0.23814 0.23851 0.23851 0.24015 0.25000

 Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

 Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

 Eigenvalues --- 0.25013 0.31446 0.33170 0.33170 0.33213

 Eigenvalues --- 0.33282 0.33282 0.33282 0.33409 0.33724

 Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

 Eigenvalues --- 0.33724 0.34318 0.34437 0.34437 0.34437

 Eigenvalues --- 0.34613 0.34923 0.35380 0.35572 0.35572

 Eigenvalues --- 0.35682 0.35682 0.35682 0.35873 0.39290

 Eigenvalues --- 0.41744 0.41744 0.42490 0.47537 0.48960

 Eigenvalues --- 0.48960 0.49463 0.50263 0.50556 0.51357

 Eigenvalues --- 0.51357 0.52367 0.53983 0.53983 0.54929

 Eigenvalues --- 0.56278 0.56331 0.56331 0.56399

 RFO step: Lambda=-3.72232765D-04 EMin= 8.77959372D-03

 Quartic linear search produced a step of 0.14147.

 Iteration 1 RMS(Cart)= 0.00492715 RMS(Int)= 0.00001533

 Iteration 2 RMS(Cart)= 0.00002827 RMS(Int)= 0.00000170

 Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000170

 ITry= 1 IFail=0 DXMaxC= 1.54D-02 DCOld= 1.00D+10 DXMaxT= 3.29D-01 DXLimC= 3.00D+00 Rises=F

 ClnCor: largest displacement from symmetrization is 3.28D-10 for atom 36.

 Variable Old X -DE/DX Delta X Delta X Delta X New X

 (Linear) (Quad) (Total)

 R1 2.57063 -0.00010 -0.00093 0.00004 -0.00089 2.56974

 R2 2.77533 0.00106 0.00175 0.00271 0.00447 2.77980

 R3 2.53220 -0.00033 -0.00088 -0.00013 -0.00101 2.53120

 R4 2.56079 -0.00108 -0.00187 -0.00182 -0.00369 2.55710

 R5 3.77253 0.00111 -0.00298 0.00889 0.00590 3.77843

 R6 2.81601 0.00261 0.00338 0.00744 0.01082 2.82683

 R7 2.52433 -0.00064 -0.00124 -0.00065 -0.00189 2.52244

 R8 2.56509 -0.00092 -0.00318 -0.00075 -0.00393 2.56117

 R9 2.80534 -0.00012 -0.00187 0.00025 -0.00163 2.80371

 R10 2.04117 0.00002 -0.00066 0.00030 -0.00036 2.04081

 R11 2.53220 -0.00033 -0.00088 -0.00013 -0.00101 2.53120

 R12 2.57063 -0.00010 -0.00093 0.00004 -0.00089 2.56974

 R13 2.77533 0.00106 0.00175 0.00271 0.00447 2.77980

 R14 2.56079 -0.00108 -0.00187 -0.00182 -0.00369 2.55710

 R15 3.77253 0.00111 -0.00298 0.00889 0.00590 3.77843

 R16 2.81601 0.00261 0.00338 0.00744 0.01082 2.82683

 R17 2.52433 -0.00064 -0.00124 -0.00065 -0.00189 2.52244

 R18 2.56509 -0.00092 -0.00318 -0.00075 -0.00393 2.56117

 R19 2.80534 -0.00012 -0.00187 0.00025 -0.00163 2.80371

 R20 2.04117 0.00002 -0.00066 0.00030 -0.00036 2.04081

 R21 2.52433 -0.00064 -0.00124 -0.00065 -0.00189 2.52244

 R22 2.56509 -0.00092 -0.00318 -0.00075 -0.00393 2.56117

 R23 2.81601 0.00261 0.00338 0.00744 0.01082 2.82683

 R24 2.80534 -0.00012 -0.00187 0.00025 -0.00163 2.80371

 R25 2.77533 0.00106 0.00175 0.00271 0.00447 2.77980

 R26 2.04117 0.00002 -0.00066 0.00030 -0.00036 2.04081

 R27 2.57063 -0.00010 -0.00093 0.00004 -0.00089 2.56974

 R28 2.53220 -0.00033 -0.00088 -0.00013 -0.00101 2.53120

 R29 2.56079 -0.00108 -0.00187 -0.00182 -0.00369 2.55710

 R30 3.77253 0.00111 -0.00298 0.00889 0.00590 3.77843

 R31 2.52433 -0.00064 -0.00124 -0.00065 -0.00189 2.52244

 R32 2.56079 -0.00108 -0.00187 -0.00182 -0.00369 2.55710

 R33 2.57063 -0.00010 -0.00093 0.00004 -0.00089 2.56974

 R34 3.77253 0.00111 -0.00298 0.00889 0.00590 3.77843

 R35 2.81601 0.00261 0.00338 0.00744 0.01082 2.82683

 R36 2.56509 -0.00092 -0.00318 -0.00075 -0.00393 2.56117

 R37 2.80534 -0.00012 -0.00187 0.00025 -0.00163 2.80371

 R38 2.77533 0.00106 0.00175 0.00271 0.00447 2.77980

 R39 2.04117 0.00002 -0.00066 0.00030 -0.00036 2.04081

 R40 2.53220 -0.00033 -0.00088 -0.00013 -0.00101 2.53120

 R41 2.06064 -0.00006 -0.00076 0.00008 -0.00068 2.05996

 R42 2.06794 0.00012 -0.00142 0.00091 -0.00051 2.06742

 R43 2.06794 0.00012 -0.00142 0.00091 -0.00051 2.06742

 R44 2.06794 0.00012 -0.00142 0.00091 -0.00051 2.06742

 R45 2.06794 0.00012 -0.00142 0.00091 -0.00051 2.06742

 R46 2.06064 -0.00006 -0.00076 0.00008 -0.00068 2.05996

 R47 2.06794 0.00012 -0.00142 0.00091 -0.00051 2.06742

 R48 2.06794 0.00012 -0.00142 0.00091 -0.00051 2.06742

 R49 2.06064 -0.00006 -0.00076 0.00008 -0.00068 2.05996

 R50 2.06794 0.00012 -0.00142 0.00091 -0.00051 2.06742

 R51 2.06794 0.00012 -0.00142 0.00091 -0.00051 2.06742

 R52 2.06064 -0.00006 -0.00076 0.00008 -0.00068 2.05996

 A1 1.89637 -0.00069 0.00071 -0.00399 -0.00328 1.89309

 A2 2.21121 0.00025 -0.00016 0.00142 0.00125 2.21247

 A3 2.17560 0.00044 -0.00055 0.00257 0.00203 2.17763

 A4 1.90438 0.00115 -0.00028 0.00561 0.00533 1.90971

 A5 2.19291 -0.00041 0.00037 -0.00182 -0.00146 2.19146

 A6 2.18589 -0.00074 -0.00008 -0.00379 -0.00388 2.18201

 A7 1.89617 -0.00069 -0.00004 -0.00340 -0.00345 1.89272

 A8 2.22553 0.00115 0.00086 0.00472 0.00558 2.23111

 A9 2.16149 -0.00046 -0.00082 -0.00132 -0.00214 2.15935

 A10 1.85113 -0.00024 0.00001 -0.00094 -0.00093 1.85020

 A11 2.17158 -0.00156 -0.00087 -0.00688 -0.00775 2.16383

 A12 2.26047 0.00180 0.00087 0.00781 0.00868 2.26915

 A13 1.87672 0.00048 -0.00039 0.00272 0.00233 1.87905

 A14 2.17827 -0.00085 0.00000 -0.00562 -0.00562 2.17264

 A15 2.22820 0.00037 0.00039 0.00290 0.00329 2.23149

 A16 2.18003 -0.00025 -0.00098 -0.00053 -0.00151 2.17852

 A17 2.21121 0.00025 -0.00016 0.00142 0.00125 2.21247

 A18 2.17560 0.00044 -0.00055 0.00257 0.00203 2.17763

 A19 1.89637 -0.00069 0.00071 -0.00399 -0.00328 1.89309

 A20 1.90438 0.00115 -0.00028 0.00561 0.00533 1.90971

 A21 2.19291 -0.00041 0.00037 -0.00182 -0.00146 2.19146

 A22 2.18589 -0.00074 -0.00008 -0.00379 -0.00388 2.18201

 A23 1.89617 -0.00069 -0.00004 -0.00340 -0.00345 1.89272

 A24 2.22553 0.00115 0.00086 0.00472 0.00558 2.23111

 A25 2.16149 -0.00046 -0.00082 -0.00132 -0.00214 2.15935

 A26 1.85113 -0.00024 0.00001 -0.00094 -0.00093 1.85020

 A27 2.17158 -0.00156 -0.00087 -0.00688 -0.00775 2.16383

 A28 2.26047 0.00180 0.00087 0.00781 0.00868 2.26915

 A29 1.87672 0.00048 -0.00039 0.00272 0.00233 1.87905

 A30 2.17827 -0.00085 0.00000 -0.00562 -0.00562 2.17264

 A31 2.22820 0.00037 0.00039 0.00290 0.00329 2.23149

 A32 2.18003 -0.00025 -0.00098 -0.00053 -0.00151 2.17852

 A33 1.85113 -0.00024 0.00001 -0.00094 -0.00093 1.85020

 A34 2.26047 0.00180 0.00087 0.00781 0.00868 2.26915

 A35 2.17158 -0.00156 -0.00087 -0.00688 -0.00775 2.16383

 A36 1.87672 0.00048 -0.00039 0.00272 0.00233 1.87905

 A37 2.22820 0.00037 0.00039 0.00290 0.00329 2.23149

 A38 2.17827 -0.00085 0.00000 -0.00562 -0.00562 2.17264

 A39 1.89637 -0.00069 0.00071 -0.00399 -0.00328 1.89309

 A40 2.17560 0.00044 -0.00055 0.00257 0.00203 2.17763

 A41 2.21121 0.00025 -0.00016 0.00142 0.00125 2.21247

 A42 1.90438 0.00115 -0.00028 0.00561 0.00533 1.90971

 A43 2.19291 -0.00041 0.00037 -0.00182 -0.00146 2.19146

 A44 2.18589 -0.00074 -0.00008 -0.00379 -0.00388 2.18201

 A45 2.16149 -0.00046 -0.00082 -0.00132 -0.00214 2.15935

 A46 2.22553 0.00115 0.00086 0.00472 0.00558 2.23111

 A47 1.89617 -0.00069 -0.00004 -0.00340 -0.00345 1.89272

 A48 2.18003 -0.00025 -0.00098 -0.00053 -0.00151 2.17852

 A49 1.90438 0.00115 -0.00028 0.00561 0.00533 1.90971

 A50 2.18589 -0.00074 -0.00008 -0.00379 -0.00388 2.18201

 A51 2.19291 -0.00041 0.00037 -0.00182 -0.00146 2.19146

 A52 2.22553 0.00115 0.00086 0.00472 0.00558 2.23111

 A53 2.16149 -0.00046 -0.00082 -0.00132 -0.00214 2.15935

 A54 1.89617 -0.00069 -0.00004 -0.00340 -0.00345 1.89272

 A55 1.85113 -0.00024 0.00001 -0.00094 -0.00093 1.85020

 A56 2.17158 -0.00156 -0.00087 -0.00688 -0.00775 2.16383

 A57 2.26047 0.00180 0.00087 0.00781 0.00868 2.26915

 A58 1.87672 0.00048 -0.00039 0.00272 0.00233 1.87905

 A59 2.22820 0.00037 0.00039 0.00290 0.00329 2.23149

 A60 2.17827 -0.00085 0.00000 -0.00562 -0.00562 2.17264

 A61 1.89637 -0.00069 0.00071 -0.00399 -0.00328 1.89309

 A62 2.21121 0.00025 -0.00016 0.00142 0.00125 2.21247

 A63 2.17560 0.00044 -0.00055 0.00257 0.00203 2.17763

 A64 2.18003 -0.00025 -0.00098 -0.00053 -0.00151 2.17852

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 A67 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

 A68 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

 A69 1.93957 0.00015 0.00059 0.00164 0.00223 1.94179

 A70 1.93379 0.00011 -0.00039 0.00052 0.00012 1.93391

 A71 1.93379 0.00011 -0.00039 0.00052 0.00012 1.93391

 A72 1.89557 -0.00002 0.00063 0.00034 0.00097 1.89654

 A73 1.89557 -0.00002 0.00063 0.00034 0.00097 1.89654

 A74 1.86331 -0.00035 -0.00109 -0.00356 -0.00465 1.85865

 A75 1.93379 0.00011 -0.00039 0.00052 0.00012 1.93391

 A76 1.93379 0.00011 -0.00039 0.00052 0.00012 1.93391

 A77 1.93957 0.00015 0.00059 0.00164 0.00223 1.94179

 A78 1.86331 -0.00035 -0.00109 -0.00356 -0.00465 1.85865

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 A80 1.89557 -0.00002 0.00063 0.00034 0.00097 1.89654

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 A83 1.93957 0.00015 0.00059 0.00164 0.00223 1.94179

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 A85 1.89557 -0.00002 0.00063 0.00034 0.00097 1.89654

 A86 1.89557 -0.00002 0.00063 0.00034 0.00097 1.89654

 A87 1.93379 0.00011 -0.00039 0.00052 0.00012 1.93391

 A88 1.93379 0.00011 -0.00039 0.00052 0.00012 1.93391

 A89 1.93957 0.00015 0.00059 0.00164 0.00223 1.94179

 A90 1.86331 -0.00035 -0.00109 -0.00356 -0.00465 1.85865

 A91 1.89557 -0.00002 0.00063 0.00034 0.00097 1.89654

 A92 1.89557 -0.00002 0.00063 0.00034 0.00097 1.89654

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 A96 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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 D4 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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 D63 1.03244 -0.00015 -0.00093 -0.00189 -0.00282 1.02962

 D64 -1.03244 0.00015 0.00093 0.00189 0.00282 -1.02962

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 D82 1.03244 -0.00015 -0.00093 -0.00189 -0.00282 1.02962

 D83 -1.03244 0.00015 0.00093 0.00189 0.00282 -1.02962

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 D109 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D110 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D111 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D112 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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 D116 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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 D119 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D120 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D121 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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 D123 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D124 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D125 1.03244 -0.00015 -0.00093 -0.00189 -0.00282 1.02962

 D126 -1.03244 0.00015 0.00093 0.00189 0.00282 -1.02962

 D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D128 -2.10915 -0.00015 -0.00093 -0.00189 -0.00282 -2.11197

 D129 2.10915 0.00015 0.00093 0.00189 0.00282 2.11197

 D130 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D131 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D132 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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 D134 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D136 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 Item Value Threshold Converged?

 Maximum Force 0.002611 0.000450 NO

 RMS Force 0.000578 0.000300 NO

 Maximum Displacement 0.015402 0.001800 NO

 RMS Displacement 0.004930 0.001200 NO

 Predicted change in Energy=-2.225845D-04

 Lowest energy point so far. Saving SCF results.

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link 103 at Fri Jul 5 21:10:25 2019, MaxMem= 1342177280 cpu: 1.5

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

 Input orientation:

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

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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

 1 6 0 -2.063828 -2.179493 0.000000

 2 7 0 -0.742942 -1.856306 0.000000

 3 6 0 -0.002647 -2.989006 0.000000

 4 6 0 -0.931567 -4.161527 0.000000

 5 6 0 -2.184803 -3.645517 0.000000

 6 7 0 1.327747 -3.097587 0.000000

 7 6 0 2.179493 -2.063828 0.000000

 8 7 0 1.856306 -0.742942 0.000000

 9 6 0 2.989006 -0.002647 0.000000

 10 6 0 4.161527 -0.931567 0.000000

 11 6 0 3.645517 -2.184803 0.000000

 12 7 0 -3.097587 -1.327747 0.000000

 13 6 0 -4.161527 0.931567 0.000000

 14 6 0 -3.645517 2.184803 0.000000

 15 6 0 -2.179493 2.063828 0.000000

 16 7 0 -1.856306 0.742942 0.000000

 17 6 0 -2.989006 0.002647 0.000000

 18 7 0 -1.327747 3.097587 0.000000

 19 7 0 0.742942 1.856306 0.000000

 20 6 0 0.002647 2.989006 0.000000

 21 6 0 0.931567 4.161527 0.000000

 22 6 0 2.184803 3.645517 0.000000

 23 6 0 2.063828 2.179493 0.000000

 24 7 0 3.097587 1.327747 0.000000

 25 30 0 0.000000 0.000000 0.000000

 26 6 0 -0.482118 -5.575472 0.000000

 27 1 0 -3.122267 -4.181668 0.000000

 28 6 0 5.575472 -0.482118 0.000000

 29 1 0 4.181668 -3.122267 0.000000

 30 6 0 -5.575472 0.482118 0.000000

 31 1 0 -4.181668 3.122267 0.000000

 32 6 0 0.482118 5.575472 0.000000

 33 1 0 3.122267 4.181668 0.000000

 34 1 0 -1.330584 -6.259866 0.000000

 35 1 0 0.137676 -5.786207 0.876559

 36 1 0 0.137676 -5.786207 -0.876559

 37 1 0 5.786207 0.137676 0.876559

 38 1 0 5.786207 0.137676 -0.876559

 39 1 0 6.259866 -1.330584 0.000000

 40 1 0 -5.786207 -0.137676 0.876559

 41 1 0 -5.786207 -0.137676 -0.876559

 42 1 0 -6.259866 1.330584 0.000000

 43 1 0 -0.137676 5.786207 0.876559

 44 1 0 -0.137676 5.786207 -0.876559

 45 1 0 1.330584 6.259866 0.000000

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

 Distance matrix (angstroms):

 1 2 3 4 5

 1 C 0.000000

 2 N 1.359849 0.000000

 3 C 2.214447 1.353161 0.000000

 4 C 2.282646 2.312926 1.495894 0.000000

 5 C 1.471006 2.297877 2.278774 1.355311 0.000000

 6 N 3.513642 2.414235 1.334818 2.497292 3.555029

 7 C 4.244897 2.929794 2.370167 3.752204 4.642071

 8 N 4.175060 2.827661 2.915563 4.411231 4.975490

 9 C 5.501798 4.166951 4.227094 5.715520 6.327621

 10 C 6.349202 4.990887 4.644718 6.030941 6.902277

 11 C 5.709347 4.400736 3.735752 4.985693 6.010517

 12 N 1.339451 2.413240 3.512611 3.566785 2.491030

 13 C 3.752204 4.411231 5.715520 6.030941 4.985693

 14 C 4.642071 4.975490 6.327621 6.902277 6.010517

 15 C 4.244897 4.175060 5.501798 6.349202 5.709347

 16 N 2.929794 2.827661 4.166951 4.990887 4.400736

 17 C 2.370167 2.915563 4.227094 4.644718 3.735752

 18 N 5.328170 4.988291 6.229165 7.269917 6.797352

 19 N 4.915855 3.998916 4.902341 6.246462 6.232314

 20 C 5.566300 4.902341 5.978014 7.211302 6.985830

 21 C 7.012911 6.246462 7.211302 8.529038 8.406051

 22 C 7.209827 6.232314 6.985830 8.406051 8.500154

 23 C 6.003191 4.915855 5.566300 7.012911 7.209827

 24 N 6.240268 4.988773 5.314679 6.809274 7.255136

 25 Zn 3.001596 1.999458 2.989007 4.264519 4.250077

 26 C 3.746262 3.728301 2.630533 1.483660 2.573687

 27 H 2.264729 3.326935 3.339831 2.190793 1.079953

 28 C 7.825599 6.466123 6.115546 7.475267 8.380272

 29 H 6.316252 5.084726 4.186437 5.217781 6.387937

 30 C 4.406339 5.368573 6.565446 6.567290 5.341723

 31 H 5.709108 6.050704 7.403504 7.976015 7.056229

 32 C 8.162189 7.532071 8.578186 9.839089 9.598912

 33 H 8.207311 7.169168 7.821998 9.275908 9.456734

 34 H 4.145731 4.442596 3.530147 2.135940 2.750365

 35 H 4.315479 4.121647 2.934686 2.133359 3.277929

 36 H 4.315479 4.121647 2.934686 2.133359 3.277929

 37 H 8.231688 6.882885 6.637419 8.023714 8.866674

 38 H 8.231688 6.882885 6.637419 8.023714 8.866674

 39 H 8.366870 7.022513 6.478382 7.728579 8.756217

 40 H 4.335145 5.399682 6.507534 6.366103 5.103275

 41 H 4.335145 5.399682 6.507534 6.366103 5.103275

 42 H 5.470592 6.371241 7.603396 7.652062 6.431774

 43 H 8.242014 7.716392 8.819918 10.017786 9.691053

 44 H 8.242014 7.716392 8.819918 10.017786 9.691053

 45 H 9.096417 8.376858 9.344470 10.664087 10.510687

 6 7 8 9 10

 6 N 0.000000

 7 C 1.339451 0.000000

 8 N 2.413240 1.359849 0.000000

 9 C 3.512611 2.214447 1.353161 0.000000

 10 C 3.566785 2.282646 2.312926 1.495894 0.000000

 11 C 2.491030 1.471006 2.297877 2.278774 1.355311

 12 N 4.766122 5.328170 4.988291 6.229165 7.269917

 13 C 6.809274 7.012911 6.246462 7.211302 8.529038

 14 C 7.255136 7.209827 6.232314 6.985830 8.406051

 15 C 6.240268 6.003191 4.915855 5.566300 7.012911

 16 N 4.988773 4.915855 3.998916 4.902341 6.246462

 17 C 5.314679 5.566300 4.902341 5.978014 7.211302

 18 N 6.740314 6.240268 4.988773 5.314679 6.809274

 19 N 4.988291 4.175060 2.827661 2.915563 4.411231

 20 C 6.229165 5.501798 4.166951 4.227094 5.715520

 21 C 7.269917 6.349202 4.990887 4.644718 6.030941

 22 C 6.797352 5.709347 4.400736 3.735752 4.985693

 23 C 5.328170 4.244897 2.929794 2.370167 3.752204

 24 N 4.766122 3.513642 2.414235 1.334818 2.497292

 25 Zn 3.370157 3.001596 1.999458 2.989007 4.264519

 26 C 3.068473 4.406339 5.368573 6.565446 6.567290

 27 H 4.580159 5.709108 6.050704 7.403504 7.976015

 28 C 4.988372 3.746262 3.728301 2.630533 1.483660

 29 H 2.854028 2.264729 3.326935 3.339831 2.190793

 30 C 7.776164 8.162189 7.532071 8.578186 9.839089

 31 H 8.309046 8.207311 7.169168 7.821998 9.275908

 32 C 8.714187 7.825599 6.466123 6.115546 7.475267

 33 H 7.497190 6.316252 5.084726 4.186437 5.217781

 34 H 4.131190 5.470592 6.371241 7.603396 7.652062

 35 H 3.068110 4.335145 5.399682 6.507534 6.366103

 36 H 3.068110 4.335145 5.399682 6.507534 6.366103

 37 H 5.577916 4.315479 4.121647 2.934686 2.133359

 38 H 5.577916 4.315479 4.121647 2.934686 2.133359

 39 H 5.239093 4.145731 4.442596 3.530147 2.135940

 40 H 7.754855 8.242014 7.716392 8.819918 10.017786

 41 H 7.754855 8.242014 7.716392 8.819918 10.017786

 42 H 8.785247 9.096417 8.376858 9.344470 10.664087

 43 H 9.046415 8.231688 6.882885 6.637419 8.023714

 44 H 9.046415 8.231688 6.882885 6.637419 8.023714

 45 H 9.357453 8.366870 7.022513 6.478382 7.728579

 11 12 13 14 15

 11 C 0.000000

 12 N 6.797352 0.000000

 13 C 8.406051 2.497292 0.000000

 14 C 8.500154 3.555029 1.355311 0.000000

 15 C 7.209827 3.513642 2.282646 1.471006 0.000000

 16 N 6.232314 2.414235 2.312926 2.297877 1.359849

 17 C 6.985830 1.334818 1.495894 2.278774 2.214447

 18 N 7.255136 4.766122 3.566785 2.491030 1.339451

 19 N 4.975490 4.988773 4.990887 4.400736 2.929794

 20 C 6.327621 5.314679 4.644718 3.735752 2.370167

 21 C 6.902277 6.809274 6.030941 4.985693 3.752204

 22 C 6.010517 7.255136 6.902277 6.010517 4.642071

 23 C 4.642071 6.240268 6.349202 5.709347 4.244897

 24 N 3.555029 6.740314 7.269917 6.797352 5.328170

 25 Zn 4.250077 3.370157 4.264519 4.250077 3.001596

 26 C 5.341723 4.988372 7.475267 8.380272 7.825599

 27 H 7.056229 2.854028 5.217781 6.387937 6.316252

 28 C 2.573687 8.714187 9.839089 9.598912 8.162189

 29 H 1.079953 7.497190 9.275908 9.456734 8.207311

 30 C 9.598912 3.068473 1.483660 2.573687 3.746262

 31 H 9.456734 4.580159 2.190793 1.079953 2.264729

 32 C 8.380272 7.776164 6.567290 5.341723 4.406339

 33 H 6.387937 8.309046 7.976015 7.056229 5.709108

 34 H 6.431774 5.239093 7.728579 8.756217 8.366870

 35 H 5.103275 5.577916 8.023714 8.866674 8.231688

 36 H 5.103275 5.577916 8.023714 8.866674 8.231688

 37 H 3.277929 9.046415 10.017786 9.691053 8.242014

 38 H 3.277929 9.046415 10.017786 9.691053 8.242014

 39 H 2.750365 9.357453 10.664087 10.510687 9.096417

 40 H 9.691053 3.068110 2.133359 3.277929 4.315479

 41 H 9.691053 3.068110 2.133359 3.277929 4.315479

 42 H 10.510687 4.131190 2.135940 2.750365 4.145731

 43 H 8.866674 7.754855 6.366103 5.103275 4.335145

 44 H 8.866674 7.754855 6.366103 5.103275 4.335145

 45 H 8.756217 8.785247 7.652062 6.431774 5.470592

 16 17 18 19 20

 16 N 0.000000

 17 C 1.353161 0.000000

 18 N 2.413240 3.512611 0.000000

 19 N 2.827661 4.166951 2.414235 0.000000

 20 C 2.915563 4.227094 1.334818 1.353161 0.000000

 21 C 4.411231 5.715520 2.497292 2.312926 1.495894

 22 C 4.975490 6.327621 3.555029 2.297877 2.278774

 23 C 4.175060 5.501798 3.513642 1.359849 2.214447

 24 N 4.988291 6.229165 4.766122 2.413240 3.512611

 25 Zn 1.999458 2.989007 3.370157 1.999458 2.989007

 26 C 6.466123 6.115546 8.714187 7.532071 8.578186

 27 H 5.084726 4.186437 7.497190 7.169168 7.821998

 28 C 7.532071 8.578186 7.776164 5.368573 6.565446

 29 H 7.169168 7.821998 8.309046 6.050704 7.403504

 30 C 3.728301 2.630533 4.988372 6.466123 6.115546

 31 H 3.326935 3.339831 2.854028 5.084726 4.186437

 32 C 5.368573 6.565446 3.068473 3.728301 2.630533

 33 H 6.050704 7.403504 4.580159 3.326935 3.339831

 34 H 7.022513 6.478382 9.357453 8.376858 9.344470

 35 H 6.882885 6.637419 9.046415 7.716392 8.819918

 36 H 6.882885 6.637419 9.046415 7.716392 8.819918

 37 H 7.716392 8.819918 7.754855 5.399682 6.507534

 38 H 7.716392 8.819918 7.754855 5.399682 6.507534

 39 H 8.376858 9.344470 8.785247 6.371241 7.603396

 40 H 4.121647 2.934686 5.577916 6.882885 6.637419

 41 H 4.121647 2.934686 5.577916 6.882885 6.637419

 42 H 4.442596 3.530147 5.239093 7.022513 6.478382

 43 H 5.399682 6.507534 3.068110 4.121647 2.934686

 44 H 5.399682 6.507534 3.068110 4.121647 2.934686

 45 H 6.371241 7.603396 4.131190 4.442596 3.530147

 21 22 23 24 25

 21 C 0.000000

 22 C 1.355311 0.000000

 23 C 2.282646 1.471006 0.000000

 24 N 3.566785 2.491030 1.339451 0.000000

 25 Zn 4.264519 4.250077 3.001596 3.370157 0.000000

 26 C 9.839089 9.598912 8.162189 7.776164 5.596278

 27 H 9.275908 9.456734 8.207311 8.309046 5.218707

 28 C 6.567290 5.341723 4.406339 3.068473 5.596278

 29 H 7.976015 7.056229 5.709108 4.580159 5.218707

 30 C 7.475267 8.380272 7.825599 8.714187 5.596278

 31 H 5.217781 6.387937 6.316252 7.497190 5.218707

 32 C 1.483660 2.573687 3.746262 4.988372 5.596278

 33 H 2.190793 1.079953 2.264729 2.854028 5.218707

 34 H 10.664087 10.510687 9.096417 8.785247 6.399716

 35 H 10.017786 9.691053 8.242014 7.754855 5.853845

 36 H 10.017786 9.691053 8.242014 7.754855 5.853845

 37 H 6.366103 5.103275 4.335145 3.068110 5.853845

 38 H 6.366103 5.103275 4.335145 3.068110 5.853845

 39 H 7.652062 6.431774 5.470592 4.131190 6.399716

 40 H 8.023714 8.866674 8.231688 9.046415 5.853845

 41 H 8.023714 8.866674 8.231688 9.046415 5.853845

 42 H 7.728579 8.756217 8.366870 9.357453 6.399716

 43 H 2.133359 3.277929 4.315479 5.577916 5.853845

 44 H 2.133359 3.277929 4.315479 5.577916 5.853845

 45 H 2.135940 2.750365 4.145731 5.239093 6.399716

 26 27 28 29 30

 26 C 0.000000

 27 H 2.985478 0.000000

 28 C 7.914333 9.451844 0.000000

 29 H 5.269641 7.380366 2.985478 0.000000

 30 C 7.914333 5.269641 11.192557 10.401605 0.000000

 31 H 9.451844 7.380366 10.401605 10.437414 2.985478

 32 C 11.192557 10.401605 7.914333 9.451844 7.914333

 33 H 10.401605 10.437414 5.269641 7.380366 9.451844

 34 H 1.090087 2.743908 9.004220 6.342669 7.967021

 35 H 1.094033 3.737664 7.646656 4.921260 8.526448

 36 H 1.094033 3.737664 7.646656 4.921260 8.526448

 37 H 8.526448 9.939115 1.094033 3.737664 11.400647

 38 H 8.526448 9.939115 1.094033 3.737664 11.400647

 39 H 7.967021 9.805768 1.090087 2.743908 11.973350

 40 H 7.646656 4.921260 11.400647 10.441967 1.094033

 41 H 7.646656 4.921260 11.400647 10.441967 1.094033

 42 H 9.004220 6.342669 11.973350 11.351366 1.090087

 43 H 11.400647 10.441967 8.526448 9.939115 7.646656

 44 H 11.400647 10.441967 8.526448 9.939115 7.646656

 45 H 11.973350 11.351366 7.967021 9.805768 9.004220

 31 32 33 34 35

 31 H 0.000000

 32 C 5.269641 0.000000

 33 H 7.380366 2.985478 0.000000

 34 H 9.805768 11.973350 11.351366 0.000000

 35 H 9.939115 11.400647 10.441967 1.774400 0.000000

 36 H 9.939115 11.400647 10.441967 1.774400 1.753117

 37 H 10.441967 7.646656 4.921260 9.609662 8.185249

 38 H 10.441967 7.646656 4.921260 9.609662 8.370885

 39 H 11.351366 9.004220 6.342669 9.050566 7.622476

 40 H 3.737664 8.526448 9.939115 7.622476 8.185249

 41 H 3.737664 8.526448 9.939115 7.622476 8.370885

 42 H 2.743908 7.967021 9.805768 9.050566 9.609662

 43 H 4.921260 1.094033 3.737664 12.136690 11.575690

 44 H 4.921260 1.094033 3.737664 12.136690 11.707690

 45 H 6.342669 1.090087 2.743908 12.799433 12.136690

 36 37 38 39 40

 36 H 0.000000

 37 H 8.370885 0.000000

 38 H 8.185249 1.753117 0.000000

 39 H 7.622476 1.774400 1.774400 0.000000

 40 H 8.370885 11.575690 11.707690 12.136690 0.000000

 41 H 8.185249 11.707690 11.575690 12.136690 1.753117

 42 H 9.609662 12.136690 12.136690 12.799433 1.774400

 43 H 11.707690 8.185249 8.370885 9.609662 8.185249

 44 H 11.575690 8.370885 8.185249 9.609662 8.370885

 45 H 12.136690 7.622476 7.622476 9.050566 9.609662

 41 42 43 44 45

 41 H 0.000000

 42 H 1.774400 0.000000

 43 H 8.370885 7.622476 0.000000

 44 H 8.185249 7.622476 1.753117 0.000000

 45 H 9.609662 9.050566 1.774400 1.774400 0.000000

 Stoichiometry C20H16N8Zn(1+,2)

 Framework group C4H[O(Zn),SGH(C20H8N8),X(H8)]

 Deg. of freedom 20

 Full point group C4H NOp 8

 RotChk: IX=0 Diff= 1.16D-03

 Largest Abelian subgroup C2H NOp 4

 Largest concise Abelian subgroup C2H NOp 4

 Standard orientation:

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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

 1 6 0 -2.181320 2.061897 0.000000

 2 7 0 -1.856963 0.741298 0.000000

 3 6 0 -2.989007 0.000000 0.000000

 4 6 0 -4.162350 0.927881 0.000000

 5 6 0 -3.647450 2.181573 0.000000

 6 7 0 -3.096410 -1.330490 0.000000

 7 6 0 -2.061897 -2.181320 0.000000

 8 7 0 -0.741298 -1.856963 0.000000

 9 6 0 0.000000 -2.989007 0.000000

 10 6 0 -0.927881 -4.162350 0.000000

 11 6 0 -2.181573 -3.647450 0.000000

 12 7 0 -1.330490 3.096410 0.000000

 13 6 0 0.927881 4.162350 0.000000

 14 6 0 2.181573 3.647450 0.000000

 15 6 0 2.061897 2.181320 0.000000

 16 7 0 0.741298 1.856963 0.000000

 17 6 0 0.000000 2.989007 0.000000

 18 7 0 3.096410 1.330490 0.000000

 19 7 0 1.856963 -0.741298 0.000000

 20 6 0 2.989007 0.000000 0.000000

 21 6 0 4.162350 -0.927881 0.000000

 22 6 0 3.647450 -2.181573 0.000000

 23 6 0 2.181320 -2.061897 0.000000

 24 7 0 1.330490 -3.096410 0.000000

 25 30 0 0.000000 0.000000 0.000000

 26 6 0 -5.575897 0.477180 0.000000

 27 1 0 -4.184432 3.118562 0.000000

 28 6 0 -0.477180 -5.575897 0.000000

 29 1 0 -3.118562 -4.184432 0.000000

 30 6 0 0.477180 5.575897 0.000000

 31 1 0 3.118562 4.184432 0.000000

 32 6 0 5.575897 -0.477180 0.000000

 33 1 0 4.184432 -3.118562 0.000000

 34 1 0 -6.261042 1.325039 0.000000

 35 1 0 -5.786083 -0.142801 0.876559

 36 1 0 -5.786083 -0.142801 -0.876559

 37 1 0 0.142801 -5.786083 0.876559

 38 1 0 0.142801 -5.786083 -0.876559

 39 1 0 -1.325039 -6.261042 0.000000

 40 1 0 -0.142801 5.786083 0.876559

 41 1 0 -0.142801 5.786083 -0.876559

 42 1 0 1.325039 6.261042 0.000000

 43 1 0 5.786083 0.142801 0.876559

 44 1 0 5.786083 0.142801 -0.876559

 45 1 0 6.261042 -1.325039 0.000000

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 Rotational constants (GHZ): 0.1830408 0.1830408 0.0917262

 Leave Link 202 at Fri Jul 5 21:10:25 2019, MaxMem= 1342177280 cpu: 0.2

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

 Basis read from rwf: (5D, 7F)

 Pseudo-potential data read from rwf file.

 There are 229 symmetry adapted cartesian basis functions of AG symmetry.

 There are 82 symmetry adapted cartesian basis functions of BG symmetry.

 There are 78 symmetry adapted cartesian basis functions of AU symmetry.

 There are 218 symmetry adapted cartesian basis functions of BU symmetry.

 There are 212 symmetry adapted basis functions of AG symmetry.

 There are 82 symmetry adapted basis functions of BG symmetry.

 There are 78 symmetry adapted basis functions of AU symmetry.

 There are 204 symmetry adapted basis functions of BU symmetry.

 576 basis functions, 1015 primitive gaussians, 607 cartesian basis functions

 102 alpha electrons 101 beta electrons

 nuclear repulsion energy 2766.8948892811 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= 45 NActive= 45 NUniq= 11 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= -0.1142324257 Hartrees.

 Nuclear repulsion after empirical dispersion term = 2766.7806568554 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= 45.

 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 = 45

 GePol: Total number of spheres = 45

 GePol: Number of exposed spheres = 45 (100.00%)

 GePol: Number of points = 3542

 GePol: Average weight of points = 0.11

 GePol: Minimum weight of points = 0.43D-11

 GePol: Maximum weight of points = 0.18390

 GePol: Number of points with low weight = 164

 GePol: Fraction of low-weight points (<1% of avg) = 4.63%

 GePol: Cavity surface area = 381.984 Ang\*\*2

 GePol: Cavity volume = 378.927 Ang\*\*3

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

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 PCM non-electrostatic energy = -0.0110740564 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 2766.7695827990 Hartrees.

 Leave Link 301 at Fri Jul 5 21:10:25 2019, MaxMem= 1342177280 cpu: 1.0

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

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

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

 One-electron integrals computed using PRISM.

 One-electron integral symmetry used in STVInt

 8 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15383 LenP2D= 41368.

 LDataN: DoStor=T MaxTD1= 5 Len= 102

 NBasis= 576 RedAO= T EigKep= 1.85D-04 NBF= 212 82 78 204

 NBsUse= 576 1.00D-06 EigRej= -1.00D+00 NBFU= 212 82 78 204

 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= 594 594 594 594 594 MxSgAt= 45 MxSgA2= 45.

 Leave Link 302 at Fri Jul 5 21:10:25 2019, MaxMem= 1342177280 cpu: 7.7

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

 DipDrv: MaxL=1.

 Leave Link 303 at Fri Jul 5 21:10:26 2019, MaxMem= 1342177280 cpu: 0.8

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

 Initial guess from the checkpoint file: "ZntAzPcation.chk"

 B after Tr= 0.000000 0.000000 0.000000

 Rot= 1.000000 0.000000 0.000000 -0.000135 Ang= -0.02 deg.

 Guess basis will be translated and rotated to current coordinates.

 JPrj=2 DoOrth=T DoCkMO=T.

 Initial guess orbital symmetries:

 Alpha Orbitals:

 Occupied (BG) (EU) (EU) (AG) (EU) (EU) (BG) (AG) (BG) (EU)

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 (AG) (EU) (EU) (AG) (BG) (AU) (EG) (EG) (AG) (EU)

 (EU) (BU) (BG) (AU) (EG) (EG) (BG) (AG) (BU) (EU)

 (EU) (BU) (AG) (EU) (EU) (BG) (AG) (EU) (EU) (EG)

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 (BU) (AU)

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

 Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7819 S= 0.5158

 Leave Link 401 at Fri Jul 5 21:10:27 2019, MaxMem= 1342177280 cpu: 21.7

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

 UHF open shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 1138797 IEndB= 1138797 NGot= 1342177280 MDV= 1341424180

 LenX= 1341424180 LenY= 1341055124

 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= 670000000 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= 37637292.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 7.99D-15 for 2086.

 Iteration 1 A\*A^-1 deviation from orthogonality is 3.20D-15 for 3536 2658.

 Iteration 1 A^-1\*A deviation from unit magnitude is 6.22D-15 for 1785.

 Iteration 1 A^-1\*A deviation from orthogonality is 3.67D-09 for 918 847.

 Iteration 2 A\*A^-1 deviation from unit magnitude is 2.89D-15 for 676.

 Iteration 2 A\*A^-1 deviation from orthogonality is 4.22D-15 for 1508 516.

 Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 58.

 Iteration 2 A^-1\*A deviation from orthogonality is 3.27D-16 for 1743 735.

 E= -1275.69927337364

 DIIS: error= 4.57D-04 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -1275.69927337364 IErMin= 1 ErrMin= 4.57D-04

 ErrMax= 4.57D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.68D-04 BMatP= 5.68D-04

 IDIUse=3 WtCom= 9.95D-01 WtEn= 4.57D-03

 Coeff-Com: 0.100D+01

 Coeff-En: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.372 Goal= None Shift= 0.000

 Gap= 0.406 Goal= None Shift= 0.000

 RMSDP=3.24D-05 MaxDP=7.63D-04 OVMax= 2.64D-03

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 3.23D-05 CP: 1.00D+00

 E= -1275.69947027645 Delta-E= -0.000196902809 Rises=F Damp=F

 DIIS: error= 1.77D-04 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -1275.69947027645 IErMin= 2 ErrMin= 1.77D-04

 ErrMax= 1.77D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.86D-05 BMatP= 5.68D-04

 IDIUse=3 WtCom= 9.98D-01 WtEn= 1.77D-03

 Coeff-Com: 0.706D-01 0.929D+00

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

 Coeff: 0.705D-01 0.930D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=1.00D-05 MaxDP=5.36D-04 DE=-1.97D-04 OVMax= 1.38D-03

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 9.97D-06 CP: 1.00D+00 9.99D-01

 E= -1275.69945947479 Delta-E= 0.000010801666 Rises=F Damp=F

 DIIS: error= 3.07D-04 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 2 EnMin= -1275.69947027645 IErMin= 2 ErrMin= 1.77D-04

 ErrMax= 3.07D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-04 BMatP= 4.86D-05

 IDIUse=3 WtCom= 3.63D-01 WtEn= 6.37D-01

 Coeff-Com: -0.278D-01 0.612D+00 0.416D+00

 Coeff-En: 0.000D+00 0.648D+00 0.352D+00

 Coeff: -0.101D-01 0.635D+00 0.375D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=5.92D-06 MaxDP=3.18D-04 DE= 1.08D-05 OVMax= 9.30D-04

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 2.07D-06 CP: 1.00D+00 1.03D+00 4.56D-01

 E= -1275.69948101980 Delta-E= -0.000021545016 Rises=F Damp=F

 DIIS: error= 2.47D-05 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -1275.69948101980 IErMin= 4 ErrMin= 2.47D-05

 ErrMax= 2.47D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.41D-07 BMatP= 4.86D-05

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

 Coeff-Com: -0.132D-01 0.199D+00 0.110D+00 0.704D+00

 Coeff: -0.132D-01 0.199D+00 0.110D+00 0.704D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

 RMSDP=7.58D-07 MaxDP=3.58D-05 DE=-2.15D-05 OVMax= 1.55D-04

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 7.11D-07 CP: 1.00D+00 1.04D+00 4.45D-01 9.91D-01

 E= -1275.69948114588 Delta-E= -0.000000126081 Rises=F Damp=F

 DIIS: error= 1.29D-05 at cycle 5 NSaved= 5.

 NSaved= 5 IEnMin= 5 EnMin= -1275.69948114588 IErMin= 5 ErrMin= 1.29D-05

 ErrMax= 1.29D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.54D-07 BMatP= 7.41D-07

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

 Coeff-Com: -0.351D-02 0.358D-01 0.130D-01 0.395D+00 0.560D+00

 Coeff: -0.351D-02 0.358D-01 0.130D-01 0.395D+00 0.560D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=3.78D-07 MaxDP=1.94D-05 DE=-1.26D-07 OVMax= 1.19D-04

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 3.17D-07 CP: 1.00D+00 1.04D+00 4.43D-01 1.06D+00 7.88D-01

 E= -1275.69948120125 Delta-E= -0.000000055368 Rises=F Damp=F

 DIIS: error= 3.63D-06 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -1275.69948120125 IErMin= 6 ErrMin= 3.63D-06

 ErrMax= 3.63D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.04D-08 BMatP= 2.54D-07

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

 Coeff-Com: -0.759D-03 0.840D-03-0.426D-03 0.124D+00 0.276D+00 0.600D+00

 Coeff: -0.759D-03 0.840D-03-0.426D-03 0.124D+00 0.276D+00 0.600D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

 RMSDP=1.61D-07 MaxDP=6.30D-06 DE=-5.54D-08 OVMax= 6.10D-05

 Cycle 7 Pass 1 IDiag 1:

 RMSU= 1.32D-07 CP: 1.00D+00 1.04D+00 4.45D-01 1.08D+00 8.75D-01

 CP: 9.27D-01

 E= -1275.69948120888 Delta-E= -0.000000007627 Rises=F Damp=F

 DIIS: error= 2.51D-06 at cycle 7 NSaved= 7.

 NSaved= 7 IEnMin= 7 EnMin= -1275.69948120888 IErMin= 7 ErrMin= 2.51D-06

 ErrMax= 2.51D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.64D-09 BMatP= 2.04D-08

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

 Coeff-Com: 0.496D-03-0.877D-02-0.252D-02-0.276D-01 0.241D-01 0.319D+00

 Coeff-Com: 0.696D+00

 Coeff: 0.496D-03-0.877D-02-0.252D-02-0.276D-01 0.241D-01 0.319D+00

 Coeff: 0.696D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=1.09D-07 MaxDP=5.54D-06 DE=-7.63D-09 OVMax= 5.16D-05

 Cycle 8 Pass 1 IDiag 1:

 RMSU= 6.68D-08 CP: 1.00D+00 1.04D+00 4.47D-01 1.10D+00 9.30D-01

 CP: 1.14D+00 1.19D+00

 E= -1275.69948121270 Delta-E= -0.000000003824 Rises=F Damp=F

 DIIS: error= 1.47D-06 at cycle 8 NSaved= 8.

 NSaved= 8 IEnMin= 8 EnMin= -1275.69948121270 IErMin= 8 ErrMin= 1.47D-06

 ErrMax= 1.47D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.87D-10 BMatP= 4.64D-09

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

 Coeff-Com: 0.119D-03 0.400D-03 0.938D-03-0.274D-01-0.596D-01-0.151D+00

 Coeff-Com: -0.107D-01 0.125D+01

 Coeff: 0.119D-03 0.400D-03 0.938D-03-0.274D-01-0.596D-01-0.151D+00

 Coeff: -0.107D-01 0.125D+01

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=1.10D-07 MaxDP=6.66D-06 DE=-3.82D-09 OVMax= 5.76D-05

 Cycle 9 Pass 1 IDiag 1:

 RMSU= 3.43D-08 CP: 1.00D+00 1.04D+00 4.48D-01 1.11D+00 9.76D-01

 CP: 1.30D+00 1.69D+00 1.67D+00

 E= -1275.69948121477 Delta-E= -0.000000002063 Rises=F Damp=F

 DIIS: error= 1.16D-06 at cycle 9 NSaved= 9.

 NSaved= 9 IEnMin= 9 EnMin= -1275.69948121477 IErMin= 9 ErrMin= 1.16D-06

 ErrMax= 1.16D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.44D-10 BMatP= 7.87D-10

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

 Coeff-Com: -0.948D-04 0.359D-02 0.138D-02-0.820D-02-0.506D-01-0.227D+00

 Coeff-Com: -0.300D+00 0.825D+00 0.756D+00

 Coeff: -0.948D-04 0.359D-02 0.138D-02-0.820D-02-0.506D-01-0.227D+00

 Coeff: -0.300D+00 0.825D+00 0.756D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=7.08D-08 MaxDP=4.38D-06 DE=-2.06D-09 OVMax= 3.24D-05

 Cycle 10 Pass 1 IDiag 1:

 RMSU= 2.26D-08 CP: 1.00D+00 1.04D+00 4.48D-01 1.11D+00 1.00D+00

 CP: 1.40D+00 1.99D+00 2.21D+00 1.31D+00

 E= -1275.69948121529 Delta-E= -0.000000000522 Rises=F Damp=F

 DIIS: error= 5.80D-07 at cycle 10 NSaved= 10.

 NSaved=10 IEnMin=10 EnMin= -1275.69948121529 IErMin=10 ErrMin= 5.80D-07

 ErrMax= 5.80D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.23D-10 BMatP= 5.44D-10

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

 Coeff-Com: -0.894D-04 0.174D-02 0.244D-03 0.663D-02-0.276D-02-0.514D-01

 Coeff-Com: -0.141D+00 0.351D-01 0.386D+00 0.765D+00

 Coeff: -0.894D-04 0.174D-02 0.244D-03 0.663D-02-0.276D-02-0.514D-01

 Coeff: -0.141D+00 0.351D-01 0.386D+00 0.765D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 21319 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

 RMSDP=2.37D-08 MaxDP=1.64D-06 DE=-5.22D-10 OVMax= 1.12D-05

 Cycle 11 Pass 1 IDiag 1:

 RMSU= 1.12D-08 CP: 1.00D+00 1.04D+00 4.48D-01 1.11D+00 1.01D+00

 CP: 1.42D+00 2.06D+00 2.41D+00 1.62D+00 1.10D+00

 E= -1275.69948121544 Delta-E= -0.000000000151 Rises=F Damp=F

 DIIS: error= 1.61D-07 at cycle 11 NSaved= 11.

 NSaved=11 IEnMin=11 EnMin= -1275.69948121544 IErMin=11 ErrMin= 1.61D-07

 ErrMax= 1.61D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.38D-11 BMatP= 1.23D-10

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

 Coeff-Com: -0.252D-04 0.347D-04-0.250D-03 0.510D-02 0.936D-02 0.273D-01

 Coeff-Com: -0.319D-02-0.186D+00 0.242D-01 0.366D+00 0.758D+00

 Coeff: -0.252D-04 0.347D-04-0.250D-03 0.510D-02 0.936D-02 0.273D-01

 Coeff: -0.319D-02-0.186D+00 0.242D-01 0.366D+00 0.758D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=1.17D-08 MaxDP=7.40D-07 DE=-1.51D-10 OVMax= 4.04D-06

 Cycle 12 Pass 1 IDiag 1:

 RMSU= 3.84D-09 CP: 1.00D+00 1.04D+00 4.48D-01 1.11D+00 1.01D+00

 CP: 1.43D+00 2.09D+00 2.48D+00 1.81D+00 1.38D+00

 CP: 1.12D+00

 E= -1275.69948121535 Delta-E= 0.000000000087 Rises=F Damp=F

 DIIS: error= 8.56D-08 at cycle 12 NSaved= 12.

 NSaved=12 IEnMin=11 EnMin= -1275.69948121544 IErMin=12 ErrMin= 8.56D-08

 ErrMax= 8.56D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.09D-12 BMatP= 2.38D-11

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

 Coeff-Com: 0.722D-05-0.376D-03-0.170D-03 0.106D-02 0.506D-02 0.247D-01

 Coeff-Com: 0.311D-01-0.949D-01-0.566D-01 0.159D-02 0.308D+00 0.781D+00

 Coeff: 0.722D-05-0.376D-03-0.170D-03 0.106D-02 0.506D-02 0.247D-01

 Coeff: 0.311D-01-0.949D-01-0.566D-01 0.159D-02 0.308D+00 0.781D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

 RMSDP=4.24D-09 MaxDP=1.83D-07 DE= 8.69D-11 OVMax= 3.43D-06

 Error on total polarization charges = 0.06023

 SCF Done: E(UB3LYP) = -1275.69948122 A.U. after 12 cycles

 NFock= 12 Conv=0.42D-08 -V/T= 1.9660

 <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7819 S= 0.5158

 <L.S>= 0.000000000000E+00

 KE= 1.320618023965D+03 PE=-8.557393733877D+03 EE= 3.194306645898D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.95

 (included in total energy above)

 Annihilation of the first spin contaminant:

 S\*\*2 before annihilation 0.7819, after 0.7509

 Leave Link 502 at Fri Jul 5 21:11:43 2019, MaxMem= 1342177280 cpu: 869.5

 (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.

 8 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15383 LenP2D= 41368.

 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 = 248

 Leave Link 701 at Fri Jul 5 21:11:47 2019, MaxMem= 1342177280 cpu: 53.5

 (Enter /apps/gaussian/g09d01/g09/l702.exe)

 L702 exits ... SP integral derivatives will be done elsewhere.

 Leave Link 702 at Fri Jul 5 21:11:47 2019, MaxMem= 1342177280 cpu: 0.2

 (Enter /apps/gaussian/g09d01/g09/l703.exe)

 Compute integral first derivatives, UseDBF=F ICtDFT= 0.

 Integral derivatives from FoFJK, PRISM(SPDF).

 Calling FoFJK, ICntrl= 2127 FMM=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 Fri Jul 5 21:11:55 2019, MaxMem= 1342177280 cpu: 92.4

 (Enter /apps/gaussian/g09d01/g09/l716.exe)

 Dipole = 1.59872116D-13 3.20188320D-13-6.66133815D-16

 \*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

 Center Atomic Forces (Hartrees/Bohr)

 Number Number X Y Z

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

 1 6 -0.000374068 -0.000168097 0.000000000

 2 7 -0.000004292 -0.000609469 0.000000000

 3 6 0.000255950 0.000759312 0.000000000

 4 6 -0.000726389 -0.000652617 0.000000000

 5 6 0.000189040 0.000241380 0.000000000

 6 7 0.000047361 0.000141149 0.000000000

 7 6 0.000168097 -0.000374068 0.000000000

 8 7 0.000609469 -0.000004292 0.000000000

 9 6 -0.000759312 0.000255950 0.000000000

 10 6 0.000652617 -0.000726389 0.000000000

 11 6 -0.000241380 0.000189040 0.000000000

 12 7 0.000141149 -0.000047361 0.000000000

 13 6 -0.000652617 0.000726389 0.000000000

 14 6 0.000241380 -0.000189040 0.000000000

 15 6 -0.000168097 0.000374068 0.000000000

 16 7 -0.000609469 0.000004292 0.000000000

 17 6 0.000759312 -0.000255950 0.000000000

 18 7 -0.000047361 -0.000141149 0.000000000

 19 7 0.000004292 0.000609469 0.000000000

 20 6 -0.000255950 -0.000759312 0.000000000

 21 6 0.000726389 0.000652617 0.000000000

 22 6 -0.000189040 -0.000241380 0.000000000

 23 6 0.000374068 0.000168097 0.000000000

 24 7 -0.000141149 0.000047361 0.000000000

 25 30 0.000000000 0.000000000 0.000000000

 26 6 0.000086281 0.000257548 0.000000000

 27 1 -0.000329970 0.000114263 0.000000000

 28 6 -0.000257548 0.000086281 0.000000000

 29 1 -0.000114263 -0.000329970 0.000000000

 30 6 0.000257548 -0.000086281 0.000000000

 31 1 0.000114263 0.000329970 0.000000000

 32 6 -0.000086281 -0.000257548 0.000000000

 33 1 0.000329970 -0.000114263 0.000000000

 34 1 -0.000115795 -0.000187393 0.000000000

 35 1 0.000157712 -0.000035209 0.000276027

 36 1 0.000157712 -0.000035209 -0.000276027

 37 1 0.000035209 0.000157712 0.000276027

 38 1 0.000035209 0.000157712 -0.000276027

 39 1 0.000187393 -0.000115795 0.000000000

 40 1 -0.000035209 -0.000157712 0.000276027

 41 1 -0.000035209 -0.000157712 -0.000276027

 42 1 -0.000187393 0.000115795 0.000000000

 43 1 -0.000157712 0.000035209 0.000276027

 44 1 -0.000157712 0.000035209 -0.000276027

 45 1 0.000115795 0.000187393 0.000000000

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

 Cartesian Forces: Max 0.000759312 RMS 0.000282857

 Leave Link 716 at Fri Jul 5 21:11:55 2019, MaxMem= 1342177280 cpu: 0.3

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

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Berny optimization.

 Using GEDIIS/GDIIS optimizer.

 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

 Internal Forces: Max 0.000737236 RMS 0.000178142

 Search for a local minimum.

 Step number 3 out of a maximum of 270

 All quantities printed in internal units (Hartrees-Bohrs-Radians)

 RMS Force = .17814D-03 SwitMx=.10000D-02 MixMth= 2

 Mixed Optimization -- En-DIIS/RFO-DIIS

 Swapping is turned off.

 Update second derivatives using D2CorX and points 1 2 3

 DE= -2.59D-04 DEPred=-2.23D-04 R= 1.16D+00

 TightC=F SS= 1.41D+00 RLast= 4.76D-02 DXNew= 5.5297D-01 1.4279D-01

 Trust test= 1.16D+00 RLast= 4.76D-02 DXMaxT set to 3.29D-01

 ITU= 1 1 0

 Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01340

 Eigenvalues --- 0.01343 0.01343 0.01343 0.01600 0.01618

 Eigenvalues --- 0.01631 0.01631 0.01776 0.01791 0.01817

 Eigenvalues --- 0.01817 0.01890 0.01906 0.01943 0.01943

 Eigenvalues --- 0.01998 0.01998 0.02045 0.02045 0.02070

 Eigenvalues --- 0.02087 0.02101 0.02112 0.02112 0.02205

 Eigenvalues --- 0.02316 0.02316 0.02352 0.02373 0.07189

 Eigenvalues --- 0.07222 0.07222 0.07222 0.07222 0.07393

 Eigenvalues --- 0.07393 0.07393 0.14163 0.14501 0.14501

 Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

 Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

 Eigenvalues --- 0.16000 0.16000 0.16000 0.16001 0.16087

 Eigenvalues --- 0.16517 0.18229 0.20271 0.22082 0.22082

 Eigenvalues --- 0.23812 0.23848 0.23848 0.24090 0.25000

 Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

 Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25005

 Eigenvalues --- 0.25827 0.31253 0.33173 0.33173 0.33215

 Eigenvalues --- 0.33282 0.33282 0.33282 0.33416 0.33724

 Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

 Eigenvalues --- 0.33724 0.34275 0.34437 0.34437 0.34437

 Eigenvalues --- 0.34536 0.35253 0.35377 0.35572 0.35572

 Eigenvalues --- 0.35682 0.35682 0.35682 0.36194 0.39286

 Eigenvalues --- 0.41750 0.41750 0.43818 0.47331 0.48967

 Eigenvalues --- 0.48967 0.49690 0.50264 0.50565 0.51356

 Eigenvalues --- 0.51356 0.53616 0.53986 0.53986 0.54931

 Eigenvalues --- 0.56276 0.56330 0.56330 0.56626

 En-DIIS/RFO-DIIS IScMMF= 0 using points: 3 2

 RFO step: Lambda=-1.99435033D-05.

 NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 2.59D-04 SmlDif= 1.00D-05

 RMS Error= 0.4057630061D-03 NUsed= 2 EDIIS=F

 DidBck=F Rises=F RFO-DIIS coefs: 1.25704 -0.25704

 Iteration 1 RMS(Cart)= 0.00277940 RMS(Int)= 0.00000457

 Iteration 2 RMS(Cart)= 0.00000778 RMS(Int)= 0.00000047

 Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000047

 ITry= 1 IFail=0 DXMaxC= 9.19D-03 DCOld= 1.00D+10 DXMaxT= 3.29D-01 DXLimC= 3.00D+00 Rises=F

 ClnCor: largest displacement from symmetrization is 1.96D-10 for atom 33.

 Variable Old X -DE/DX Delta X Delta X Delta X New X

 (Linear) (Quad) (Total)

 R1 2.56974 0.00012 -0.00023 0.00018 -0.00005 2.56969

 R2 2.77980 -0.00003 0.00115 -0.00054 0.00061 2.78041

 R3 2.53120 -0.00009 -0.00026 -0.00003 -0.00029 2.53091

 R4 2.55710 -0.00034 -0.00095 -0.00060 -0.00154 2.55556

 R5 3.77843 0.00036 0.00152 0.00038 0.00190 3.78033

 R6 2.82683 0.00058 0.00278 0.00068 0.00346 2.83029

 R7 2.52244 0.00015 -0.00048 0.00056 0.00007 2.52251

 R8 2.56117 0.00028 -0.00101 0.00093 -0.00008 2.56108

 R9 2.80371 0.00013 -0.00042 0.00040 -0.00002 2.80369

 R10 2.04081 0.00022 -0.00009 0.00068 0.00059 2.04141

 R11 2.53120 -0.00009 -0.00026 -0.00003 -0.00029 2.53091

 R12 2.56974 0.00012 -0.00023 0.00018 -0.00005 2.56969

 R13 2.77980 -0.00003 0.00115 -0.00054 0.00061 2.78041

 R14 2.55710 -0.00034 -0.00095 -0.00060 -0.00154 2.55556

 R15 3.77843 0.00036 0.00152 0.00038 0.00190 3.78033

 R16 2.82683 0.00058 0.00278 0.00068 0.00346 2.83029

 R17 2.52244 0.00015 -0.00048 0.00056 0.00007 2.52251

 R18 2.56117 0.00028 -0.00101 0.00093 -0.00008 2.56108

 R19 2.80371 0.00013 -0.00042 0.00040 -0.00002 2.80369

 R20 2.04081 0.00022 -0.00009 0.00068 0.00059 2.04141

 R21 2.52244 0.00015 -0.00048 0.00056 0.00007 2.52251

 R22 2.56117 0.00028 -0.00101 0.00093 -0.00008 2.56108

 R23 2.82683 0.00058 0.00278 0.00068 0.00346 2.83029

 R24 2.80371 0.00013 -0.00042 0.00040 -0.00002 2.80369

 R25 2.77980 -0.00003 0.00115 -0.00054 0.00061 2.78041

 R26 2.04081 0.00022 -0.00009 0.00068 0.00059 2.04141

 R27 2.56974 0.00012 -0.00023 0.00018 -0.00005 2.56969

 R28 2.53120 -0.00009 -0.00026 -0.00003 -0.00029 2.53091

 R29 2.55710 -0.00034 -0.00095 -0.00060 -0.00154 2.55556

 R30 3.77843 0.00036 0.00152 0.00038 0.00190 3.78033

 R31 2.52244 0.00015 -0.00048 0.00056 0.00007 2.52251

 R32 2.55710 -0.00034 -0.00095 -0.00060 -0.00154 2.55556

 R33 2.56974 0.00012 -0.00023 0.00018 -0.00005 2.56969

 R34 3.77843 0.00036 0.00152 0.00038 0.00190 3.78033

 R35 2.82683 0.00058 0.00278 0.00068 0.00346 2.83029

 R36 2.56117 0.00028 -0.00101 0.00093 -0.00008 2.56108

 R37 2.80371 0.00013 -0.00042 0.00040 -0.00002 2.80369

 R38 2.77980 -0.00003 0.00115 -0.00054 0.00061 2.78041

 R39 2.04081 0.00022 -0.00009 0.00068 0.00059 2.04141

 R40 2.53120 -0.00009 -0.00026 -0.00003 -0.00029 2.53091

 R41 2.05996 0.00019 -0.00017 0.00064 0.00046 2.06043

 R42 2.06742 0.00033 -0.00013 0.00101 0.00088 2.06830

 R43 2.06742 0.00033 -0.00013 0.00101 0.00088 2.06830

 R44 2.06742 0.00033 -0.00013 0.00101 0.00088 2.06830

 R45 2.06742 0.00033 -0.00013 0.00101 0.00088 2.06830

 R46 2.05996 0.00019 -0.00017 0.00064 0.00046 2.06043

 R47 2.06742 0.00033 -0.00013 0.00101 0.00088 2.06830

 R48 2.06742 0.00033 -0.00013 0.00101 0.00088 2.06830

 R49 2.05996 0.00019 -0.00017 0.00064 0.00046 2.06043

 R50 2.06742 0.00033 -0.00013 0.00101 0.00088 2.06830

 R51 2.06742 0.00033 -0.00013 0.00101 0.00088 2.06830

 R52 2.05996 0.00019 -0.00017 0.00064 0.00046 2.06043

 A1 1.89309 0.00007 -0.00084 0.00086 0.00002 1.89311

 A2 2.21247 -0.00017 0.00032 -0.00109 -0.00077 2.21170

 A3 2.17763 0.00010 0.00052 0.00023 0.00075 2.17838

 A4 1.90971 0.00012 0.00137 -0.00043 0.00094 1.91066

 A5 2.19146 0.00000 -0.00037 0.00042 0.00004 2.19150

 A6 2.18201 -0.00012 -0.00100 0.00001 -0.00098 2.18103

 A7 1.89272 -0.00003 -0.00089 0.00030 -0.00059 1.89214

 A8 2.23111 0.00012 0.00144 -0.00040 0.00104 2.23215

 A9 2.15935 -0.00010 -0.00055 0.00010 -0.00045 2.15890

 A10 1.85020 -0.00012 -0.00024 -0.00019 -0.00043 1.84977

 A11 2.16383 -0.00061 -0.00199 -0.00178 -0.00377 2.16006

 A12 2.26915 0.00074 0.00223 0.00197 0.00420 2.27335

 A13 1.87905 -0.00004 0.00060 -0.00054 0.00005 1.87911

 A14 2.17264 -0.00022 -0.00145 -0.00075 -0.00219 2.17045

 A15 2.23149 0.00026 0.00085 0.00129 0.00214 2.23363

 A16 2.17852 0.00017 -0.00039 0.00106 0.00068 2.17920

 A17 2.21247 -0.00017 0.00032 -0.00109 -0.00077 2.21170

 A18 2.17763 0.00010 0.00052 0.00023 0.00075 2.17838

 A19 1.89309 0.00007 -0.00084 0.00086 0.00002 1.89311

 A20 1.90971 0.00012 0.00137 -0.00043 0.00094 1.91066

 A21 2.19146 0.00000 -0.00037 0.00042 0.00004 2.19150

 A22 2.18201 -0.00012 -0.00100 0.00001 -0.00098 2.18103

 A23 1.89272 -0.00003 -0.00089 0.00030 -0.00059 1.89214

 A24 2.23111 0.00012 0.00144 -0.00040 0.00104 2.23215

 A25 2.15935 -0.00010 -0.00055 0.00010 -0.00045 2.15890

 A26 1.85020 -0.00012 -0.00024 -0.00019 -0.00043 1.84977

 A27 2.16383 -0.00061 -0.00199 -0.00178 -0.00377 2.16006

 A28 2.26915 0.00074 0.00223 0.00197 0.00420 2.27335

 A29 1.87905 -0.00004 0.00060 -0.00054 0.00005 1.87911

 A30 2.17264 -0.00022 -0.00145 -0.00075 -0.00219 2.17045

 A31 2.23149 0.00026 0.00085 0.00129 0.00214 2.23363

 A32 2.17852 0.00017 -0.00039 0.00106 0.00068 2.17920

 A33 1.85020 -0.00012 -0.00024 -0.00019 -0.00043 1.84977

 A34 2.26915 0.00074 0.00223 0.00197 0.00420 2.27335

 A35 2.16383 -0.00061 -0.00199 -0.00178 -0.00377 2.16006

 A36 1.87905 -0.00004 0.00060 -0.00054 0.00005 1.87911

 A37 2.23149 0.00026 0.00085 0.00129 0.00214 2.23363

 A38 2.17264 -0.00022 -0.00145 -0.00075 -0.00219 2.17045

 A39 1.89309 0.00007 -0.00084 0.00086 0.00002 1.89311

 A40 2.17763 0.00010 0.00052 0.00023 0.00075 2.17838

 A41 2.21247 -0.00017 0.00032 -0.00109 -0.00077 2.21170

 A42 1.90971 0.00012 0.00137 -0.00043 0.00094 1.91066

 A43 2.19146 0.00000 -0.00037 0.00042 0.00004 2.19150

 A44 2.18201 -0.00012 -0.00100 0.00001 -0.00098 2.18103

 A45 2.15935 -0.00010 -0.00055 0.00010 -0.00045 2.15890

 A46 2.23111 0.00012 0.00144 -0.00040 0.00104 2.23215

 A47 1.89272 -0.00003 -0.00089 0.00030 -0.00059 1.89214

 A48 2.17852 0.00017 -0.00039 0.00106 0.00068 2.17920

 A49 1.90971 0.00012 0.00137 -0.00043 0.00094 1.91066

 A50 2.18201 -0.00012 -0.00100 0.00001 -0.00098 2.18103

 A51 2.19146 0.00000 -0.00037 0.00042 0.00004 2.19150

 A52 2.23111 0.00012 0.00144 -0.00040 0.00104 2.23215

 A53 2.15935 -0.00010 -0.00055 0.00010 -0.00045 2.15890

 A54 1.89272 -0.00003 -0.00089 0.00030 -0.00059 1.89214

 A55 1.85020 -0.00012 -0.00024 -0.00019 -0.00043 1.84977

 A56 2.16383 -0.00061 -0.00199 -0.00178 -0.00377 2.16006

 A57 2.26915 0.00074 0.00223 0.00197 0.00420 2.27335

 A58 1.87905 -0.00004 0.00060 -0.00054 0.00005 1.87911

 A59 2.23149 0.00026 0.00085 0.00129 0.00214 2.23363

 A60 2.17264 -0.00022 -0.00145 -0.00075 -0.00219 2.17045

 A61 1.89309 0.00007 -0.00084 0.00086 0.00002 1.89311

 A62 2.21247 -0.00017 0.00032 -0.00109 -0.00077 2.21170

 A63 2.17763 0.00010 0.00052 0.00023 0.00075 2.17838

 A64 2.17852 0.00017 -0.00039 0.00106 0.00068 2.17920

 A65 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

 A66 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

 A67 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

 A68 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

 A69 1.94179 0.00017 0.00057 0.00113 0.00170 1.94349

 A70 1.93391 -0.00007 0.00003 -0.00071 -0.00068 1.93324

 A71 1.93391 -0.00007 0.00003 -0.00071 -0.00068 1.93324

 A72 1.89654 -0.00003 0.00025 -0.00017 0.00008 1.89662

 A73 1.89654 -0.00003 0.00025 -0.00017 0.00008 1.89662

 A74 1.85865 0.00003 -0.00120 0.00062 -0.00058 1.85808

 A75 1.93391 -0.00007 0.00003 -0.00071 -0.00068 1.93324

 A76 1.93391 -0.00007 0.00003 -0.00071 -0.00068 1.93324

 A77 1.94179 0.00017 0.00057 0.00113 0.00170 1.94349

 A78 1.85865 0.00003 -0.00120 0.00062 -0.00058 1.85808

 A79 1.89654 -0.00003 0.00025 -0.00017 0.00008 1.89662

 A80 1.89654 -0.00003 0.00025 -0.00017 0.00008 1.89662

 A81 1.93391 -0.00007 0.00003 -0.00071 -0.00068 1.93324

 A82 1.93391 -0.00007 0.00003 -0.00071 -0.00068 1.93324

 A83 1.94179 0.00017 0.00057 0.00113 0.00170 1.94349

 A84 1.85865 0.00003 -0.00120 0.00062 -0.00058 1.85808

 A85 1.89654 -0.00003 0.00025 -0.00017 0.00008 1.89662

 A86 1.89654 -0.00003 0.00025 -0.00017 0.00008 1.89662

 A87 1.93391 -0.00007 0.00003 -0.00071 -0.00068 1.93324

 A88 1.93391 -0.00007 0.00003 -0.00071 -0.00068 1.93324

 A89 1.94179 0.00017 0.00057 0.00113 0.00170 1.94349

 A90 1.85865 0.00003 -0.00120 0.00062 -0.00058 1.85808

 A91 1.89654 -0.00003 0.00025 -0.00017 0.00008 1.89662

 A92 1.89654 -0.00003 0.00025 -0.00017 0.00008 1.89662

 A93 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 A94 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 A95 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 A96 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D2 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D3 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D4 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D6 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D7 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D9 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D10 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D11 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D12 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D13 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D14 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D15 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D16 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D17 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D18 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D19 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D20 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D21 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D22 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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 D124 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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 D126 -1.02962 0.00003 0.00072 0.00006 0.00079 -1.02884

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 D128 -2.11197 -0.00003 -0.00072 -0.00006 -0.00079 -2.11275

 D129 2.11197 0.00003 0.00072 0.00006 0.00079 2.11275

 D130 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D131 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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 D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D136 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 Item Value Threshold Converged?

 Maximum Force 0.000737 0.000450 NO

 RMS Force 0.000178 0.000300 YES

 Maximum Displacement 0.009191 0.001800 NO

 RMS Displacement 0.002782 0.001200 NO

 Predicted change in Energy=-2.338147D-05

 Lowest energy point so far. Saving SCF results.

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link 103 at Fri Jul 5 21:11:55 2019, MaxMem= 1342177280 cpu: 1.3

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

 Input orientation:

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -2.065782 -2.178940 0.000000

 2 7 0 -0.744697 -1.856686 0.000000

 3 6 0 -0.004578 -2.988525 0.000000

 4 6 0 -0.935041 -4.162161 0.000000

 5 6 0 -2.187838 -3.645198 0.000000

 6 7 0 1.325768 -3.098169 0.000000

 7 6 0 2.178940 -2.065782 0.000000

 8 7 0 1.856686 -0.744697 0.000000

 9 6 0 2.988525 -0.004578 0.000000

 10 6 0 4.162161 -0.935041 0.000000

 11 6 0 3.645198 -2.187838 0.000000

 12 7 0 -3.098169 -1.325768 0.000000

 13 6 0 -4.162161 0.935041 0.000000

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 17 6 0 -2.988525 0.004578 0.000000

 18 7 0 -1.325768 3.098169 0.000000

 19 7 0 0.744697 1.856686 0.000000

 20 6 0 0.004578 2.988525 0.000000

 21 6 0 0.935041 4.162161 0.000000

 22 6 0 2.187838 3.645198 0.000000

 23 6 0 2.065782 2.178940 0.000000

 24 7 0 3.098169 1.325768 0.000000

 25 30 0 0.000000 0.000000 0.000000

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 27 1 0 -3.127131 -4.178773 0.000000

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 31 1 0 -4.178773 3.127131 0.000000

 32 6 0 0.480756 5.574549 0.000000

 33 1 0 3.127131 4.178773 0.000000

 34 1 0 -1.325896 -6.263435 0.000000

 35 1 0 0.140592 -5.782337 0.876742

 36 1 0 0.140592 -5.782337 -0.876742

 37 1 0 5.782337 0.140592 0.876742

 38 1 0 5.782337 0.140592 -0.876742

 39 1 0 6.263435 -1.325896 0.000000

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 41 1 0 -5.782337 -0.140592 -0.876742

 42 1 0 -6.263435 1.325896 0.000000

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 45 1 0 1.325896 6.263435 0.000000

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 Distance matrix (angstroms):

 1 2 3 4 5

 1 C 0.000000

 2 N 1.359821 0.000000

 3 C 2.214496 1.352345 0.000000

 4 C 2.282923 2.313319 1.497726 0.000000

 5 C 1.471329 2.298137 2.279878 1.355267 0.000000

 6 N 3.513915 2.414147 1.334857 2.498668 3.555935

 7 C 4.246231 2.931105 2.370487 3.753889 4.643631

 8 N 4.176459 2.829083 2.915316 4.412800 4.977056

 9 C 5.502170 4.167404 4.226418 5.716631 6.328416

 10 C 6.350949 4.992663 4.645267 6.032891 6.904161

 11 C 5.710987 4.402368 3.736571 4.987639 6.012338

 12 N 1.339300 2.412614 3.512131 3.567106 2.491678

 13 C 3.753889 4.412800 5.716631 6.032891 4.987639

 14 C 4.643631 4.977056 6.328416 6.904161 6.012338

 15 C 4.246231 4.176459 5.502170 6.350949 5.710987

 16 N 2.931105 2.829083 4.167404 4.992663 4.402368

 17 C 2.370487 2.915316 4.226418 4.645267 3.736571

 18 N 5.328743 4.988811 6.228434 7.270836 6.798247

 19 N 4.917832 4.000928 4.902804 6.248843 6.234620

 20 C 5.566785 4.902804 5.977058 7.212156 6.986628

 21 C 7.015305 6.248843 7.212156 8.531796 8.408759

 22 C 7.212065 6.234620 6.986628 8.408759 8.502730

 23 C 6.005077 4.917832 5.566785 7.015305 7.212065

 24 N 6.240944 4.989553 5.314148 6.810591 7.256196

 25 Zn 3.002539 2.000464 2.988529 4.265898 4.251365

 26 C 3.747328 3.727220 2.629499 1.483649 2.576145

 27 H 2.264021 3.326873 3.341710 2.192152 1.080265

 28 C 7.826780 6.467306 6.116826 7.478469 8.382622

 29 H 6.316133 5.084741 4.185647 5.217508 6.387655

 30 C 4.402889 5.365734 6.562050 6.563666 5.337913

 31 H 5.711315 6.052381 7.404401 7.978444 7.058914

 32 C 8.160972 7.531599 8.576817 9.839106 9.598184

 33 H 8.208951 7.170622 7.821622 9.277523 9.458511

 34 H 4.150967 4.444910 3.531418 2.137316 2.756467

 35 H 4.315233 4.118635 2.931746 2.133222 3.279882

 36 H 4.315233 4.118635 2.931746 2.133222 3.279882

 37 H 8.230546 6.881858 6.636900 8.025306 8.867050

 38 H 8.230546 6.881858 6.636900 8.025306 8.867050

 39 H 8.372786 7.028204 6.484776 7.737083 8.763742

 40 H 4.328547 5.393651 6.500916 6.359085 5.096211

 41 H 4.328547 5.393651 6.500916 6.359085 5.096211

 42 H 5.468470 6.370659 7.601810 7.649218 6.428240

 43 H 8.237535 7.712865 8.815623 10.014633 9.687018

 44 H 8.237535 7.712865 8.815623 10.014633 9.687018

 45 H 9.098197 8.379959 9.347135 10.667937 10.513198

 6 7 8 9 10

 6 N 0.000000

 7 C 1.339300 0.000000

 8 N 2.412614 1.359821 0.000000

 9 C 3.512131 2.214496 1.352345 0.000000

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 13 C 6.810591 7.015305 6.248843 7.212156 8.531796

 14 C 7.256196 7.212065 6.234620 6.986628 8.408759

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 19 N 4.988811 4.176459 2.829083 2.915316 4.412800

 20 C 6.228434 5.502170 4.167404 4.226418 5.716631

 21 C 7.270836 6.350949 4.992663 4.645267 6.032891

 22 C 6.798247 5.710987 4.402368 3.736571 4.987639

 23 C 5.328743 4.246231 2.931105 2.370487 3.753889

 24 N 4.765777 3.513915 2.414147 1.334857 2.498668

 25 Zn 3.369913 3.002539 2.000464 2.988529 4.265898

 26 C 3.065288 4.402889 5.365734 6.562050 6.563666

 27 H 4.582141 5.711315 6.052381 7.404401 7.978444

 28 C 4.990289 3.747328 3.727220 2.629499 1.483649

 29 H 2.853152 2.264021 3.326873 3.341710 2.192152

 30 C 7.773229 8.160972 7.531599 8.576817 9.839106

 31 H 8.309894 8.208951 7.170622 7.821622 9.277523

 32 C 8.713787 7.826780 6.467306 6.116826 7.478469

 33 H 7.496586 6.316133 5.084741 4.185647 5.217508

 34 H 4.129192 5.468470 6.370659 7.601810 7.649218

 35 H 3.062365 4.328547 5.393651 6.500916 6.359085

 36 H 3.062365 4.328547 5.393651 6.500916 6.359085

 37 H 5.578464 4.315233 4.118635 2.931746 2.133222

 38 H 5.578464 4.315233 4.118635 2.931746 2.133222

 39 H 5.246094 4.150967 4.444910 3.531418 2.137316

 40 H 7.748619 8.237535 7.712865 8.815623 10.014633

 41 H 7.748619 8.237535 7.712865 8.815623 10.014633

 42 H 8.784552 9.098197 8.379959 9.347135 10.667937

 43 H 9.043356 8.230546 6.881858 6.636900 8.025306

 44 H 9.043356 8.230546 6.881858 6.636900 8.025306

 45 H 9.361604 8.372786 7.028204 6.484776 7.737083

 11 12 13 14 15

 11 C 0.000000

 12 N 6.798247 0.000000

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 17 C 6.986628 1.334857 1.497726 2.279878 2.214496

 18 N 7.256196 4.765777 3.567106 2.491678 1.339300

 19 N 4.977056 4.989553 4.992663 4.402368 2.931105

 20 C 6.328416 5.314148 4.645267 3.736571 2.370487

 21 C 6.904161 6.810591 6.032891 4.987639 3.753889

 22 C 6.012338 7.256196 6.904161 6.012338 4.643631

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 24 N 3.555935 6.739826 7.270836 6.798247 5.328743

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 26 C 5.337913 4.990289 7.478469 8.382622 7.826780

 27 H 7.058914 2.853152 5.217508 6.387655 6.316133

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 34 H 6.428240 5.246094 7.737083 8.763742 8.372786

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 37 H 3.279882 9.043356 10.014633 9.687018 8.237535

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 40 H 9.687018 3.062365 2.133222 3.279882 4.315233

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 42 H 10.513198 4.129192 2.137316 2.756467 4.150967

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 44 H 8.867050 7.748619 6.359085 5.096211 4.328547

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 19 N 2.829083 4.167404 2.414147 0.000000

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 21 C 4.412800 5.716631 2.498668 2.313319 1.497726

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 23 C 4.176459 5.502170 3.513915 1.359821 2.214496

 24 N 4.988811 6.228434 4.765777 2.412614 3.512131

 25 Zn 2.000464 2.988529 3.369913 2.000464 2.988529

 26 C 6.467306 6.116826 8.713787 7.531599 8.576817

 27 H 5.084741 4.185647 7.496586 7.170622 7.821622

 28 C 7.531599 8.576817 7.773229 5.365734 6.562050

 29 H 7.170622 7.821622 8.309894 6.052381 7.404401

 30 C 3.727220 2.629499 4.990289 6.467306 6.116826

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 34 H 7.028204 6.484776 9.361604 8.379959 9.347135

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 41 H 4.118635 2.931746 5.578464 6.881858 6.636900

 42 H 4.444910 3.531418 5.246094 7.028204 6.484776

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 44 H 5.393651 6.500916 3.062365 4.118635 2.931746

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 21 22 23 24 25

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 35 H 10.014633 9.687018 8.237535 7.748619 5.850117

 36 H 10.014633 9.687018 8.237535 7.748619 5.850117

 37 H 6.359085 5.096211 4.328547 3.062365 5.850117

 38 H 6.359085 5.096211 4.328547 3.062365 5.850117

 39 H 7.649218 6.428240 5.468470 4.129192 6.402235

 40 H 8.025306 8.867050 8.230546 9.043356 5.850117

 41 H 8.025306 8.867050 8.230546 9.043356 5.850117

 42 H 7.737083 8.763742 8.372786 9.361604 6.402235

 43 H 2.133222 3.279882 4.315233 5.578464 5.850117

 44 H 2.133222 3.279882 4.315233 5.578464 5.850117

 45 H 2.137316 2.756467 4.150967 5.246094 6.402235

 26 27 28 29 30

 26 C 0.000000

 27 H 2.991904 0.000000

 28 C 7.912866 9.454870 0.000000

 29 H 5.263181 7.381205 2.991904 0.000000

 30 C 7.912866 5.263181 11.190482 10.399238 0.000000

 31 H 9.454870 7.381205 10.399238 10.438600 2.991904

 32 C 11.190482 10.399238 7.912866 9.454870 7.912866

 33 H 10.399238 10.438600 5.263181 7.381205 9.454870

 34 H 1.090332 2.755043 9.003083 6.335439 7.970895

 35 H 1.094498 3.744076 7.642207 4.911792 8.523958

 36 H 1.094498 3.744076 7.642207 4.911792 8.523958

 37 H 8.523958 9.940031 1.094498 3.744076 11.395756

 38 H 8.523958 9.940031 1.094498 3.744076 11.395756

 39 H 7.970895 9.814359 1.090332 2.755043 11.975051

 40 H 7.642207 4.911792 11.395756 10.436082 1.094498

 41 H 7.642207 4.911792 11.395756 10.436082 1.094498

 42 H 9.003083 6.335439 11.975051 11.352055 1.090332

 43 H 11.395756 10.436082 8.523958 9.940031 7.642207

 44 H 11.395756 10.436082 8.523958 9.940031 7.642207

 45 H 11.975051 11.352055 7.970895 9.814359 9.003083

 31 32 33 34 35

 31 H 0.000000

 32 C 5.263181 0.000000

 33 H 7.381205 2.991904 0.000000

 34 H 9.814359 11.975051 11.352055 0.000000

 35 H 9.940031 11.395756 10.436082 1.775026 0.000000

 36 H 9.940031 11.395756 10.436082 1.775026 1.753485

 37 H 10.436082 7.642207 4.911792 9.607664 8.179876

 38 H 10.436082 7.642207 4.911792 9.607664 8.365709

 39 H 11.352055 9.003083 6.335439 9.054128 7.623500

 40 H 3.744076 8.523958 9.940031 7.623500 8.179876

 41 H 3.744076 8.523958 9.940031 7.623500 8.365709

 42 H 2.755043 7.970895 9.814359 9.054128 9.607664

 43 H 4.911792 1.094498 3.744076 12.135660 11.568092

 44 H 4.911792 1.094498 3.744076 12.135660 11.700234

 45 H 6.335439 1.090332 2.755043 12.804471 12.135660

 36 37 38 39 40

 36 H 0.000000

 37 H 8.365709 0.000000

 38 H 8.179876 1.753485 0.000000

 39 H 7.623500 1.775026 1.775026 0.000000

 40 H 8.365709 11.568092 11.700234 12.135660 0.000000

 41 H 8.179876 11.700234 11.568092 12.135660 1.753485

 42 H 9.607664 12.135660 12.135660 12.804471 1.775026

 43 H 11.700234 8.179876 8.365709 9.607664 8.179876

 44 H 11.568092 8.365709 8.179876 9.607664 8.365709

 45 H 12.135660 7.623500 7.623500 9.054128 9.607664

 41 42 43 44 45

 41 H 0.000000

 42 H 1.775026 0.000000

 43 H 8.365709 7.623500 0.000000

 44 H 8.179876 7.623500 1.753485 0.000000

 45 H 9.607664 9.054128 1.775026 1.775026 0.000000

 Stoichiometry C20H16N8Zn(1+,2)

 Framework group C4H[O(Zn),SGH(C20H8N8),X(H8)]

 Deg. of freedom 20

 Full point group C4H NOp 8

 RotChk: IX=0 Diff= 9.14D-04

 Largest Abelian subgroup C2H NOp 4

 Largest concise Abelian subgroup C2H NOp 4

 Standard orientation:

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

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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

 1 6 0 -2.182102 2.062442 0.000000

 2 7 0 -1.857824 0.741852 0.000000

 3 6 0 -2.988529 0.000000 0.000000

 4 6 0 -4.163588 0.928665 0.000000

 5 6 0 -3.648545 2.182252 0.000000

 6 7 0 -3.096135 -1.330513 0.000000

 7 6 0 -2.062442 -2.182102 0.000000

 8 7 0 -0.741852 -1.857824 0.000000

 9 6 0 0.000000 -2.988529 0.000000

 10 6 0 -0.928665 -4.163588 0.000000

 11 6 0 -2.182252 -3.648545 0.000000

 12 7 0 -1.330513 3.096135 0.000000

 13 6 0 0.928665 4.163588 0.000000

 14 6 0 2.182252 3.648545 0.000000

 15 6 0 2.062442 2.182102 0.000000

 16 7 0 0.741852 1.857824 0.000000

 17 6 0 0.000000 2.988529 0.000000

 18 7 0 3.096135 1.330513 0.000000

 19 7 0 1.857824 -0.741852 0.000000

 20 6 0 2.988529 0.000000 0.000000

 21 6 0 4.163588 -0.928665 0.000000

 22 6 0 3.648545 -2.182252 0.000000

 23 6 0 2.182102 -2.062442 0.000000

 24 7 0 1.330513 -3.096135 0.000000

 25 30 0 0.000000 0.000000 0.000000

 26 6 0 -5.575279 0.472217 0.000000

 27 1 0 -4.183559 3.120726 0.000000

 28 6 0 -0.472217 -5.575279 0.000000

 29 1 0 -3.120726 -4.183559 0.000000

 30 6 0 0.472217 5.575279 0.000000

 31 1 0 3.120726 4.183559 0.000000

 32 6 0 5.575279 -0.472217 0.000000

 33 1 0 4.183559 -3.120726 0.000000

 34 1 0 -6.265459 1.316300 0.000000

 35 1 0 -5.782115 -0.149449 0.876742

 36 1 0 -5.782115 -0.149449 -0.876742

 37 1 0 0.149449 -5.782115 0.876742

 38 1 0 0.149449 -5.782115 -0.876742

 39 1 0 -1.316300 -6.265459 0.000000

 40 1 0 -0.149449 5.782115 0.876742

 41 1 0 -0.149449 5.782115 -0.876742

 42 1 0 1.316300 6.265459 0.000000

 43 1 0 5.782115 0.149449 0.876742

 44 1 0 5.782115 0.149449 -0.876742

 45 1 0 6.265459 -1.316300 0.000000

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 Rotational constants (GHZ): 0.1830207 0.1830207 0.0917162

 Leave Link 202 at Fri Jul 5 21:11:55 2019, MaxMem= 1342177280 cpu: 0.2

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

 Basis read from rwf: (5D, 7F)

 Pseudo-potential data read from rwf file.

 There are 229 symmetry adapted cartesian basis functions of AG symmetry.

 There are 82 symmetry adapted cartesian basis functions of BG symmetry.

 There are 78 symmetry adapted cartesian basis functions of AU symmetry.

 There are 218 symmetry adapted cartesian basis functions of BU symmetry.

 There are 212 symmetry adapted basis functions of AG symmetry.

 There are 82 symmetry adapted basis functions of BG symmetry.

 There are 78 symmetry adapted basis functions of AU symmetry.

 There are 204 symmetry adapted basis functions of BU symmetry.

 576 basis functions, 1015 primitive gaussians, 607 cartesian basis functions

 102 alpha electrons 101 beta electrons

 nuclear repulsion energy 2766.6354236876 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= 45 NActive= 45 NUniq= 11 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= -0.1142374744 Hartrees.

 Nuclear repulsion after empirical dispersion term = 2766.5211862132 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= 45.

 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 = 45

 GePol: Total number of spheres = 45

 GePol: Number of exposed spheres = 45 (100.00%)

 GePol: Number of points = 3538

 GePol: Average weight of points = 0.11

 GePol: Minimum weight of points = 0.76D-11

 GePol: Maximum weight of points = 0.18390

 GePol: Number of points with low weight = 160

 GePol: Fraction of low-weight points (<1% of avg) = 4.52%

 GePol: Cavity surface area = 382.113 Ang\*\*2

 GePol: Cavity volume = 379.112 Ang\*\*3

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

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 PCM non-electrostatic energy = -0.0110968490 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 2766.5100893642 Hartrees.

 Leave Link 301 at Fri Jul 5 21:11:56 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

 8 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15383 LenP2D= 41364.

 LDataN: DoStor=T MaxTD1= 5 Len= 102

 NBasis= 576 RedAO= T EigKep= 1.86D-04 NBF= 212 82 78 204

 NBsUse= 576 1.00D-06 EigRej= -1.00D+00 NBFU= 212 82 78 204

 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= 594 594 594 594 594 MxSgAt= 45 MxSgA2= 45.

 Leave Link 302 at Fri Jul 5 21:11:56 2019, MaxMem= 1342177280 cpu: 7.8

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

 DipDrv: MaxL=1.

 Leave Link 303 at Fri Jul 5 21:11:57 2019, MaxMem= 1342177280 cpu: 0.8

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

 Initial guess from the checkpoint file: "ZntAzPcation.chk"

 B after Tr= 0.000000 0.000000 0.000000

 Rot= 1.000000 0.000000 0.000000 -0.000186 Ang= -0.02 deg.

 Guess basis will be translated and rotated to current coordinates.

 JPrj=2 DoOrth=T DoCkMO=T.

 Initial guess orbital symmetries:

 Alpha Orbitals:

 Occupied (BG) (EU) (EU) (AG) (EU) (EU) (BG) (AG) (BG) (EU)

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

 Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7819 S= 0.5158

 Leave Link 401 at Fri Jul 5 21:11:59 2019, MaxMem= 1342177280 cpu: 23.1

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

 UHF open shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 1138797 IEndB= 1138797 NGot= 1342177280 MDV= 1341424180

 LenX= 1341424180 LenY= 1341055124

 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= 670000000 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= 37552332.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 7.11D-15 for 273.

 Iteration 1 A\*A^-1 deviation from orthogonality is 5.41D-15 for 3160 849.

 Iteration 1 A^-1\*A deviation from unit magnitude is 7.55D-15 for 861.

 Iteration 1 A^-1\*A deviation from orthogonality is 2.24D-15 for 1949 1905.

 E= -1275.69945994435

 DIIS: error= 2.61D-04 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -1275.69945994435 IErMin= 1 ErrMin= 2.61D-04

 ErrMax= 2.61D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-04 BMatP= 1.04D-04

 IDIUse=3 WtCom= 9.97D-01 WtEn= 2.61D-03

 Coeff-Com: 0.100D+01

 Coeff-En: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.372 Goal= None Shift= 0.000

 Gap= 0.406 Goal= None Shift= 0.000

 RMSDP=1.33D-05 MaxDP=4.39D-04 OVMax= 1.52D-03

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 1.32D-05 CP: 1.00D+00

 E= -1275.69949984038 Delta-E= -0.000039896028 Rises=F Damp=F

 DIIS: error= 5.80D-05 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -1275.69949984038 IErMin= 2 ErrMin= 5.80D-05

 ErrMax= 5.80D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.23D-06 BMatP= 1.04D-04

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

 Coeff-Com: 0.356D-01 0.964D+00

 Coeff: 0.356D-01 0.964D+00

 Gap= 0.104 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=3.96D-06 MaxDP=1.76D-04 DE=-3.99D-05 OVMax= 5.88D-04

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 3.95D-06 CP: 1.00D+00 1.00D+00

 E= -1275.69949833130 Delta-E= 0.000001509076 Rises=F Damp=F

 DIIS: error= 1.01D-04 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 2 EnMin= -1275.69949984038 IErMin= 2 ErrMin= 5.80D-05

 ErrMax= 1.01D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D-05 BMatP= 6.23D-06

 IDIUse=3 WtCom= 4.99D-01 WtEn= 5.01D-01

 Coeff-Com: -0.313D-01 0.619D+00 0.412D+00

 Coeff-En: 0.000D+00 0.646D+00 0.354D+00

 Coeff: -0.156D-01 0.633D+00 0.383D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=2.39D-06 MaxDP=1.03D-04 DE= 1.51D-06 OVMax= 4.90D-04

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 1.01D-06 CP: 1.00D+00 1.03D+00 4.63D-01

 E= -1275.69950151749 Delta-E= -0.000003186193 Rises=F Damp=F

 DIIS: error= 7.41D-06 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -1275.69950151749 IErMin= 4 ErrMin= 7.41D-06

 ErrMax= 7.41D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.99D-08 BMatP= 6.23D-06

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

 Coeff-Com: -0.135D-01 0.168D+00 0.120D+00 0.725D+00

 Coeff: -0.135D-01 0.168D+00 0.120D+00 0.725D+00

 Gap= 0.104 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 31774 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

 Gap= 0.083 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328219 trying DSYEV.

 RMSDP=3.42D-07 MaxDP=1.77D-05 DE=-3.19D-06 OVMax= 1.45D-04

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 3.25D-07 CP: 1.00D+00 1.04D+00 4.61D-01 1.03D+00

 E= -1275.69950154127 Delta-E= -0.000000023778 Rises=F Damp=F

 DIIS: error= 5.39D-06 at cycle 5 NSaved= 5.

 NSaved= 5 IEnMin= 5 EnMin= -1275.69950154127 IErMin= 5 ErrMin= 5.39D-06

 ErrMax= 5.39D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.83D-08 BMatP= 8.99D-08

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

 Coeff-Com: -0.381D-02 0.330D-01 0.313D-01 0.360D+00 0.580D+00

 Coeff: -0.381D-02 0.330D-01 0.313D-01 0.360D+00 0.580D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=1.72D-07 MaxDP=6.94D-06 DE=-2.38D-08 OVMax= 8.24D-05

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 1.54D-07 CP: 1.00D+00 1.04D+00 4.70D-01 1.09D+00 9.23D-01

 E= -1275.69950155045 Delta-E= -0.000000009183 Rises=F Damp=F

 DIIS: error= 2.44D-06 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -1275.69950155045 IErMin= 6 ErrMin= 2.44D-06

 ErrMax= 2.44D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.32D-09 BMatP= 2.83D-08

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

 Coeff-Com: 0.163D-04-0.839D-02 0.110D-02 0.538D-01 0.270D+00 0.683D+00

 Coeff: 0.163D-04-0.839D-02 0.110D-02 0.538D-01 0.270D+00 0.683D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=9.84D-08 MaxDP=4.00D-06 DE=-9.18D-09 OVMax= 5.67D-05

 Cycle 7 Pass 1 IDiag 1:

 RMSU= 6.32D-08 CP: 1.00D+00 1.04D+00 4.74D-01 1.13D+00 1.10D+00

 CP: 1.07D+00

 E= -1275.69950155332 Delta-E= -0.000000002867 Rises=F Damp=F

 DIIS: error= 1.31D-06 at cycle 7 NSaved= 7.

 NSaved= 7 IEnMin= 7 EnMin= -1275.69950155332 IErMin= 7 ErrMin= 1.31D-06

 ErrMax= 1.31D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.39D-09 BMatP= 4.32D-09

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

 Coeff-Com: 0.105D-02-0.141D-01-0.619D-02-0.603D-01 0.255D-01 0.381D+00

 Coeff-Com: 0.673D+00

 Coeff: 0.105D-02-0.141D-01-0.619D-02-0.603D-01 0.255D-01 0.381D+00

 Coeff: 0.673D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=6.92D-08 MaxDP=3.43D-06 DE=-2.87D-09 OVMax= 4.15D-05

 Cycle 8 Pass 1 IDiag 1:

 RMSU= 3.09D-08 CP: 1.00D+00 1.04D+00 4.77D-01 1.16D+00 1.20D+00

 CP: 1.34D+00 1.33D+00

 E= -1275.69950155474 Delta-E= -0.000000001423 Rises=F Damp=F

 DIIS: error= 8.14D-07 at cycle 8 NSaved= 8.

 NSaved= 8 IEnMin= 8 EnMin= -1275.69950155474 IErMin= 8 ErrMin= 8.14D-07

 ErrMax= 8.14D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.50D-10 BMatP= 1.39D-09

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

 Coeff-Com: 0.152D-03 0.122D-02-0.538D-03-0.352D-01-0.115D+00-0.262D+00

 Coeff-Com: 0.146D+00 0.126D+01

 Coeff: 0.152D-03 0.122D-02-0.538D-03-0.352D-01-0.115D+00-0.262D+00

 Coeff: 0.146D+00 0.126D+01

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=8.29D-08 MaxDP=4.64D-06 DE=-1.42D-09 OVMax= 4.04D-05

 Cycle 9 Pass 1 IDiag 1:

 RMSU= 2.12D-08 CP: 1.00D+00 1.04D+00 4.80D-01 1.18D+00 1.31D+00

 CP: 1.60D+00 2.08D+00 1.67D+00

 E= -1275.69950155563 Delta-E= -0.000000000882 Rises=F Damp=F

 DIIS: error= 3.95D-07 at cycle 9 NSaved= 9.

 NSaved= 9 IEnMin= 9 EnMin= -1275.69950155563 IErMin= 9 ErrMin= 3.95D-07

 ErrMax= 3.95D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.56D-10 BMatP= 3.50D-10

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

 Coeff-Com: -0.159D-03 0.422D-02 0.111D-02-0.471D-02-0.725D-01-0.239D+00

 Coeff-Com: -0.886D-01 0.751D+00 0.648D+00

 Coeff: -0.159D-03 0.422D-02 0.111D-02-0.471D-02-0.725D-01-0.239D+00

 Coeff: -0.886D-01 0.751D+00 0.648D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=2.84D-08 MaxDP=1.68D-06 DE=-8.82D-10 OVMax= 1.24D-05

 Cycle 10 Pass 1 IDiag 1:

 RMSU= 1.22D-08 CP: 1.00D+00 1.04D+00 4.80D-01 1.19D+00 1.34D+00

 CP: 1.68D+00 2.31D+00 2.05D+00 1.22D+00

 E= -1275.69950155563 Delta-E= 0.000000000000 Rises=F Damp=F

 DIIS: error= 2.77D-07 at cycle 10 NSaved= 10.

 NSaved=10 IEnMin=10 EnMin= -1275.69950155563 IErMin=10 ErrMin= 2.77D-07

 ErrMax= 2.77D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.45D-11 BMatP= 1.56D-10

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

 Coeff-Com: -0.146D-03 0.181D-02 0.678D-03 0.118D-01 0.841D-02-0.386D-02

 Coeff-Com: -0.982D-01-0.897D-01 0.299D+00 0.870D+00

 Coeff: -0.146D-03 0.181D-02 0.678D-03 0.118D-01 0.841D-02-0.386D-02

 Coeff: -0.982D-01-0.897D-01 0.299D+00 0.870D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=1.41D-08 MaxDP=8.91D-07 DE=-4.55D-13 OVMax= 6.31D-06

 Cycle 11 Pass 1 IDiag 1:

 RMSU= 5.27D-09 CP: 1.00D+00 1.04D+00 4.80D-01 1.19D+00 1.34D+00

 CP: 1.70D+00 2.40D+00 2.25D+00 1.66D+00 1.25D+00

 E= -1275.69950155577 Delta-E= -0.000000000141 Rises=F Damp=F

 DIIS: error= 1.02D-07 at cycle 11 NSaved= 11.

 NSaved=11 IEnMin=11 EnMin= -1275.69950155577 IErMin=11 ErrMin= 1.02D-07

 ErrMax= 1.02D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.91D-12 BMatP= 3.45D-11

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

 Coeff-Com: -0.327D-04-0.119D-03-0.515D-04 0.625D-02 0.184D-01 0.508D-01

 Coeff-Com: -0.340D-01-0.211D+00 0.752D-02 0.447D+00 0.715D+00

 Coeff: -0.327D-04-0.119D-03-0.515D-04 0.625D-02 0.184D-01 0.508D-01

 Coeff: -0.340D-01-0.211D+00 0.752D-02 0.447D+00 0.715D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=6.66D-09 MaxDP=3.94D-07 DE=-1.41D-10 OVMax= 3.22D-06

 Error on total polarization charges = 0.06026

 SCF Done: E(UB3LYP) = -1275.69950156 A.U. after 11 cycles

 NFock= 11 Conv=0.67D-08 -V/T= 1.9660

 <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7819 S= 0.5158

 <L.S>= 0.000000000000E+00

 KE= 1.320599904401D+03 PE=-8.556853724139D+03 EE= 3.194044228819D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.96

 (included in total energy above)

 Annihilation of the first spin contaminant:

 S\*\*2 before annihilation 0.7819, after 0.7509

 Leave Link 502 at Fri Jul 5 21:13:06 2019, MaxMem= 1342177280 cpu: 775.3

 (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.

 8 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15383 LenP2D= 41364.

 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 = 248

 Leave Link 701 at Fri Jul 5 21:13:11 2019, MaxMem= 1342177280 cpu: 53.4

 (Enter /apps/gaussian/g09d01/g09/l702.exe)

 L702 exits ... SP integral derivatives will be done elsewhere.

 Leave Link 702 at Fri Jul 5 21:13:11 2019, MaxMem= 1342177280 cpu: 0.2

 (Enter /apps/gaussian/g09d01/g09/l703.exe)

 Compute integral first derivatives, UseDBF=F ICtDFT= 0.

 Integral derivatives from FoFJK, PRISM(SPDF).

 Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

 FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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 Fri Jul 5 21:13:18 2019, MaxMem= 1342177280 cpu: 92.4

 (Enter /apps/gaussian/g09d01/g09/l716.exe)

 Dipole =-9.23705556D-14 1.32782674D-13-4.44089210D-16

 \*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

 Center Atomic Forces (Hartrees/Bohr)

 Number Number X Y Z

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

 1 6 -0.000315832 -0.000245734 0.000000000

 2 7 0.000181903 0.000062597 0.000000000

 3 6 -0.000184370 -0.000064551 0.000000000

 4 6 0.000037715 -0.000057082 0.000000000

 5 6 -0.000060278 0.000311643 0.000000000

 6 7 0.000119418 0.000038493 0.000000000

 7 6 0.000245734 -0.000315832 0.000000000

 8 7 -0.000062597 0.000181903 0.000000000

 9 6 0.000064551 -0.000184370 0.000000000

 10 6 0.000057082 0.000037715 0.000000000

 11 6 -0.000311643 -0.000060278 0.000000000

 12 7 0.000038493 -0.000119418 0.000000000

 13 6 -0.000057082 -0.000037715 0.000000000

 14 6 0.000311643 0.000060278 0.000000000

 15 6 -0.000245734 0.000315832 0.000000000

 16 7 0.000062597 -0.000181903 0.000000000

 17 6 -0.000064551 0.000184370 0.000000000

 18 7 -0.000119418 -0.000038493 0.000000000

 19 7 -0.000181903 -0.000062597 0.000000000

 20 6 0.000184370 0.000064551 0.000000000

 21 6 -0.000037715 0.000057082 0.000000000

 22 6 0.000060278 -0.000311643 0.000000000

 23 6 0.000315832 0.000245734 0.000000000

 24 7 -0.000038493 0.000119418 0.000000000

 25 30 0.000000000 0.000000000 0.000000000

 26 6 0.000069864 0.000021063 0.000000000

 27 1 -0.000047920 0.000054089 0.000000000

 28 6 -0.000021063 0.000069864 0.000000000

 29 1 -0.000054089 -0.000047920 0.000000000

 30 6 0.000021063 -0.000069864 0.000000000

 31 1 0.000054089 0.000047920 0.000000000

 32 6 -0.000069864 -0.000021063 0.000000000

 33 1 0.000047920 -0.000054089 0.000000000

 34 1 -0.000034500 -0.000025249 0.000000000

 35 1 -0.000029083 0.000012860 0.000051071

 36 1 -0.000029083 0.000012860 -0.000051071

 37 1 -0.000012860 -0.000029083 0.000051071

 38 1 -0.000012860 -0.000029083 -0.000051071

 39 1 0.000025249 -0.000034500 0.000000000

 40 1 0.000012860 0.000029083 0.000051071

 41 1 0.000012860 0.000029083 -0.000051071

 42 1 -0.000025249 0.000034500 0.000000000

 43 1 0.000029083 -0.000012860 0.000051071

 44 1 0.000029083 -0.000012860 -0.000051071

 45 1 0.000034500 0.000025249 0.000000000

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

 Cartesian Forces: Max 0.000315832 RMS 0.000105563

 Leave Link 716 at Fri Jul 5 21:13:18 2019, MaxMem= 1342177280 cpu: 0.3

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

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Berny optimization.

 Using GEDIIS/GDIIS optimizer.

 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

 GSVD: received Info= 1 from GESDD.

 Internal Forces: Max 0.000207042 RMS 0.000055295

 Search for a local minimum.

 Step number 4 out of a maximum of 270

 All quantities printed in internal units (Hartrees-Bohrs-Radians)

 RMS Force = .55295D-04 SwitMx=.10000D-02 MixMth= 2

 Mixed Optimization -- En-DIIS/RFO-DIIS

 Swapping is turned off.

 Update second derivatives using D2CorX and points 1 2 3 4

 DE= -2.03D-05 DEPred=-2.34D-05 R= 8.70D-01

 TightC=F SS= 1.41D+00 RLast= 1.72D-02 DXNew= 5.5297D-01 5.1496D-02

 Trust test= 8.70D-01 RLast= 1.72D-02 DXMaxT set to 3.29D-01

 ITU= 1 1 1 0

 Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01342

 Eigenvalues --- 0.01345 0.01345 0.01345 0.01600 0.01618

 Eigenvalues --- 0.01631 0.01631 0.01777 0.01792 0.01819

 Eigenvalues --- 0.01819 0.01890 0.01906 0.01943 0.01943

 Eigenvalues --- 0.01998 0.01999 0.02045 0.02045 0.02070

 Eigenvalues --- 0.02087 0.02102 0.02113 0.02113 0.02205

 Eigenvalues --- 0.02316 0.02316 0.02352 0.02374 0.07179

 Eigenvalues --- 0.07212 0.07212 0.07212 0.07212 0.07401

 Eigenvalues --- 0.07401 0.07401 0.12607 0.14501 0.14501

 Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

 Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

 Eigenvalues --- 0.16000 0.16000 0.16000 0.16003 0.16087

 Eigenvalues --- 0.16516 0.18181 0.20215 0.22084 0.22084

 Eigenvalues --- 0.23811 0.23848 0.23848 0.24128 0.25000

 Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

 Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25002

 Eigenvalues --- 0.25887 0.32167 0.33173 0.33173 0.33215

 Eigenvalues --- 0.33282 0.33282 0.33282 0.33433 0.33724

 Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

 Eigenvalues --- 0.33724 0.34154 0.34437 0.34437 0.34437

 Eigenvalues --- 0.34493 0.35379 0.35449 0.35574 0.35574

 Eigenvalues --- 0.35682 0.35682 0.35682 0.36047 0.39287

 Eigenvalues --- 0.41754 0.41754 0.42763 0.47097 0.48969

 Eigenvalues --- 0.48969 0.49606 0.50265 0.50567 0.51356

 Eigenvalues --- 0.51356 0.52275 0.53984 0.53984 0.54930

 Eigenvalues --- 0.56277 0.56331 0.56331 0.56433

 En-DIIS/RFO-DIIS IScMMF= 0 using points: 4 3 2

 RFO step: Lambda=-1.56511822D-06.

 NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=F DC= 2.59D-04 SmlDif= 1.00D-05

 RMS Error= 0.1037808339D-03 NUsed= 3 EDIIS=F

 DidBck=F Rises=F RFO-DIIS coefs: 1.24858 -0.29634 0.04776

 Iteration 1 RMS(Cart)= 0.00085191 RMS(Int)= 0.00000035

 Iteration 2 RMS(Cart)= 0.00000050 RMS(Int)= 0.00000009

 ITry= 1 IFail=0 DXMaxC= 2.90D-03 DCOld= 1.00D+10 DXMaxT= 3.29D-01 DXLimC= 3.00D+00 Rises=F

 ClnCor: largest displacement from symmetrization is 2.02D-10 for atom 36.

 Variable Old X -DE/DX Delta X Delta X Delta X New X

 (Linear) (Quad) (Total)

 R1 2.56969 0.00018 0.00003 0.00038 0.00041 2.57010

 R2 2.78041 -0.00021 -0.00006 -0.00052 -0.00059 2.77982

 R3 2.53091 -0.00006 -0.00002 -0.00014 -0.00017 2.53074

 R4 2.55556 -0.00001 -0.00021 0.00004 -0.00017 2.55539

 R5 3.78033 0.00001 0.00019 -0.00016 0.00003 3.78036

 R6 2.83029 -0.00008 0.00034 -0.00036 -0.00002 2.83028

 R7 2.52251 0.00012 0.00011 0.00012 0.00023 2.52274

 R8 2.56108 0.00017 0.00017 0.00013 0.00030 2.56138

 R9 2.80369 0.00002 0.00007 -0.00008 -0.00001 2.80369

 R10 2.04141 0.00000 0.00016 -0.00015 0.00001 2.04142

 R11 2.53091 -0.00006 -0.00002 -0.00014 -0.00017 2.53074

 R12 2.56969 0.00018 0.00003 0.00038 0.00041 2.57010

 R13 2.78041 -0.00021 -0.00006 -0.00052 -0.00059 2.77982

 R14 2.55556 -0.00001 -0.00021 0.00004 -0.00017 2.55539

 R15 3.78033 0.00001 0.00019 -0.00016 0.00003 3.78036

 R16 2.83029 -0.00008 0.00034 -0.00036 -0.00002 2.83028

 R17 2.52251 0.00012 0.00011 0.00012 0.00023 2.52274

 R18 2.56108 0.00017 0.00017 0.00013 0.00030 2.56138

 R19 2.80369 0.00002 0.00007 -0.00008 -0.00001 2.80369

 R20 2.04141 0.00000 0.00016 -0.00015 0.00001 2.04142

 R21 2.52251 0.00012 0.00011 0.00012 0.00023 2.52274

 R22 2.56108 0.00017 0.00017 0.00013 0.00030 2.56138

 R23 2.83029 -0.00008 0.00034 -0.00036 -0.00002 2.83028

 R24 2.80369 0.00002 0.00007 -0.00008 -0.00001 2.80369

 R25 2.78041 -0.00021 -0.00006 -0.00052 -0.00059 2.77982

 R26 2.04141 0.00000 0.00016 -0.00015 0.00001 2.04142

 R27 2.56969 0.00018 0.00003 0.00038 0.00041 2.57010

 R28 2.53091 -0.00006 -0.00002 -0.00014 -0.00017 2.53074

 R29 2.55556 -0.00001 -0.00021 0.00004 -0.00017 2.55539

 R30 3.78033 0.00001 0.00019 -0.00016 0.00003 3.78036

 R31 2.52251 0.00012 0.00011 0.00012 0.00023 2.52274

 R32 2.55556 -0.00001 -0.00021 0.00004 -0.00017 2.55539

 R33 2.56969 0.00018 0.00003 0.00038 0.00041 2.57010

 R34 3.78033 0.00001 0.00019 -0.00016 0.00003 3.78036

 R35 2.83029 -0.00008 0.00034 -0.00036 -0.00002 2.83028

 R36 2.56108 0.00017 0.00017 0.00013 0.00030 2.56138

 R37 2.80369 0.00002 0.00007 -0.00008 -0.00001 2.80369

 R38 2.78041 -0.00021 -0.00006 -0.00052 -0.00059 2.77982

 R39 2.04141 0.00000 0.00016 -0.00015 0.00001 2.04142

 R40 2.53091 -0.00006 -0.00002 -0.00014 -0.00017 2.53074

 R41 2.06043 0.00002 0.00015 -0.00008 0.00007 2.06050

 R42 2.06830 0.00004 0.00024 -0.00012 0.00013 2.06843

 R43 2.06830 0.00004 0.00024 -0.00012 0.00013 2.06843

 R44 2.06830 0.00004 0.00024 -0.00012 0.00013 2.06843

 R45 2.06830 0.00004 0.00024 -0.00012 0.00013 2.06843

 R46 2.06043 0.00002 0.00015 -0.00008 0.00007 2.06050

 R47 2.06830 0.00004 0.00024 -0.00012 0.00013 2.06843

 R48 2.06830 0.00004 0.00024 -0.00012 0.00013 2.06843

 R49 2.06043 0.00002 0.00015 -0.00008 0.00007 2.06050

 R50 2.06830 0.00004 0.00024 -0.00012 0.00013 2.06843

 R51 2.06830 0.00004 0.00024 -0.00012 0.00013 2.06843

 R52 2.06043 0.00002 0.00015 -0.00008 0.00007 2.06050

 A1 1.89311 0.00000 0.00016 -0.00019 -0.00003 1.89308

 A2 2.21170 -0.00004 -0.00025 0.00006 -0.00019 2.21150

 A3 2.17838 0.00004 0.00009 0.00013 0.00022 2.17860

 A4 1.91066 -0.00002 -0.00002 -0.00001 -0.00003 1.91062

 A5 2.19150 0.00001 0.00008 0.00000 0.00008 2.19158

 A6 2.18103 0.00001 -0.00006 0.00001 -0.00005 2.18098

 A7 1.89214 0.00002 0.00002 0.00002 0.00004 1.89218

 A8 2.23215 0.00001 -0.00001 0.00014 0.00013 2.23228

 A9 2.15890 -0.00003 -0.00001 -0.00016 -0.00017 2.15873

 A10 1.84977 -0.00002 -0.00006 -0.00007 -0.00013 1.84964

 A11 2.16006 -0.00017 -0.00057 -0.00046 -0.00103 2.15904

 A12 2.27335 0.00019 0.00063 0.00053 0.00116 2.27451

 A13 1.87911 0.00002 -0.00010 0.00024 0.00014 1.87925

 A14 2.17045 -0.00006 -0.00028 -0.00027 -0.00054 2.16991

 A15 2.23363 0.00003 0.00037 0.00003 0.00040 2.23403

 A16 2.17920 0.00000 0.00024 -0.00021 0.00003 2.17923

 A17 2.21170 -0.00004 -0.00025 0.00006 -0.00019 2.21150

 A18 2.17838 0.00004 0.00009 0.00013 0.00022 2.17860

 A19 1.89311 0.00000 0.00016 -0.00019 -0.00003 1.89308

 A20 1.91066 -0.00002 -0.00002 -0.00001 -0.00003 1.91062

 A21 2.19150 0.00001 0.00008 0.00000 0.00008 2.19158

 A22 2.18103 0.00001 -0.00006 0.00001 -0.00005 2.18098

 A23 1.89214 0.00002 0.00002 0.00002 0.00004 1.89218

 A24 2.23215 0.00001 -0.00001 0.00014 0.00013 2.23228

 A25 2.15890 -0.00003 -0.00001 -0.00016 -0.00017 2.15873

 A26 1.84977 -0.00002 -0.00006 -0.00007 -0.00013 1.84964

 A27 2.16006 -0.00017 -0.00057 -0.00046 -0.00103 2.15904

 A28 2.27335 0.00019 0.00063 0.00053 0.00116 2.27451

 A29 1.87911 0.00002 -0.00010 0.00024 0.00014 1.87925

 A30 2.17045 -0.00006 -0.00028 -0.00027 -0.00054 2.16991

 A31 2.23363 0.00003 0.00037 0.00003 0.00040 2.23403

 A32 2.17920 0.00000 0.00024 -0.00021 0.00003 2.17923

 A33 1.84977 -0.00002 -0.00006 -0.00007 -0.00013 1.84964

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 A37 2.23363 0.00003 0.00037 0.00003 0.00040 2.23403

 A38 2.17045 -0.00006 -0.00028 -0.00027 -0.00054 2.16991

 A39 1.89311 0.00000 0.00016 -0.00019 -0.00003 1.89308

 A40 2.17838 0.00004 0.00009 0.00013 0.00022 2.17860

 A41 2.21170 -0.00004 -0.00025 0.00006 -0.00019 2.21150

 A42 1.91066 -0.00002 -0.00002 -0.00001 -0.00003 1.91062

 A43 2.19150 0.00001 0.00008 0.00000 0.00008 2.19158

 A44 2.18103 0.00001 -0.00006 0.00001 -0.00005 2.18098

 A45 2.15890 -0.00003 -0.00001 -0.00016 -0.00017 2.15873

 A46 2.23215 0.00001 -0.00001 0.00014 0.00013 2.23228

 A47 1.89214 0.00002 0.00002 0.00002 0.00004 1.89218

 A48 2.17920 0.00000 0.00024 -0.00021 0.00003 2.17923

 A49 1.91066 -0.00002 -0.00002 -0.00001 -0.00003 1.91062

 A50 2.18103 0.00001 -0.00006 0.00001 -0.00005 2.18098

 A51 2.19150 0.00001 0.00008 0.00000 0.00008 2.19158

 A52 2.23215 0.00001 -0.00001 0.00014 0.00013 2.23228

 A53 2.15890 -0.00003 -0.00001 -0.00016 -0.00017 2.15873

 A54 1.89214 0.00002 0.00002 0.00002 0.00004 1.89218

 A55 1.84977 -0.00002 -0.00006 -0.00007 -0.00013 1.84964

 A56 2.16006 -0.00017 -0.00057 -0.00046 -0.00103 2.15904

 A57 2.27335 0.00019 0.00063 0.00053 0.00116 2.27451

 A58 1.87911 0.00002 -0.00010 0.00024 0.00014 1.87925

 A59 2.23363 0.00003 0.00037 0.00003 0.00040 2.23403

 A60 2.17045 -0.00006 -0.00028 -0.00027 -0.00054 2.16991

 A61 1.89311 0.00000 0.00016 -0.00019 -0.00003 1.89308

 A62 2.21170 -0.00004 -0.00025 0.00006 -0.00019 2.21150

 A63 2.17838 0.00004 0.00009 0.00013 0.00022 2.17860

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 A65 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

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 A67 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

 A68 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

 A69 1.94349 0.00004 0.00032 0.00010 0.00042 1.94391

 A70 1.93324 -0.00004 -0.00017 -0.00016 -0.00033 1.93291

 A71 1.93324 -0.00004 -0.00017 -0.00016 -0.00033 1.93291

 A72 1.89662 0.00000 -0.00003 0.00001 -0.00002 1.89660

 A73 1.89662 0.00000 -0.00003 0.00001 -0.00002 1.89660

 A74 1.85808 0.00004 0.00008 0.00020 0.00028 1.85835

 A75 1.93324 -0.00004 -0.00017 -0.00016 -0.00033 1.93291

 A76 1.93324 -0.00004 -0.00017 -0.00016 -0.00033 1.93291

 A77 1.94349 0.00004 0.00032 0.00010 0.00042 1.94391

 A78 1.85808 0.00004 0.00008 0.00020 0.00028 1.85835

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 A80 1.89662 0.00000 -0.00003 0.00001 -0.00002 1.89660

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 A83 1.94349 0.00004 0.00032 0.00010 0.00042 1.94391

 A84 1.85808 0.00004 0.00008 0.00020 0.00028 1.85835

 A85 1.89662 0.00000 -0.00003 0.00001 -0.00002 1.89660

 A86 1.89662 0.00000 -0.00003 0.00001 -0.00002 1.89660

 A87 1.93324 -0.00004 -0.00017 -0.00016 -0.00033 1.93291

 A88 1.93324 -0.00004 -0.00017 -0.00016 -0.00033 1.93291

 A89 1.94349 0.00004 0.00032 0.00010 0.00042 1.94391

 A90 1.85808 0.00004 0.00008 0.00020 0.00028 1.85835

 A91 1.89662 0.00000 -0.00003 0.00001 -0.00002 1.89660

 A92 1.89662 0.00000 -0.00003 0.00001 -0.00002 1.89660

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 A96 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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 D31 -1.02884 0.00000 0.00006 -0.00002 0.00004 -1.02880

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 D64 -1.02884 0.00000 0.00006 -0.00002 0.00004 -1.02880

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 D67 2.11275 0.00000 0.00006 -0.00002 0.00004 2.11279

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 D80 2.11275 0.00000 0.00006 -0.00002 0.00004 2.11279

 D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D82 1.02884 0.00000 -0.00006 0.00002 -0.00004 1.02880

 D83 -1.02884 0.00000 0.00006 -0.00002 0.00004 -1.02880

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 D123 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D124 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D125 1.02884 0.00000 -0.00006 0.00002 -0.00004 1.02880

 D126 -1.02884 0.00000 0.00006 -0.00002 0.00004 -1.02880

 D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D128 -2.11275 0.00000 -0.00006 0.00002 -0.00004 -2.11279

 D129 2.11275 0.00000 0.00006 -0.00002 0.00004 2.11279

 D130 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D131 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

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 D133 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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 D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D136 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 Item Value Threshold Converged?

 Maximum Force 0.000207 0.000450 YES

 RMS Force 0.000055 0.000300 YES

 Maximum Displacement 0.002896 0.001800 NO

 RMS Displacement 0.000852 0.001200 YES

 Predicted change in Energy=-1.518488D-06

 Lowest energy point so far. Saving SCF results.

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Leave Link 103 at Fri Jul 5 21:13:19 2019, MaxMem= 1342177280 cpu: 1.4

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

 Input orientation:

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

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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

 1 6 0 -2.066415 -2.178693 0.000000

 2 7 0 -0.745079 -1.856552 0.000000

 3 6 0 -0.005184 -2.988429 0.000000

 4 6 0 -0.935773 -4.161954 0.000000

 5 6 0 -2.188591 -3.644629 0.000000

 6 7 0 1.325250 -3.098463 0.000000

 7 6 0 2.178693 -2.066415 0.000000

 8 7 0 1.856552 -0.745079 0.000000

 9 6 0 2.988429 -0.005184 0.000000

 10 6 0 4.161954 -0.935773 0.000000

 11 6 0 3.644629 -2.188591 0.000000

 12 7 0 -3.098463 -1.325250 0.000000

 13 6 0 -4.161954 0.935773 0.000000

 14 6 0 -3.644629 2.188591 0.000000

 15 6 0 -2.178693 2.066415 0.000000

 16 7 0 -1.856552 0.745079 0.000000

 17 6 0 -2.988429 0.005184 0.000000

 18 7 0 -1.325250 3.098463 0.000000

 19 7 0 0.745079 1.856552 0.000000

 20 6 0 0.005184 2.988429 0.000000

 21 6 0 0.935773 4.161954 0.000000

 22 6 0 2.188591 3.644629 0.000000

 23 6 0 2.066415 2.178693 0.000000

 24 7 0 3.098463 1.325250 0.000000

 25 30 0 0.000000 0.000000 0.000000

 26 6 0 -0.480197 -5.573923 0.000000

 27 1 0 -3.128232 -4.177604 0.000000

 28 6 0 5.573923 -0.480197 0.000000

 29 1 0 4.177604 -3.128232 0.000000

 30 6 0 -5.573923 0.480197 0.000000

 31 1 0 -4.177604 3.128232 0.000000

 32 6 0 0.480197 5.573923 0.000000

 33 1 0 3.128232 4.177604 0.000000

 34 1 0 -1.324446 -6.263958 0.000000

 35 1 0 0.141368 -5.780804 0.876886

 36 1 0 0.141368 -5.780804 -0.876886

 37 1 0 5.780804 0.141368 0.876886

 38 1 0 5.780804 0.141368 -0.876886

 39 1 0 6.263958 -1.324446 0.000000

 40 1 0 -5.780804 -0.141368 0.876886

 41 1 0 -5.780804 -0.141368 -0.876886

 42 1 0 -6.263958 1.324446 0.000000

 43 1 0 -0.141368 5.780804 0.876886

 44 1 0 -0.141368 5.780804 -0.876886

 45 1 0 1.324446 6.263958 0.000000

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

 Distance matrix (angstroms):

 1 2 3 4 5

 1 C 0.000000

 2 N 1.360038 0.000000

 3 C 2.214576 1.352254 0.000000

 4 C 2.282910 2.313276 1.497717 0.000000

 5 C 1.471019 2.298031 2.279882 1.355425 0.000000

 6 N 3.514167 2.414251 1.334977 2.498647 3.556033

 7 C 4.246592 2.931294 2.370534 3.753822 4.643697

 8 N 4.176711 2.829108 2.915250 4.412722 4.977004

 9 C 5.502326 4.167330 4.226283 5.716476 6.328277

 10 C 6.351176 4.992675 4.645260 6.032832 6.904152

 11 C 5.711053 4.402248 3.736426 4.987409 6.012196

 12 N 1.339212 2.412613 3.512057 3.567088 2.491463

 13 C 3.753822 4.412722 5.716476 6.032832 4.987409

 14 C 4.643697 4.977004 6.328277 6.904152 6.012196

 15 C 4.246592 4.176711 5.502326 6.351176 5.711053

 16 N 2.931294 2.829108 4.167330 4.992675 4.402248

 17 C 2.370534 2.915250 4.226283 4.645260 3.736426

 18 N 5.328949 4.988865 6.228389 7.270856 6.798136

 19 N 4.918099 4.000963 4.902727 6.248814 6.234533

 20 C 5.566927 4.902727 5.976867 7.212030 6.986423

 21 C 7.015478 6.248814 7.212030 8.531714 8.408590

 22 C 7.212222 6.234533 6.986423 8.408590 8.502529

 23 C 6.005588 4.918099 5.566927 7.015478 7.212222

 24 N 6.241280 4.989657 5.314175 6.810615 7.256214

 25 Zn 3.002794 2.000481 2.988434 4.265857 4.251265

 26 C 3.747489 3.726797 2.628767 1.483646 2.576972

 27 H 2.263427 3.326665 3.341791 2.192515 1.080272

 28 C 7.826855 6.467159 6.116998 7.478735 8.382735

 29 H 6.315805 5.084287 4.185124 5.216819 6.387104

 30 C 4.401399 5.364525 6.560657 6.562165 5.336166

 31 H 5.711442 6.052297 7.404231 7.978489 7.058883

 32 C 8.160165 7.530820 8.576099 9.838307 9.597090

 33 H 8.208950 7.170325 7.821146 9.277088 9.458115

 34 H 4.152097 4.445323 3.531223 2.137635 2.758193

 35 H 4.314910 4.117582 2.930489 2.133035 3.280378

 36 H 4.314910 4.117582 2.930489 2.133035 3.280378

 37 H 8.229852 6.880971 6.636432 8.024957 8.866452

 38 H 8.229852 6.880971 6.636432 8.024957 8.866452

 39 H 8.374058 7.029205 6.486215 7.738706 8.765205

 40 H 4.326235 5.391597 6.498652 6.356758 5.093699

 41 H 4.326235 5.391597 6.498652 6.356758 5.093699

 42 H 5.467298 6.369989 7.600864 7.647884 6.426532

 43 H 8.235796 7.711200 8.814019 10.012915 9.684981

 44 H 8.235796 7.711200 8.814019 10.012915 9.684981

 45 H 9.098147 8.380072 9.347437 10.668094 10.512921

 6 7 8 9 10

 6 N 0.000000

 7 C 1.339212 0.000000

 8 N 2.412613 1.360038 0.000000

 9 C 3.512057 2.214576 1.352254 0.000000

 10 C 3.567088 2.282910 2.313276 1.497717 0.000000

 11 C 2.491463 1.471019 2.298031 2.279882 1.355425

 12 N 4.765871 5.328949 4.988865 6.228389 7.270856

 13 C 6.810615 7.015478 6.248814 7.212030 8.531714

 14 C 7.256214 7.212222 6.234533 6.986423 8.408590

 15 C 6.241280 6.005588 4.918099 5.566927 7.015478

 16 N 4.989657 4.918099 4.000963 4.902727 6.248814

 17 C 5.314175 5.566927 4.902727 5.976867 7.212030

 18 N 6.739959 6.241280 4.989657 5.314175 6.810615

 19 N 4.988865 4.176711 2.829108 2.915250 4.412722

 20 C 6.228389 5.502326 4.167330 4.226283 5.716476

 21 C 7.270856 6.351176 4.992675 4.645260 6.032832

 22 C 6.798136 5.711053 4.402248 3.736426 4.987409

 23 C 5.328949 4.246592 2.931294 2.370534 3.753822

 24 N 4.765871 3.514167 2.414251 1.334977 2.498647

 25 Zn 3.369980 3.002794 2.000481 2.988434 4.265857

 26 C 3.063909 4.401399 5.364525 6.560657 6.562165

 27 H 4.582363 5.711442 6.052297 7.404231 7.978489

 28 C 4.990646 3.747489 3.726797 2.628767 1.483646

 29 H 2.852509 2.263427 3.326665 3.341791 2.192515

 30 C 7.772091 8.160165 7.530820 8.576099 9.838307

 31 H 8.309822 8.208950 7.170325 7.821146 9.277088

 32 C 8.713461 7.826855 6.467159 6.116998 7.478735

 33 H 7.496125 6.315805 5.084287 4.185124 5.216819

 34 H 4.128104 5.467298 6.369989 7.600864 7.647884

 35 H 3.060304 4.326235 5.391597 6.498652 6.356758

 36 H 3.060304 4.326235 5.391597 6.498652 6.356758

 37 H 5.578298 4.314910 4.117582 2.930489 2.133035

 38 H 5.578298 4.314910 4.117582 2.930489 2.133035

 39 H 5.247664 4.152097 4.445323 3.531223 2.137635

 40 H 7.746570 8.235796 7.711200 8.814019 10.012915

 41 H 7.746570 8.235796 7.711200 8.814019 10.012915

 42 H 8.783974 9.098147 8.380072 9.347437 10.668094

 43 H 9.042195 8.229852 6.880971 6.636432 8.024957

 44 H 9.042195 8.229852 6.880971 6.636432 8.024957

 45 H 9.362421 8.374058 7.029205 6.486215 7.738706

 11 12 13 14 15

 11 C 0.000000

 12 N 6.798136 0.000000

 13 C 8.408590 2.498647 0.000000

 14 C 8.502529 3.556033 1.355425 0.000000

 15 C 7.212222 3.514167 2.282910 1.471019 0.000000

 16 N 6.234533 2.414251 2.313276 2.298031 1.360038

 17 C 6.986423 1.334977 1.497717 2.279882 2.214576

 18 N 7.256214 4.765871 3.567088 2.491463 1.339212

 19 N 4.977004 4.989657 4.992675 4.402248 2.931294

 20 C 6.328277 5.314175 4.645260 3.736426 2.370534

 21 C 6.904152 6.810615 6.032832 4.987409 3.753822

 22 C 6.012196 7.256214 6.904152 6.012196 4.643697

 23 C 4.643697 6.241280 6.351176 5.711053 4.246592

 24 N 3.556033 6.739959 7.270856 6.798136 5.328949

 25 Zn 4.251265 3.369980 4.265857 4.251265 3.002794

 26 C 5.336166 4.990646 7.478735 8.382735 7.826855

 27 H 7.058883 2.852509 5.216819 6.387104 6.315805

 28 C 2.576972 8.713461 9.838307 9.597090 8.160165

 29 H 1.080272 7.496125 9.277088 9.458115 8.208950

 30 C 9.597090 3.063909 1.483646 2.576972 3.747489

 31 H 9.458115 4.582363 2.192515 1.080272 2.263427

 32 C 8.382735 7.772091 6.562165 5.336166 4.401399

 33 H 6.387104 8.309822 7.978489 7.058883 5.711442

 34 H 6.426532 5.247664 7.738706 8.765205 8.374058

 35 H 5.093699 5.578298 8.024957 8.866452 8.229852

 36 H 5.093699 5.578298 8.024957 8.866452 8.229852

 37 H 3.280378 9.042195 10.012915 9.684981 8.235796

 38 H 3.280378 9.042195 10.012915 9.684981 8.235796

 39 H 2.758193 9.362421 10.668094 10.512921 9.098147

 40 H 9.684981 3.060304 2.133035 3.280378 4.314910

 41 H 9.684981 3.060304 2.133035 3.280378 4.314910

 42 H 10.512921 4.128104 2.137635 2.758193 4.152097

 43 H 8.866452 7.746570 6.356758 5.093699 4.326235

 44 H 8.866452 7.746570 6.356758 5.093699 4.326235

 45 H 8.765205 8.783974 7.647884 6.426532 5.467298

 16 17 18 19 20

 16 N 0.000000

 17 C 1.352254 0.000000

 18 N 2.412613 3.512057 0.000000

 19 N 2.829108 4.167330 2.414251 0.000000

 20 C 2.915250 4.226283 1.334977 1.352254 0.000000

 21 C 4.412722 5.716476 2.498647 2.313276 1.497717

 22 C 4.977004 6.328277 3.556033 2.298031 2.279882

 23 C 4.176711 5.502326 3.514167 1.360038 2.214576

 24 N 4.988865 6.228389 4.765871 2.412613 3.512057

 25 Zn 2.000481 2.988434 3.369980 2.000481 2.988434

 26 C 6.467159 6.116998 8.713461 7.530820 8.576099

 27 H 5.084287 4.185124 7.496125 7.170325 7.821146

 28 C 7.530820 8.576099 7.772091 5.364525 6.560657

 29 H 7.170325 7.821146 8.309822 6.052297 7.404231

 30 C 3.726797 2.628767 4.990646 6.467159 6.116998

 31 H 3.326665 3.341791 2.852509 5.084287 4.185124

 32 C 5.364525 6.560657 3.063909 3.726797 2.628767

 33 H 6.052297 7.404231 4.582363 3.326665 3.341791

 34 H 7.029205 6.486215 9.362421 8.380072 9.347437

 35 H 6.880971 6.636432 9.042195 7.711200 8.814019

 36 H 6.880971 6.636432 9.042195 7.711200 8.814019

 37 H 7.711200 8.814019 7.746570 5.391597 6.498652

 38 H 7.711200 8.814019 7.746570 5.391597 6.498652

 39 H 8.380072 9.347437 8.783974 6.369989 7.600864

 40 H 4.117582 2.930489 5.578298 6.880971 6.636432

 41 H 4.117582 2.930489 5.578298 6.880971 6.636432

 42 H 4.445323 3.531223 5.247664 7.029205 6.486215

 43 H 5.391597 6.498652 3.060304 4.117582 2.930489

 44 H 5.391597 6.498652 3.060304 4.117582 2.930489

 45 H 6.369989 7.600864 4.128104 4.445323 3.531223

 21 22 23 24 25

 21 C 0.000000

 22 C 1.355425 0.000000

 23 C 2.282910 1.471019 0.000000

 24 N 3.567088 2.491463 1.339212 0.000000

 25 Zn 4.265857 4.251265 3.002794 3.369980 0.000000

 26 C 9.838307 9.597090 8.160165 7.772091 5.594570

 27 H 9.277088 9.458115 8.208950 8.309822 5.219024

 28 C 6.562165 5.336166 4.401399 3.063909 5.594570

 29 H 7.978489 7.058883 5.711442 4.582363 5.219024

 30 C 7.478735 8.382735 7.826855 8.713461 5.594570

 31 H 5.216819 6.387104 6.315805 7.496125 5.219024

 32 C 1.483646 2.576972 3.747489 4.990646 5.594570

 33 H 2.192515 1.080272 2.263427 2.852509 5.219024

 34 H 10.668094 10.512921 9.098147 8.783974 6.402446

 35 H 10.012915 9.684981 8.235796 7.746570 5.848642

 36 H 10.012915 9.684981 8.235796 7.746570 5.848642

 37 H 6.356758 5.093699 4.326235 3.060304 5.848642

 38 H 6.356758 5.093699 4.326235 3.060304 5.848642

 39 H 7.647884 6.426532 5.467298 4.128104 6.402446

 40 H 8.024957 8.866452 8.229852 9.042195 5.848642

 41 H 8.024957 8.866452 8.229852 9.042195 5.848642

 42 H 7.738706 8.765205 8.374058 9.362421 6.402446

 43 H 2.133035 3.280378 4.314910 5.578298 5.848642

 44 H 2.133035 3.280378 4.314910 5.578298 5.848642

 45 H 2.137635 2.758193 4.152097 5.247664 6.402446

 26 27 28 29 30

 26 C 0.000000

 27 H 2.993627 0.000000

 28 C 7.911916 9.455069 0.000000

 29 H 5.260847 7.380814 2.993627 0.000000

 30 C 7.911916 5.260847 11.189139 10.397742 0.000000

 31 H 9.455069 7.380814 10.397742 10.438048 2.993627

 32 C 11.189139 10.397742 7.911916 9.455069 7.911916

 33 H 10.397742 10.438048 5.260847 7.380814 9.455069

 34 H 1.090368 2.757992 9.002188 6.332876 7.971304

 35 H 1.094565 3.745594 7.640551 4.908794 8.522536

 36 H 1.094565 3.745594 7.640551 4.908794 8.522536

 37 H 8.522536 9.939486 1.094565 3.745594 11.393576

 38 H 8.522536 9.939486 1.094565 3.745594 11.393576

 39 H 7.971304 9.815994 1.090368 2.757992 11.974646

 40 H 7.640551 4.908794 11.393576 10.433608 1.094565

 41 H 7.640551 4.908794 11.393576 10.433608 1.094565

 42 H 9.002188 6.332876 11.974646 11.351323 1.090368

 43 H 11.393576 10.433608 8.522536 9.939486 7.640551

 44 H 11.393576 10.433608 8.522536 9.939486 7.640551

 45 H 11.974646 11.351323 7.971304 9.815994 9.002188

 31 32 33 34 35

 31 H 0.000000

 32 C 5.260847 0.000000

 33 H 7.380814 2.993627 0.000000

 34 H 9.815994 11.974646 11.351323 0.000000

 35 H 9.939486 11.393576 10.433608 1.775099 0.000000

 36 H 9.939486 11.393576 10.433608 1.775099 1.753773

 37 H 10.433608 7.640551 4.908794 9.606337 8.177736

 38 H 10.433608 7.640551 4.908794 9.606337 8.363677

 39 H 11.351323 9.002188 6.332876 9.054427 7.623265

 40 H 3.745594 8.522536 9.939486 7.623265 8.177736

 41 H 3.745594 8.522536 9.939486 7.623265 8.363677

 42 H 2.757992 7.971304 9.815994 9.054427 9.606337

 43 H 4.908794 1.094565 3.745594 12.134451 11.565066

 44 H 4.908794 1.094565 3.745594 12.134451 11.697284

 45 H 6.332876 1.090368 2.757992 12.804893 12.134451

 36 37 38 39 40

 36 H 0.000000

 37 H 8.363677 0.000000

 38 H 8.177736 1.753773 0.000000

 39 H 7.623265 1.775099 1.775099 0.000000

 40 H 8.363677 11.565066 11.697284 12.134451 0.000000

 41 H 8.177736 11.697284 11.565066 12.134451 1.753773

 42 H 9.606337 12.134451 12.134451 12.804893 1.775099

 43 H 11.697284 8.177736 8.363677 9.606337 8.177736

 44 H 11.565066 8.363677 8.177736 9.606337 8.363677

 45 H 12.134451 7.623265 7.623265 9.054427 9.606337

 41 42 43 44 45

 41 H 0.000000

 42 H 1.775099 0.000000

 43 H 8.363677 7.623265 0.000000

 44 H 8.177736 7.623265 1.753773 0.000000

 45 H 9.606337 9.054427 1.775099 1.775099 0.000000

 Stoichiometry C20H16N8Zn(1+,2)

 Framework group C4H[O(Zn),SGH(C20H8N8),X(H8)]

 Deg. of freedom 20

 Full point group C4H NOp 8

 RotChk: IX=0 Diff= 2.87D-04

 Largest Abelian subgroup C2H NOp 4

 Largest concise Abelian subgroup C2H NOp 4

 Standard orientation:

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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

 1 6 0 -2.182274 2.062632 0.000000

 2 7 0 -1.857841 0.741857 0.000000

 3 6 0 -2.988434 0.000000 0.000000

 4 6 0 -4.163571 0.928552 0.000000

 5 6 0 -3.648420 2.182265 0.000000

 6 7 0 -3.096160 -1.330623 0.000000

 7 6 0 -2.062632 -2.182274 0.000000

 8 7 0 -0.741857 -1.857841 0.000000

 9 6 0 0.000000 -2.988434 0.000000

 10 6 0 -0.928552 -4.163571 0.000000

 11 6 0 -2.182265 -3.648420 0.000000

 12 7 0 -1.330623 3.096160 0.000000

 13 6 0 0.928552 4.163571 0.000000

 14 6 0 2.182265 3.648420 0.000000

 15 6 0 2.062632 2.182274 0.000000

 16 7 0 0.741857 1.857841 0.000000

 17 6 0 0.000000 2.988434 0.000000

 18 7 0 3.096160 1.330623 0.000000

 19 7 0 1.857841 -0.741857 0.000000

 20 6 0 2.988434 0.000000 0.000000

 21 6 0 4.163571 -0.928552 0.000000

 22 6 0 3.648420 -2.182265 0.000000

 23 6 0 2.182274 -2.062632 0.000000

 24 7 0 1.330623 -3.096160 0.000000

 25 30 0 0.000000 0.000000 0.000000

 26 6 0 -5.574748 0.470527 0.000000

 27 1 0 -4.183024 3.120980 0.000000

 28 6 0 -0.470527 -5.574748 0.000000

 29 1 0 -3.120980 -4.183024 0.000000

 30 6 0 0.470527 5.574748 0.000000

 31 1 0 3.120980 4.183024 0.000000

 32 6 0 5.574748 -0.470527 0.000000

 33 1 0 4.183024 -3.120980 0.000000

 34 1 0 -6.266246 1.313577 0.000000

 35 1 0 -5.780551 -0.151397 0.876886

 36 1 0 -5.780551 -0.151397 -0.876886

 37 1 0 0.151397 -5.780551 0.876886

 38 1 0 0.151397 -5.780551 -0.876886

 39 1 0 -1.313577 -6.266246 0.000000

 40 1 0 -0.151397 5.780551 0.876886

 41 1 0 -0.151397 5.780551 -0.876886

 42 1 0 1.313577 6.266246 0.000000

 43 1 0 5.780551 0.151397 0.876886

 44 1 0 5.780551 0.151397 -0.876886

 45 1 0 6.266246 -1.313577 0.000000

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

 Rotational constants (GHZ): 0.1830366 0.1830366 0.0917243

 Leave Link 202 at Fri Jul 5 21:13:19 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 229 symmetry adapted cartesian basis functions of AG symmetry.

 There are 82 symmetry adapted cartesian basis functions of BG symmetry.

 There are 78 symmetry adapted cartesian basis functions of AU symmetry.

 There are 218 symmetry adapted cartesian basis functions of BU symmetry.

 There are 212 symmetry adapted basis functions of AG symmetry.

 There are 82 symmetry adapted basis functions of BG symmetry.

 There are 78 symmetry adapted basis functions of AU symmetry.

 There are 204 symmetry adapted basis functions of BU symmetry.

 576 basis functions, 1015 primitive gaussians, 607 cartesian basis functions

 102 alpha electrons 101 beta electrons

 nuclear repulsion energy 2766.6963647715 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= 45 NActive= 45 NUniq= 11 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= -0.1142450957 Hartrees.

 Nuclear repulsion after empirical dispersion term = 2766.5821196758 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= 45.

 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 = 45

 GePol: Total number of spheres = 45

 GePol: Number of exposed spheres = 45 (100.00%)

 GePol: Number of points = 3538

 GePol: Average weight of points = 0.11

 GePol: Minimum weight of points = 0.69D-11

 GePol: Maximum weight of points = 0.18390

 GePol: Number of points with low weight = 160

 GePol: Fraction of low-weight points (<1% of avg) = 4.52%

 GePol: Cavity surface area = 382.114 Ang\*\*2

 GePol: Cavity volume = 379.149 Ang\*\*3

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

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 PCM non-electrostatic energy = -0.0110998430 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 2766.5710198328 Hartrees.

 Leave Link 301 at Fri Jul 5 21:13:19 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

 One-electron integrals computed using PRISM.

 One-electron integral symmetry used in STVInt

 8 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15383 LenP2D= 41364.

 LDataN: DoStor=T MaxTD1= 5 Len= 102

 NBasis= 576 RedAO= T EigKep= 1.86D-04 NBF= 212 82 78 204

 NBsUse= 576 1.00D-06 EigRej= -1.00D+00 NBFU= 212 82 78 204

 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= 594 594 594 594 594 MxSgAt= 45 MxSgA2= 45.

 Leave Link 302 at Fri Jul 5 21:13:19 2019, MaxMem= 1342177280 cpu: 7.7

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

 DipDrv: MaxL=1.

 Leave Link 303 at Fri Jul 5 21:13:20 2019, MaxMem= 1342177280 cpu: 1.1

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

 Initial guess from the checkpoint file: "ZntAzPcation.chk"

 B after Tr= 0.000000 0.000000 0.000000

 Rot= 1.000000 0.000000 0.000000 -0.000064 Ang= -0.01 deg.

 Guess basis will be translated and rotated to current coordinates.

 JPrj=2 DoOrth=T DoCkMO=T.

 Initial guess orbital symmetries:

 Alpha Orbitals:

 Occupied (BG) (EU) (EU) (AG) (EU) (EU) (BG) (AG) (BG) (EU)

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

 Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7819 S= 0.5158

 Leave Link 401 at Fri Jul 5 21:13:21 2019, MaxMem= 1342177280 cpu: 21.7

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

 UHF open shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 1138797 IEndB= 1138797 NGot= 1342177280 MDV= 1341424180

 LenX= 1341424180 LenY= 1341055124

 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= 670000000 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= 37552332.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 7.55D-15 for 252.

 Iteration 1 A\*A^-1 deviation from orthogonality is 3.56D-15 for 3161 850.

 Iteration 1 A^-1\*A deviation from unit magnitude is 8.10D-15 for 553.

 Iteration 1 A^-1\*A deviation from orthogonality is 1.10D-14 for 1948 1904.

 E= -1275.69949886719

 DIIS: error= 7.23D-05 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -1275.69949886719 IErMin= 1 ErrMin= 7.23D-05

 ErrMax= 7.23D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.57D-06 BMatP= 6.57D-06

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

 Coeff-Com: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.372 Goal= None Shift= 0.000

 Gap= 0.406 Goal= None Shift= 0.000

 RMSDP=3.54D-06 MaxDP=1.19D-04 OVMax= 6.55D-04

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 3.54D-06 CP: 1.00D+00

 E= -1275.69950154482 Delta-E= -0.000002677623 Rises=F Damp=F

 DIIS: error= 1.58D-05 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -1275.69950154482 IErMin= 2 ErrMin= 1.58D-05

 ErrMax= 1.58D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.56D-07 BMatP= 6.57D-06

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

 Coeff-Com: 0.271D-01 0.973D+00

 Coeff: 0.271D-01 0.973D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=9.14D-07 MaxDP=4.00D-05 DE=-2.68D-06 OVMax= 1.88D-04

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 9.06D-07 CP: 1.00D+00 1.03D+00

 E= -1275.69950148951 Delta-E= 0.000000055305 Rises=F Damp=F

 DIIS: error= 2.59D-05 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 2 EnMin= -1275.69950154482 IErMin= 2 ErrMin= 1.58D-05

 ErrMax= 2.59D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.70D-07 BMatP= 3.56D-07

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

 Coeff-Com: -0.290D-01 0.600D+00 0.429D+00

 Coeff: -0.290D-01 0.600D+00 0.429D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=5.81D-07 MaxDP=2.59D-05 DE= 5.53D-08 OVMax= 1.42D-04

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 3.31D-07 CP: 1.00D+00 1.05D+00 4.81D-01

 E= -1275.69950164832 Delta-E= -0.000000158807 Rises=F Damp=F

 DIIS: error= 4.92D-06 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -1275.69950164832 IErMin= 4 ErrMin= 4.92D-06

 ErrMax= 4.92D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.27D-08 BMatP= 3.56D-07

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

 Coeff-Com: -0.142D-01 0.169D+00 0.205D+00 0.640D+00

 Coeff: -0.142D-01 0.169D+00 0.205D+00 0.640D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=1.24D-07 MaxDP=4.52D-06 DE=-1.59D-07 OVMax= 5.73D-05

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 1.09D-07 CP: 1.00D+00 1.06D+00 5.37D-01 9.46D-01

 E= -1275.69950165430 Delta-E= -0.000000005978 Rises=F Damp=F

 DIIS: error= 1.24D-06 at cycle 5 NSaved= 5.

 NSaved= 5 IEnMin= 5 EnMin= -1275.69950165430 IErMin= 5 ErrMin= 1.24D-06

 ErrMax= 1.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.96D-09 BMatP= 2.27D-08

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

 Coeff-Com: -0.468D-02 0.390D-01 0.771D-01 0.297D+00 0.592D+00

 Coeff: -0.468D-02 0.390D-01 0.771D-01 0.297D+00 0.592D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=5.11D-08 MaxDP=2.08D-06 DE=-5.98D-09 OVMax= 3.42D-05

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 3.73D-08 CP: 1.00D+00 1.06D+00 5.54D-01 1.04D+00 1.05D+00

 E= -1275.69950165539 Delta-E= -0.000000001096 Rises=F Damp=F

 DIIS: error= 8.71D-07 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -1275.69950165539 IErMin= 6 ErrMin= 8.71D-07

 ErrMax= 8.71D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.54D-10 BMatP= 1.96D-09

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

 Coeff-Com: 0.184D-02-0.289D-01-0.142D-01-0.449D-01 0.214D+00 0.872D+00

 Coeff: 0.184D-02-0.289D-01-0.142D-01-0.449D-01 0.214D+00 0.872D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=4.69D-08 MaxDP=1.89D-06 DE=-1.10D-09 OVMax= 3.62D-05

 Cycle 7 Pass 1 IDiag 1:

 RMSU= 2.32D-08 CP: 1.00D+00 1.06D+00 5.69D-01 1.11D+00 1.30D+00

 CP: 1.28D+00

 E= -1275.69950165571 Delta-E= -0.000000000316 Rises=F Damp=F

 DIIS: error= 5.33D-07 at cycle 7 NSaved= 7.

 NSaved= 7 IEnMin= 7 EnMin= -1275.69950165571 IErMin= 7 ErrMin= 5.33D-07

 ErrMax= 5.33D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.57D-10 BMatP= 3.54D-10

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

 Coeff-Com: 0.203D-02-0.261D-01-0.229D-01-0.859D-01 0.130D-01 0.523D+00

 Coeff-Com: 0.597D+00

 Coeff: 0.203D-02-0.261D-01-0.229D-01-0.859D-01 0.130D-01 0.523D+00

 Coeff: 0.597D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=2.22D-08 MaxDP=1.05D-06 DE=-3.16D-10 OVMax= 1.46D-05

 Cycle 8 Pass 1 IDiag 1:

 RMSU= 1.07D-08 CP: 1.00D+00 1.06D+00 5.75D-01 1.14D+00 1.40D+00

 CP: 1.57D+00 1.16D+00

 E= -1275.69950165577 Delta-E= -0.000000000061 Rises=F Damp=F

 DIIS: error= 2.49D-07 at cycle 8 NSaved= 8.

 NSaved= 8 IEnMin= 8 EnMin= -1275.69950165577 IErMin= 8 ErrMin= 2.49D-07

 ErrMax= 2.49D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.53D-11 BMatP= 1.57D-10

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

 Coeff-Com: -0.216D-03 0.635D-02 0.212D-03-0.824D-02-0.123D+00-0.284D+00

 Coeff-Com: 0.274D+00 0.113D+01

 Coeff: -0.216D-03 0.635D-02 0.212D-03-0.824D-02-0.123D+00-0.284D+00

 Coeff: 0.274D+00 0.113D+01

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=2.46D-08 MaxDP=1.33D-06 DE=-6.09D-11 OVMax= 1.35D-05

 Cycle 9 Pass 1 IDiag 1:

 RMSU= 7.17D-09 CP: 1.00D+00 1.06D+00 5.79D-01 1.16D+00 1.50D+00

 CP: 1.87D+00 1.70D+00 1.54D+00

 E= -1275.69950165586 Delta-E= -0.000000000094 Rises=F Damp=F

 DIIS: error= 1.25D-07 at cycle 9 NSaved= 9.

 NSaved= 9 IEnMin= 9 EnMin= -1275.69950165586 IErMin= 9 ErrMin= 1.25D-07

 ErrMax= 1.25D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.43D-12 BMatP= 3.53D-11

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

 Coeff-Com: -0.394D-03 0.624D-02 0.377D-02 0.112D-01-0.357D-01-0.159D+00

 Coeff-Com: 0.135D-01 0.318D+00 0.843D+00

 Coeff: -0.394D-03 0.624D-02 0.377D-02 0.112D-01-0.357D-01-0.159D+00

 Coeff: 0.135D-01 0.318D+00 0.843D+00

 Gap= 0.104 Goal= None Shift= 0.000

 Gap= 0.083 Goal= None Shift= 0.000

 RMSDP=6.35D-09 MaxDP=4.11D-07 DE=-9.37D-11 OVMax= 3.11D-06

 Error on total polarization charges = 0.06026

 SCF Done: E(UB3LYP) = -1275.69950166 A.U. after 9 cycles

 NFock= 9 Conv=0.64D-08 -V/T= 1.9660

 <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.5000 <S\*\*2>= 0.7819 S= 0.5158

 <L.S>= 0.000000000000E+00

 KE= 1.320598028643D+03 PE=-8.556975834555D+03 EE= 3.194107284423D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.97

 (included in total energy above)

 Annihilation of the first spin contaminant:

 S\*\*2 before annihilation 0.7819, after 0.7509

 Leave Link 502 at Fri Jul 5 21:14:19 2019, MaxMem= 1342177280 cpu: 657.7

 (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.

 8 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 19306 NPrTT= 91506 LenC2= 15383 LenP2D= 41364.

 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 = 248

 Leave Link 701 at Fri Jul 5 21:14:24 2019, MaxMem= 1342177280 cpu: 53.3

 (Enter /apps/gaussian/g09d01/g09/l702.exe)

 L702 exits ... SP integral derivatives will be done elsewhere.

 Leave Link 702 at Fri Jul 5 21:14:24 2019, MaxMem= 1342177280 cpu: 0.2

 (Enter /apps/gaussian/g09d01/g09/l703.exe)

 Compute integral first derivatives, UseDBF=F ICtDFT= 0.

 Integral derivatives from FoFJK, PRISM(SPDF).

 Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

 FoFJK: IHMeth= 1 ICntrl= 2127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

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

 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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 Fri Jul 5 21:14:32 2019, MaxMem= 1342177280 cpu: 92.4

 (Enter /apps/gaussian/g09d01/g09/l716.exe)

 Dipole = 4.05009359D-13 2.04281037D-13 0.00000000D+00

 \*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

 Center Atomic Forces (Hartrees/Bohr)

 Number Number X Y Z

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

 1 6 -0.000135460 -0.000083215 0.000000000

 2 7 0.000147749 0.000070182 0.000000000

 3 6 -0.000166317 -0.000012274 0.000000000

 4 6 -0.000002228 0.000012154 0.000000000

 5 6 -0.000025779 0.000080556 0.000000000

 6 7 0.000067498 0.000023114 0.000000000

 7 6 0.000083215 -0.000135460 0.000000000

 8 7 -0.000070182 0.000147749 0.000000000

 9 6 0.000012274 -0.000166317 0.000000000

 10 6 -0.000012154 -0.000002228 0.000000000

 11 6 -0.000080556 -0.000025779 0.000000000

 12 7 0.000023114 -0.000067498 0.000000000

 13 6 0.000012154 0.000002228 0.000000000

 14 6 0.000080556 0.000025779 0.000000000

 15 6 -0.000083215 0.000135460 0.000000000

 16 7 0.000070182 -0.000147749 0.000000000

 17 6 -0.000012274 0.000166317 0.000000000

 18 7 -0.000067498 -0.000023114 0.000000000

 19 7 -0.000147749 -0.000070182 0.000000000

 20 6 0.000166317 0.000012274 0.000000000

 21 6 0.000002228 -0.000012154 0.000000000

 22 6 0.000025779 -0.000080556 0.000000000

 23 6 0.000135460 0.000083215 0.000000000

 24 7 -0.000023114 0.000067498 0.000000000

 25 30 0.000000000 0.000000000 0.000000000

 26 6 -0.000004128 -0.000010487 0.000000000

 27 1 -0.000021841 0.000010315 0.000000000

 28 6 0.000010487 -0.000004128 0.000000000

 29 1 -0.000010315 -0.000021841 0.000000000

 30 6 -0.000010487 0.000004128 0.000000000

 31 1 0.000010315 0.000021841 0.000000000

 32 6 0.000004128 0.000010487 0.000000000

 33 1 0.000021841 -0.000010315 0.000000000

 34 1 -0.000029422 0.000005172 0.000000000

 35 1 -0.000037997 0.000006278 -0.000002224

 36 1 -0.000037997 0.000006278 0.000002224

 37 1 -0.000006278 -0.000037997 -0.000002224

 38 1 -0.000006278 -0.000037997 0.000002224

 39 1 -0.000005172 -0.000029422 0.000000000

 40 1 0.000006278 0.000037997 -0.000002224

 41 1 0.000006278 0.000037997 0.000002224

 42 1 0.000005172 0.000029422 0.000000000

 43 1 0.000037997 -0.000006278 -0.000002224

 44 1 0.000037997 -0.000006278 0.000002224

 45 1 0.000029422 -0.000005172 0.000000000

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

 Cartesian Forces: Max 0.000166317 RMS 0.000053560

 Leave Link 716 at Fri Jul 5 21:14:32 2019, MaxMem= 1342177280 cpu: 0.3

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

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Berny optimization.

 Using GEDIIS/GDIIS optimizer.

 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

 GSVD: received Info= 1 from GESDD.

 Internal Forces: Max 0.000096381 RMS 0.000019584

 Search for a local minimum.

 Step number 5 out of a maximum of 270

 All quantities printed in internal units (Hartrees-Bohrs-Radians)

 RMS Force = .19584D-04 SwitMx=.10000D-02 MixMth= 2

 Mixed Optimization -- En-DIIS/RFO-DIIS

 Swapping is turned off.

 Update second derivatives using D2CorX and points 1 2 3 4 5

 DE= -1.00D-07 DEPred=-1.52D-06 R= 6.59D-02

 Trust test= 6.59D-02 RLast= 4.12D-03 DXMaxT set to 1.64D-01

 ITU= -1 1 1 1 0

 Eigenvalues --- 0.00878 0.00878 0.00878 0.00878 0.01343

 Eigenvalues --- 0.01345 0.01345 0.01345 0.01600 0.01618

 Eigenvalues --- 0.01631 0.01631 0.01777 0.01792 0.01819

 Eigenvalues --- 0.01819 0.01890 0.01906 0.01943 0.01943

 Eigenvalues --- 0.01998 0.01999 0.02045 0.02045 0.02070

 Eigenvalues --- 0.02088 0.02102 0.02113 0.02113 0.02205

 Eigenvalues --- 0.02316 0.02316 0.02352 0.02374 0.07152

 Eigenvalues --- 0.07210 0.07210 0.07210 0.07210 0.07404

 Eigenvalues --- 0.07404 0.07404 0.12187 0.14501 0.14501

 Eigenvalues --- 0.15897 0.16000 0.16000 0.16000 0.16000

 Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000

 Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16007

 Eigenvalues --- 0.16516 0.17929 0.20123 0.22084 0.22084

 Eigenvalues --- 0.23767 0.23811 0.23847 0.23847 0.24544

 Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

 Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000

 Eigenvalues --- 0.25058 0.30893 0.33173 0.33173 0.33215

 Eigenvalues --- 0.33282 0.33282 0.33282 0.33448 0.33718

 Eigenvalues --- 0.33724 0.33724 0.33724 0.33724 0.33724

 Eigenvalues --- 0.33724 0.33724 0.34353 0.34437 0.34437

 Eigenvalues --- 0.34437 0.35176 0.35379 0.35573 0.35573

 Eigenvalues --- 0.35682 0.35682 0.35682 0.36240 0.39287

 Eigenvalues --- 0.41753 0.41753 0.42576 0.45927 0.48969

 Eigenvalues --- 0.48969 0.49008 0.50265 0.50567 0.51356

 Eigenvalues --- 0.51356 0.52270 0.53984 0.53984 0.54930

 Eigenvalues --- 0.56214 0.56277 0.56331 0.56331

 En-DIIS/RFO-DIIS IScMMF= 0 using points: 5 4 3 2

 RFO step: Lambda=-1.99512507D-07.

 NNeg= 0 NP= 4 Switch= 2.50D-03 Rises=F DC= 2.59D-04 SmlDif= 1.00D-05

 RMS Error= 0.3698654048D-04 NUsed= 4 EDIIS=F

 DidBck=F Rises=F RFO-DIIS coefs: 1.28243 -0.28403 -0.01157 0.01316

 Iteration 1 RMS(Cart)= 0.00021472 RMS(Int)= 0.00000003

 Iteration 2 RMS(Cart)= 0.00000003 RMS(Int)= 0.00000003

 ITry= 1 IFail=0 DXMaxC= 8.23D-04 DCOld= 1.00D+10 DXMaxT= 1.64D-01 DXLimC= 3.00D+00 Rises=F

 ClnCor: largest displacement from symmetrization is 5.07D-10 for atom 40.

 Variable Old X -DE/DX Delta X Delta X Delta X New X

 (Linear) (Quad) (Total)

 R1 2.57010 0.00010 0.00013 0.00017 0.00029 2.57039

 R2 2.77982 -0.00005 -0.00023 0.00001 -0.00022 2.77960

 R3 2.53074 -0.00003 -0.00003 -0.00005 -0.00008 2.53066

 R4 2.55539 -0.00003 0.00000 -0.00010 -0.00010 2.55529

 R5 3.78036 -0.00003 -0.00007 -0.00010 -0.00018 3.78019

 R6 2.83028 -0.00003 -0.00015 0.00005 -0.00010 2.83017

 R7 2.52274 0.00008 0.00009 0.00010 0.00019 2.52293

 R8 2.56138 0.00002 0.00014 -0.00007 0.00006 2.56144

 R9 2.80369 0.00000 0.00002 0.00000 0.00002 2.80371

 R10 2.04142 0.00000 0.00001 0.00001 0.00001 2.04143

 R11 2.53074 -0.00003 -0.00003 -0.00005 -0.00008 2.53066

 R12 2.57010 0.00010 0.00013 0.00017 0.00029 2.57039

 R13 2.77982 -0.00005 -0.00023 0.00001 -0.00022 2.77960

 R14 2.55539 -0.00003 0.00000 -0.00010 -0.00010 2.55529

 R15 3.78036 -0.00003 -0.00007 -0.00010 -0.00018 3.78019

 R16 2.83028 -0.00003 -0.00015 0.00005 -0.00010 2.83017

 R17 2.52274 0.00008 0.00009 0.00010 0.00019 2.52293

 R18 2.56138 0.00002 0.00014 -0.00007 0.00006 2.56144

 R19 2.80369 0.00000 0.00002 0.00000 0.00002 2.80371

 R20 2.04142 0.00000 0.00001 0.00001 0.00001 2.04143

 R21 2.52274 0.00008 0.00009 0.00010 0.00019 2.52293

 R22 2.56138 0.00002 0.00014 -0.00007 0.00006 2.56144

 R23 2.83028 -0.00003 -0.00015 0.00005 -0.00010 2.83017

 R24 2.80369 0.00000 0.00002 0.00000 0.00002 2.80371

 R25 2.77982 -0.00005 -0.00023 0.00001 -0.00022 2.77960

 R26 2.04142 0.00000 0.00001 0.00001 0.00001 2.04143

 R27 2.57010 0.00010 0.00013 0.00017 0.00029 2.57039

 R28 2.53074 -0.00003 -0.00003 -0.00005 -0.00008 2.53066

 R29 2.55539 -0.00003 0.00000 -0.00010 -0.00010 2.55529

 R30 3.78036 -0.00003 -0.00007 -0.00010 -0.00018 3.78019

 R31 2.52274 0.00008 0.00009 0.00010 0.00019 2.52293

 R32 2.55539 -0.00003 0.00000 -0.00010 -0.00010 2.55529

 R33 2.57010 0.00010 0.00013 0.00017 0.00029 2.57039

 R34 3.78036 -0.00003 -0.00007 -0.00010 -0.00018 3.78019

 R35 2.83028 -0.00003 -0.00015 0.00005 -0.00010 2.83017

 R36 2.56138 0.00002 0.00014 -0.00007 0.00006 2.56144

 R37 2.80369 0.00000 0.00002 0.00000 0.00002 2.80371

 R38 2.77982 -0.00005 -0.00023 0.00001 -0.00022 2.77960

 R39 2.04142 0.00000 0.00001 0.00001 0.00001 2.04143

 R40 2.53074 -0.00003 -0.00003 -0.00005 -0.00008 2.53066

 R41 2.06050 0.00000 0.00003 -0.00002 0.00000 2.06050

 R42 2.06843 -0.00001 0.00004 -0.00005 -0.00001 2.06842

 R43 2.06843 -0.00001 0.00004 -0.00005 -0.00001 2.06842

 R44 2.06843 -0.00001 0.00004 -0.00005 -0.00001 2.06842

 R45 2.06843 -0.00001 0.00004 -0.00005 -0.00001 2.06842

 R46 2.06050 0.00000 0.00003 -0.00002 0.00000 2.06050

 R47 2.06843 -0.00001 0.00004 -0.00005 -0.00001 2.06842

 R48 2.06843 -0.00001 0.00004 -0.00005 -0.00001 2.06842

 R49 2.06050 0.00000 0.00003 -0.00002 0.00000 2.06050

 R50 2.06843 -0.00001 0.00004 -0.00005 -0.00001 2.06842

 R51 2.06843 -0.00001 0.00004 -0.00005 -0.00001 2.06842

 R52 2.06050 0.00000 0.00003 -0.00002 0.00000 2.06050

 A1 1.89308 0.00001 0.00004 0.00001 0.00005 1.89313

 A2 2.21150 -0.00002 -0.00007 -0.00005 -0.00012 2.21138

 A3 2.17860 0.00002 0.00003 0.00004 0.00007 2.17867

 A4 1.91062 -0.00004 -0.00008 -0.00008 -0.00016 1.91047

 A5 2.19158 0.00001 0.00004 0.00001 0.00005 2.19163

 A6 2.18098 0.00003 0.00004 0.00007 0.00010 2.18109

 A7 1.89218 0.00003 0.00006 0.00007 0.00013 1.89231

 A8 2.23228 -0.00002 -0.00004 -0.00002 -0.00006 2.23221

 A9 2.15873 -0.00001 -0.00002 -0.00004 -0.00006 2.15866

 A10 1.84964 0.00000 -0.00002 0.00000 -0.00003 1.84962

 A11 2.15904 -0.00003 -0.00018 -0.00004 -0.00023 2.15881

 A12 2.27451 0.00002 0.00021 0.00005 0.00025 2.27476

 A13 1.87925 0.00000 0.00001 0.00000 0.00001 1.87926

 A14 2.16991 0.00001 -0.00008 0.00006 -0.00002 2.16989

 A15 2.23403 0.00000 0.00007 -0.00006 0.00001 2.23404

 A16 2.17923 0.00000 0.00003 0.00000 0.00002 2.17926

 A17 2.21150 -0.00002 -0.00007 -0.00005 -0.00012 2.21138

 A18 2.17860 0.00002 0.00003 0.00004 0.00007 2.17867

 A19 1.89308 0.00001 0.00004 0.00001 0.00005 1.89313

 A20 1.91062 -0.00004 -0.00008 -0.00008 -0.00016 1.91047

 A21 2.19158 0.00001 0.00004 0.00001 0.00005 2.19163

 A22 2.18098 0.00003 0.00004 0.00007 0.00010 2.18109

 A23 1.89218 0.00003 0.00006 0.00007 0.00013 1.89231

 A24 2.23228 -0.00002 -0.00004 -0.00002 -0.00006 2.23221

 A25 2.15873 -0.00001 -0.00002 -0.00004 -0.00006 2.15866

 A26 1.84964 0.00000 -0.00002 0.00000 -0.00003 1.84962

 A27 2.15904 -0.00003 -0.00018 -0.00004 -0.00023 2.15881

 A28 2.27451 0.00002 0.00021 0.00005 0.00025 2.27476

 A29 1.87925 0.00000 0.00001 0.00000 0.00001 1.87926

 A30 2.16991 0.00001 -0.00008 0.00006 -0.00002 2.16989

 A31 2.23403 0.00000 0.00007 -0.00006 0.00001 2.23404

 A32 2.17923 0.00000 0.00003 0.00000 0.00002 2.17926

 A33 1.84964 0.00000 -0.00002 0.00000 -0.00003 1.84962

 A34 2.27451 0.00002 0.00021 0.00005 0.00025 2.27476

 A35 2.15904 -0.00003 -0.00018 -0.00004 -0.00023 2.15881

 A36 1.87925 0.00000 0.00001 0.00000 0.00001 1.87926

 A37 2.23403 0.00000 0.00007 -0.00006 0.00001 2.23404

 A38 2.16991 0.00001 -0.00008 0.00006 -0.00002 2.16989

 A39 1.89308 0.00001 0.00004 0.00001 0.00005 1.89313

 A40 2.17860 0.00002 0.00003 0.00004 0.00007 2.17867

 A41 2.21150 -0.00002 -0.00007 -0.00005 -0.00012 2.21138

 A42 1.91062 -0.00004 -0.00008 -0.00008 -0.00016 1.91047

 A43 2.19158 0.00001 0.00004 0.00001 0.00005 2.19163

 A44 2.18098 0.00003 0.00004 0.00007 0.00010 2.18109

 A45 2.15873 -0.00001 -0.00002 -0.00004 -0.00006 2.15866

 A46 2.23228 -0.00002 -0.00004 -0.00002 -0.00006 2.23221

 A47 1.89218 0.00003 0.00006 0.00007 0.00013 1.89231

 A48 2.17923 0.00000 0.00003 0.00000 0.00002 2.17926

 A49 1.91062 -0.00004 -0.00008 -0.00008 -0.00016 1.91047

 A50 2.18098 0.00003 0.00004 0.00007 0.00010 2.18109

 A51 2.19158 0.00001 0.00004 0.00001 0.00005 2.19163

 A52 2.23228 -0.00002 -0.00004 -0.00002 -0.00006 2.23221

 A53 2.15873 -0.00001 -0.00002 -0.00004 -0.00006 2.15866

 A54 1.89218 0.00003 0.00006 0.00007 0.00013 1.89231

 A55 1.84964 0.00000 -0.00002 0.00000 -0.00003 1.84962

 A56 2.15904 -0.00003 -0.00018 -0.00004 -0.00023 2.15881

 A57 2.27451 0.00002 0.00021 0.00005 0.00025 2.27476

 A58 1.87925 0.00000 0.00001 0.00000 0.00001 1.87926

 A59 2.23403 0.00000 0.00007 -0.00006 0.00001 2.23404

 A60 2.16991 0.00001 -0.00008 0.00006 -0.00002 2.16989

 A61 1.89308 0.00001 0.00004 0.00001 0.00005 1.89313

 A62 2.21150 -0.00002 -0.00007 -0.00005 -0.00012 2.21138

 A63 2.17860 0.00002 0.00003 0.00004 0.00007 2.17867

 A64 2.17923 0.00000 0.00003 0.00000 0.00002 2.17926

 A65 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

 A66 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

 A67 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

 A68 1.57080 0.00000 0.00000 0.00000 0.00000 1.57080

 A69 1.94391 0.00001 0.00009 0.00002 0.00010 1.94401

 A70 1.93291 -0.00001 -0.00009 -0.00001 -0.00010 1.93281

 A71 1.93291 -0.00001 -0.00009 -0.00001 -0.00010 1.93281

 A72 1.89660 0.00000 -0.00002 0.00002 0.00000 1.89661

 A73 1.89660 0.00000 -0.00002 0.00002 0.00000 1.89661

 A74 1.85835 0.00001 0.00014 -0.00005 0.00009 1.85845

 A75 1.93291 -0.00001 -0.00009 -0.00001 -0.00010 1.93281

 A76 1.93291 -0.00001 -0.00009 -0.00001 -0.00010 1.93281

 A77 1.94391 0.00001 0.00009 0.00002 0.00010 1.94401

 A78 1.85835 0.00001 0.00014 -0.00005 0.00009 1.85845

 A79 1.89660 0.00000 -0.00002 0.00002 0.00000 1.89661

 A80 1.89660 0.00000 -0.00002 0.00002 0.00000 1.89661

 A81 1.93291 -0.00001 -0.00009 -0.00001 -0.00010 1.93281

 A82 1.93291 -0.00001 -0.00009 -0.00001 -0.00010 1.93281

 A83 1.94391 0.00001 0.00009 0.00002 0.00010 1.94401

 A84 1.85835 0.00001 0.00014 -0.00005 0.00009 1.85845

 A85 1.89660 0.00000 -0.00002 0.00002 0.00000 1.89661

 A86 1.89660 0.00000 -0.00002 0.00002 0.00000 1.89661

 A87 1.93291 -0.00001 -0.00009 -0.00001 -0.00010 1.93281

 A88 1.93291 -0.00001 -0.00009 -0.00001 -0.00010 1.93281

 A89 1.94391 0.00001 0.00009 0.00002 0.00010 1.94401

 A90 1.85835 0.00001 0.00014 -0.00005 0.00009 1.85845

 A91 1.89660 0.00000 -0.00002 0.00002 0.00000 1.89661

 A92 1.89660 0.00000 -0.00002 0.00002 0.00000 1.89661

 A93 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 A94 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 A95 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 A96 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D2 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D3 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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 D26 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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 D28 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D29 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D30 1.02880 0.00000 0.00003 -0.00003 -0.00001 1.02880

 D31 -1.02880 0.00000 -0.00003 0.00003 0.00001 -1.02880

 D32 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D33 -2.11279 0.00000 0.00003 -0.00003 -0.00001 -2.11280

 D34 2.11279 0.00000 -0.00003 0.00003 0.00001 2.11280

 D35 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D36 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D37 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D38 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D39 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D40 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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 D50 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

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 D61 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D62 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D63 1.02880 0.00000 0.00003 -0.00003 -0.00001 1.02880

 D64 -1.02880 0.00000 -0.00003 0.00003 0.00001 -1.02880

 D65 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D66 -2.11279 0.00000 0.00003 -0.00003 -0.00001 -2.11280

 D67 2.11279 0.00000 -0.00003 0.00003 0.00001 2.11280

 D68 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D69 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D70 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D71 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D72 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D73 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D74 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D75 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D76 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D77 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D78 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D79 -2.11279 0.00000 0.00003 -0.00003 -0.00001 -2.11280

 D80 2.11279 0.00000 -0.00003 0.00003 0.00001 2.11280

 D81 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D82 1.02880 0.00000 0.00003 -0.00003 -0.00001 1.02880

 D83 -1.02880 0.00000 -0.00003 0.00003 0.00001 -1.02880

 D84 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D85 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D86 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D87 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D88 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D89 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D90 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D91 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D92 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D93 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D94 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D95 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D96 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D97 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D98 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D99 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D100 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D101 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D102 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D103 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D104 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D105 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D106 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D107 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D108 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D109 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D110 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D111 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D112 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D113 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D114 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D115 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D116 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D117 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D118 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D119 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D120 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D121 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D122 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D123 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D124 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D125 1.02880 0.00000 0.00003 -0.00003 -0.00001 1.02880

 D126 -1.02880 0.00000 -0.00003 0.00003 0.00001 -1.02880

 D127 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D128 -2.11279 0.00000 0.00003 -0.00003 -0.00001 -2.11280

 D129 2.11279 0.00000 -0.00003 0.00003 0.00001 2.11280

 D130 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D131 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D132 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D133 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 D134 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D135 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

 D136 3.14159 0.00000 0.00000 0.00000 0.00000 3.14159

 Item Value Threshold Converged?

 Maximum Force 0.000096 0.000450 YES

 RMS Force 0.000020 0.000300 YES

 Maximum Displacement 0.000823 0.001800 YES

 RMS Displacement 0.000215 0.001200 YES

 Predicted change in Energy=-1.935777D-07

 Optimization completed.

 -- Stationary point found.

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 ! Optimized Parameters !

 ! (Angstroms and Degrees) !

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 ! Name Definition Value Derivative Info. !

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 ! R1 R(1,2) 1.36 -DE/DX = 0.0001 !

 ! R2 R(1,5) 1.471 -DE/DX = -0.0001 !

 ! R3 R(1,12) 1.3392 -DE/DX = 0.0 !

 ! R4 R(2,3) 1.3523 -DE/DX = 0.0 !

 ! R5 R(2,25) 2.0005 -DE/DX = 0.0 !

 ! R6 R(3,4) 1.4977 -DE/DX = 0.0 !

 ! R7 R(3,6) 1.335 -DE/DX = 0.0001 !

 ! R8 R(4,5) 1.3554 -DE/DX = 0.0 !

 ! R9 R(4,26) 1.4836 -DE/DX = 0.0 !

 ! R10 R(5,27) 1.0803 -DE/DX = 0.0 !

 ! R11 R(6,7) 1.3392 -DE/DX = 0.0 !

 ! R12 R(7,8) 1.36 -DE/DX = 0.0001 !

 ! R13 R(7,11) 1.471 -DE/DX = -0.0001 !

 ! R14 R(8,9) 1.3523 -DE/DX = 0.0 !

 ! R15 R(8,25) 2.0005 -DE/DX = 0.0 !

 ! R16 R(9,10) 1.4977 -DE/DX = 0.0 !

 ! R17 R(9,24) 1.335 -DE/DX = 0.0001 !

 ! R18 R(10,11) 1.3554 -DE/DX = 0.0 !

 ! R19 R(10,28) 1.4836 -DE/DX = 0.0 !

 ! R20 R(11,29) 1.0803 -DE/DX = 0.0 !

 ! R21 R(12,17) 1.335 -DE/DX = 0.0001 !

 ! R22 R(13,14) 1.3554 -DE/DX = 0.0 !

 ! R23 R(13,17) 1.4977 -DE/DX = 0.0 !

 ! R24 R(13,30) 1.4836 -DE/DX = 0.0 !

 ! R25 R(14,15) 1.471 -DE/DX = -0.0001 !

 ! R26 R(14,31) 1.0803 -DE/DX = 0.0 !

 ! R27 R(15,16) 1.36 -DE/DX = 0.0001 !

 ! R28 R(15,18) 1.3392 -DE/DX = 0.0 !

 ! R29 R(16,17) 1.3523 -DE/DX = 0.0 !

 ! R30 R(16,25) 2.0005 -DE/DX = 0.0 !

 ! R31 R(18,20) 1.335 -DE/DX = 0.0001 !

 ! R32 R(19,20) 1.3523 -DE/DX = 0.0 !

 ! R33 R(19,23) 1.36 -DE/DX = 0.0001 !

 ! R34 R(19,25) 2.0005 -DE/DX = 0.0 !

 ! R35 R(20,21) 1.4977 -DE/DX = 0.0 !

 ! R36 R(21,22) 1.3554 -DE/DX = 0.0 !

 ! R37 R(21,32) 1.4836 -DE/DX = 0.0 !

 ! R38 R(22,23) 1.471 -DE/DX = -0.0001 !

 ! R39 R(22,33) 1.0803 -DE/DX = 0.0 !

 ! R40 R(23,24) 1.3392 -DE/DX = 0.0 !

 ! R41 R(26,34) 1.0904 -DE/DX = 0.0 !

 ! R42 R(26,35) 1.0946 -DE/DX = 0.0 !

 ! R43 R(26,36) 1.0946 -DE/DX = 0.0 !

 ! R44 R(28,37) 1.0946 -DE/DX = 0.0 !

 ! R45 R(28,38) 1.0946 -DE/DX = 0.0 !

 ! R46 R(28,39) 1.0904 -DE/DX = 0.0 !

 ! R47 R(30,40) 1.0946 -DE/DX = 0.0 !

 ! R48 R(30,41) 1.0946 -DE/DX = 0.0 !

 ! R49 R(30,42) 1.0904 -DE/DX = 0.0 !

 ! R50 R(32,43) 1.0946 -DE/DX = 0.0 !

 ! R51 R(32,44) 1.0946 -DE/DX = 0.0 !

 ! R52 R(32,45) 1.0904 -DE/DX = 0.0 !

 ! A1 A(2,1,5) 108.4656 -DE/DX = 0.0 !

 ! A2 A(2,1,12) 126.7099 -DE/DX = 0.0 !

 ! A3 A(5,1,12) 124.8245 -DE/DX = 0.0 !

 ! A4 A(1,2,3) 109.4707 -DE/DX = 0.0 !

 ! A5 A(1,2,25) 125.5682 -DE/DX = 0.0 !

 ! A6 A(3,2,25) 124.9611 -DE/DX = 0.0 !

 ! A7 A(2,3,4) 108.4139 -DE/DX = 0.0 !

 ! A8 A(2,3,6) 127.9001 -DE/DX = 0.0 !

 ! A9 A(4,3,6) 123.686 -DE/DX = 0.0 !

 ! A10 A(3,4,5) 105.9768 -DE/DX = 0.0 !

 ! A11 A(3,4,26) 123.7036 -DE/DX = 0.0 !

 ! A12 A(5,4,26) 130.3196 -DE/DX = 0.0 !

 ! A13 A(1,5,4) 107.673 -DE/DX = 0.0 !

 ! A14 A(1,5,27) 124.3265 -DE/DX = 0.0 !

 ! A15 A(4,5,27) 128.0005 -DE/DX = 0.0 !

 ! A16 A(3,6,7) 124.8608 -DE/DX = 0.0 !

 ! A17 A(6,7,8) 126.7099 -DE/DX = 0.0 !

 ! A18 A(6,7,11) 124.8245 -DE/DX = 0.0 !

 ! A19 A(8,7,11) 108.4656 -DE/DX = 0.0 !

 ! A20 A(7,8,9) 109.4707 -DE/DX = 0.0 !

 ! A21 A(7,8,25) 125.5682 -DE/DX = 0.0 !

 ! A22 A(9,8,25) 124.9611 -DE/DX = 0.0 !

 ! A23 A(8,9,10) 108.4139 -DE/DX = 0.0 !

 ! A24 A(8,9,24) 127.9001 -DE/DX = 0.0 !

 ! A25 A(10,9,24) 123.686 -DE/DX = 0.0 !

 ! A26 A(9,10,11) 105.9768 -DE/DX = 0.0 !

 ! A27 A(9,10,28) 123.7036 -DE/DX = 0.0 !

 ! A28 A(11,10,28) 130.3196 -DE/DX = 0.0 !

 ! A29 A(7,11,10) 107.673 -DE/DX = 0.0 !

 ! A30 A(7,11,29) 124.3265 -DE/DX = 0.0 !

 ! A31 A(10,11,29) 128.0005 -DE/DX = 0.0 !

 ! A32 A(1,12,17) 124.8608 -DE/DX = 0.0 !

 ! A33 A(14,13,17) 105.9768 -DE/DX = 0.0 !

 ! A34 A(14,13,30) 130.3196 -DE/DX = 0.0 !

 ! A35 A(17,13,30) 123.7036 -DE/DX = 0.0 !

 ! A36 A(13,14,15) 107.673 -DE/DX = 0.0 !

 ! A37 A(13,14,31) 128.0005 -DE/DX = 0.0 !

 ! A38 A(15,14,31) 124.3265 -DE/DX = 0.0 !

 ! A39 A(14,15,16) 108.4656 -DE/DX = 0.0 !

 ! A40 A(14,15,18) 124.8245 -DE/DX = 0.0 !

 ! A41 A(16,15,18) 126.7099 -DE/DX = 0.0 !

 ! A42 A(15,16,17) 109.4707 -DE/DX = 0.0 !

 ! A43 A(15,16,25) 125.5682 -DE/DX = 0.0 !

 ! A44 A(17,16,25) 124.9611 -DE/DX = 0.0 !

 ! A45 A(12,17,13) 123.686 -DE/DX = 0.0 !

 ! A46 A(12,17,16) 127.9001 -DE/DX = 0.0 !

 ! A47 A(13,17,16) 108.4139 -DE/DX = 0.0 !

 ! A48 A(15,18,20) 124.8608 -DE/DX = 0.0 !

 ! A49 A(20,19,23) 109.4707 -DE/DX = 0.0 !

 ! A50 A(20,19,25) 124.9611 -DE/DX = 0.0 !

 ! A51 A(23,19,25) 125.5682 -DE/DX = 0.0 !

 ! A52 A(18,20,19) 127.9001 -DE/DX = 0.0 !

 ! A53 A(18,20,21) 123.686 -DE/DX = 0.0 !

 ! A54 A(19,20,21) 108.4139 -DE/DX = 0.0 !

 ! A55 A(20,21,22) 105.9768 -DE/DX = 0.0 !

 ! A56 A(20,21,32) 123.7036 -DE/DX = 0.0 !

 ! A57 A(22,21,32) 130.3196 -DE/DX = 0.0 !

 ! A58 A(21,22,23) 107.673 -DE/DX = 0.0 !

 ! A59 A(21,22,33) 128.0005 -DE/DX = 0.0 !

 ! A60 A(23,22,33) 124.3265 -DE/DX = 0.0 !

 ! A61 A(19,23,22) 108.4656 -DE/DX = 0.0 !

 ! A62 A(19,23,24) 126.7099 -DE/DX = 0.0 !

 ! A63 A(22,23,24) 124.8245 -DE/DX = 0.0 !

 ! A64 A(9,24,23) 124.8608 -DE/DX = 0.0 !

 ! A65 A(2,25,8) 90.0 -DE/DX = 0.0 !

 ! A66 A(2,25,16) 90.0 -DE/DX = 0.0 !

 ! A67 A(8,25,19) 90.0 -DE/DX = 0.0 !

 ! A68 A(16,25,19) 90.0 -DE/DX = 0.0 !

 ! A69 A(4,26,34) 111.3779 -DE/DX = 0.0 !

 ! A70 A(4,26,35) 110.7474 -DE/DX = 0.0 !

 ! A71 A(4,26,36) 110.7474 -DE/DX = 0.0 !

 ! A72 A(34,26,35) 108.6673 -DE/DX = 0.0 !

 ! A73 A(34,26,36) 108.6673 -DE/DX = 0.0 !

 ! A74 A(35,26,36) 106.4758 -DE/DX = 0.0 !

 ! A75 A(10,28,37) 110.7474 -DE/DX = 0.0 !

 ! A76 A(10,28,38) 110.7474 -DE/DX = 0.0 !

 ! A77 A(10,28,39) 111.3779 -DE/DX = 0.0 !

 ! A78 A(37,28,38) 106.4758 -DE/DX = 0.0 !

 ! A79 A(37,28,39) 108.6673 -DE/DX = 0.0 !

 ! A80 A(38,28,39) 108.6673 -DE/DX = 0.0 !

 ! A81 A(13,30,40) 110.7474 -DE/DX = 0.0 !

 ! A82 A(13,30,41) 110.7474 -DE/DX = 0.0 !

 ! A83 A(13,30,42) 111.3779 -DE/DX = 0.0 !

 ! A84 A(40,30,41) 106.4758 -DE/DX = 0.0 !

 ! A85 A(40,30,42) 108.6673 -DE/DX = 0.0 !

 ! A86 A(41,30,42) 108.6673 -DE/DX = 0.0 !

 ! A87 A(21,32,43) 110.7474 -DE/DX = 0.0 !

 ! A88 A(21,32,44) 110.7474 -DE/DX = 0.0 !

 ! A89 A(21,32,45) 111.3779 -DE/DX = 0.0 !

 ! A90 A(43,32,44) 106.4758 -DE/DX = 0.0 !

 ! A91 A(43,32,45) 108.6673 -DE/DX = 0.0 !

 ! A92 A(44,32,45) 108.6673 -DE/DX = 0.0 !

 ! A93 L(2,25,19,16,-1) 180.0 -DE/DX = 0.0 !

 ! A94 L(8,25,16,19,-1) 180.0 -DE/DX = 0.0 !

 ! A95 L(2,25,19,16,-2) 180.0 -DE/DX = 0.0 !

 ! A96 L(8,25,16,19,-2) 180.0 -DE/DX = 0.0 !

 ! D1 D(5,1,2,3) 0.0 -DE/DX = 0.0 !

 ! D2 D(5,1,2,25) 180.0 -DE/DX = 0.0 !

 ! D3 D(12,1,2,3) 180.0 -DE/DX = 0.0 !

 ! D4 D(12,1,2,25) 0.0 -DE/DX = 0.0 !

 ! D5 D(2,1,5,4) 0.0 -DE/DX = 0.0 !

 ! D6 D(2,1,5,27) 180.0 -DE/DX = 0.0 !

 ! D7 D(12,1,5,4) 180.0 -DE/DX = 0.0 !

 ! D8 D(12,1,5,27) 0.0 -DE/DX = 0.0 !

 ! D9 D(2,1,12,17) 0.0 -DE/DX = 0.0 !

 ! D10 D(5,1,12,17) 180.0 -DE/DX = 0.0 !

 ! D11 D(1,2,3,4) 0.0 -DE/DX = 0.0 !

 ! D12 D(1,2,3,6) 180.0 -DE/DX = 0.0 !

 ! D13 D(25,2,3,4) 180.0 -DE/DX = 0.0 !

 ! D14 D(25,2,3,6) 0.0 -DE/DX = 0.0 !

 ! D15 D(1,2,25,8) 180.0 -DE/DX = 0.0 !

 ! D16 D(1,2,25,16) 0.0 -DE/DX = 0.0 !

 ! D17 D(3,2,25,8) 0.0 -DE/DX = 0.0 !

 ! D18 D(3,2,25,16) 180.0 -DE/DX = 0.0 !

 ! D19 D(2,3,4,5) 0.0 -DE/DX = 0.0 !

 ! D20 D(2,3,4,26) 180.0 -DE/DX = 0.0 !

 ! D21 D(6,3,4,5) 180.0 -DE/DX = 0.0 !

 ! D22 D(6,3,4,26) 0.0 -DE/DX = 0.0 !

 ! D23 D(2,3,6,7) 0.0 -DE/DX = 0.0 !

 ! D24 D(4,3,6,7) 180.0 -DE/DX = 0.0 !

 ! D25 D(3,4,5,1) 0.0 -DE/DX = 0.0 !

 ! D26 D(3,4,5,27) 180.0 -DE/DX = 0.0 !

 ! D27 D(26,4,5,1) 180.0 -DE/DX = 0.0 !

 ! D28 D(26,4,5,27) 0.0 -DE/DX = 0.0 !

 ! D29 D(3,4,26,34) 180.0 -DE/DX = 0.0 !

 ! D30 D(3,4,26,35) 58.9461 -DE/DX = 0.0 !

 ! D31 D(3,4,26,36) -58.9461 -DE/DX = 0.0 !

 ! D32 D(5,4,26,34) 0.0 -DE/DX = 0.0 !

 ! D33 D(5,4,26,35) -121.0539 -DE/DX = 0.0 !

 ! D34 D(5,4,26,36) 121.0539 -DE/DX = 0.0 !

 ! D35 D(3,6,7,8) 0.0 -DE/DX = 0.0 !

 ! D36 D(3,6,7,11) 180.0 -DE/DX = 0.0 !

 ! D37 D(6,7,8,9) 180.0 -DE/DX = 0.0 !

 ! D38 D(6,7,8,25) 0.0 -DE/DX = 0.0 !

 ! D39 D(11,7,8,9) 0.0 -DE/DX = 0.0 !

 ! D40 D(11,7,8,25) 180.0 -DE/DX = 0.0 !

 ! D41 D(6,7,11,10) 180.0 -DE/DX = 0.0 !

 ! D42 D(6,7,11,29) 0.0 -DE/DX = 0.0 !

 ! D43 D(8,7,11,10) 0.0 -DE/DX = 0.0 !

 ! D44 D(8,7,11,29) 180.0 -DE/DX = 0.0 !

 ! D45 D(7,8,9,10) 0.0 -DE/DX = 0.0 !

 ! D46 D(7,8,9,24) 180.0 -DE/DX = 0.0 !

 ! D47 D(25,8,9,10) 180.0 -DE/DX = 0.0 !

 ! D48 D(25,8,9,24) 0.0 -DE/DX = 0.0 !

 ! D49 D(7,8,25,2) 0.0 -DE/DX = 0.0 !

 ! D50 D(7,8,25,19) 180.0 -DE/DX = 0.0 !

 ! D51 D(9,8,25,2) 180.0 -DE/DX = 0.0 !

 ! D52 D(9,8,25,19) 0.0 -DE/DX = 0.0 !

 ! D53 D(8,9,10,11) 0.0 -DE/DX = 0.0 !

 ! D54 D(8,9,10,28) 180.0 -DE/DX = 0.0 !

 ! D55 D(24,9,10,11) 180.0 -DE/DX = 0.0 !

 ! D56 D(24,9,10,28) 0.0 -DE/DX = 0.0 !

 ! D57 D(8,9,24,23) 0.0 -DE/DX = 0.0 !

 ! D58 D(10,9,24,23) 180.0 -DE/DX = 0.0 !

 ! D59 D(9,10,11,7) 0.0 -DE/DX = 0.0 !

 ! D60 D(9,10,11,29) 180.0 -DE/DX = 0.0 !

 ! D61 D(28,10,11,7) 180.0 -DE/DX = 0.0 !

 ! D62 D(28,10,11,29) 0.0 -DE/DX = 0.0 !

 ! D63 D(9,10,28,37) 58.9461 -DE/DX = 0.0 !

 ! D64 D(9,10,28,38) -58.9461 -DE/DX = 0.0 !

 ! D65 D(9,10,28,39) 180.0 -DE/DX = 0.0 !

 ! D66 D(11,10,28,37) -121.0539 -DE/DX = 0.0 !

 ! D67 D(11,10,28,38) 121.0539 -DE/DX = 0.0 !

 ! D68 D(11,10,28,39) 0.0 -DE/DX = 0.0 !

 ! D69 D(1,12,17,13) 180.0 -DE/DX = 0.0 !

 ! D70 D(1,12,17,16) 0.0 -DE/DX = 0.0 !

 ! D71 D(17,13,14,15) 0.0 -DE/DX = 0.0 !

 ! D72 D(17,13,14,31) 180.0 -DE/DX = 0.0 !

 ! D73 D(30,13,14,15) 180.0 -DE/DX = 0.0 !

 ! D74 D(30,13,14,31) 0.0 -DE/DX = 0.0 !

 ! D75 D(14,13,17,12) 180.0 -DE/DX = 0.0 !

 ! D76 D(14,13,17,16) 0.0 -DE/DX = 0.0 !

 ! D77 D(30,13,17,12) 0.0 -DE/DX = 0.0 !

 ! D78 D(30,13,17,16) 180.0 -DE/DX = 0.0 !

 ! D79 D(14,13,30,40) -121.0539 -DE/DX = 0.0 !

 ! D80 D(14,13,30,41) 121.0539 -DE/DX = 0.0 !

 ! D81 D(14,13,30,42) 0.0 -DE/DX = 0.0 !

 ! D82 D(17,13,30,40) 58.9461 -DE/DX = 0.0 !

 ! D83 D(17,13,30,41) -58.9461 -DE/DX = 0.0 !

 ! D84 D(17,13,30,42) 180.0 -DE/DX = 0.0 !

 ! D85 D(13,14,15,16) 0.0 -DE/DX = 0.0 !

 ! D86 D(13,14,15,18) 180.0 -DE/DX = 0.0 !

 ! D87 D(31,14,15,16) 180.0 -DE/DX = 0.0 !

 ! D88 D(31,14,15,18) 0.0 -DE/DX = 0.0 !

 ! D89 D(14,15,16,17) 0.0 -DE/DX = 0.0 !

 ! D90 D(14,15,16,25) 180.0 -DE/DX = 0.0 !

 ! D91 D(18,15,16,17) 180.0 -DE/DX = 0.0 !

 ! D92 D(18,15,16,25) 0.0 -DE/DX = 0.0 !

 ! D93 D(14,15,18,20) 180.0 -DE/DX = 0.0 !

 ! D94 D(16,15,18,20) 0.0 -DE/DX = 0.0 !

 ! D95 D(15,16,17,12) 180.0 -DE/DX = 0.0 !

 ! D96 D(15,16,17,13) 0.0 -DE/DX = 0.0 !

 ! D97 D(25,16,17,12) 0.0 -DE/DX = 0.0 !

 ! D98 D(25,16,17,13) 180.0 -DE/DX = 0.0 !

 ! D99 D(15,16,25,2) 180.0 -DE/DX = 0.0 !

 ! D100 D(15,16,25,19) 0.0 -DE/DX = 0.0 !

 ! D101 D(17,16,25,2) 0.0 -DE/DX = 0.0 !

 ! D102 D(17,16,25,19) 180.0 -DE/DX = 0.0 !

 ! D103 D(15,18,20,19) 0.0 -DE/DX = 0.0 !

 ! D104 D(15,18,20,21) 180.0 -DE/DX = 0.0 !

 ! D105 D(23,19,20,18) 180.0 -DE/DX = 0.0 !

 ! D106 D(23,19,20,21) 0.0 -DE/DX = 0.0 !

 ! D107 D(25,19,20,18) 0.0 -DE/DX = 0.0 !

 ! D108 D(25,19,20,21) 180.0 -DE/DX = 0.0 !

 ! D109 D(20,19,23,22) 0.0 -DE/DX = 0.0 !

 ! D110 D(20,19,23,24) 180.0 -DE/DX = 0.0 !

 ! D111 D(25,19,23,22) 180.0 -DE/DX = 0.0 !

 ! D112 D(25,19,23,24) 0.0 -DE/DX = 0.0 !

 ! D113 D(20,19,25,8) 180.0 -DE/DX = 0.0 !

 ! D114 D(20,19,25,16) 0.0 -DE/DX = 0.0 !

 ! D115 D(23,19,25,8) 0.0 -DE/DX = 0.0 !

 ! D116 D(23,19,25,16) 180.0 -DE/DX = 0.0 !

 ! D117 D(18,20,21,22) 180.0 -DE/DX = 0.0 !

 ! D118 D(18,20,21,32) 0.0 -DE/DX = 0.0 !

 ! D119 D(19,20,21,22) 0.0 -DE/DX = 0.0 !

 ! D120 D(19,20,21,32) 180.0 -DE/DX = 0.0 !

 ! D121 D(20,21,22,23) 0.0 -DE/DX = 0.0 !

 ! D122 D(20,21,22,33) 180.0 -DE/DX = 0.0 !

 ! D123 D(32,21,22,23) 180.0 -DE/DX = 0.0 !

 ! D124 D(32,21,22,33) 0.0 -DE/DX = 0.0 !

 ! D125 D(20,21,32,43) 58.9461 -DE/DX = 0.0 !

 ! D126 D(20,21,32,44) -58.9461 -DE/DX = 0.0 !

 ! D127 D(20,21,32,45) 180.0 -DE/DX = 0.0 !

 ! D128 D(22,21,32,43) -121.0539 -DE/DX = 0.0 !

 ! D129 D(22,21,32,44) 121.0539 -DE/DX = 0.0 !

 ! D130 D(22,21,32,45) 0.0 -DE/DX = 0.0 !

 ! D131 D(21,22,23,19) 0.0 -DE/DX = 0.0 !

 ! D132 D(21,22,23,24) 180.0 -DE/DX = 0.0 !

 ! D133 D(33,22,23,19) 180.0 -DE/DX = 0.0 !

 ! D134 D(33,22,23,24) 0.0 -DE/DX = 0.0 !

 ! D135 D(19,23,24,9) 0.0 -DE/DX = 0.0 !

 ! D136 D(22,23,24,9) 180.0 -DE/DX = 0.0 !

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

 Lowest energy point so far. Saving SCF results.

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

 Largest change from initial coordinates is atom 40 0.033 Angstoms.

 Leave Link 103 at Fri Jul 5 21:14:32 2019, MaxMem= 1342177280 cpu: 1.4

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

 Input orientation:

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -2.066415 -2.178693 0.000000

 2 7 0 -0.745079 -1.856552 0.000000

 3 6 0 -0.005184 -2.988429 0.000000

 4 6 0 -0.935773 -4.161954 0.000000

 5 6 0 -2.188591 -3.644629 0.000000

 6 7 0 1.325250 -3.098463 0.000000

 7 6 0 2.178693 -2.066415 0.000000

 8 7 0 1.856552 -0.745079 0.000000

 9 6 0 2.988429 -0.005184 0.000000

 10 6 0 4.161954 -0.935773 0.000000

 11 6 0 3.644629 -2.188591 0.000000

 12 7 0 -3.098463 -1.325250 0.000000

 13 6 0 -4.161954 0.935773 0.000000

 14 6 0 -3.644629 2.188591 0.000000

 15 6 0 -2.178693 2.066415 0.000000

 16 7 0 -1.856552 0.745079 0.000000

 17 6 0 -2.988429 0.005184 0.000000

 18 7 0 -1.325250 3.098463 0.000000

 19 7 0 0.745079 1.856552 0.000000

 20 6 0 0.005184 2.988429 0.000000

 21 6 0 0.935773 4.161954 0.000000

 22 6 0 2.188591 3.644629 0.000000

 23 6 0 2.066415 2.178693 0.000000

 24 7 0 3.098463 1.325250 0.000000

 25 30 0 0.000000 0.000000 0.000000

 26 6 0 -0.480197 -5.573923 0.000000

 27 1 0 -3.128232 -4.177604 0.000000

 28 6 0 5.573923 -0.480197 0.000000

 29 1 0 4.177604 -3.128232 0.000000

 30 6 0 -5.573923 0.480197 0.000000

 31 1 0 -4.177604 3.128232 0.000000

 32 6 0 0.480197 5.573923 0.000000

 33 1 0 3.128232 4.177604 0.000000

 34 1 0 -1.324446 -6.263958 0.000000

 35 1 0 0.141368 -5.780804 0.876886

 36 1 0 0.141368 -5.780804 -0.876886

 37 1 0 5.780804 0.141368 0.876886

 38 1 0 5.780804 0.141368 -0.876886

 39 1 0 6.263958 -1.324446 0.000000

 40 1 0 -5.780804 -0.141368 0.876886

 41 1 0 -5.780804 -0.141368 -0.876886

 42 1 0 -6.263958 1.324446 0.000000

 43 1 0 -0.141368 5.780804 0.876886

 44 1 0 -0.141368 5.780804 -0.876886

 45 1 0 1.324446 6.263958 0.000000

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 Distance matrix (angstroms):

 1 2 3 4 5

 1 C 0.000000

 2 N 1.360038 0.000000

 3 C 2.214576 1.352254 0.000000

 4 C 2.282910 2.313276 1.497717 0.000000

 5 C 1.471019 2.298031 2.279882 1.355425 0.000000

 6 N 3.514167 2.414251 1.334977 2.498647 3.556033

 7 C 4.246592 2.931294 2.370534 3.753822 4.643697

 8 N 4.176711 2.829108 2.915250 4.412722 4.977004

 9 C 5.502326 4.167330 4.226283 5.716476 6.328277

 10 C 6.351176 4.992675 4.645260 6.032832 6.904152

 11 C 5.711053 4.402248 3.736426 4.987409 6.012196

 12 N 1.339212 2.412613 3.512057 3.567088 2.491463

 13 C 3.753822 4.412722 5.716476 6.032832 4.987409

 14 C 4.643697 4.977004 6.328277 6.904152 6.012196

 15 C 4.246592 4.176711 5.502326 6.351176 5.711053

 16 N 2.931294 2.829108 4.167330 4.992675 4.402248

 17 C 2.370534 2.915250 4.226283 4.645260 3.736426

 18 N 5.328949 4.988865 6.228389 7.270856 6.798136

 19 N 4.918099 4.000963 4.902727 6.248814 6.234533

 20 C 5.566927 4.902727 5.976867 7.212030 6.986423

 21 C 7.015478 6.248814 7.212030 8.531714 8.408590

 22 C 7.212222 6.234533 6.986423 8.408590 8.502529

 23 C 6.005588 4.918099 5.566927 7.015478 7.212222

 24 N 6.241280 4.989657 5.314175 6.810615 7.256214

 25 Zn 3.002794 2.000481 2.988434 4.265857 4.251265

 26 C 3.747489 3.726797 2.628767 1.483646 2.576972

 27 H 2.263427 3.326665 3.341791 2.192515 1.080272

 28 C 7.826855 6.467159 6.116998 7.478735 8.382735

 29 H 6.315805 5.084287 4.185124 5.216819 6.387104

 30 C 4.401399 5.364525 6.560657 6.562165 5.336166

 31 H 5.711442 6.052297 7.404231 7.978489 7.058883

 32 C 8.160165 7.530820 8.576099 9.838307 9.597090

 33 H 8.208950 7.170325 7.821146 9.277088 9.458115

 34 H 4.152097 4.445323 3.531223 2.137635 2.758193

 35 H 4.314910 4.117582 2.930489 2.133035 3.280378

 36 H 4.314910 4.117582 2.930489 2.133035 3.280378

 37 H 8.229852 6.880971 6.636432 8.024957 8.866452

 38 H 8.229852 6.880971 6.636432 8.024957 8.866452

 39 H 8.374058 7.029205 6.486215 7.738706 8.765205

 40 H 4.326235 5.391597 6.498652 6.356758 5.093699

 41 H 4.326235 5.391597 6.498652 6.356758 5.093699

 42 H 5.467298 6.369989 7.600864 7.647884 6.426532

 43 H 8.235796 7.711200 8.814019 10.012915 9.684981

 44 H 8.235796 7.711200 8.814019 10.012915 9.684981

 45 H 9.098147 8.380072 9.347437 10.668094 10.512921

 6 7 8 9 10

 6 N 0.000000

 7 C 1.339212 0.000000

 8 N 2.412613 1.360038 0.000000

 9 C 3.512057 2.214576 1.352254 0.000000

 10 C 3.567088 2.282910 2.313276 1.497717 0.000000

 11 C 2.491463 1.471019 2.298031 2.279882 1.355425

 12 N 4.765871 5.328949 4.988865 6.228389 7.270856

 13 C 6.810615 7.015478 6.248814 7.212030 8.531714

 14 C 7.256214 7.212222 6.234533 6.986423 8.408590

 15 C 6.241280 6.005588 4.918099 5.566927 7.015478

 16 N 4.989657 4.918099 4.000963 4.902727 6.248814

 17 C 5.314175 5.566927 4.902727 5.976867 7.212030

 18 N 6.739959 6.241280 4.989657 5.314175 6.810615

 19 N 4.988865 4.176711 2.829108 2.915250 4.412722

 20 C 6.228389 5.502326 4.167330 4.226283 5.716476

 21 C 7.270856 6.351176 4.992675 4.645260 6.032832

 22 C 6.798136 5.711053 4.402248 3.736426 4.987409

 23 C 5.328949 4.246592 2.931294 2.370534 3.753822

 24 N 4.765871 3.514167 2.414251 1.334977 2.498647

 25 Zn 3.369980 3.002794 2.000481 2.988434 4.265857

 26 C 3.063909 4.401399 5.364525 6.560657 6.562165

 27 H 4.582363 5.711442 6.052297 7.404231 7.978489

 28 C 4.990646 3.747489 3.726797 2.628767 1.483646

 29 H 2.852509 2.263427 3.326665 3.341791 2.192515

 30 C 7.772091 8.160165 7.530820 8.576099 9.838307

 31 H 8.309822 8.208950 7.170325 7.821146 9.277088

 32 C 8.713461 7.826855 6.467159 6.116998 7.478735

 33 H 7.496125 6.315805 5.084287 4.185124 5.216819

 34 H 4.128104 5.467298 6.369989 7.600864 7.647884

 35 H 3.060304 4.326235 5.391597 6.498652 6.356758

 36 H 3.060304 4.326235 5.391597 6.498652 6.356758

 37 H 5.578298 4.314910 4.117582 2.930489 2.133035

 38 H 5.578298 4.314910 4.117582 2.930489 2.133035

 39 H 5.247664 4.152097 4.445323 3.531223 2.137635

 40 H 7.746570 8.235796 7.711200 8.814019 10.012915

 41 H 7.746570 8.235796 7.711200 8.814019 10.012915

 42 H 8.783974 9.098147 8.380072 9.347437 10.668094

 43 H 9.042195 8.229852 6.880971 6.636432 8.024957

 44 H 9.042195 8.229852 6.880971 6.636432 8.024957

 45 H 9.362421 8.374058 7.029205 6.486215 7.738706

 11 12 13 14 15

 11 C 0.000000

 12 N 6.798136 0.000000

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 16 N 6.234533 2.414251 2.313276 2.298031 1.360038

 17 C 6.986423 1.334977 1.497717 2.279882 2.214576

 18 N 7.256214 4.765871 3.567088 2.491463 1.339212

 19 N 4.977004 4.989657 4.992675 4.402248 2.931294

 20 C 6.328277 5.314175 4.645260 3.736426 2.370534

 21 C 6.904152 6.810615 6.032832 4.987409 3.753822

 22 C 6.012196 7.256214 6.904152 6.012196 4.643697

 23 C 4.643697 6.241280 6.351176 5.711053 4.246592

 24 N 3.556033 6.739959 7.270856 6.798136 5.328949

 25 Zn 4.251265 3.369980 4.265857 4.251265 3.002794

 26 C 5.336166 4.990646 7.478735 8.382735 7.826855

 27 H 7.058883 2.852509 5.216819 6.387104 6.315805

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 29 H 1.080272 7.496125 9.277088 9.458115 8.208950

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 31 H 9.458115 4.582363 2.192515 1.080272 2.263427

 32 C 8.382735 7.772091 6.562165 5.336166 4.401399

 33 H 6.387104 8.309822 7.978489 7.058883 5.711442

 34 H 6.426532 5.247664 7.738706 8.765205 8.374058

 35 H 5.093699 5.578298 8.024957 8.866452 8.229852

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 37 H 3.280378 9.042195 10.012915 9.684981 8.235796

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 39 H 2.758193 9.362421 10.668094 10.512921 9.098147

 40 H 9.684981 3.060304 2.133035 3.280378 4.314910

 41 H 9.684981 3.060304 2.133035 3.280378 4.314910

 42 H 10.512921 4.128104 2.137635 2.758193 4.152097

 43 H 8.866452 7.746570 6.356758 5.093699 4.326235

 44 H 8.866452 7.746570 6.356758 5.093699 4.326235

 45 H 8.765205 8.783974 7.647884 6.426532 5.467298

 16 17 18 19 20

 16 N 0.000000

 17 C 1.352254 0.000000

 18 N 2.412613 3.512057 0.000000

 19 N 2.829108 4.167330 2.414251 0.000000

 20 C 2.915250 4.226283 1.334977 1.352254 0.000000

 21 C 4.412722 5.716476 2.498647 2.313276 1.497717

 22 C 4.977004 6.328277 3.556033 2.298031 2.279882

 23 C 4.176711 5.502326 3.514167 1.360038 2.214576

 24 N 4.988865 6.228389 4.765871 2.412613 3.512057

 25 Zn 2.000481 2.988434 3.369980 2.000481 2.988434

 26 C 6.467159 6.116998 8.713461 7.530820 8.576099

 27 H 5.084287 4.185124 7.496125 7.170325 7.821146

 28 C 7.530820 8.576099 7.772091 5.364525 6.560657

 29 H 7.170325 7.821146 8.309822 6.052297 7.404231

 30 C 3.726797 2.628767 4.990646 6.467159 6.116998

 31 H 3.326665 3.341791 2.852509 5.084287 4.185124

 32 C 5.364525 6.560657 3.063909 3.726797 2.628767

 33 H 6.052297 7.404231 4.582363 3.326665 3.341791

 34 H 7.029205 6.486215 9.362421 8.380072 9.347437

 35 H 6.880971 6.636432 9.042195 7.711200 8.814019

 36 H 6.880971 6.636432 9.042195 7.711200 8.814019

 37 H 7.711200 8.814019 7.746570 5.391597 6.498652

 38 H 7.711200 8.814019 7.746570 5.391597 6.498652

 39 H 8.380072 9.347437 8.783974 6.369989 7.600864

 40 H 4.117582 2.930489 5.578298 6.880971 6.636432

 41 H 4.117582 2.930489 5.578298 6.880971 6.636432

 42 H 4.445323 3.531223 5.247664 7.029205 6.486215

 43 H 5.391597 6.498652 3.060304 4.117582 2.930489

 44 H 5.391597 6.498652 3.060304 4.117582 2.930489

 45 H 6.369989 7.600864 4.128104 4.445323 3.531223

 21 22 23 24 25

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 22 C 1.355425 0.000000

 23 C 2.282910 1.471019 0.000000

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 25 Zn 4.265857 4.251265 3.002794 3.369980 0.000000

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 27 H 9.277088 9.458115 8.208950 8.309822 5.219024

 28 C 6.562165 5.336166 4.401399 3.063909 5.594570

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 31 H 5.216819 6.387104 6.315805 7.496125 5.219024

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 33 H 2.192515 1.080272 2.263427 2.852509 5.219024

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 35 H 10.012915 9.684981 8.235796 7.746570 5.848642

 36 H 10.012915 9.684981 8.235796 7.746570 5.848642

 37 H 6.356758 5.093699 4.326235 3.060304 5.848642

 38 H 6.356758 5.093699 4.326235 3.060304 5.848642

 39 H 7.647884 6.426532 5.467298 4.128104 6.402446

 40 H 8.024957 8.866452 8.229852 9.042195 5.848642

 41 H 8.024957 8.866452 8.229852 9.042195 5.848642

 42 H 7.738706 8.765205 8.374058 9.362421 6.402446

 43 H 2.133035 3.280378 4.314910 5.578298 5.848642

 44 H 2.133035 3.280378 4.314910 5.578298 5.848642

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 26 27 28 29 30

 26 C 0.000000

 27 H 2.993627 0.000000

 28 C 7.911916 9.455069 0.000000

 29 H 5.260847 7.380814 2.993627 0.000000

 30 C 7.911916 5.260847 11.189139 10.397742 0.000000

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 32 C 11.189139 10.397742 7.911916 9.455069 7.911916

 33 H 10.397742 10.438048 5.260847 7.380814 9.455069

 34 H 1.090368 2.757992 9.002188 6.332876 7.971304

 35 H 1.094565 3.745594 7.640551 4.908794 8.522536

 36 H 1.094565 3.745594 7.640551 4.908794 8.522536

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 38 H 8.522536 9.939486 1.094565 3.745594 11.393576

 39 H 7.971304 9.815994 1.090368 2.757992 11.974646

 40 H 7.640551 4.908794 11.393576 10.433608 1.094565

 41 H 7.640551 4.908794 11.393576 10.433608 1.094565

 42 H 9.002188 6.332876 11.974646 11.351323 1.090368

 43 H 11.393576 10.433608 8.522536 9.939486 7.640551

 44 H 11.393576 10.433608 8.522536 9.939486 7.640551

 45 H 11.974646 11.351323 7.971304 9.815994 9.002188

 31 32 33 34 35

 31 H 0.000000

 32 C 5.260847 0.000000

 33 H 7.380814 2.993627 0.000000

 34 H 9.815994 11.974646 11.351323 0.000000

 35 H 9.939486 11.393576 10.433608 1.775099 0.000000

 36 H 9.939486 11.393576 10.433608 1.775099 1.753773

 37 H 10.433608 7.640551 4.908794 9.606337 8.177736

 38 H 10.433608 7.640551 4.908794 9.606337 8.363677

 39 H 11.351323 9.002188 6.332876 9.054427 7.623265

 40 H 3.745594 8.522536 9.939486 7.623265 8.177736

 41 H 3.745594 8.522536 9.939486 7.623265 8.363677

 42 H 2.757992 7.971304 9.815994 9.054427 9.606337

 43 H 4.908794 1.094565 3.745594 12.134451 11.565066

 44 H 4.908794 1.094565 3.745594 12.134451 11.697284

 45 H 6.332876 1.090368 2.757992 12.804893 12.134451

 36 37 38 39 40

 36 H 0.000000

 37 H 8.363677 0.000000

 38 H 8.177736 1.753773 0.000000

 39 H 7.623265 1.775099 1.775099 0.000000

 40 H 8.363677 11.565066 11.697284 12.134451 0.000000

 41 H 8.177736 11.697284 11.565066 12.134451 1.753773

 42 H 9.606337 12.134451 12.134451 12.804893 1.775099

 43 H 11.697284 8.177736 8.363677 9.606337 8.177736

 44 H 11.565066 8.363677 8.177736 9.606337 8.363677

 45 H 12.134451 7.623265 7.623265 9.054427 9.606337

 41 42 43 44 45

 41 H 0.000000

 42 H 1.775099 0.000000

 43 H 8.363677 7.623265 0.000000

 44 H 8.177736 7.623265 1.753773 0.000000

 45 H 9.606337 9.054427 1.775099 1.775099 0.000000

 Stoichiometry C20H16N8Zn(1+,2)

 Framework group C4H[O(Zn),SGH(C20H8N8),X(H8)]

 Deg. of freedom 20

 Full point group C4H NOp 8

 RotChk: IX=0 Diff= 3.14D-16

 Largest Abelian subgroup C2H NOp 4

 Largest concise Abelian subgroup C2H NOp 4

 Standard orientation:

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 2 7 0 -1.857841 0.741857 0.000000

 3 6 0 -2.988434 0.000000 0.000000

 4 6 0 -4.163571 0.928552 0.000000

 5 6 0 -3.648420 2.182265 0.000000

 6 7 0 -3.096160 -1.330623 0.000000

 7 6 0 -2.062632 -2.182274 0.000000

 8 7 0 -0.741857 -1.857841 0.000000

 9 6 0 0.000000 -2.988434 0.000000

 10 6 0 -0.928552 -4.163571 0.000000

 11 6 0 -2.182265 -3.648420 0.000000

 12 7 0 -1.330623 3.096160 0.000000

 13 6 0 0.928552 4.163571 0.000000

 14 6 0 2.182265 3.648420 0.000000

 15 6 0 2.062632 2.182274 0.000000

 16 7 0 0.741857 1.857841 0.000000

 17 6 0 0.000000 2.988434 0.000000

 18 7 0 3.096160 1.330623 0.000000

 19 7 0 1.857841 -0.741857 0.000000

 20 6 0 2.988434 0.000000 0.000000

 21 6 0 4.163571 -0.928552 0.000000

 22 6 0 3.648420 -2.182265 0.000000

 23 6 0 2.182274 -2.062632 0.000000

 24 7 0 1.330623 -3.096160 0.000000

 25 30 0 0.000000 0.000000 0.000000

 26 6 0 -5.574748 0.470527 0.000000

 27 1 0 -4.183024 3.120980 0.000000

 28 6 0 -0.470527 -5.574748 0.000000

 29 1 0 -3.120980 -4.183024 0.000000

 30 6 0 0.470527 5.574748 0.000000

 31 1 0 3.120980 4.183024 0.000000

 32 6 0 5.574748 -0.470527 0.000000

 33 1 0 4.183024 -3.120980 0.000000

 34 1 0 -6.266246 1.313577 0.000000

 35 1 0 -5.780551 -0.151397 0.876886

 36 1 0 -5.780551 -0.151397 -0.876886

 37 1 0 0.151397 -5.780551 0.876886

 38 1 0 0.151397 -5.780551 -0.876886

 39 1 0 -1.313577 -6.266246 0.000000

 40 1 0 -0.151397 5.780551 0.876886

 41 1 0 -0.151397 5.780551 -0.876886

 42 1 0 1.313577 6.266246 0.000000

 43 1 0 5.780551 0.151397 0.876886

 44 1 0 5.780551 0.151397 -0.876886

 45 1 0 6.266246 -1.313577 0.000000

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

 Rotational constants (GHZ): 0.1830366 0.1830366 0.0917243

 Leave Link 202 at Fri Jul 5 21:14:32 2019, MaxMem= 1342177280 cpu: 0.2

 (Enter /apps/gaussian/g09d01/g09/l601.exe)

 Copying SCF densities to generalized density rwf, IOpCl= 1 IROHF=0.

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

 Population analysis using the SCF density.

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 Orbital symmetries:

 Alpha Orbitals:

 Occupied (BG) (EU) (EU) (AG) (EU) (EU) (BG) (AG) (BG) (EU)

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 Beta Orbitals:

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 The electronic state is 2-AU.

 Alpha occ. eigenvalues -- -14.34226 -14.34226 -14.34226 -14.34225 -14.32977

 Alpha occ. eigenvalues -- -14.32977 -14.32977 -14.32977 -10.28499 -10.28499

 Alpha occ. eigenvalues -- -10.28499 -10.28499 -10.28381 -10.28381 -10.28381

 Alpha occ. eigenvalues -- -10.28381 -10.21287 -10.21287 -10.21287 -10.21287

 Alpha occ. eigenvalues -- -10.19258 -10.19258 -10.19258 -10.19258 -10.17130

 Alpha occ. eigenvalues -- -10.17130 -10.17130 -10.17130 -1.03362 -1.01930

 Alpha occ. eigenvalues -- -1.01930 -0.99149 -0.96932 -0.92699 -0.92699

 Alpha occ. eigenvalues -- -0.89350 -0.81967 -0.81463 -0.81463 -0.81213

 Alpha occ. eigenvalues -- -0.77755 -0.74051 -0.74051 -0.71953 -0.70731

 Alpha occ. eigenvalues -- -0.69972 -0.69972 -0.65919 -0.63258 -0.61124

 Alpha occ. eigenvalues -- -0.59685 -0.59412 -0.58855 -0.58855 -0.57368

 Alpha occ. eigenvalues -- -0.57368 -0.56582 -0.56543 -0.56543 -0.56192

 Alpha occ. eigenvalues -- -0.53867 -0.52552 -0.52552 -0.51765 -0.50505

 Alpha occ. eigenvalues -- -0.48690 -0.46988 -0.46988 -0.45944 -0.45029

 Alpha occ. eigenvalues -- -0.45029 -0.44585 -0.44389 -0.41813 -0.41707

 Alpha occ. eigenvalues -- -0.41707 -0.41604 -0.41522 -0.41255 -0.40743

 Alpha occ. eigenvalues -- -0.40743 -0.39670 -0.39567 -0.39248 -0.39248

 Alpha occ. eigenvalues -- -0.38538 -0.38070 -0.34921 -0.34921 -0.34336

 Alpha occ. eigenvalues -- -0.34336 -0.32921 -0.30187 -0.30187 -0.28442

 Alpha occ. eigenvalues -- -0.28123 -0.27896 -0.27075 -0.27075 -0.26886

 Alpha occ. eigenvalues -- -0.26830 -0.23632

 Alpha virt. eigenvalues -- -0.13274 -0.13274 -0.06528 0.00129 0.02493

 Alpha virt. eigenvalues -- 0.02493 0.02729 0.03921 0.04044 0.04044

 Alpha virt. eigenvalues -- 0.04894 0.06533 0.06725 0.07433 0.07860

 Alpha virt. eigenvalues -- 0.07860 0.08559 0.08856 0.09000 0.09000

 Alpha virt. eigenvalues -- 0.09591 0.09591 0.09667 0.12414 0.13091

 Alpha virt. eigenvalues -- 0.13133 0.13133 0.13218 0.13284 0.13284

 Alpha virt. eigenvalues -- 0.13702 0.16758 0.18572 0.18940 0.19522

 Alpha virt. eigenvalues -- 0.19522 0.19606 0.19762 0.19762 0.21083

 Alpha virt. eigenvalues -- 0.21266 0.21519 0.21600 0.21600 0.23619

 Alpha virt. eigenvalues -- 0.25841 0.26555 0.26555 0.27370 0.27407

 Alpha virt. eigenvalues -- 0.27951 0.27951 0.28598 0.30631 0.30631

 Alpha virt. eigenvalues -- 0.30691 0.30781 0.30866 0.30866 0.31359

 Alpha virt. eigenvalues -- 0.31686 0.33751 0.34174 0.34174 0.34735

 Alpha virt. eigenvalues -- 0.36194 0.36194 0.36208 0.37406 0.37507

 Alpha virt. eigenvalues -- 0.37507 0.38524 0.38902 0.38902 0.39307

 Alpha virt. eigenvalues -- 0.40402 0.42197 0.42197 0.42255 0.42486

 Alpha virt. eigenvalues -- 0.42804 0.44428 0.45219 0.45219 0.45402

 Alpha virt. eigenvalues -- 0.46787 0.47672 0.47672 0.47949 0.48011

 Alpha virt. eigenvalues -- 0.48011 0.48118 0.49883 0.50470 0.50644

 Alpha virt. eigenvalues -- 0.50644 0.51904 0.52740 0.53170 0.53170

 Alpha virt. eigenvalues -- 0.53864 0.55059 0.55059 0.55453 0.55583

 Alpha virt. eigenvalues -- 0.56550 0.56550 0.56559 0.57592 0.57676

 Alpha virt. eigenvalues -- 0.57676 0.57857 0.58511 0.58511 0.58925

 Alpha virt. eigenvalues -- 0.59784 0.60125 0.61405 0.61783 0.61783

 Alpha virt. eigenvalues -- 0.62217 0.62217 0.62293 0.63829 0.64232

 Alpha virt. eigenvalues -- 0.64232 0.66845 0.67269 0.67811 0.67920

 Alpha virt. eigenvalues -- 0.67920 0.68170 0.68170 0.68503 0.69530

 Alpha virt. eigenvalues -- 0.70426 0.72032 0.72349 0.72349 0.73484

 Alpha virt. eigenvalues -- 0.74006 0.74778 0.74778 0.76591 0.76591

 Alpha virt. eigenvalues -- 0.77899 0.78391 0.78662 0.79588 0.79588

 Alpha virt. eigenvalues -- 0.80064 0.80175 0.80175 0.81273 0.81393

 Alpha virt. eigenvalues -- 0.84085 0.84085 0.84109 0.86081 0.87152

 Alpha virt. eigenvalues -- 0.87762 0.87762 0.88495 0.93266 0.95112

 Alpha virt. eigenvalues -- 0.95112 0.96554 0.96935 0.98806 0.99083

 Alpha virt. eigenvalues -- 0.99083 1.01722 1.01722 1.03453 1.03810

 Alpha virt. eigenvalues -- 1.03810 1.05384 1.06730 1.06730 1.07084

 Alpha virt. eigenvalues -- 1.08698 1.09416 1.11673 1.11709 1.11709

 Alpha virt. eigenvalues -- 1.11908 1.12364 1.12477 1.12932 1.12932

 Alpha virt. eigenvalues -- 1.12952 1.16647 1.16993 1.17709 1.17709

 Alpha virt. eigenvalues -- 1.18967 1.18967 1.19180 1.22137 1.22305

 Alpha virt. eigenvalues -- 1.26214 1.26390 1.27574 1.27574 1.28836

 Alpha virt. eigenvalues -- 1.34360 1.34360 1.35453 1.36481 1.37389

 Alpha virt. eigenvalues -- 1.38517 1.39337 1.39337 1.40476 1.40476

 Alpha virt. eigenvalues -- 1.42038 1.42785 1.47715 1.48164 1.48164

 Alpha virt. eigenvalues -- 1.50218 1.50248 1.50248 1.50398 1.50398

 Alpha virt. eigenvalues -- 1.50562 1.50574 1.51537 1.51655 1.53659

 Alpha virt. eigenvalues -- 1.53659 1.54430 1.54903 1.54903 1.55872

 Alpha virt. eigenvalues -- 1.57137 1.59139 1.59251 1.59251 1.60290

 Alpha virt. eigenvalues -- 1.61270 1.61416 1.61416 1.65615 1.65711

 Alpha virt. eigenvalues -- 1.66756 1.66756 1.67632 1.67632 1.68523

 Alpha virt. eigenvalues -- 1.69373 1.69373 1.69602 1.72571 1.73207

 Alpha virt. eigenvalues -- 1.73887 1.73887 1.78532 1.78627 1.78627

 Alpha virt. eigenvalues -- 1.78652 1.83592 1.84912 1.85084 1.85084

 Alpha virt. eigenvalues -- 1.87150 1.88048 1.88048 1.89208 1.89377

 Alpha virt. eigenvalues -- 1.91791 1.93621 1.94335 1.94624 1.94624

 Alpha virt. eigenvalues -- 2.00347 2.00369 2.00486 2.00553 2.00553

 Alpha virt. eigenvalues -- 2.00567 2.00663 2.00663 2.03573 2.05552

 Alpha virt. eigenvalues -- 2.05943 2.07154 2.07154 2.10555 2.10555

 Alpha virt. eigenvalues -- 2.13126 2.13996 2.13996 2.15539 2.15783

 Alpha virt. eigenvalues -- 2.18068 2.26319 2.26830 2.27854 2.28238

 Alpha virt. eigenvalues -- 2.28238 2.28795 2.31525 2.31525 2.34105

 Alpha virt. eigenvalues -- 2.34272 2.34272 2.35734 2.35734 2.35766

 Alpha virt. eigenvalues -- 2.36714 2.37691 2.37966 2.37966 2.38237

 Alpha virt. eigenvalues -- 2.42164 2.46244 2.46524 2.46524 2.46622

 Alpha virt. eigenvalues -- 2.46627 2.46627 2.47448 2.47741 2.54298

 Alpha virt. eigenvalues -- 2.54350 2.54350 2.55050 2.56467 2.56467

 Alpha virt. eigenvalues -- 2.57410 2.58473 2.58473 2.61355 2.62124

 Alpha virt. eigenvalues -- 2.63085 2.64737 2.66163 2.68882 2.68882

 Alpha virt. eigenvalues -- 2.69942 2.70997 2.70997 2.71198 2.73356

 Alpha virt. eigenvalues -- 2.73356 2.74513 2.77008 2.80946 2.81634

 Alpha virt. eigenvalues -- 2.81634 2.81839 2.82554 2.83036 2.83525

 Alpha virt. eigenvalues -- 2.83525 2.89601 2.89601 2.91291 2.91683

 Alpha virt. eigenvalues -- 2.94592 2.94819 2.94819 2.99091 3.00662

 Alpha virt. eigenvalues -- 3.02430 3.02430 3.03286 3.10241 3.11028

 Alpha virt. eigenvalues -- 3.12040 3.12040 3.12592 3.13099 3.13099

 Alpha virt. eigenvalues -- 3.13419 3.13665 3.15259 3.15259 3.17351

 Alpha virt. eigenvalues -- 3.18885 3.18885 3.19104 3.20708 3.23067

 Alpha virt. eigenvalues -- 3.25362 3.26302 3.26699 3.26699 3.28533

 Alpha virt. eigenvalues -- 3.28533 3.33955 3.36693 3.37513 3.37513

 Alpha virt. eigenvalues -- 3.37786 3.50715 3.55223 3.55223 3.68190

 Alpha virt. eigenvalues -- 3.70191 3.71002 3.71002 3.74458 3.76421

 Alpha virt. eigenvalues -- 3.76583 3.76583 3.77476 3.79212 3.80013

 Alpha virt. eigenvalues -- 3.80013 3.85208 3.86011 3.86011 3.86084

 Alpha virt. eigenvalues -- 3.89130 4.03224 4.03224 4.03826 4.04031

 Alpha virt. eigenvalues -- 4.09816 4.10641 4.10641 4.16632 4.26313

 Alpha virt. eigenvalues -- 4.33578 4.33578 4.35673 4.44687 4.49420

 Alpha virt. eigenvalues -- 4.59242 4.59242 4.97039 5.00483 5.00483

 Alpha virt. eigenvalues -- 5.09582 5.12987 5.31099 5.31099 5.48051

 Alpha virt. eigenvalues -- 7.76920 7.76920 7.88201 7.93902 8.21953

 Alpha virt. eigenvalues -- 11.19162 23.41254 23.43512 23.43512 23.44809

 Alpha virt. eigenvalues -- 23.66671 23.67097 23.67106 23.67106 23.76920

 Alpha virt. eigenvalues -- 23.78302 23.78302 23.79795 23.83272 23.84487

 Alpha virt. eigenvalues -- 23.84487 23.84781 24.11966 24.12473 24.12473

 Alpha virt. eigenvalues -- 24.13183 35.54490 35.59108 35.59108 35.60369

 Alpha virt. eigenvalues -- 35.65663 35.66960 35.66960 35.67373

 Beta occ. eigenvalues -- -14.34371 -14.34371 -14.34371 -14.34371 -14.33075

 Beta occ. eigenvalues -- -14.33075 -14.33075 -14.33075 -10.28227 -10.28227

 Beta occ. eigenvalues -- -10.28227 -10.28227 -10.28110 -10.28110 -10.28110

 Beta occ. eigenvalues -- -10.28110 -10.21219 -10.21219 -10.21219 -10.21219

 Beta occ. eigenvalues -- -10.19282 -10.19282 -10.19282 -10.19282 -10.17131

 Beta occ. eigenvalues -- -10.17131 -10.17131 -10.17131 -1.03160 -1.01728

 Beta occ. eigenvalues -- -1.01728 -0.98937 -0.96840 -0.92678 -0.92678

 Beta occ. eigenvalues -- -0.89524 -0.81861 -0.81385 -0.81385 -0.81143

 Beta occ. eigenvalues -- -0.77184 -0.73774 -0.73774 -0.71913 -0.70591

 Beta occ. eigenvalues -- -0.69750 -0.69750 -0.65633 -0.63026 -0.61072

 Beta occ. eigenvalues -- -0.59585 -0.59374 -0.58706 -0.58706 -0.57389

 Beta occ. eigenvalues -- -0.57389 -0.56475 -0.56382 -0.56382 -0.56160

 Beta occ. eigenvalues -- -0.53748 -0.52461 -0.52461 -0.51660 -0.50431

 Beta occ. eigenvalues -- -0.47951 -0.46234 -0.46234 -0.45912 -0.44994

 Beta occ. eigenvalues -- -0.44994 -0.44344 -0.43951 -0.41656 -0.41522

 Beta occ. eigenvalues -- -0.41503 -0.41503 -0.41483 -0.40636 -0.40636

 Beta occ. eigenvalues -- -0.40585 -0.39459 -0.39205 -0.39205 -0.39189

 Beta occ. eigenvalues -- -0.38487 -0.37985 -0.34917 -0.34917 -0.33593

 Beta occ. eigenvalues -- -0.33593 -0.33005 -0.30280 -0.30280 -0.28556

 Beta occ. eigenvalues -- -0.28033 -0.27944 -0.27744 -0.27059 -0.27059

 Beta occ. eigenvalues -- -0.26813

 Beta virt. eigenvalues -- -0.18531 -0.11856 -0.11856 -0.05874 0.01328

 Beta virt. eigenvalues -- 0.02966 0.03338 0.03338 0.04097 0.04097

 Beta virt. eigenvalues -- 0.04706 0.04904 0.06535 0.06740 0.07892

 Beta virt. eigenvalues -- 0.07892 0.08200 0.08874 0.08950 0.09606

 Beta virt. eigenvalues -- 0.09606 0.09720 0.09752 0.09752 0.12421

 Beta virt. eigenvalues -- 0.13148 0.13148 0.13200 0.13226 0.13455

 Beta virt. eigenvalues -- 0.13455 0.13874 0.17010 0.18774 0.19217

 Beta virt. eigenvalues -- 0.19781 0.19781 0.19786 0.19958 0.19958

 Beta virt. eigenvalues -- 0.21195 0.21343 0.21765 0.21874 0.21874

 Beta virt. eigenvalues -- 0.23933 0.26144 0.26675 0.26675 0.27490

 Beta virt. eigenvalues -- 0.27804 0.28175 0.28175 0.28769 0.30758

 Beta virt. eigenvalues -- 0.30799 0.30799 0.30860 0.30929 0.30929

 Beta virt. eigenvalues -- 0.31447 0.31780 0.33810 0.34371 0.34371

 Beta virt. eigenvalues -- 0.34888 0.36326 0.36326 0.36394 0.37728

 Beta virt. eigenvalues -- 0.38180 0.38180 0.38669 0.39054 0.39054

 Beta virt. eigenvalues -- 0.39470 0.40856 0.42335 0.42335 0.42672

 Beta virt. eigenvalues -- 0.42948 0.43314 0.44583 0.45439 0.45439

 Beta virt. eigenvalues -- 0.45571 0.46922 0.47834 0.47834 0.48154

 Beta virt. eigenvalues -- 0.48154 0.48220 0.48241 0.50021 0.50748

 Beta virt. eigenvalues -- 0.50998 0.50998 0.52357 0.52877 0.53240

 Beta virt. eigenvalues -- 0.53240 0.53924 0.55131 0.55131 0.55533

 Beta virt. eigenvalues -- 0.55667 0.56632 0.56632 0.56877 0.57633

 Beta virt. eigenvalues -- 0.57807 0.57807 0.57913 0.58580 0.58580

 Beta virt. eigenvalues -- 0.58973 0.59855 0.60213 0.61538 0.61964

 Beta virt. eigenvalues -- 0.61964 0.62338 0.62572 0.62572 0.63918

 Beta virt. eigenvalues -- 0.64289 0.64289 0.67154 0.67417 0.67890

 Beta virt. eigenvalues -- 0.68020 0.68020 0.68054 0.68054 0.68643

 Beta virt. eigenvalues -- 0.69664 0.70437 0.72151 0.72497 0.72497

 Beta virt. eigenvalues -- 0.73572 0.74204 0.74875 0.74875 0.76723

 Beta virt. eigenvalues -- 0.76723 0.77881 0.78280 0.78870 0.79502

 Beta virt. eigenvalues -- 0.79502 0.79877 0.80285 0.80285 0.81358

 Beta virt. eigenvalues -- 0.81453 0.84175 0.84183 0.84183 0.86155

 Beta virt. eigenvalues -- 0.87211 0.87833 0.87833 0.88591 0.93420

 Beta virt. eigenvalues -- 0.95167 0.95167 0.96762 0.97018 0.99194

 Beta virt. eigenvalues -- 0.99194 0.99223 1.02056 1.02056 1.03510

 Beta virt. eigenvalues -- 1.03972 1.03972 1.05568 1.07142 1.07142

 Beta virt. eigenvalues -- 1.07203 1.09060 1.09418 1.11735 1.12337

 Beta virt. eigenvalues -- 1.12353 1.12353 1.12477 1.12931 1.13039

 Beta virt. eigenvalues -- 1.13039 1.13508 1.17207 1.17265 1.17743

 Beta virt. eigenvalues -- 1.17743 1.19368 1.19423 1.19423 1.22181

 Beta virt. eigenvalues -- 1.22335 1.26296 1.26830 1.27712 1.27712

 Beta virt. eigenvalues -- 1.28880 1.34849 1.34849 1.35635 1.37075

 Beta virt. eigenvalues -- 1.37467 1.38971 1.39414 1.39414 1.40610

 Beta virt. eigenvalues -- 1.40610 1.42285 1.42935 1.47710 1.48214

 Beta virt. eigenvalues -- 1.48214 1.50294 1.50321 1.50321 1.50375

 Beta virt. eigenvalues -- 1.50375 1.50508 1.50615 1.51630 1.52105

 Beta virt. eigenvalues -- 1.53771 1.53771 1.54486 1.55058 1.55058

 Beta virt. eigenvalues -- 1.56089 1.57367 1.59217 1.59526 1.59526

 Beta virt. eigenvalues -- 1.60373 1.61475 1.61537 1.61537 1.65681

 Beta virt. eigenvalues -- 1.66094 1.66922 1.66922 1.67731 1.67731

 Beta virt. eigenvalues -- 1.68717 1.69718 1.69887 1.69887 1.72733

 Beta virt. eigenvalues -- 1.73866 1.74054 1.74054 1.78827 1.78845

 Beta virt. eigenvalues -- 1.78849 1.78849 1.83705 1.85162 1.85234

 Beta virt. eigenvalues -- 1.85234 1.87256 1.88399 1.88399 1.89383

 Beta virt. eigenvalues -- 1.89729 1.92076 1.93921 1.94510 1.94963

 Beta virt. eigenvalues -- 1.94963 2.00506 2.00657 2.00717 2.00717

 Beta virt. eigenvalues -- 2.00720 2.00786 2.01176 2.01176 2.03656

 Beta virt. eigenvalues -- 2.05955 2.05971 2.07211 2.07211 2.10608

 Beta virt. eigenvalues -- 2.10608 2.13250 2.14306 2.14306 2.15652

 Beta virt. eigenvalues -- 2.16226 2.18220 2.26372 2.27108 2.27904

 Beta virt. eigenvalues -- 2.28271 2.28271 2.28826 2.31626 2.31626

 Beta virt. eigenvalues -- 2.34148 2.34332 2.34332 2.35816 2.36071

 Beta virt. eigenvalues -- 2.36071 2.36748 2.37763 2.37995 2.37995

 Beta virt. eigenvalues -- 2.38645 2.42208 2.46155 2.46650 2.46650

 Beta virt. eigenvalues -- 2.46691 2.46691 2.46753 2.47697 2.47827

 Beta virt. eigenvalues -- 2.54232 2.54237 2.54237 2.55049 2.56460

 Beta virt. eigenvalues -- 2.56460 2.57854 2.58893 2.58893 2.61666

 Beta virt. eigenvalues -- 2.62041 2.62963 2.65063 2.66160 2.69089

 Beta virt. eigenvalues -- 2.69089 2.70119 2.70938 2.70938 2.71156

 Beta virt. eigenvalues -- 2.74149 2.74149 2.75250 2.77916 2.81503

 Beta virt. eigenvalues -- 2.82304 2.82304 2.82601 2.82654 2.83069

 Beta virt. eigenvalues -- 2.83596 2.83596 2.89686 2.89686 2.91408

 Beta virt. eigenvalues -- 2.92122 2.94658 2.95411 2.95411 2.99810

 Beta virt. eigenvalues -- 3.00756 3.02517 3.02517 3.03377 3.10278

 Beta virt. eigenvalues -- 3.11082 3.12106 3.12106 3.12669 3.13192

 Beta virt. eigenvalues -- 3.13192 3.13516 3.13800 3.15327 3.15327

 Beta virt. eigenvalues -- 3.17392 3.18944 3.18944 3.19168 3.20728

 Beta virt. eigenvalues -- 3.23130 3.25417 3.26375 3.26760 3.26760

 Beta virt. eigenvalues -- 3.28606 3.28606 3.34039 3.36716 3.37538

 Beta virt. eigenvalues -- 3.37538 3.37817 3.50866 3.55361 3.55361

 Beta virt. eigenvalues -- 3.68306 3.70321 3.71149 3.71149 3.74570

 Beta virt. eigenvalues -- 3.76590 3.76718 3.76718 3.77616 3.78732

 Beta virt. eigenvalues -- 3.79632 3.79632 3.84892 3.85625 3.85625

 Beta virt. eigenvalues -- 3.85637 3.88814 4.03342 4.03342 4.03943

 Beta virt. eigenvalues -- 4.04158 4.09810 4.10688 4.10688 4.16747

 Beta virt. eigenvalues -- 4.26364 4.33742 4.33742 4.35912 4.44748

 Beta virt. eigenvalues -- 4.49430 4.59267 4.59267 4.97210 5.00658

 Beta virt. eigenvalues -- 5.00658 5.09779 5.13145 5.31287 5.31287

 Beta virt. eigenvalues -- 5.48241 7.76902 7.76902 7.88201 7.93897

 Beta virt. eigenvalues -- 8.21949 11.19152 23.41301 23.43552 23.43552

 Beta virt. eigenvalues -- 23.44845 23.66691 23.67108 23.67119 23.67119

 Beta virt. eigenvalues -- 23.77191 23.78591 23.78591 23.80091 23.83585

 Beta virt. eigenvalues -- 23.84799 23.84799 23.85096 24.11994 24.12501

 Beta virt. eigenvalues -- 24.12501 24.13212 35.54366 35.58995 35.58995

 Beta virt. eigenvalues -- 35.60268 35.65512 35.66821 35.66821 35.67245

 Condensed to atoms (all electrons):

 1 2 3 4 5 6

 1 C 4.568765 0.403219 -0.128854 -0.047235 0.402264 -0.001888

 2 N 0.403219 7.120889 0.389900 -0.063537 -0.092361 -0.077874

 3 C -0.128854 0.389900 4.604148 0.375381 -0.064669 0.557042

 4 C -0.047235 -0.063537 0.375381 5.030996 0.632645 -0.069900

 5 C 0.402264 -0.092361 -0.064669 0.632645 5.081045 0.004157

 6 N -0.001888 -0.077874 0.557042 -0.069900 0.004157 6.567016

 7 C -0.001135 -0.005058 -0.089215 0.004496 -0.000309 0.514663

 8 N 0.000720 -0.018783 -0.005858 -0.000169 -0.000203 -0.071319

 9 C -0.000007 0.000616 -0.000909 0.000023 -0.000004 0.000086

 10 C -0.000003 -0.000111 0.000062 0.000013 0.000000 0.003231

 11 C 0.000023 0.000207 0.004124 -0.000235 0.000010 -0.040392

 12 N 0.514663 -0.071319 0.000086 0.003231 -0.040392 -0.000150

 13 C 0.004496 -0.000169 0.000023 0.000013 -0.000235 0.000000

 14 C -0.000309 -0.000203 -0.000004 0.000000 0.000010 0.000000

 15 C -0.001135 0.000720 -0.000007 -0.000003 0.000023 -0.000001

 16 N -0.005058 -0.018783 0.000616 -0.000111 0.000207 -0.000004

 17 C -0.089215 -0.005858 -0.000909 0.000062 0.004124 -0.000025

 18 N -0.000019 -0.000004 -0.000001 0.000000 0.000000 0.000000

 19 N 0.000164 -0.003650 0.000224 0.000002 0.000003 -0.000004

 20 C -0.000053 0.000224 -0.000011 0.000000 0.000000 -0.000001

 21 C 0.000000 0.000002 0.000000 0.000000 0.000000 0.000000

 22 C 0.000000 0.000003 0.000000 0.000000 0.000000 0.000000

 23 C -0.000004 0.000164 -0.000053 0.000000 0.000000 -0.000019

 24 N -0.000001 -0.000004 -0.000025 0.000000 0.000000 -0.000150

 25 Zn -0.015454 0.104850 -0.016767 -0.000991 -0.001118 -0.004938

 26 C 0.009024 0.008228 -0.068843 0.271786 -0.052086 0.013058

 27 H -0.046094 0.005535 0.009196 -0.040614 0.395502 -0.000010

 28 C 0.000000 0.000000 0.000002 0.000000 0.000000 -0.000020

 29 H 0.000001 0.000065 -0.000224 -0.000129 -0.000003 0.005477

 30 C -0.000507 0.000059 0.000000 0.000000 -0.000046 0.000000

 31 H 0.000012 0.000001 0.000000 0.000000 0.000000 0.000000

 32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 33 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 34 H 0.000203 -0.000232 0.006189 -0.039530 -0.005559 0.000056

 35 H -0.000186 0.000409 -0.005251 -0.042909 -0.000326 0.003632

 36 H -0.000186 0.000409 -0.005251 -0.042909 -0.000326 0.003632

 37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000007

 38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000007

 39 H 0.000000 0.000000 0.000001 0.000000 0.000000 -0.000009

 40 H -0.000045 0.000013 0.000000 0.000000 -0.000020 0.000000

 41 H -0.000045 0.000013 0.000000 0.000000 -0.000020 0.000000

 42 H 0.000038 0.000000 0.000000 0.000000 -0.000001 0.000000

 43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 7 8 9 10 11 12

 1 C -0.001135 0.000720 -0.000007 -0.000003 0.000023 0.514663

 2 N -0.005058 -0.018783 0.000616 -0.000111 0.000207 -0.071319

 3 C -0.089215 -0.005858 -0.000909 0.000062 0.004124 0.000086

 4 C 0.004496 -0.000169 0.000023 0.000013 -0.000235 0.003231

 5 C -0.000309 -0.000203 -0.000004 0.000000 0.000010 -0.040392

 6 N 0.514663 -0.071319 0.000086 0.003231 -0.040392 -0.000150

 7 C 4.568765 0.403219 -0.128854 -0.047235 0.402264 -0.000019

 8 N 0.403219 7.120889 0.389900 -0.063537 -0.092361 -0.000004

 9 C -0.128854 0.389900 4.604148 0.375381 -0.064669 -0.000001

 10 C -0.047235 -0.063537 0.375381 5.030996 0.632645 0.000000

 11 C 0.402264 -0.092361 -0.064669 0.632645 5.081045 0.000000

 12 N -0.000019 -0.000004 -0.000001 0.000000 0.000000 6.567016

 13 C 0.000000 0.000002 0.000000 0.000000 0.000000 -0.069900

 14 C 0.000000 0.000003 0.000000 0.000000 0.000000 0.004157

 15 C -0.000004 0.000164 -0.000053 0.000000 0.000000 -0.001888

 16 N 0.000164 -0.003650 0.000224 0.000002 0.000003 -0.077874

 17 C -0.000053 0.000224 -0.000011 0.000000 0.000000 0.557042

 18 N -0.000001 -0.000004 -0.000025 0.000000 0.000000 -0.000150

 19 N 0.000720 -0.018783 -0.005858 -0.000169 -0.000203 -0.000004

 20 C -0.000007 0.000616 -0.000909 0.000023 -0.000004 -0.000025

 21 C -0.000003 -0.000111 0.000062 0.000013 0.000000 0.000000

 22 C 0.000023 0.000207 0.004124 -0.000235 0.000010 0.000000

 23 C -0.001135 -0.005058 -0.089215 0.004496 -0.000309 -0.000001

 24 N -0.001888 -0.077874 0.557042 -0.069900 0.004157 0.000000

 25 Zn -0.015454 0.104850 -0.016767 -0.000991 -0.001118 -0.004938

 26 C -0.000507 0.000059 0.000000 0.000000 -0.000046 -0.000020

 27 H 0.000012 0.000001 0.000000 0.000000 0.000000 0.005477

 28 C 0.009024 0.008228 -0.068843 0.271786 -0.052086 0.000000

 29 H -0.046094 0.005535 0.009196 -0.040614 0.395502 0.000000

 30 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.013058

 31 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000010

 32 C 0.000000 0.000000 0.000002 0.000000 0.000000 0.000000

 33 H 0.000001 0.000065 -0.000224 -0.000129 -0.000003 0.000000

 34 H 0.000038 0.000000 0.000000 0.000000 -0.000001 -0.000009

 35 H -0.000045 0.000013 0.000000 0.000000 -0.000020 0.000007

 36 H -0.000045 0.000013 0.000000 0.000000 -0.000020 0.000007

 37 H -0.000186 0.000409 -0.005251 -0.042909 -0.000326 0.000000

 38 H -0.000186 0.000409 -0.005251 -0.042909 -0.000326 0.000000

 39 H 0.000203 -0.000232 0.006189 -0.039530 -0.005559 0.000000

 40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.003632

 41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.003632

 42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000056

 43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 45 H 0.000000 0.000000 0.000001 0.000000 0.000000 0.000000

 13 14 15 16 17 18

 1 C 0.004496 -0.000309 -0.001135 -0.005058 -0.089215 -0.000019

 2 N -0.000169 -0.000203 0.000720 -0.018783 -0.005858 -0.000004

 3 C 0.000023 -0.000004 -0.000007 0.000616 -0.000909 -0.000001

 4 C 0.000013 0.000000 -0.000003 -0.000111 0.000062 0.000000

 5 C -0.000235 0.000010 0.000023 0.000207 0.004124 0.000000

 6 N 0.000000 0.000000 -0.000001 -0.000004 -0.000025 0.000000

 7 C 0.000000 0.000000 -0.000004 0.000164 -0.000053 -0.000001

 8 N 0.000002 0.000003 0.000164 -0.003650 0.000224 -0.000004

 9 C 0.000000 0.000000 -0.000053 0.000224 -0.000011 -0.000025

 10 C 0.000000 0.000000 0.000000 0.000002 0.000000 0.000000

 11 C 0.000000 0.000000 0.000000 0.000003 0.000000 0.000000

 12 N -0.069900 0.004157 -0.001888 -0.077874 0.557042 -0.000150

 13 C 5.030996 0.632645 -0.047235 -0.063537 0.375381 0.003231

 14 C 0.632645 5.081045 0.402264 -0.092361 -0.064669 -0.040392

 15 C -0.047235 0.402264 4.568765 0.403219 -0.128854 0.514663

 16 N -0.063537 -0.092361 0.403219 7.120889 0.389900 -0.071319

 17 C 0.375381 -0.064669 -0.128854 0.389900 4.604148 0.000086

 18 N 0.003231 -0.040392 0.514663 -0.071319 0.000086 6.567016

 19 N -0.000111 0.000207 -0.005058 -0.018783 0.000616 -0.077874

 20 C 0.000062 0.004124 -0.089215 -0.005858 -0.000909 0.557042

 21 C 0.000013 -0.000235 0.004496 -0.000169 0.000023 -0.069900

 22 C 0.000000 0.000010 -0.000309 -0.000203 -0.000004 0.004157

 23 C -0.000003 0.000023 -0.001135 0.000720 -0.000007 -0.001888

 24 N 0.000000 0.000000 -0.000019 -0.000004 -0.000001 -0.000150

 25 Zn -0.000991 -0.001118 -0.015454 0.104850 -0.016767 -0.004938

 26 C 0.000000 0.000000 0.000000 0.000000 0.000002 0.000000

 27 H -0.000129 -0.000003 0.000001 0.000065 -0.000224 0.000000

 28 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 29 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 30 C 0.271786 -0.052086 0.009024 0.008228 -0.068843 -0.000020

 31 H -0.040614 0.395502 -0.046094 0.005535 0.009196 0.005477

 32 C 0.000000 -0.000046 -0.000507 0.000059 0.000000 0.013058

 33 H 0.000000 0.000000 0.000012 0.000001 0.000000 -0.000010

 34 H 0.000000 0.000000 0.000000 0.000000 0.000001 0.000000

 35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 40 H -0.042909 -0.000326 -0.000186 0.000409 -0.005251 0.000007

 41 H -0.042909 -0.000326 -0.000186 0.000409 -0.005251 0.000007

 42 H -0.039530 -0.005559 0.000203 -0.000232 0.006189 -0.000009

 43 H 0.000000 -0.000020 -0.000045 0.000013 0.000000 0.003632

 44 H 0.000000 -0.000020 -0.000045 0.000013 0.000000 0.003632

 45 H 0.000000 -0.000001 0.000038 0.000000 0.000000 0.000056

 19 20 21 22 23 24

 1 C 0.000164 -0.000053 0.000000 0.000000 -0.000004 -0.000001

 2 N -0.003650 0.000224 0.000002 0.000003 0.000164 -0.000004

 3 C 0.000224 -0.000011 0.000000 0.000000 -0.000053 -0.000025

 4 C 0.000002 0.000000 0.000000 0.000000 0.000000 0.000000

 5 C 0.000003 0.000000 0.000000 0.000000 0.000000 0.000000

 6 N -0.000004 -0.000001 0.000000 0.000000 -0.000019 -0.000150

 7 C 0.000720 -0.000007 -0.000003 0.000023 -0.001135 -0.001888

 8 N -0.018783 0.000616 -0.000111 0.000207 -0.005058 -0.077874

 9 C -0.005858 -0.000909 0.000062 0.004124 -0.089215 0.557042

 10 C -0.000169 0.000023 0.000013 -0.000235 0.004496 -0.069900

 11 C -0.000203 -0.000004 0.000000 0.000010 -0.000309 0.004157

 12 N -0.000004 -0.000025 0.000000 0.000000 -0.000001 0.000000

 13 C -0.000111 0.000062 0.000013 0.000000 -0.000003 0.000000

 14 C 0.000207 0.004124 -0.000235 0.000010 0.000023 0.000000

 15 C -0.005058 -0.089215 0.004496 -0.000309 -0.001135 -0.000019

 16 N -0.018783 -0.005858 -0.000169 -0.000203 0.000720 -0.000004

 17 C 0.000616 -0.000909 0.000023 -0.000004 -0.000007 -0.000001

 18 N -0.077874 0.557042 -0.069900 0.004157 -0.001888 -0.000150

 19 N 7.120889 0.389900 -0.063537 -0.092361 0.403219 -0.071319

 20 C 0.389900 4.604148 0.375381 -0.064669 -0.128854 0.000086

 21 C -0.063537 0.375381 5.030996 0.632645 -0.047235 0.003231

 22 C -0.092361 -0.064669 0.632645 5.081045 0.402264 -0.040392

 23 C 0.403219 -0.128854 -0.047235 0.402264 4.568765 0.514663

 24 N -0.071319 0.000086 0.003231 -0.040392 0.514663 6.567016

 25 Zn 0.104850 -0.016767 -0.000991 -0.001118 -0.015454 -0.004938

 26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 28 C 0.000059 0.000000 0.000000 -0.000046 -0.000507 0.013058

 29 H 0.000001 0.000000 0.000000 0.000000 0.000012 -0.000010

 30 C 0.000000 0.000002 0.000000 0.000000 0.000000 0.000000

 31 H 0.000065 -0.000224 -0.000129 -0.000003 0.000001 0.000000

 32 C 0.008228 -0.068843 0.271786 -0.052086 0.009024 -0.000020

 33 H 0.005535 0.009196 -0.040614 0.395502 -0.046094 0.005477

 34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 37 H 0.000013 0.000000 0.000000 -0.000020 -0.000045 0.003632

 38 H 0.000013 0.000000 0.000000 -0.000020 -0.000045 0.003632

 39 H 0.000000 0.000000 0.000000 -0.000001 0.000038 0.000056

 40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 42 H 0.000000 0.000001 0.000000 0.000000 0.000000 0.000000

 43 H 0.000409 -0.005251 -0.042909 -0.000326 -0.000186 0.000007

 44 H 0.000409 -0.005251 -0.042909 -0.000326 -0.000186 0.000007

 45 H -0.000232 0.006189 -0.039530 -0.005559 0.000203 -0.000009

 25 26 27 28 29 30

 1 C -0.015454 0.009024 -0.046094 0.000000 0.000001 -0.000507

 2 N 0.104850 0.008228 0.005535 0.000000 0.000065 0.000059

 3 C -0.016767 -0.068843 0.009196 0.000002 -0.000224 0.000000

 4 C -0.000991 0.271786 -0.040614 0.000000 -0.000129 0.000000

 5 C -0.001118 -0.052086 0.395502 0.000000 -0.000003 -0.000046

 6 N -0.004938 0.013058 -0.000010 -0.000020 0.005477 0.000000

 7 C -0.015454 -0.000507 0.000012 0.009024 -0.046094 0.000000

 8 N 0.104850 0.000059 0.000001 0.008228 0.005535 0.000000

 9 C -0.016767 0.000000 0.000000 -0.068843 0.009196 0.000000

 10 C -0.000991 0.000000 0.000000 0.271786 -0.040614 0.000000

 11 C -0.001118 -0.000046 0.000000 -0.052086 0.395502 0.000000

 12 N -0.004938 -0.000020 0.005477 0.000000 0.000000 0.013058

 13 C -0.000991 0.000000 -0.000129 0.000000 0.000000 0.271786

 14 C -0.001118 0.000000 -0.000003 0.000000 0.000000 -0.052086

 15 C -0.015454 0.000000 0.000001 0.000000 0.000000 0.009024

 16 N 0.104850 0.000000 0.000065 0.000000 0.000000 0.008228

 17 C -0.016767 0.000002 -0.000224 0.000000 0.000000 -0.068843

 18 N -0.004938 0.000000 0.000000 0.000000 0.000000 -0.000020

 19 N 0.104850 0.000000 0.000000 0.000059 0.000001 0.000000

 20 C -0.016767 0.000000 0.000000 0.000000 0.000000 0.000002

 21 C -0.000991 0.000000 0.000000 0.000000 0.000000 0.000000

 22 C -0.001118 0.000000 0.000000 -0.000046 0.000000 0.000000

 23 C -0.015454 0.000000 0.000000 -0.000507 0.000012 0.000000

 24 N -0.004938 0.000000 0.000000 0.013058 -0.000010 0.000000

 25 Zn 10.188336 0.000411 0.000025 0.000411 0.000025 0.000411

 26 C 0.000411 5.357168 -0.004283 0.000000 0.000058 0.000000

 27 H 0.000025 -0.004283 0.426033 0.000000 0.000000 0.000058

 28 C 0.000411 0.000000 0.000000 5.357168 -0.004283 0.000000

 29 H 0.000025 0.000058 0.000000 -0.004283 0.426033 0.000000

 30 C 0.000411 0.000000 0.000058 0.000000 0.000000 5.357168

 31 H 0.000025 0.000000 0.000000 0.000000 0.000000 -0.004283

 32 C 0.000411 0.000000 0.000000 0.000000 0.000000 0.000000

 33 H 0.000025 0.000000 0.000000 0.000058 0.000000 0.000000

 34 H 0.000051 0.388481 0.001240 0.000000 0.000000 0.000000

 35 H 0.000075 0.386967 -0.000100 0.000000 0.000032 0.000000

 36 H 0.000075 0.386967 -0.000100 0.000000 0.000032 0.000000

 37 H 0.000075 0.000000 0.000000 0.386967 -0.000100 0.000000

 38 H 0.000075 0.000000 0.000000 0.386967 -0.000100 0.000000

 39 H 0.000051 0.000000 0.000000 0.388481 0.001240 0.000000

 40 H 0.000075 0.000000 0.000032 0.000000 0.000000 0.386967

 41 H 0.000075 0.000000 0.000032 0.000000 0.000000 0.386967

 42 H 0.000051 0.000000 0.000000 0.000000 0.000000 0.388481

 43 H 0.000075 0.000000 0.000000 0.000000 0.000000 0.000000

 44 H 0.000075 0.000000 0.000000 0.000000 0.000000 0.000000

 45 H 0.000051 0.000000 0.000000 0.000000 0.000000 0.000000

 31 32 33 34 35 36

 1 C 0.000012 0.000000 0.000000 0.000203 -0.000186 -0.000186

 2 N 0.000001 0.000000 0.000000 -0.000232 0.000409 0.000409

 3 C 0.000000 0.000000 0.000000 0.006189 -0.005251 -0.005251

 4 C 0.000000 0.000000 0.000000 -0.039530 -0.042909 -0.042909

 5 C 0.000000 0.000000 0.000000 -0.005559 -0.000326 -0.000326

 6 N 0.000000 0.000000 0.000000 0.000056 0.003632 0.003632

 7 C 0.000000 0.000000 0.000001 0.000038 -0.000045 -0.000045

 8 N 0.000000 0.000000 0.000065 0.000000 0.000013 0.000013

 9 C 0.000000 0.000002 -0.000224 0.000000 0.000000 0.000000

 10 C 0.000000 0.000000 -0.000129 0.000000 0.000000 0.000000

 11 C 0.000000 0.000000 -0.000003 -0.000001 -0.000020 -0.000020

 12 N -0.000010 0.000000 0.000000 -0.000009 0.000007 0.000007

 13 C -0.040614 0.000000 0.000000 0.000000 0.000000 0.000000

 14 C 0.395502 -0.000046 0.000000 0.000000 0.000000 0.000000

 15 C -0.046094 -0.000507 0.000012 0.000000 0.000000 0.000000

 16 N 0.005535 0.000059 0.000001 0.000000 0.000000 0.000000

 17 C 0.009196 0.000000 0.000000 0.000001 0.000000 0.000000

 18 N 0.005477 0.013058 -0.000010 0.000000 0.000000 0.000000

 19 N 0.000065 0.008228 0.005535 0.000000 0.000000 0.000000

 20 C -0.000224 -0.068843 0.009196 0.000000 0.000000 0.000000

 21 C -0.000129 0.271786 -0.040614 0.000000 0.000000 0.000000

 22 C -0.000003 -0.052086 0.395502 0.000000 0.000000 0.000000

 23 C 0.000001 0.009024 -0.046094 0.000000 0.000000 0.000000

 24 N 0.000000 -0.000020 0.005477 0.000000 0.000000 0.000000

 25 Zn 0.000025 0.000411 0.000025 0.000051 0.000075 0.000075

 26 C 0.000000 0.000000 0.000000 0.388481 0.386967 0.386967

 27 H 0.000000 0.000000 0.000000 0.001240 -0.000100 -0.000100

 28 C 0.000000 0.000000 0.000058 0.000000 0.000000 0.000000

 29 H 0.000000 0.000000 0.000000 0.000000 0.000032 0.000032

 30 C -0.004283 0.000000 0.000000 0.000000 0.000000 0.000000

 31 H 0.426033 0.000058 0.000000 0.000000 0.000000 0.000000

 32 C 0.000058 5.357168 -0.004283 0.000000 0.000000 0.000000

 33 H 0.000000 -0.004283 0.426033 0.000000 0.000000 0.000000

 34 H 0.000000 0.000000 0.000000 0.446962 -0.023873 -0.023873

 35 H 0.000000 0.000000 0.000000 -0.023873 0.457354 -0.027507

 36 H 0.000000 0.000000 0.000000 -0.023873 -0.027507 0.457354

 37 H 0.000000 0.000000 0.000032 0.000000 0.000000 0.000000

 38 H 0.000000 0.000000 0.000032 0.000000 0.000000 0.000000

 39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 40 H -0.000100 0.000000 0.000000 0.000000 0.000000 0.000000

 41 H -0.000100 0.000000 0.000000 0.000000 0.000000 0.000000

 42 H 0.001240 0.000000 0.000000 0.000000 0.000000 0.000000

 43 H 0.000032 0.386967 -0.000100 0.000000 0.000000 0.000000

 44 H 0.000032 0.386967 -0.000100 0.000000 0.000000 0.000000

 45 H 0.000000 0.388481 0.001240 0.000000 0.000000 0.000000

 37 38 39 40 41 42

 1 C 0.000000 0.000000 0.000000 -0.000045 -0.000045 0.000038

 2 N 0.000000 0.000000 0.000000 0.000013 0.000013 0.000000

 3 C 0.000000 0.000000 0.000001 0.000000 0.000000 0.000000

 4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 5 C 0.000000 0.000000 0.000000 -0.000020 -0.000020 -0.000001

 6 N 0.000007 0.000007 -0.000009 0.000000 0.000000 0.000000

 7 C -0.000186 -0.000186 0.000203 0.000000 0.000000 0.000000

 8 N 0.000409 0.000409 -0.000232 0.000000 0.000000 0.000000

 9 C -0.005251 -0.005251 0.006189 0.000000 0.000000 0.000000

 10 C -0.042909 -0.042909 -0.039530 0.000000 0.000000 0.000000

 11 C -0.000326 -0.000326 -0.005559 0.000000 0.000000 0.000000

 12 N 0.000000 0.000000 0.000000 0.003632 0.003632 0.000056

 13 C 0.000000 0.000000 0.000000 -0.042909 -0.042909 -0.039530

 14 C 0.000000 0.000000 0.000000 -0.000326 -0.000326 -0.005559

 15 C 0.000000 0.000000 0.000000 -0.000186 -0.000186 0.000203

 16 N 0.000000 0.000000 0.000000 0.000409 0.000409 -0.000232

 17 C 0.000000 0.000000 0.000000 -0.005251 -0.005251 0.006189

 18 N 0.000000 0.000000 0.000000 0.000007 0.000007 -0.000009

 19 N 0.000013 0.000013 0.000000 0.000000 0.000000 0.000000

 20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000001

 21 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 22 C -0.000020 -0.000020 -0.000001 0.000000 0.000000 0.000000

 23 C -0.000045 -0.000045 0.000038 0.000000 0.000000 0.000000

 24 N 0.003632 0.003632 0.000056 0.000000 0.000000 0.000000

 25 Zn 0.000075 0.000075 0.000051 0.000075 0.000075 0.000051

 26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 27 H 0.000000 0.000000 0.000000 0.000032 0.000032 0.000000

 28 C 0.386967 0.386967 0.388481 0.000000 0.000000 0.000000

 29 H -0.000100 -0.000100 0.001240 0.000000 0.000000 0.000000

 30 C 0.000000 0.000000 0.000000 0.386967 0.386967 0.388481

 31 H 0.000000 0.000000 0.000000 -0.000100 -0.000100 0.001240

 32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 33 H 0.000032 0.000032 0.000000 0.000000 0.000000 0.000000

 34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 37 H 0.457354 -0.027507 -0.023873 0.000000 0.000000 0.000000

 38 H -0.027507 0.457354 -0.023873 0.000000 0.000000 0.000000

 39 H -0.023873 -0.023873 0.446962 0.000000 0.000000 0.000000

 40 H 0.000000 0.000000 0.000000 0.457354 -0.027507 -0.023873

 41 H 0.000000 0.000000 0.000000 -0.027507 0.457354 -0.023873

 42 H 0.000000 0.000000 0.000000 -0.023873 -0.023873 0.446962

 43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 43 44 45

 1 C 0.000000 0.000000 0.000000

 2 N 0.000000 0.000000 0.000000

 3 C 0.000000 0.000000 0.000000

 4 C 0.000000 0.000000 0.000000

 5 C 0.000000 0.000000 0.000000

 6 N 0.000000 0.000000 0.000000

 7 C 0.000000 0.000000 0.000000

 8 N 0.000000 0.000000 0.000000

 9 C 0.000000 0.000000 0.000001

 10 C 0.000000 0.000000 0.000000

 11 C 0.000000 0.000000 0.000000

 12 N 0.000000 0.000000 0.000000

 13 C 0.000000 0.000000 0.000000

 14 C -0.000020 -0.000020 -0.000001

 15 C -0.000045 -0.000045 0.000038

 16 N 0.000013 0.000013 0.000000

 17 C 0.000000 0.000000 0.000000

 18 N 0.003632 0.003632 0.000056

 19 N 0.000409 0.000409 -0.000232

 20 C -0.005251 -0.005251 0.006189

 21 C -0.042909 -0.042909 -0.039530

 22 C -0.000326 -0.000326 -0.005559

 23 C -0.000186 -0.000186 0.000203

 24 N 0.000007 0.000007 -0.000009

 25 Zn 0.000075 0.000075 0.000051

 26 C 0.000000 0.000000 0.000000

 27 H 0.000000 0.000000 0.000000

 28 C 0.000000 0.000000 0.000000

 29 H 0.000000 0.000000 0.000000

 30 C 0.000000 0.000000 0.000000

 31 H 0.000032 0.000032 0.000000

 32 C 0.386967 0.386967 0.388481

 33 H -0.000100 -0.000100 0.001240

 34 H 0.000000 0.000000 0.000000

 35 H 0.000000 0.000000 0.000000

 36 H 0.000000 0.000000 0.000000

 37 H 0.000000 0.000000 0.000000

 38 H 0.000000 0.000000 0.000000

 39 H 0.000000 0.000000 0.000000

 40 H 0.000000 0.000000 0.000000

 41 H 0.000000 0.000000 0.000000

 42 H 0.000000 0.000000 0.000000

 43 H 0.457354 -0.027507 -0.023873

 44 H -0.027507 0.457354 -0.023873

 45 H -0.023873 -0.023873 0.446962

 Atomic-Atomic Spin Densities.

 1 2 3 4 5 6

 1 C 0.186572 0.004047 -0.012472 -0.008705 0.012937 0.000169

 2 N 0.004047 -0.058325 -0.001696 -0.001549 0.000340 0.001073

 3 C -0.012472 -0.001696 0.187465 0.021020 -0.005928 -0.000109

 4 C -0.008705 -0.001549 0.021020 0.052292 -0.008087 -0.000676

 5 C 0.012937 0.000340 -0.005928 -0.008087 -0.019601 -0.000079

 6 N 0.000169 0.001073 -0.000109 -0.000676 -0.000079 -0.082611

 7 C 0.000185 0.000026 -0.011385 -0.000417 0.000033 0.002345

 8 N 0.000033 0.000221 -0.000327 -0.000014 0.000000 0.000690

 9 C -0.000007 0.000021 0.000200 0.000002 0.000000 0.000077

 10 C 0.000000 -0.000002 0.000058 0.000000 0.000000 0.000019

 11 C 0.000001 -0.000003 -0.000286 0.000009 0.000000 0.000204

 12 N 0.002345 0.000690 0.000077 0.000019 0.000204 0.000002

 13 C -0.000417 -0.000014 0.000002 0.000000 0.000009 0.000000

 14 C 0.000033 0.000000 0.000000 0.000000 0.000000 0.000000

 15 C 0.000185 0.000033 -0.000007 0.000000 0.000001 0.000000

 16 N 0.000026 0.000221 0.000021 -0.000002 -0.000003 0.000000

 17 C -0.011385 -0.000327 0.000200 0.000058 -0.000286 0.000000

 18 N 0.000000 -0.000001 0.000000 0.000000 0.000000 0.000000

 19 N 0.000001 0.000013 -0.000001 0.000000 0.000000 -0.000001

 20 C -0.000007 -0.000001 0.000002 0.000000 0.000000 0.000000

 21 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 22 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 23 C 0.000002 0.000001 -0.000007 0.000000 0.000000 0.000000

 24 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000002

 25 Zn 0.000254 0.001164 -0.000481 -0.000055 0.000014 -0.000107

 26 C 0.000003 0.000007 -0.001251 -0.003629 0.001244 0.000322

 27 H 0.000042 -0.000020 -0.000085 0.000331 0.000337 -0.000002

 28 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000001

 29 H 0.000000 0.000001 -0.000005 0.000000 0.000000 0.000082

 30 C 0.000035 0.000000 0.000000 0.000000 0.000001 0.000000

 31 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 33 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 34 H 0.000011 0.000000 0.000033 -0.000175 0.000008 -0.000001

 35 H 0.000026 0.000008 -0.000462 -0.001159 0.000076 0.000021

 36 H 0.000026 0.000008 -0.000462 -0.001159 0.000076 0.000021

 37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 40 H 0.000028 0.000000 0.000000 0.000000 0.000002 0.000000

 41 H 0.000028 0.000000 0.000000 0.000000 0.000002 0.000000

 42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 7 8 9 10 11 12

 1 C 0.000185 0.000033 -0.000007 0.000000 0.000001 0.002345

 2 N 0.000026 0.000221 0.000021 -0.000002 -0.000003 0.000690

 3 C -0.011385 -0.000327 0.000200 0.000058 -0.000286 0.000077

 4 C -0.000417 -0.000014 0.000002 0.000000 0.000009 0.000019

 5 C 0.000033 0.000000 0.000000 0.000000 0.000000 0.000204

 6 N 0.002345 0.000690 0.000077 0.000019 0.000204 0.000002

 7 C 0.186572 0.004047 -0.012472 -0.008705 0.012937 0.000000

 8 N 0.004047 -0.058325 -0.001696 -0.001549 0.000340 -0.000001

 9 C -0.012472 -0.001696 0.187465 0.021020 -0.005928 0.000000

 10 C -0.008705 -0.001549 0.021020 0.052292 -0.008087 0.000000

 11 C 0.012937 0.000340 -0.005928 -0.008087 -0.019601 0.000000

 12 N 0.000000 -0.000001 0.000000 0.000000 0.000000 -0.082611

 13 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000676

 14 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000079

 15 C 0.000002 0.000001 -0.000007 0.000000 0.000000 0.000169

 16 N 0.000001 0.000013 -0.000001 0.000000 0.000000 0.001073

 17 C -0.000007 -0.000001 0.000002 0.000000 0.000000 -0.000109

 18 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000002

 19 N 0.000033 0.000221 -0.000327 -0.000014 0.000000 0.000000

 20 C -0.000007 0.000021 0.000200 0.000002 0.000000 0.000000

 21 C 0.000000 -0.000002 0.000058 0.000000 0.000000 0.000000

 22 C 0.000001 -0.000003 -0.000286 0.000009 0.000000 0.000000

 23 C 0.000185 0.000026 -0.011385 -0.000417 0.000033 0.000000

 24 N 0.000169 0.001073 -0.000109 -0.000676 -0.000079 0.000000

 25 Zn 0.000254 0.001164 -0.000481 -0.000055 0.000014 -0.000107

 26 C 0.000035 0.000000 0.000000 0.000000 0.000001 0.000001

 27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000082

 28 C 0.000003 0.000007 -0.001251 -0.003629 0.001244 0.000000

 29 H 0.000042 -0.000020 -0.000085 0.000331 0.000337 0.000000

 30 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000322

 31 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

 32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 33 H 0.000000 0.000001 -0.000005 0.000000 0.000000 0.000000

 34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 35 H 0.000028 0.000000 0.000000 0.000000 0.000002 0.000000

 36 H 0.000028 0.000000 0.000000 0.000000 0.000002 0.000000

 37 H 0.000026 0.000008 -0.000462 -0.001159 0.000076 0.000000

 38 H 0.000026 0.000008 -0.000462 -0.001159 0.000076 0.000000

 39 H 0.000011 0.000000 0.000033 -0.000175 0.000008 0.000000

 40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000021

 41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000021

 42 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000001

 43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 13 14 15 16 17 18

 1 C -0.000417 0.000033 0.000185 0.000026 -0.011385 0.000000

 2 N -0.000014 0.000000 0.000033 0.000221 -0.000327 -0.000001

 3 C 0.000002 0.000000 -0.000007 0.000021 0.000200 0.000000

 4 C 0.000000 0.000000 0.000000 -0.000002 0.000058 0.000000

 5 C 0.000009 0.000000 0.000001 -0.000003 -0.000286 0.000000

 6 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 7 C 0.000000 0.000000 0.000002 0.000001 -0.000007 0.000000

 8 N 0.000000 0.000000 0.000001 0.000013 -0.000001 0.000000

 9 C 0.000000 0.000000 -0.000007 -0.000001 0.000002 0.000000

 10 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 11 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 12 N -0.000676 -0.000079 0.000169 0.001073 -0.000109 0.000002

 13 C 0.052292 -0.008087 -0.008705 -0.001549 0.021020 0.000019

 14 C -0.008087 -0.019601 0.012937 0.000340 -0.005928 0.000204

 15 C -0.008705 0.012937 0.186572 0.004047 -0.012472 0.002345

 16 N -0.001549 0.000340 0.004047 -0.058325 -0.001696 0.000690

 17 C 0.021020 -0.005928 -0.012472 -0.001696 0.187465 0.000077

 18 N 0.000019 0.000204 0.002345 0.000690 0.000077 -0.082611

 19 N -0.000002 -0.000003 0.000026 0.000221 0.000021 0.001073

 20 C 0.000058 -0.000286 -0.011385 -0.000327 0.000200 -0.000109

 21 C 0.000000 0.000009 -0.000417 -0.000014 0.000002 -0.000676

 22 C 0.000000 0.000000 0.000033 0.000000 0.000000 -0.000079

 23 C 0.000000 0.000001 0.000185 0.000033 -0.000007 0.000169

 24 N 0.000000 0.000000 0.000000 -0.000001 0.000000 0.000002

 25 Zn -0.000055 0.000014 0.000254 0.001164 -0.000481 -0.000107

 26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 27 H 0.000000 0.000000 0.000000 0.000001 -0.000005 0.000000

 28 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 29 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 30 C -0.003629 0.001244 0.000003 0.000007 -0.001251 0.000001

 31 H 0.000331 0.000337 0.000042 -0.000020 -0.000085 0.000082

 32 C 0.000000 0.000001 0.000035 0.000000 0.000000 0.000322

 33 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

 34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 40 H -0.001159 0.000076 0.000026 0.000008 -0.000462 0.000000

 41 H -0.001159 0.000076 0.000026 0.000008 -0.000462 0.000000

 42 H -0.000175 0.000008 0.000011 0.000000 0.000033 0.000000

 43 H 0.000000 0.000002 0.000028 0.000000 0.000000 0.000021

 44 H 0.000000 0.000002 0.000028 0.000000 0.000000 0.000021

 45 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000001

 19 20 21 22 23 24

 1 C 0.000001 -0.000007 0.000000 0.000000 0.000002 0.000000

 2 N 0.000013 -0.000001 0.000000 0.000000 0.000001 0.000000

 3 C -0.000001 0.000002 0.000000 0.000000 -0.000007 0.000000

 4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 5 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 6 N -0.000001 0.000000 0.000000 0.000000 0.000000 0.000002

 7 C 0.000033 -0.000007 0.000000 0.000001 0.000185 0.000169

 8 N 0.000221 0.000021 -0.000002 -0.000003 0.000026 0.001073

 9 C -0.000327 0.000200 0.000058 -0.000286 -0.011385 -0.000109

 10 C -0.000014 0.000002 0.000000 0.000009 -0.000417 -0.000676

 11 C 0.000000 0.000000 0.000000 0.000000 0.000033 -0.000079

 12 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 13 C -0.000002 0.000058 0.000000 0.000000 0.000000 0.000000

 14 C -0.000003 -0.000286 0.000009 0.000000 0.000001 0.000000

 15 C 0.000026 -0.011385 -0.000417 0.000033 0.000185 0.000000

 16 N 0.000221 -0.000327 -0.000014 0.000000 0.000033 -0.000001

 17 C 0.000021 0.000200 0.000002 0.000000 -0.000007 0.000000

 18 N 0.001073 -0.000109 -0.000676 -0.000079 0.000169 0.000002

 19 N -0.058325 -0.001696 -0.001549 0.000340 0.004047 0.000690

 20 C -0.001696 0.187465 0.021020 -0.005928 -0.012472 0.000077

 21 C -0.001549 0.021020 0.052292 -0.008087 -0.008705 0.000019

 22 C 0.000340 -0.005928 -0.008087 -0.019601 0.012937 0.000204

 23 C 0.004047 -0.012472 -0.008705 0.012937 0.186572 0.002345

 24 N 0.000690 0.000077 0.000019 0.000204 0.002345 -0.082611

 25 Zn 0.001164 -0.000481 -0.000055 0.000014 0.000254 -0.000107

 26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 28 C 0.000000 0.000000 0.000000 0.000001 0.000035 0.000322

 29 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000002

 30 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 31 H 0.000001 -0.000005 0.000000 0.000000 0.000000 0.000000

 32 C 0.000007 -0.001251 -0.003629 0.001244 0.000003 0.000001

 33 H -0.000020 -0.000085 0.000331 0.000337 0.000042 0.000082

 34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 37 H 0.000000 0.000000 0.000000 0.000002 0.000028 0.000021

 38 H 0.000000 0.000000 0.000000 0.000002 0.000028 0.000021

 39 H 0.000000 0.000000 0.000000 0.000000 0.000000 -0.000001

 40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 43 H 0.000008 -0.000462 -0.001159 0.000076 0.000026 0.000000

 44 H 0.000008 -0.000462 -0.001159 0.000076 0.000026 0.000000

 45 H 0.000000 0.000033 -0.000175 0.000008 0.000011 0.000000

 25 26 27 28 29 30

 1 C 0.000254 0.000003 0.000042 0.000000 0.000000 0.000035

 2 N 0.001164 0.000007 -0.000020 0.000000 0.000001 0.000000

 3 C -0.000481 -0.001251 -0.000085 0.000000 -0.000005 0.000000

 4 C -0.000055 -0.003629 0.000331 0.000000 0.000000 0.000000

 5 C 0.000014 0.001244 0.000337 0.000000 0.000000 0.000001

 6 N -0.000107 0.000322 -0.000002 0.000001 0.000082 0.000000

 7 C 0.000254 0.000035 0.000000 0.000003 0.000042 0.000000

 8 N 0.001164 0.000000 0.000000 0.000007 -0.000020 0.000000

 9 C -0.000481 0.000000 0.000000 -0.001251 -0.000085 0.000000

 10 C -0.000055 0.000000 0.000000 -0.003629 0.000331 0.000000

 11 C 0.000014 0.000001 0.000000 0.001244 0.000337 0.000000

 12 N -0.000107 0.000001 0.000082 0.000000 0.000000 0.000322

 13 C -0.000055 0.000000 0.000000 0.000000 0.000000 -0.003629

 14 C 0.000014 0.000000 0.000000 0.000000 0.000000 0.001244

 15 C 0.000254 0.000000 0.000000 0.000000 0.000000 0.000003

 16 N 0.001164 0.000000 0.000001 0.000000 0.000000 0.000007

 17 C -0.000481 0.000000 -0.000005 0.000000 0.000000 -0.001251

 18 N -0.000107 0.000000 0.000000 0.000000 0.000000 0.000001

 19 N 0.001164 0.000000 0.000000 0.000000 0.000000 0.000000

 20 C -0.000481 0.000000 0.000000 0.000000 0.000000 0.000000

 21 C -0.000055 0.000000 0.000000 0.000000 0.000000 0.000000

 22 C 0.000014 0.000000 0.000000 0.000001 0.000000 0.000000

 23 C 0.000254 0.000000 0.000000 0.000035 0.000000 0.000000

 24 N -0.000107 0.000000 0.000000 0.000322 -0.000002 0.000000

 25 Zn -0.000493 0.000000 0.000000 0.000000 0.000000 0.000000

 26 C 0.000000 -0.002651 0.000125 0.000000 0.000000 0.000000

 27 H 0.000000 0.000125 -0.000588 0.000000 0.000000 0.000000

 28 C 0.000000 0.000000 0.000000 -0.002651 0.000125 0.000000

 29 H 0.000000 0.000000 0.000000 0.000125 -0.000588 0.000000

 30 C 0.000000 0.000000 0.000000 0.000000 0.000000 -0.002651

 31 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000125

 32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 33 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 34 H 0.000002 0.000265 -0.000037 0.000000 0.000000 0.000000

 35 H 0.000000 0.001674 0.000001 0.000000 0.000000 0.000000

 36 H 0.000000 0.001674 0.000001 0.000000 0.000000 0.000000

 37 H 0.000000 0.000000 0.000000 0.001674 0.000001 0.000000

 38 H 0.000000 0.000000 0.000000 0.001674 0.000001 0.000000

 39 H 0.000002 0.000000 0.000000 0.000265 -0.000037 0.000000

 40 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.001674

 41 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.001674

 42 H 0.000002 0.000000 0.000000 0.000000 0.000000 0.000265

 43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 45 H 0.000002 0.000000 0.000000 0.000000 0.000000 0.000000

 31 32 33 34 35 36

 1 C 0.000000 0.000000 0.000000 0.000011 0.000026 0.000026

 2 N 0.000000 0.000000 0.000000 0.000000 0.000008 0.000008

 3 C 0.000000 0.000000 0.000000 0.000033 -0.000462 -0.000462

 4 C 0.000000 0.000000 0.000000 -0.000175 -0.001159 -0.001159

 5 C 0.000000 0.000000 0.000000 0.000008 0.000076 0.000076

 6 N 0.000000 0.000000 0.000000 -0.000001 0.000021 0.000021

 7 C 0.000000 0.000000 0.000000 0.000000 0.000028 0.000028

 8 N 0.000000 0.000000 0.000001 0.000000 0.000000 0.000000

 9 C 0.000000 0.000000 -0.000005 0.000000 0.000000 0.000000

 10 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 11 C 0.000000 0.000000 0.000000 0.000000 0.000002 0.000002

 12 N -0.000002 0.000000 0.000000 0.000000 0.000000 0.000000

 13 C 0.000331 0.000000 0.000000 0.000000 0.000000 0.000000

 14 C 0.000337 0.000001 0.000000 0.000000 0.000000 0.000000

 15 C 0.000042 0.000035 0.000000 0.000000 0.000000 0.000000

 16 N -0.000020 0.000000 0.000000 0.000000 0.000000 0.000000

 17 C -0.000085 0.000000 0.000000 0.000000 0.000000 0.000000

 18 N 0.000082 0.000322 -0.000002 0.000000 0.000000 0.000000

 19 N 0.000001 0.000007 -0.000020 0.000000 0.000000 0.000000

 20 C -0.000005 -0.001251 -0.000085 0.000000 0.000000 0.000000

 21 C 0.000000 -0.003629 0.000331 0.000000 0.000000 0.000000

 22 C 0.000000 0.001244 0.000337 0.000000 0.000000 0.000000

 23 C 0.000000 0.000003 0.000042 0.000000 0.000000 0.000000

 24 N 0.000000 0.000001 0.000082 0.000000 0.000000 0.000000

 25 Zn 0.000000 0.000000 0.000000 0.000002 0.000000 0.000000

 26 C 0.000000 0.000000 0.000000 0.000265 0.001674 0.001674

 27 H 0.000000 0.000000 0.000000 -0.000037 0.000001 0.000001

 28 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 29 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 30 C 0.000125 0.000000 0.000000 0.000000 0.000000 0.000000

 31 H -0.000588 0.000000 0.000000 0.000000 0.000000 0.000000

 32 C 0.000000 -0.002651 0.000125 0.000000 0.000000 0.000000

 33 H 0.000000 0.000125 -0.000588 0.000000 0.000000 0.000000

 34 H 0.000000 0.000000 0.000000 -0.000398 -0.000002 -0.000002

 35 H 0.000000 0.000000 0.000000 -0.000002 0.003991 -0.000830

 36 H 0.000000 0.000000 0.000000 -0.000002 -0.000830 0.003991

 37 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 38 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 39 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 40 H 0.000001 0.000000 0.000000 0.000000 0.000000 0.000000

 41 H 0.000001 0.000000 0.000000 0.000000 0.000000 0.000000

 42 H -0.000037 0.000000 0.000000 0.000000 0.000000 0.000000

 43 H 0.000000 0.001674 0.000001 0.000000 0.000000 0.000000

 44 H 0.000000 0.001674 0.000001 0.000000 0.000000 0.000000

 45 H 0.000000 0.000265 -0.000037 0.000000 0.000000 0.000000

 37 38 39 40 41 42

 1 C 0.000000 0.000000 0.000000 0.000028 0.000028 0.000000

 2 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 3 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 4 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 5 C 0.000000 0.000000 0.000000 0.000002 0.000002 0.000000

 6 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 7 C 0.000026 0.000026 0.000011 0.000000 0.000000 0.000000

 8 N 0.000008 0.000008 0.000000 0.000000 0.000000 0.000000

 9 C -0.000462 -0.000462 0.000033 0.000000 0.000000 0.000000

 10 C -0.001159 -0.001159 -0.000175 0.000000 0.000000 0.000000

 11 C 0.000076 0.000076 0.000008 0.000000 0.000000 0.000000

 12 N 0.000000 0.000000 0.000000 0.000021 0.000021 -0.000001

 13 C 0.000000 0.000000 0.000000 -0.001159 -0.001159 -0.000175

 14 C 0.000000 0.000000 0.000000 0.000076 0.000076 0.000008

 15 C 0.000000 0.000000 0.000000 0.000026 0.000026 0.000011

 16 N 0.000000 0.000000 0.000000 0.000008 0.000008 0.000000

 17 C 0.000000 0.000000 0.000000 -0.000462 -0.000462 0.000033

 18 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 19 N 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 20 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 21 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 22 C 0.000002 0.000002 0.000000 0.000000 0.000000 0.000000

 23 C 0.000028 0.000028 0.000000 0.000000 0.000000 0.000000

 24 N 0.000021 0.000021 -0.000001 0.000000 0.000000 0.000000

 25 Zn 0.000000 0.000000 0.000002 0.000000 0.000000 0.000002

 26 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 27 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 28 C 0.001674 0.001674 0.000265 0.000000 0.000000 0.000000

 29 H 0.000001 0.000001 -0.000037 0.000000 0.000000 0.000000

 30 C 0.000000 0.000000 0.000000 0.001674 0.001674 0.000265

 31 H 0.000000 0.000000 0.000000 0.000001 0.000001 -0.000037

 32 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 33 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 34 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 35 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 36 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 37 H 0.003991 -0.000830 -0.000002 0.000000 0.000000 0.000000

 38 H -0.000830 0.003991 -0.000002 0.000000 0.000000 0.000000

 39 H -0.000002 -0.000002 -0.000398 0.000000 0.000000 0.000000

 40 H 0.000000 0.000000 0.000000 0.003991 -0.000830 -0.000002

 41 H 0.000000 0.000000 0.000000 -0.000830 0.003991 -0.000002

 42 H 0.000000 0.000000 0.000000 -0.000002 -0.000002 -0.000398

 43 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 45 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

 43 44 45

 1 C 0.000000 0.000000 0.000000

 2 N 0.000000 0.000000 0.000000

 3 C 0.000000 0.000000 0.000000

 4 C 0.000000 0.000000 0.000000

 5 C 0.000000 0.000000 0.000000

 6 N 0.000000 0.000000 0.000000

 7 C 0.000000 0.000000 0.000000

 8 N 0.000000 0.000000 0.000000

 9 C 0.000000 0.000000 0.000000

 10 C 0.000000 0.000000 0.000000

 11 C 0.000000 0.000000 0.000000

 12 N 0.000000 0.000000 0.000000

 13 C 0.000000 0.000000 0.000000

 14 C 0.000002 0.000002 0.000000

 15 C 0.000028 0.000028 0.000000

 16 N 0.000000 0.000000 0.000000

 17 C 0.000000 0.000000 0.000000

 18 N 0.000021 0.000021 -0.000001

 19 N 0.000008 0.000008 0.000000

 20 C -0.000462 -0.000462 0.000033

 21 C -0.001159 -0.001159 -0.000175

 22 C 0.000076 0.000076 0.000008

 23 C 0.000026 0.000026 0.000011

 24 N 0.000000 0.000000 0.000000

 25 Zn 0.000000 0.000000 0.000002

 26 C 0.000000 0.000000 0.000000

 27 H 0.000000 0.000000 0.000000

 28 C 0.000000 0.000000 0.000000

 29 H 0.000000 0.000000 0.000000

 30 C 0.000000 0.000000 0.000000

 31 H 0.000000 0.000000 0.000000

 32 C 0.001674 0.001674 0.000265

 33 H 0.000001 0.000001 -0.000037

 34 H 0.000000 0.000000 0.000000

 35 H 0.000000 0.000000 0.000000

 36 H 0.000000 0.000000 0.000000

 37 H 0.000000 0.000000 0.000000

 38 H 0.000000 0.000000 0.000000

 39 H 0.000000 0.000000 0.000000

 40 H 0.000000 0.000000 0.000000

 41 H 0.000000 0.000000 0.000000

 42 H 0.000000 0.000000 0.000000

 43 H 0.003991 -0.000830 -0.000002

 44 H -0.000830 0.003991 -0.000002

 45 H -0.000002 -0.000002 -0.000398

 Mulliken charges and spin densities:

 1 2

 1 C 0.433843 0.173993

 2 N -0.677583 -0.054062

 3 C 0.439856 0.174112

 4 C 0.029623 0.048102

 5 C -0.262311 -0.018704

 6 N -0.405360 -0.078558

 7 C 0.433843 0.173993

 8 N -0.677583 -0.054062

 9 C 0.439856 0.174112

 10 C 0.029623 0.048102

 11 C -0.262311 -0.018704

 12 N -0.405360 -0.078558

 13 C 0.029623 0.048102

 14 C -0.262311 -0.018704

 15 C 0.433843 0.173993

 16 N -0.677583 -0.054062

 17 C 0.439856 0.174112

 18 N -0.405360 -0.078558

 19 N -0.677583 -0.054062

 20 C 0.439856 0.174112

 21 C 0.029623 0.048102

 22 C -0.262311 -0.018704

 23 C 0.433843 0.173993

 24 N -0.405360 -0.078558

 25 Zn 1.546788 0.002669

 26 C -0.696424 -0.002180

 27 H 0.248348 0.000182

 28 C -0.696424 -0.002180

 29 H 0.248348 0.000182

 30 C -0.696424 -0.002180

 31 H 0.248348 0.000182

 32 C -0.696424 -0.002180

 33 H 0.248348 0.000182

 34 H 0.249855 -0.000296

 35 H 0.251728 0.003372

 36 H 0.251728 0.003372

 37 H 0.251728 0.003372

 38 H 0.251728 0.003372

 39 H 0.249855 -0.000296

 40 H 0.251728 0.003372

 41 H 0.251728 0.003372

 42 H 0.249855 -0.000296

 43 H 0.251728 0.003372

 44 H 0.251728 0.003372

 45 H 0.249855 -0.000296

 Sum of Mulliken charges = 1.00000 1.00000

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

 1 2

 1 C 0.433843 0.173993

 2 N -0.677583 -0.054062

 3 C 0.439856 0.174112

 4 C 0.029623 0.048102

 5 C -0.013963 -0.018522

 6 N -0.405360 -0.078558

 7 C 0.433843 0.173993

 8 N -0.677583 -0.054062

 9 C 0.439856 0.174112

 10 C 0.029623 0.048102

 11 C -0.013963 -0.018522

 12 N -0.405360 -0.078558

 13 C 0.029623 0.048102

 14 C -0.013963 -0.018522

 15 C 0.433843 0.173993

 16 N -0.677583 -0.054062

 17 C 0.439856 0.174112

 18 N -0.405360 -0.078558

 19 N -0.677583 -0.054062

 20 C 0.439856 0.174112

 21 C 0.029623 0.048102

 22 C -0.013963 -0.018522

 23 C 0.433843 0.173993

 24 N -0.405360 -0.078558

 25 Zn 1.546788 0.002669

 26 C 0.056888 0.004269

 28 C 0.056888 0.004269

 30 C 0.056888 0.004269

 32 C 0.056888 0.004269

 Electronic spatial extent (au): <R\*\*2>= 11120.7464

 Charge= 1.0000 electrons

 Dipole moment (field-independent basis, Debye):

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

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

 XX= -120.7059 YY= -120.7059 ZZ= -167.3012

 XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

 XX= 15.5318 YY= 15.5318 ZZ= -31.0636

 XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

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

 XXY= 0.0000 XXZ= 0.0000 XZZ= 0.0000 YZZ= 0.0000

 YYZ= 0.0000 XYZ= 0.0000

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

 XXXX= -6205.4855 YYYY= -6205.4855 ZZZZ= -197.4556 XXXY= -311.7629

 XXXZ= 0.0000 YYYX= 311.7629 YYYZ= 0.0000 ZZZX= 0.0000

 ZZZY= 0.0000 XXYY= -2259.0663 XXZZ= -1318.2789 YYZZ= -1318.2789

 XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

 N-N= 2.766571019833D+03 E-N=-8.556975833456D+03 KE= 1.320598028643D+03

 Symmetry AG KE= 6.514027370571D+02

 Symmetry BG KE= 6.561836078981D+01

 Symmetry AU KE= 2.129681930232D+01

 Symmetry BU KE= 5.822801114940D+02

 Isotropic Fermi Contact Couplings

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

 1 C(13) 0.01423 15.99742 5.70828 5.33616

 2 N(14) -0.00856 -2.76423 -0.98635 -0.92205

 3 C(13) 0.01289 14.48747 5.16949 4.83250

 4 C(13) -0.00061 -0.69099 -0.24656 -0.23049

 5 C(13) -0.00590 -6.63232 -2.36658 -2.21230

 6 N(14) -0.01198 -3.86977 -1.38083 -1.29082

 7 C(13) 0.01423 15.99742 5.70828 5.33616

 8 N(14) -0.00856 -2.76423 -0.98635 -0.92205

 9 C(13) 0.01289 14.48747 5.16949 4.83250

 10 C(13) -0.00061 -0.69099 -0.24656 -0.23049

 11 C(13) -0.00590 -6.63232 -2.36658 -2.21230

 12 N(14) -0.01198 -3.86977 -1.38083 -1.29082

 13 C(13) -0.00061 -0.69099 -0.24656 -0.23049

 14 C(13) -0.00590 -6.63232 -2.36658 -2.21230

 15 C(13) 0.01423 15.99742 5.70828 5.33616

 16 N(14) -0.00856 -2.76423 -0.98635 -0.92205

 17 C(13) 0.01289 14.48747 5.16949 4.83250

 18 N(14) -0.01198 -3.86977 -1.38083 -1.29082

 19 N(14) -0.00856 -2.76423 -0.98635 -0.92205

 20 C(13) 0.01289 14.48747 5.16949 4.83250

 21 C(13) -0.00061 -0.69099 -0.24656 -0.23049

 22 C(13) -0.00590 -6.63232 -2.36658 -2.21230

 23 C(13) 0.01423 15.99742 5.70828 5.33616

 24 N(14) -0.01198 -3.86977 -1.38083 -1.29082

 25 Zn(67) 0.00000 0.00000 0.00000 0.00000

 26 C(13) -0.00201 -2.26473 -0.80811 -0.75543

 27 H(1) -0.00005 -0.22891 -0.08168 -0.07636

 28 C(13) -0.00201 -2.26473 -0.80811 -0.75543

 29 H(1) -0.00005 -0.22891 -0.08168 -0.07636

 30 C(13) -0.00201 -2.26473 -0.80811 -0.75543

 31 H(1) -0.00005 -0.22891 -0.08168 -0.07636

 32 C(13) -0.00201 -2.26473 -0.80811 -0.75543

 33 H(1) -0.00005 -0.22891 -0.08168 -0.07636

 34 H(1) -0.00010 -0.44657 -0.15935 -0.14896

 35 H(1) 0.00213 9.53262 3.40148 3.17974

 36 H(1) 0.00213 9.53262 3.40148 3.17974

 37 H(1) 0.00213 9.53262 3.40148 3.17974

 38 H(1) 0.00213 9.53262 3.40148 3.17974

 39 H(1) -0.00010 -0.44657 -0.15935 -0.14896

 40 H(1) 0.00213 9.53262 3.40148 3.17974

 41 H(1) 0.00213 9.53262 3.40148 3.17974

 42 H(1) -0.00010 -0.44657 -0.15935 -0.14896

 43 H(1) 0.00213 9.53262 3.40148 3.17974

 44 H(1) 0.00213 9.53262 3.40148 3.17974

 45 H(1) -0.00010 -0.44657 -0.15935 -0.14896

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

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

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 1 Atom -0.104371 -0.109217 0.213589

 2 Atom 0.044839 0.046658 -0.091497

 3 Atom -0.107200 -0.108935 0.216135

 4 Atom -0.029822 -0.035403 0.065224

 5 Atom 0.003736 0.005238 -0.008974

 6 Atom 0.064339 0.075328 -0.139666

 7 Atom -0.109217 -0.104371 0.213589

 8 Atom 0.046658 0.044839 -0.091497

 9 Atom -0.108935 -0.107200 0.216135

 10 Atom -0.035403 -0.029822 0.065224

 11 Atom 0.005238 0.003736 -0.008974

 12 Atom 0.075328 0.064339 -0.139666

 13 Atom -0.035403 -0.029822 0.065224

 14 Atom 0.005238 0.003736 -0.008974

 15 Atom -0.109217 -0.104371 0.213589

 16 Atom 0.046658 0.044839 -0.091497

 17 Atom -0.108935 -0.107200 0.216135

 18 Atom 0.064339 0.075328 -0.139666

 19 Atom 0.044839 0.046658 -0.091497

 20 Atom -0.107200 -0.108935 0.216135

 21 Atom -0.029822 -0.035403 0.065224

 22 Atom 0.003736 0.005238 -0.008974

 23 Atom -0.104371 -0.109217 0.213589

 24 Atom 0.075328 0.064339 -0.139666

 25 Atom 0.003569 0.003569 -0.007137

 26 Atom 0.000695 -0.004231 0.003536

 27 Atom 0.001925 0.000030 -0.001955

 28 Atom -0.004231 0.000695 0.003536

 29 Atom 0.000030 0.001925 -0.001955

 30 Atom -0.004231 0.000695 0.003536

 31 Atom 0.000030 0.001925 -0.001955

 32 Atom 0.000695 -0.004231 0.003536

 33 Atom 0.001925 0.000030 -0.001955

 34 Atom 0.001813 -0.000715 -0.001097

 35 Atom 0.001952 -0.000839 -0.001113

 36 Atom 0.001952 -0.000839 -0.001113

 37 Atom -0.000839 0.001952 -0.001113

 38 Atom -0.000839 0.001952 -0.001113

 39 Atom -0.000715 0.001813 -0.001097

 40 Atom -0.000839 0.001952 -0.001113

 41 Atom -0.000839 0.001952 -0.001113

 42 Atom -0.000715 0.001813 -0.001097

 43 Atom 0.001952 -0.000839 -0.001113

 44 Atom 0.001952 -0.000839 -0.001113

 45 Atom 0.001813 -0.000715 -0.001097

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 XY XZ YZ

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 1 Atom -0.000174 0.000000 0.000000

 2 Atom 0.001555 0.000000 0.000000

 3 Atom -0.004051 0.000000 0.000000

 4 Atom -0.000543 0.000000 0.000000

 5 Atom -0.001395 0.000000 0.000000

 6 Atom -0.005715 0.000000 0.000000

 7 Atom 0.000174 0.000000 0.000000

 8 Atom -0.001555 0.000000 0.000000

 9 Atom 0.004051 0.000000 0.000000

 10 Atom 0.000543 0.000000 0.000000

 11 Atom 0.001395 0.000000 0.000000

 12 Atom 0.005715 0.000000 0.000000

 13 Atom 0.000543 0.000000 0.000000

 14 Atom 0.001395 0.000000 0.000000

 15 Atom 0.000174 0.000000 0.000000

 16 Atom -0.001555 0.000000 0.000000

 17 Atom 0.004051 0.000000 0.000000

 18 Atom -0.005715 0.000000 0.000000

 19 Atom 0.001555 0.000000 0.000000

 20 Atom -0.004051 0.000000 0.000000

 21 Atom -0.000543 0.000000 0.000000

 22 Atom -0.001395 0.000000 0.000000

 23 Atom -0.000174 0.000000 0.000000

 24 Atom 0.005715 0.000000 0.000000

 25 Atom 0.000000 0.000000 0.000000

 26 Atom -0.000289 0.000000 0.000000

 27 Atom -0.002116 0.000000 0.000000

 28 Atom 0.000289 0.000000 0.000000

 29 Atom 0.002116 0.000000 0.000000

 30 Atom 0.000289 0.000000 0.000000

 31 Atom 0.002116 0.000000 0.000000

 32 Atom -0.000289 0.000000 0.000000

 33 Atom -0.002116 0.000000 0.000000

 34 Atom -0.000965 0.000000 0.000000

 35 Atom 0.000827 -0.001044 -0.000875

 36 Atom 0.000827 0.001044 0.000875

 37 Atom -0.000827 0.000875 -0.001044

 38 Atom -0.000827 -0.000875 0.001044

 39 Atom 0.000965 0.000000 0.000000

 40 Atom -0.000827 -0.000875 0.001044

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 42 Atom 0.000965 0.000000 0.000000

 43 Atom 0.000827 0.001044 0.000875

 44 Atom 0.000827 -0.001044 -0.000875

 45 Atom -0.000965 0.000000 0.000000

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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 -0.1092 -14.657 -5.230 -4.889 0.0359 0.9994 0.0000

 1 C(13) Bbb -0.1044 -14.005 -4.997 -4.671 0.9994 -0.0359 0.0000

 Bcc 0.2136 28.662 10.227 9.560 0.0000 0.0000 1.0000

 Baa -0.0915 -3.529 -1.259 -1.177 0.0000 0.0000 1.0000

 2 N(14) Bbb 0.0439 1.695 0.605 0.565 0.8675 -0.4975 0.0000

 Bcc 0.0476 1.834 0.654 0.612 0.4975 0.8675 0.0000

 Baa -0.1122 -15.058 -5.373 -5.023 0.6287 0.7776 0.0000

 3 C(13) Bbb -0.1039 -13.946 -4.976 -4.652 0.7776 -0.6287 0.0000

 Bcc 0.2161 29.003 10.349 9.674 0.0000 0.0000 1.0000

 Baa -0.0355 -4.758 -1.698 -1.587 0.0960 0.9954 0.0000

 4 C(13) Bbb -0.0298 -3.995 -1.425 -1.333 0.9954 -0.0960 0.0000

 Bcc 0.0652 8.752 3.123 2.920 0.0000 0.0000 1.0000

 Baa -0.0090 -1.204 -0.430 -0.402 0.0000 0.0000 1.0000

 5 C(13) Bbb 0.0029 0.389 0.139 0.130 0.8584 0.5129 0.0000

 Bcc 0.0061 0.815 0.291 0.272 -0.5129 0.8584 0.0000

 Baa -0.1397 -5.387 -1.922 -1.797 0.0000 0.0000 1.0000

 6 N(14) Bbb 0.0619 2.388 0.852 0.796 0.9201 0.3917 0.0000

 Bcc 0.0778 2.999 1.070 1.000 -0.3917 0.9201 0.0000

 Baa -0.1092 -14.657 -5.230 -4.889 0.9994 -0.0359 0.0000

 7 C(13) Bbb -0.1044 -14.005 -4.997 -4.671 0.0359 0.9994 0.0000

 Bcc 0.2136 28.662 10.227 9.560 0.0000 0.0000 1.0000

 Baa -0.0915 -3.529 -1.259 -1.177 0.0000 0.0000 1.0000

 8 N(14) Bbb 0.0439 1.695 0.605 0.565 0.4975 0.8675 0.0000

 Bcc 0.0476 1.834 0.654 0.612 0.8675 -0.4975 0.0000

 Baa -0.1122 -15.058 -5.373 -5.023 0.7776 -0.6287 0.0000

 9 C(13) Bbb -0.1039 -13.946 -4.976 -4.652 0.6287 0.7776 0.0000

 Bcc 0.2161 29.003 10.349 9.674 0.0000 0.0000 1.0000

 Baa -0.0355 -4.758 -1.698 -1.587 0.9954 -0.0960 0.0000

 10 C(13) Bbb -0.0298 -3.995 -1.425 -1.333 0.0960 0.9954 0.0000

 Bcc 0.0652 8.752 3.123 2.920 0.0000 0.0000 1.0000

 Baa -0.0090 -1.204 -0.430 -0.402 0.0000 0.0000 1.0000

 11 C(13) Bbb 0.0029 0.389 0.139 0.130 -0.5129 0.8584 0.0000

 Bcc 0.0061 0.815 0.291 0.272 0.8584 0.5129 0.0000

 Baa -0.1397 -5.387 -1.922 -1.797 0.0000 0.0000 1.0000

 12 N(14) Bbb 0.0619 2.388 0.852 0.796 -0.3917 0.9201 0.0000

 Bcc 0.0778 2.999 1.070 1.000 0.9201 0.3917 0.0000

 Baa -0.0355 -4.758 -1.698 -1.587 0.9954 -0.0960 0.0000

 13 C(13) Bbb -0.0298 -3.995 -1.425 -1.333 0.0960 0.9954 0.0000

 Bcc 0.0652 8.752 3.123 2.920 0.0000 0.0000 1.0000

 Baa -0.0090 -1.204 -0.430 -0.402 0.0000 0.0000 1.0000

 14 C(13) Bbb 0.0029 0.389 0.139 0.130 -0.5129 0.8584 0.0000

 Bcc 0.0061 0.815 0.291 0.272 0.8584 0.5129 0.0000

 Baa -0.1092 -14.657 -5.230 -4.889 0.9994 -0.0359 0.0000

 15 C(13) Bbb -0.1044 -14.005 -4.997 -4.671 0.0359 0.9994 0.0000

 Bcc 0.2136 28.662 10.227 9.560 0.0000 0.0000 1.0000

 Baa -0.0915 -3.529 -1.259 -1.177 0.0000 0.0000 1.0000

 16 N(14) Bbb 0.0439 1.695 0.605 0.565 0.4975 0.8675 0.0000

 Bcc 0.0476 1.834 0.654 0.612 0.8675 -0.4975 0.0000

 Baa -0.1122 -15.058 -5.373 -5.023 0.7776 -0.6287 0.0000

 17 C(13) Bbb -0.1039 -13.946 -4.976 -4.652 0.6287 0.7776 0.0000

 Bcc 0.2161 29.003 10.349 9.674 0.0000 0.0000 1.0000

 Baa -0.1397 -5.387 -1.922 -1.797 0.0000 0.0000 1.0000

 18 N(14) Bbb 0.0619 2.388 0.852 0.796 0.9201 0.3917 0.0000

 Bcc 0.0778 2.999 1.070 1.000 -0.3917 0.9201 0.0000

 Baa -0.0915 -3.529 -1.259 -1.177 0.0000 0.0000 1.0000

 19 N(14) Bbb 0.0439 1.695 0.605 0.565 0.8675 -0.4975 0.0000

 Bcc 0.0476 1.834 0.654 0.612 0.4975 0.8675 0.0000

 Baa -0.1122 -15.058 -5.373 -5.023 0.6287 0.7776 0.0000

 20 C(13) Bbb -0.1039 -13.946 -4.976 -4.652 0.7776 -0.6287 0.0000

 Bcc 0.2161 29.003 10.349 9.674 0.0000 0.0000 1.0000

 Baa -0.0355 -4.758 -1.698 -1.587 0.0960 0.9954 0.0000

 21 C(13) Bbb -0.0298 -3.995 -1.425 -1.333 0.9954 -0.0960 0.0000

 Bcc 0.0652 8.752 3.123 2.920 0.0000 0.0000 1.0000

 Baa -0.0090 -1.204 -0.430 -0.402 0.0000 0.0000 1.0000

 22 C(13) Bbb 0.0029 0.389 0.139 0.130 0.8584 0.5129 0.0000

 Bcc 0.0061 0.815 0.291 0.272 -0.5129 0.8584 0.0000

 Baa -0.1092 -14.657 -5.230 -4.889 0.0359 0.9994 0.0000

 23 C(13) Bbb -0.1044 -14.005 -4.997 -4.671 0.9994 -0.0359 0.0000

 Bcc 0.2136 28.662 10.227 9.560 0.0000 0.0000 1.0000

 Baa -0.1397 -5.387 -1.922 -1.797 0.0000 0.0000 1.0000

 24 N(14) Bbb 0.0619 2.388 0.852 0.796 -0.3917 0.9201 0.0000

 Bcc 0.0778 2.999 1.070 1.000 0.9201 0.3917 0.0000

 Baa -0.0071 -0.239 -0.085 -0.080 0.0000 0.0000 1.0000

 25 Zn(67) Bbb 0.0036 0.119 0.043 0.040 1.0000 -0.0029 0.0000

 Bcc 0.0036 0.119 0.043 0.040 0.0029 1.0000 0.0000

 Baa -0.0042 -0.570 -0.203 -0.190 0.0584 0.9983 0.0000

 26 C(13) Bbb 0.0007 0.096 0.034 0.032 0.9983 -0.0584 0.0000

 Bcc 0.0035 0.474 0.169 0.158 0.0000 0.0000 1.0000

 Baa -0.0020 -1.043 -0.372 -0.348 0.0000 0.0000 1.0000

 27 H(1) Bbb -0.0013 -0.716 -0.255 -0.239 0.5438 0.8392 0.0000

 Bcc 0.0033 1.759 0.627 0.587 0.8392 -0.5438 0.0000

 Baa -0.0042 -0.570 -0.203 -0.190 0.9983 -0.0584 0.0000

 28 C(13) Bbb 0.0007 0.096 0.034 0.032 0.0584 0.9983 0.0000

 Bcc 0.0035 0.474 0.169 0.158 0.0000 0.0000 1.0000

 Baa -0.0020 -1.043 -0.372 -0.348 0.0000 0.0000 1.0000

 29 H(1) Bbb -0.0013 -0.716 -0.255 -0.239 0.8392 -0.5438 0.0000

 Bcc 0.0033 1.759 0.627 0.587 0.5438 0.8392 0.0000

 Baa -0.0042 -0.570 -0.203 -0.190 0.9983 -0.0584 0.0000

 30 C(13) Bbb 0.0007 0.096 0.034 0.032 0.0584 0.9983 0.0000

 Bcc 0.0035 0.474 0.169 0.158 0.0000 0.0000 1.0000

 Baa -0.0020 -1.043 -0.372 -0.348 0.0000 0.0000 1.0000

 31 H(1) Bbb -0.0013 -0.716 -0.255 -0.239 0.8392 -0.5438 0.0000

 Bcc 0.0033 1.759 0.627 0.587 0.5438 0.8392 0.0000

 Baa -0.0042 -0.570 -0.203 -0.190 0.0584 0.9983 0.0000

 32 C(13) Bbb 0.0007 0.096 0.034 0.032 0.9983 -0.0584 0.0000

 Bcc 0.0035 0.474 0.169 0.158 0.0000 0.0000 1.0000

 Baa -0.0020 -1.043 -0.372 -0.348 0.0000 0.0000 1.0000

 33 H(1) Bbb -0.0013 -0.716 -0.255 -0.239 0.5438 0.8392 0.0000

 Bcc 0.0033 1.759 0.627 0.587 0.8392 -0.5438 0.0000

 Baa -0.0011 -0.585 -0.209 -0.195 0.0000 0.0000 1.0000

 34 H(1) Bbb -0.0010 -0.556 -0.198 -0.185 0.3202 0.9473 0.0000

 Bcc 0.0021 1.141 0.407 0.381 0.9473 -0.3202 0.0000

 Baa -0.0019 -1.005 -0.359 -0.335 0.0880 0.5976 0.7969

 35 H(1) Bbb -0.0007 -0.383 -0.137 -0.128 -0.4304 0.7443 -0.5106

 Bcc 0.0026 1.388 0.495 0.463 0.8984 0.2980 -0.3227

 Baa -0.0019 -1.005 -0.359 -0.335 -0.0880 -0.5976 0.7969

 36 H(1) Bbb -0.0007 -0.383 -0.137 -0.128 -0.4304 0.7443 0.5106

 Bcc 0.0026 1.388 0.495 0.463 0.8984 0.2980 0.3227

 Baa -0.0019 -1.005 -0.359 -0.335 -0.5976 0.0880 0.7969

 37 H(1) Bbb -0.0007 -0.383 -0.137 -0.128 0.7443 0.4304 0.5106

 Bcc 0.0026 1.388 0.495 0.463 -0.2980 0.8984 -0.3227

 Baa -0.0019 -1.005 -0.359 -0.335 0.5976 -0.0880 0.7969

 38 H(1) Bbb -0.0007 -0.383 -0.137 -0.128 0.7443 0.4304 -0.5106

 Bcc 0.0026 1.388 0.495 0.463 -0.2980 0.8984 0.3227

 Baa -0.0011 -0.585 -0.209 -0.195 0.0000 0.0000 1.0000

 39 H(1) Bbb -0.0010 -0.556 -0.198 -0.185 0.9473 -0.3202 0.0000

 Bcc 0.0021 1.141 0.407 0.381 0.3202 0.9473 0.0000

 Baa -0.0019 -1.005 -0.359 -0.335 0.5976 -0.0880 0.7969

 40 H(1) Bbb -0.0007 -0.383 -0.137 -0.128 0.7443 0.4304 -0.5106

 Bcc 0.0026 1.388 0.495 0.463 -0.2980 0.8984 0.3227

 Baa -0.0019 -1.005 -0.359 -0.335 -0.5976 0.0880 0.7969

 41 H(1) Bbb -0.0007 -0.383 -0.137 -0.128 0.7443 0.4304 0.5106

 Bcc 0.0026 1.388 0.495 0.463 -0.2980 0.8984 -0.3227

 Baa -0.0011 -0.585 -0.209 -0.195 0.0000 0.0000 1.0000

 42 H(1) Bbb -0.0010 -0.556 -0.198 -0.185 0.9473 -0.3202 0.0000

 Bcc 0.0021 1.141 0.407 0.381 0.3202 0.9473 0.0000

 Baa -0.0019 -1.005 -0.359 -0.335 -0.0880 -0.5976 0.7969

 43 H(1) Bbb -0.0007 -0.383 -0.137 -0.128 -0.4304 0.7443 0.5106

 Bcc 0.0026 1.388 0.495 0.463 0.8984 0.2980 0.3227

 Baa -0.0019 -1.005 -0.359 -0.335 0.0880 0.5976 0.7969

 44 H(1) Bbb -0.0007 -0.383 -0.137 -0.128 -0.4304 0.7443 -0.5106

 Bcc 0.0026 1.388 0.495 0.463 0.8984 0.2980 -0.3227

 Baa -0.0011 -0.585 -0.209 -0.195 0.0000 0.0000 1.0000

 45 H(1) Bbb -0.0010 -0.556 -0.198 -0.185 0.3202 0.9473 0.0000

 Bcc 0.0021 1.141 0.407 0.381 0.9473 -0.3202 0.0000

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 No NMR shielding tensors so no spin-rotation constants.

 Leave Link 601 at Fri Jul 5 21:14:33 2019, MaxMem= 1342177280 cpu: 16.8

 (Enter /apps/gaussian/g09d01/g09/l9999.exe)

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 9\0\\#p opt b3lyp/genecp scrf=(solvent=dmso,smd) empiricaldispersion=g

 d3bj\\ZntAzPcation\\1,2\C,-2.0664148636,-2.178692856,0.\N,-0.745078814

 6,-1.8565515165,0.\C,-0.0051842407,-2.9884292162,0.\C,-0.9357731084,-4

 .1619541754,0.\C,-2.1885905894,-3.644629236,0.\N,1.3252498579,-3.09846

 33064,0.\C,2.178692856,-2.0664148636,0.\N,1.8565515165,-0.7450788146,0

 .\C,2.9884292162,-0.0051842407,0.\C,4.1619541754,-0.9357731084,0.\C,3.

 644629236,-2.1885905894,0.\N,-3.0984633064,-1.3252498579,0.\C,-4.16195

 41754,0.9357731084,0.\C,-3.644629236,2.1885905894,0.\C,-2.178692856,2.

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 2407,0.\N,-1.3252498579,3.0984633064,0.\N,0.7450788146,1.8565515165,0.

 \C,0.0051842407,2.9884292162,0.\C,0.9357731084,4.1619541754,0.\C,2.188

 5905894,3.644629236,0.\C,2.0664148636,2.178692856,0.\N,3.0984633064,1.

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 82323304,0.\C,-5.5739233198,0.48019691,0.\H,-4.1776035649,3.1282323304

 ,0.\C,0.48019691,5.5739233198,0.\H,3.1282323304,4.1776035649,0.\H,-1.3

 244455274,-6.2639575518,0.\H,0.1413683654,-5.78080446,0.876886323\H,0.

 1413683654,-5.78080446,-0.876886323\H,5.78080446,0.1413683654,0.876886

 323\H,5.78080446,0.1413683654,-0.876886323\H,6.2639575518,-1.324445527

 4,0.\H,-5.78080446,-0.1413683654,0.876886323\H,-5.78080446,-0.14136836

 54,-0.876886323\H,-6.2639575518,1.3244455274,0.\H,-0.1413683654,5.7808

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 4H [O(Zn1),SGH(C20H8N8),X(H8)]\\@

 THE NUMBERS ARE MEANINGLESS, BUT THE TRENDS ARE IMPORTANT.

 -- LARRY BURGGRAF

 Job cpu time: 0 days 1 hours 27 minutes 43.7 seconds.

 File lengths (MBytes): RWF= 700 Int= 0 D2E= 0 Chk= 35 Scr= 2

 Normal termination of Gaussian 09 at Fri Jul 5 21:14:34 2019.