Entering Gaussian System, Link 0=g09

 Input=ZntAzP0td.com

 Output=ZntAzP0td.log

 Initial command:

 /home/blab/g09/l1.exe "/home/blab/g09/scratch/Gau-47163.inp" -scrdir="/home/blab/g09/scratch/"

 Entering Link 1 = /home/blab/g09/l1.exe PID= 47170.

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 Cite this work as:

 Gaussian 09, Revision E.01,

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

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

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

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

 Gaussian 09: ES64L-G09RevE.01 30-Nov-2015

 19-Sep-2019

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

 %nprocshared=9

 Will use up to 9 processors via shared memory.

 %mem=10GB

 %chk=ZntAz0td.chk

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

 #p td(root=1,nstates=10) b3lyp/genecp scrf=(solvent=dmso,smd) empirica

 ldispersion=gd3bj IOp(9/40=3)

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

 1/38=1/1;

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

 3/5=7,11=9,16=1,17=8,25=1,30=1,70=32201,72=21,74=-5,124=41/1,2,8,3;

 4//1;

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

 8/6=1,10=1,107=1,108=10/1;

 9/8=1,40=3,41=10,42=1,70=2/14;

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

 99/5=1,9=1/99;

 Leave Link 1 at Thu Sep 19 00:35:33 2019, MaxMem= 1342177280 cpu: 0.7

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

 --------

 ZntAz0td

 --------

 Symbolic Z-matrix:

 Charge = 0 Multiplicity = 1

 C -2.18491 2.06614 0.

 N -1.86235 0.74398 0.

 C -2.99981 0. 0.

 C -4.15743 0.91558 0.

 C -3.64193 2.17904 0.

 N -3.09962 -1.33308 0.

 C -2.06614 -2.18491 0.

 N -0.74398 -1.86235 0.

 C 0. -2.99981 0.

 C -0.91558 -4.15743 0.

 C -2.17904 -3.64193 0.

 N -1.33308 3.09962 0.

 C 0.91558 4.15743 0.

 C 2.17904 3.64193 0.

 C 2.06614 2.18491 0.

 N 0.74398 1.86235 0.

 C 0. 2.99981 0.

 N 3.09962 1.33308 0.

 N 1.86235 -0.74398 0.

 C 2.99981 0. 0.

 C 4.15743 -0.91558 0.

 C 3.64193 -2.17904 0.

 C 2.18491 -2.06614 0.

 N 1.33308 -3.09962 0.

 Zn 0. 0. 0.

 C -5.58015 0.47492 0.

 H -4.18613 3.11339 0.

 C -0.47492 -5.58015 0.

 H -3.11339 -4.18613 0.

 C 0.47492 5.58015 0.

 H 3.11339 4.18613 0.

 C 5.58015 -0.47492 0.

 H 4.18613 -3.11339 0.

 H -6.25986 1.32868 0.

 H -5.80321 -0.14056 0.87714

 H -5.80321 -0.14056 -0.87714

 H 0.14056 -5.80321 0.87714

 H 0.14056 -5.80321 -0.87714

 H -1.32868 -6.25986 0.

 H -0.14056 5.80321 0.87714

 H -0.14056 5.80321 -0.87714

 H 1.32868 6.25986 0.

 H 5.80321 0.14056 0.87714

 H 5.80321 0.14056 -0.87714

 H 6.25986 -1.32868 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 Thu Sep 19 00:35:33 2019, MaxMem= 1342177280 cpu: 0.7

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

 Input orientation:

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

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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

 1 6 0 -2.184914 2.066138 0.000000

 2 7 0 -1.862347 0.743984 0.000000

 3 6 0 -2.999810 0.000000 0.000000

 4 6 0 -4.157430 0.915580 0.000000

 5 6 0 -3.641934 2.179040 0.000000

 6 7 0 -3.099620 -1.333079 0.000000

 7 6 0 -2.066138 -2.184914 0.000000

 8 7 0 -0.743984 -1.862347 0.000000

 9 6 0 0.000000 -2.999810 0.000000

 10 6 0 -0.915580 -4.157430 0.000000

 11 6 0 -2.179040 -3.641934 0.000000

 12 7 0 -1.333079 3.099620 0.000000

 13 6 0 0.915580 4.157430 0.000000

 14 6 0 2.179040 3.641934 0.000000

 15 6 0 2.066138 2.184914 0.000000

 16 7 0 0.743984 1.862347 0.000000

 17 6 0 0.000000 2.999810 0.000000

 18 7 0 3.099620 1.333079 0.000000

 19 7 0 1.862347 -0.743984 0.000000

 20 6 0 2.999810 0.000000 0.000000

 21 6 0 4.157430 -0.915580 0.000000

 22 6 0 3.641934 -2.179040 0.000000

 23 6 0 2.184914 -2.066138 0.000000

 24 7 0 1.333079 -3.099620 0.000000

 25 30 0 0.000000 0.000000 0.000000

 26 6 0 -5.580146 0.474920 0.000000

 27 1 0 -4.186125 3.113387 0.000000

 28 6 0 -0.474920 -5.580146 0.000000

 29 1 0 -3.113387 -4.186125 0.000000

 30 6 0 0.474920 5.580146 0.000000

 31 1 0 3.113387 4.186125 0.000000

 32 6 0 5.580146 -0.474920 0.000000

 33 1 0 4.186125 -3.113387 0.000000

 34 1 0 -6.259862 1.328678 0.000000

 35 1 0 -5.803210 -0.140560 0.877139

 36 1 0 -5.803210 -0.140560 -0.877139

 37 1 0 0.140560 -5.803210 0.877139

 38 1 0 0.140560 -5.803210 -0.877139

 39 1 0 -1.328678 -6.259862 0.000000

 40 1 0 -0.140560 5.803210 0.877139

 41 1 0 -0.140560 5.803210 -0.877139

 42 1 0 1.328678 6.259862 0.000000

 43 1 0 5.803210 0.140560 0.877139

 44 1 0 5.803210 0.140560 -0.877139

 45 1 0 6.259862 -1.328678 0.000000

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

 Distance matrix (angstroms):

 1 2 3 4 5

 1 C 0.000000

 2 N 1.360934 0.000000

 3 C 2.221032 1.359167 0.000000

 4 C 2.283551 2.301489 1.475930 0.000000

 5 C 1.461388 2.286114 2.271682 1.364576 0.000000

 6 N 3.520137 2.417651 1.336810 2.485041 3.553742

 7 C 4.252711 2.935979 2.376046 3.739862 4.639744

 8 N 4.184408 2.836141 2.925250 4.400965 4.973020

 9 C 5.517035 4.181427 4.242372 5.710911 6.331206

 10 C 6.351693 4.992016 4.650617 6.020384 6.898105

 11 C 5.708075 4.397337 3.733276 4.968396 6.001983

 12 N 1.339294 2.414362 3.519323 3.570293 2.485614

 13 C 3.739862 4.400965 5.710911 6.020384 4.968396

 14 C 4.639744 4.973020 6.331206 6.898105 6.001983

 15 C 4.252711 4.184408 5.517035 6.351693 5.708075

 16 N 2.935979 2.836141 4.181427 4.992016 4.397337

 17 C 2.376046 2.925250 4.242372 4.650617 3.733276

 18 N 5.335136 4.996814 6.243408 7.269049 6.794424

 19 N 4.927180 4.010909 4.918748 6.244347 6.232269

 20 C 5.581244 4.918748 5.999620 7.215565 6.990063

 21 C 7.008279 6.244347 7.215565 8.514109 8.390873

 22 C 7.209278 6.232269 6.990063 8.390873 8.488085

 23 C 6.014242 4.927180 5.581244 7.008279 7.209278

 24 N 6.249906 4.998404 5.327436 6.802023 7.253620

 25 Zn 3.007121 2.005455 2.999810 4.257054 4.244043

 26 C 3.749610 3.727523 2.623677 1.489397 2.580831

 27 H 2.258667 3.318737 3.331745 2.197994 1.081272

 28 C 7.835160 6.474533 6.124794 7.466950 8.380629

 29 H 6.320827 5.086362 4.187665 5.207439 6.387072

 30 C 4.407150 5.371339 6.573567 6.573952 5.340038

 31 H 5.706692 6.050311 7.409104 7.972531 7.047180

 32 C 8.170259 7.541646 8.593090 9.836355 9.596367

 33 H 8.210823 7.173794 7.831401 9.265392 9.449248

 34 H 4.141141 4.436215 3.520415 2.142632 2.752574

 35 H 4.327927 4.133061 2.940779 2.143221 3.289534

 36 H 4.327927 4.133061 2.940779 2.143221 3.289534

 37 H 8.252505 6.902663 6.656466 8.023978 8.876539

 38 H 8.252505 6.902663 6.656466 8.023978 8.876539

 39 H 8.369911 7.024148 6.479086 7.712899 8.750213

 40 H 4.349076 5.415689 6.528547 6.386982 5.115037

 41 H 4.349076 5.415689 6.528547 6.386982 5.115037

 42 H 5.471074 6.372405 7.610629 7.658899 6.431181

 43 H 8.263616 7.739138 8.847728 10.029176 9.702346

 44 H 8.263616 7.739138 8.847728 10.029176 9.702346

 45 H 9.101594 8.382494 9.354513 10.656297 10.504744

 6 7 8 9 10

 6 N 0.000000

 7 C 1.339294 0.000000

 8 N 2.414362 1.360934 0.000000

 9 C 3.519323 2.221032 1.359167 0.000000

 10 C 3.570293 2.283551 2.301489 1.475930 0.000000

 11 C 2.485614 1.461388 2.286114 2.271682 1.364576

 12 N 4.771738 5.335136 4.996814 6.243408 7.269049

 13 C 6.802023 7.008279 6.244347 7.215565 8.514109

 14 C 7.253620 7.209278 6.232269 6.990063 8.390873

 15 C 6.249906 6.014242 4.927180 5.581244 7.008279

 16 N 4.998404 4.927180 4.010909 4.918748 6.244347

 17 C 5.327436 5.581244 4.918748 5.999620 7.215565

 18 N 6.748257 6.249906 4.998404 5.327436 6.802023

 19 N 4.996814 4.184408 2.836141 2.925250 4.400965

 20 C 6.243408 5.517035 4.181427 4.242372 5.710911

 21 C 7.269049 6.351693 4.992016 4.650617 6.020384

 22 C 6.794424 5.708075 4.397337 3.733276 4.968396

 23 C 5.335136 4.252711 2.935979 2.376046 3.739862

 24 N 4.771738 3.520137 2.417651 1.336810 2.485041

 25 Zn 3.374129 3.007121 2.005455 2.999810 4.257054

 26 C 3.069506 4.407150 5.371339 6.573567 6.573952

 27 H 4.577287 5.706692 6.050311 7.409104 7.972531

 28 C 4.992657 3.749610 3.727523 2.623677 1.489397

 29 H 2.853079 2.258667 3.318737 3.331745 2.197994

 30 C 7.782674 8.170259 7.541646 8.593090 9.836355

 31 H 8.310419 8.210823 7.173794 7.831401 9.265392

 32 C 8.722085 7.835160 6.474533 6.124794 7.466950

 33 H 7.500105 6.320827 5.086362 4.187665 5.207439

 34 H 4.131837 5.471074 6.372405 7.610629 7.658899

 35 H 3.082349 4.349076 5.415689 6.528547 6.386982

 36 H 3.082349 4.349076 5.415689 6.528547 6.386982

 37 H 5.590189 4.327927 4.133061 2.940779 2.143221

 38 H 5.590189 4.327927 4.133061 2.940779 2.143221

 39 H 5.235401 4.141141 4.436215 3.520415 2.142632

 40 H 7.775090 8.263616 7.739138 8.847728 10.029176

 41 H 7.775090 8.263616 7.739138 8.847728 10.029176

 42 H 8.789913 9.101594 8.382494 9.354513 10.656297

 43 H 9.066497 8.252505 6.902663 6.656466 8.023978

 44 H 9.066497 8.252505 6.902663 6.656466 8.023978

 45 H 9.359483 8.369911 7.024148 6.479086 7.712899

 11 12 13 14 15

 11 C 0.000000

 12 N 6.794424 0.000000

 13 C 8.390873 2.485041 0.000000

 14 C 8.488085 3.553742 1.364576 0.000000

 15 C 7.209278 3.520137 2.283551 1.461388 0.000000

 16 N 6.232269 2.417651 2.301489 2.286114 1.360934

 17 C 6.990063 1.336810 1.475930 2.271682 2.221032

 18 N 7.253620 4.771738 3.570293 2.485614 1.339294

 19 N 4.973020 4.998404 4.992016 4.397337 2.935979

 20 C 6.331206 5.327436 4.650617 3.733276 2.376046

 21 C 6.898105 6.802023 6.020384 4.968396 3.739862

 22 C 6.001983 7.253620 6.898105 6.001983 4.639744

 23 C 4.639744 6.249906 6.351693 5.708075 4.252711

 24 N 3.553742 6.748257 7.269049 6.794424 5.335136

 25 Zn 4.244043 3.374129 4.257054 4.244043 3.007121

 26 C 5.340038 4.992657 7.466950 8.380629 7.835160

 27 H 7.047180 2.853079 5.207439 6.387072 6.320827

 28 C 2.580831 8.722085 9.836355 9.596367 8.170259

 29 H 1.081272 7.500105 9.265392 9.449248 8.210823

 30 C 9.596367 3.069506 1.489397 2.580831 3.749610

 31 H 9.449248 4.577287 2.197994 1.081272 2.258667

 32 C 8.380629 7.782674 6.573952 5.340038 4.407150

 33 H 6.387072 8.310419 7.972531 7.047180 5.706692

 34 H 6.431181 5.235401 7.712899 8.750213 8.369911

 35 H 5.115037 5.590189 8.023978 8.876539 8.252505

 36 H 5.115037 5.590189 8.023978 8.876539 8.252505

 37 H 3.289534 9.066497 10.029176 9.702346 8.263616

 38 H 3.289534 9.066497 10.029176 9.702346 8.263616

 39 H 2.752574 9.359483 10.656297 10.504744 9.101594

 40 H 9.702346 3.082349 2.143221 3.289534 4.327927

 41 H 9.702346 3.082349 2.143221 3.289534 4.327927

 42 H 10.504744 4.131837 2.142632 2.752574 4.141141

 43 H 8.876539 7.775090 6.386982 5.115037 4.349076

 44 H 8.876539 7.775090 6.386982 5.115037 4.349076

 45 H 8.750213 8.789913 7.658899 6.431181 5.471074

 16 17 18 19 20

 16 N 0.000000

 17 C 1.359167 0.000000

 18 N 2.414362 3.519323 0.000000

 19 N 2.836141 4.181427 2.417651 0.000000

 20 C 2.925250 4.242372 1.336810 1.359167 0.000000

 21 C 4.400965 5.710911 2.485041 2.301489 1.475930

 22 C 4.973020 6.331206 3.553742 2.286114 2.271682

 23 C 4.184408 5.517035 3.520137 1.360934 2.221032

 24 N 4.996814 6.243408 4.771738 2.414362 3.519323

 25 Zn 2.005455 2.999810 3.374129 2.005455 2.999810

 26 C 6.474533 6.124794 8.722085 7.541646 8.593090

 27 H 5.086362 4.187665 7.500105 7.173794 7.831401

 28 C 7.541646 8.593090 7.782674 5.371339 6.573567

 29 H 7.173794 7.831401 8.310419 6.050311 7.409104

 30 C 3.727523 2.623677 4.992657 6.474533 6.124794

 31 H 3.318737 3.331745 2.853079 5.086362 4.187665

 32 C 5.371339 6.573567 3.069506 3.727523 2.623677

 33 H 6.050311 7.409104 4.577287 3.318737 3.331745

 34 H 7.024148 6.479086 9.359483 8.382494 9.354513

 35 H 6.902663 6.656466 9.066497 7.739138 8.847728

 36 H 6.902663 6.656466 9.066497 7.739138 8.847728

 37 H 7.739138 8.847728 7.775090 5.415689 6.528547

 38 H 7.739138 8.847728 7.775090 5.415689 6.528547

 39 H 8.382494 9.354513 8.789913 6.372405 7.610629

 40 H 4.133061 2.940779 5.590189 6.902663 6.656466

 41 H 4.133061 2.940779 5.590189 6.902663 6.656466

 42 H 4.436215 3.520415 5.235401 7.024148 6.479086

 43 H 5.415689 6.528547 3.082349 4.133061 2.940779

 44 H 5.415689 6.528547 3.082349 4.133061 2.940779

 45 H 6.372405 7.610629 4.131837 4.436215 3.520415

 21 22 23 24 25

 21 C 0.000000

 22 C 1.364576 0.000000

 23 C 2.283551 1.461388 0.000000

 24 N 3.570293 2.485614 1.339294 0.000000

 25 Zn 4.257054 4.244043 3.007121 3.374129 0.000000

 26 C 9.836355 9.596367 8.170259 7.782674 5.600319

 27 H 9.265392 9.449248 8.210823 8.310419 5.216974

 28 C 6.573952 5.340038 4.407150 3.069506 5.600319

 29 H 7.972531 7.047180 5.706692 4.577287 5.216974

 30 C 7.466950 8.380629 7.835160 8.722085 5.600319

 31 H 5.207439 6.387072 6.320827 7.500105 5.216974

 32 C 1.489397 2.580831 3.749610 4.992657 5.600319

 33 H 2.197994 1.081272 2.258667 2.853079 5.216974

 34 H 10.656297 10.504744 9.101594 8.789913 6.399317

 35 H 10.029176 9.702346 8.263616 7.775090 5.870807

 36 H 10.029176 9.702346 8.263616 7.775090 5.870807

 37 H 6.386982 5.115037 4.349076 3.082349 5.870807

 38 H 6.386982 5.115037 4.349076 3.082349 5.870807

 39 H 7.658899 6.431181 5.471074 4.131837 6.399317

 40 H 8.023978 8.876539 8.252505 9.066497 5.870807

 41 H 8.023978 8.876539 8.252505 9.066497 5.870807

 42 H 7.712899 8.750213 8.369911 9.359483 6.399317

 43 H 2.143221 3.289534 4.327927 5.590189 5.870807

 44 H 2.143221 3.289534 4.327927 5.590189 5.870807

 45 H 2.142632 2.752574 4.141141 5.235401 6.399317

 26 27 28 29 30

 26 C 0.000000

 27 H 2.984092 0.000000

 28 C 7.920048 9.452542 0.000000

 29 H 5.273542 7.377916 2.984092 0.000000

 30 C 7.920048 5.273542 11.200639 10.404614 0.000000

 31 H 9.452542 7.377916 10.404614 10.433949 2.984092

 32 C 11.200639 10.404614 7.920048 9.452542 7.920048

 33 H 10.404614 10.433949 5.273542 7.377916 9.452542

 34 H 1.091291 2.735977 9.010960 6.349280 7.964438

 35 H 1.094507 3.737982 7.664799 4.936711 8.538780

 36 H 1.094507 3.737982 7.664799 4.936711 8.538780

 37 H 8.538780 9.949637 1.094507 3.737982 11.421995

 38 H 8.538780 9.949637 1.094507 3.737982 11.421995

 39 H 7.964438 9.799122 1.091291 2.735977 11.976592

 40 H 7.664799 4.936711 11.421995 10.459153 1.094507

 41 H 7.664799 4.936711 11.421995 10.459153 1.094507

 42 H 9.010960 6.349280 11.976592 11.351237 1.091291

 43 H 11.421995 10.459153 8.538780 9.949637 7.664799

 44 H 11.421995 10.459153 8.538780 9.949637 7.664799

 45 H 11.976592 11.351237 7.964438 9.799122 9.010960

 31 32 33 34 35

 31 H 0.000000

 32 C 5.273542 0.000000

 33 H 7.377916 2.984092 0.000000

 34 H 9.799122 11.976592 11.351237 0.000000

 35 H 9.949637 11.421995 10.459153 1.771035 0.000000

 36 H 9.949637 11.421995 10.459153 1.771035 1.754278

 37 H 10.459153 7.664799 4.936711 9.622817 8.209385

 38 H 10.459153 7.664799 4.936711 9.622817 8.394730

 39 H 11.351237 9.010960 6.349280 9.050001 7.631295

 40 H 3.737982 8.538780 9.949637 7.631295 8.209385

 41 H 3.737982 8.538780 9.949637 7.631295 8.394730

 42 H 2.735977 7.964438 9.799122 9.050001 9.622817

 43 H 4.936711 1.094507 3.737982 12.153136 11.609824

 44 H 4.936711 1.094507 3.737982 12.153136 11.741614

 45 H 6.349280 1.091291 2.735977 12.798634 12.153136

 36 37 38 39 40

 36 H 0.000000

 37 H 8.394730 0.000000

 38 H 8.209385 1.754278 0.000000

 39 H 7.631295 1.771035 1.771035 0.000000

 40 H 8.394730 11.609824 11.741614 12.153136 0.000000

 41 H 8.209385 11.741614 11.609824 12.153136 1.754278

 42 H 9.622817 12.153136 12.153136 12.798634 1.771035

 43 H 11.741614 8.209385 8.394730 9.622817 8.209385

 44 H 11.609824 8.394730 8.209385 9.622817 8.394730

 45 H 12.153136 7.631295 7.631295 9.050001 9.622817

 41 42 43 44 45

 41 H 0.000000

 42 H 1.771035 0.000000

 43 H 8.394730 7.631295 0.000000

 44 H 8.209385 7.631295 1.754278 0.000000

 45 H 9.622817 9.050001 1.771035 1.771035 0.000000

 Stoichiometry C20H16N8Zn

 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:

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

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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

 1 6 0 1.108140 2.795497 0.000000

 2 7 0 0.000000 2.005455 0.000000

 3 6 0 -1.112870 2.785746 0.000000

 4 6 0 -0.692079 4.200421 0.000000

 5 6 0 0.672460 4.190429 0.000000

 6 7 0 -2.387849 2.383888 0.000000

 7 6 0 -2.795497 1.108140 0.000000

 8 7 0 -2.005455 0.000000 0.000000

 9 6 0 -2.785746 -1.112870 0.000000

 10 6 0 -4.200421 -0.692079 0.000000

 11 6 0 -4.190429 0.672460 0.000000

 12 7 0 2.383888 2.387849 0.000000

 13 6 0 4.200421 0.692079 0.000000

 14 6 0 4.190429 -0.672460 0.000000

 15 6 0 2.795497 -1.108140 0.000000

 16 7 0 2.005455 -0.000000 0.000000

 17 6 0 2.785746 1.112870 0.000000

 18 7 0 2.387849 -2.383888 0.000000

 19 7 0 -0.000000 -2.005455 0.000000

 20 6 0 1.112870 -2.785746 0.000000

 21 6 0 0.692079 -4.200421 0.000000

 22 6 0 -0.672460 -4.190429 0.000000

 23 6 0 -1.108140 -2.795497 0.000000

 24 7 0 -2.383888 -2.387849 0.000000

 25 30 0 0.000000 0.000000 0.000000

 26 6 0 -1.629094 5.358137 0.000000

 27 1 0 1.338249 5.042411 0.000000

 28 6 0 -5.358137 -1.629094 0.000000

 29 1 0 -5.042411 1.338249 0.000000

 30 6 0 5.358137 1.629094 0.000000

 31 1 0 5.042411 -1.338249 0.000000

 32 6 0 1.629094 -5.358137 0.000000

 33 1 0 -1.338249 -5.042411 0.000000

 34 1 0 -1.088420 6.306076 0.000000

 35 1 0 -2.283406 5.336952 0.877139

 36 1 0 -2.283406 5.336952 -0.877139

 37 1 0 -5.336952 -2.283406 0.877139

 38 1 0 -5.336952 -2.283406 -0.877139

 39 1 0 -6.306076 -1.088420 0.000000

 40 1 0 5.336952 2.283406 0.877139

 41 1 0 5.336952 2.283406 -0.877139

 42 1 0 6.306076 1.088420 0.000000

 43 1 0 2.283406 -5.336952 0.877139

 44 1 0 2.283406 -5.336952 -0.877139

 45 1 0 1.088420 -6.306076 0.000000

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 Rotational constants (GHZ): 0.1828513 0.1828513 0.0916313

 Leave Link 202 at Thu Sep 19 00:35:34 2019, MaxMem= 1342177280 cpu: 0.1

 (Enter /home/blab/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\*

 \*\*\*\*

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

 Pseudopotential Parameters

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

 Center Atomic Valence Angular Power

 Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

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

 1 6

 No pseudopotential on this center.

 2 7

 No pseudopotential on this center.

 3 6

 No pseudopotential on this center.

 4 6

 No pseudopotential on this center.

 5 6

 No pseudopotential on this center.

 6 7

 No pseudopotential on this center.

 7 6

 No pseudopotential on this center.

 8 7

 No pseudopotential on this center.

 9 6

 No pseudopotential on this center.

 10 6

 No pseudopotential on this center.

 11 6

 No pseudopotential on this center.

 12 7

 No pseudopotential on this center.

 13 6

 No pseudopotential on this center.

 14 6

 No pseudopotential on this center.

 15 6

 No pseudopotential on this center.

 16 7

 No pseudopotential on this center.

 17 6

 No pseudopotential on this center.

 18 7

 No pseudopotential on this center.

 19 7

 No pseudopotential on this center.

 20 6

 No pseudopotential on this center.

 21 6

 No pseudopotential on this center.

 22 6

 No pseudopotential on this center.

 23 6

 No pseudopotential on this center.

 24 7

 No pseudopotential on this center.

 25 30 12

 F and up

 1 386.7379660 -18.00000000 0.00000000

 2 72.8587359 -124.35274030 0.00000000

 2 15.9066170 -30.66018220 0.00000000

 2 4.3502340 -10.63589890 0.00000000

 2 1.2842199 -0.76836230 0.00000000

 S - F

 0 19.0867858 3.00000000 0.00000000

 1 5.0231080 22.52342250 0.00000000

 2 1.2701744 48.44659420 0.00000000

 2 1.0671287 -44.55601190 0.00000000

 2 0.9264190 12.99839580 0.00000000

 P - F

 0 43.4927750 5.00000000 0.00000000

 1 20.8692669 20.74355890 0.00000000

 2 21.7118378 90.30271580 0.00000000

 2 6.3616915 74.66103160 0.00000000

 2 1.2291195 9.88944240 0.00000000

 D - F

 2 13.5851800 -4.84903590 0.00000000

 2 9.8373050 3.69133790 0.00000000

 2 0.8373113 -0.50373190 0.00000000

 26 6

 No pseudopotential on this center.

 27 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

 No pseudopotential on this center.

 37 1

 No pseudopotential on this center.

 38 1

 No pseudopotential on this center.

 39 1

 No pseudopotential on this center.

 40 1

 No pseudopotential on this center.

 41 1

 No pseudopotential on this center.

 42 1

 No pseudopotential on this center.

 43 1

 No pseudopotential on this center.

 44 1

 No pseudopotential on this center.

 45 1

 No pseudopotential on this center.

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

 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 102 beta electrons

 nuclear repulsion energy 2765.4879751323 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.

 Regular integral format.

 Two-electron integral symmetry is turned on.

 R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1141862501 Hartrees.

 Nuclear repulsion after empirical dispersion term = 2765.3737888822 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: York/Karplus (Gamma=1.0000).

 Polarization charges: spherical gaussians, with

 point-specific exponents (IZeta= 3).

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

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

 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 = 3490

 GePol: Average weight of points = 0.11

 GePol: Minimum weight of points = 0.43D-08

 GePol: Maximum weight of points = 0.18390

 GePol: Number of points with low weight = 128

 GePol: Fraction of low-weight points (<1% of avg) = 3.67%

 GePol: Cavity surface area = 381.474 Ang\*\*2

 GePol: Cavity volume = 378.535 Ang\*\*3

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

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 PCM non-electrostatic energy = -0.0108334690 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 2765.3629554132 Hartrees.

 Leave Link 301 at Thu Sep 19 00:35:34 2019, MaxMem= 1342177280 cpu: 1.1

 (Enter /home/blab/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= 15331 LenP2D= 41292.

 LDataN: DoStor=T MaxTD1= 5 Len= 102

 NBasis= 576 RedAO= T EigKep= 1.80D-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 Thu Sep 19 00:35:34 2019, MaxMem= 1342177280 cpu: 6.6

 (Enter /home/blab/g09/l308.exe)

 Leave Link 308 at Thu Sep 19 00:35:35 2019, MaxMem= 1342177280 cpu: 1.2

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

 DipDrv: MaxL=1.

 Leave Link 303 at Thu Sep 19 00:35:35 2019, MaxMem= 1342177280 cpu: 0.8

 (Enter /home/blab/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= -1276.20063471339

 JPrj=0 DoOrth=F DoCkMO=F.

 Initial guess orbital symmetries:

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

 The electronic state of the initial guess is 1-AG.

 Leave Link 401 at Thu Sep 19 00:35:36 2019, MaxMem= 1342177280 cpu: 10.4

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

 Closed shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 1136976 IEndB= 1136976 NGot= 1342177280 MDV= 1341426001

 LenX= 1341426001 LenY= 1341056945

 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= 0 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= 36540300.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 6.88D-15 for 3474.

 Iteration 1 A\*A^-1 deviation from orthogonality is 3.32D-15 for 3130 3062.

 Iteration 1 A^-1\*A deviation from unit magnitude is 6.88D-15 for 3474.

 Iteration 1 A^-1\*A deviation from orthogonality is 2.10D-14 for 3266 3131.

 E= -1275.19089292008

 DIIS: error= 9.10D-02 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -1275.19089292008 IErMin= 1 ErrMin= 9.10D-02

 ErrMax= 9.10D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.93D-01 BMatP= 9.93D-01

 IDIUse=3 WtCom= 9.04D-02 WtEn= 9.10D-01

 Coeff-Com: 0.100D+01

 Coeff-En: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.111 Goal= None Shift= 0.000

 GapD= 0.111 DampG=1.000 DampE=0.250 DampFc=0.2500 IDamp=-1.

 Damping current iteration by 2.50D-01

 RMSDP=2.65D-03 MaxDP=1.29D-01 OVMax= 1.75D-01

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 6.60D-04 CP: 9.93D-01

 E= -1275.44651239658 Delta-E= -0.255619476496 Rises=F Damp=T

 DIIS: error= 3.78D-02 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -1275.44651239658 IErMin= 2 ErrMin= 3.78D-02

 ErrMax= 3.78D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.54D-01 BMatP= 9.93D-01

 IDIUse=3 WtCom= 6.22D-01 WtEn= 3.78D-01

 Coeff-Com: -0.890D+00 0.189D+01

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

 Coeff: -0.554D+00 0.155D+01

 Gap= 0.135 Goal= None Shift= 0.000

 RMSDP=9.56D-04 MaxDP=4.57D-02 DE=-2.56D-01 OVMax= 9.87D-02

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 4.73D-04 CP: 9.83D-01 2.25D+00

 E= -1275.86907706429 Delta-E= -0.422564667718 Rises=F Damp=F

 DIIS: error= 7.81D-03 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 3 EnMin= -1275.86907706429 IErMin= 3 ErrMin= 7.81D-03

 ErrMax= 7.81D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.44D-02 BMatP= 2.54D-01

 IDIUse=3 WtCom= 9.22D-01 WtEn= 7.81D-02

 Coeff-Com: -0.586D-01 0.318D+00 0.741D+00

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

 Coeff: -0.540D-01 0.293D+00 0.761D+00

 Gap= 0.096 Goal= None Shift= 0.000

 RMSDP=3.60D-04 MaxDP=1.71D-02 DE=-4.23D-01 OVMax= 3.25D-02

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 2.19D-04 CP: 9.86D-01 1.87D+00 7.31D-01

 E= -1275.88817998846 Delta-E= -0.019102924166 Rises=F Damp=F

 DIIS: error= 3.44D-03 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -1275.88817998846 IErMin= 4 ErrMin= 3.44D-03

 ErrMax= 3.44D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.94D-03 BMatP= 2.44D-02

 IDIUse=3 WtCom= 9.66D-01 WtEn= 3.44D-02

 Coeff-Com: 0.598D-01-0.323D-01 0.406D+00 0.567D+00

 Coeff-En: 0.000D+00 0.000D+00 0.727D-01 0.927D+00

 Coeff: 0.577D-01-0.312D-01 0.394D+00 0.579D+00

 Gap= 0.096 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 409 IAlg= 4 N= 204 NDim= 576 NE2= 2328222 trying DSYEV.

 RMSDP=1.25D-04 MaxDP=5.44D-03 DE=-1.91D-02 OVMax= 2.00D-02

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 6.61D-05 CP: 9.86D-01 1.91D+00 8.37D-01 5.97D-01

 E= -1275.89227113786 Delta-E= -0.004091149403 Rises=F Damp=F

 DIIS: error= 1.47D-03 at cycle 5 NSaved= 5.

 NSaved= 5 IEnMin= 5 EnMin= -1275.89227113786 IErMin= 5 ErrMin= 1.47D-03

 ErrMax= 1.47D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.81D-04 BMatP= 4.94D-03

 IDIUse=3 WtCom= 9.85D-01 WtEn= 1.47D-02

 Coeff-Com: 0.382D-01-0.431D-01 0.174D+00 0.335D+00 0.496D+00

 Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.240D-01 0.976D+00

 Coeff: 0.376D-01-0.424D-01 0.172D+00 0.330D+00 0.503D+00

 Gap= 0.095 Goal= None Shift= 0.000

 RMSDP=4.05D-05 MaxDP=1.95D-03 DE=-4.09D-03 OVMax= 6.61D-03

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 1.78D-05 CP: 9.85D-01 1.92D+00 8.36D-01 6.60D-01 4.98D-01

 E= -1275.89277551604 Delta-E= -0.000504378178 Rises=F Damp=F

 DIIS: error= 4.49D-04 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -1275.89277551604 IErMin= 6 ErrMin= 4.49D-04

 ErrMax= 4.49D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.63D-05 BMatP= 5.81D-04

 IDIUse=3 WtCom= 9.96D-01 WtEn= 4.49D-03

 Coeff-Com: 0.154D-01-0.205D-01 0.567D-01 0.120D+00 0.266D+00 0.562D+00

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

 Coeff: 0.154D-01-0.204D-01 0.564D-01 0.120D+00 0.265D+00 0.563D+00

 Gap= 0.095 Goal= None Shift= 0.000

 RMSDP=8.71D-06 MaxDP=3.57D-04 DE=-5.04D-04 OVMax= 1.07D-03

 Cycle 7 Pass 1 IDiag 1:

 RMSU= 6.57D-06 CP: 9.85D-01 1.92D+00 8.41D-01 6.54D-01 5.33D-01

 CP: 7.66D-01

 E= -1275.89279980322 Delta-E= -0.000024287179 Rises=F Damp=F

 DIIS: error= 1.08D-04 at cycle 7 NSaved= 7.

 NSaved= 7 IEnMin= 7 EnMin= -1275.89279980322 IErMin= 7 ErrMin= 1.08D-04

 ErrMax= 1.08D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.76D-06 BMatP= 3.63D-05

 IDIUse=3 WtCom= 9.99D-01 WtEn= 1.08D-03

 Coeff-Com: 0.536D-02-0.751D-02 0.178D-01 0.398D-01 0.112D+00 0.327D+00

 Coeff-Com: 0.505D+00

 Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.228D-01

 Coeff-En: 0.977D+00

 Coeff: 0.536D-02-0.750D-02 0.178D-01 0.397D-01 0.112D+00 0.327D+00

 Coeff: 0.506D+00

 Gap= 0.095 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 21319 IAlg= 4 N= 204 NDim= 576 NE2= 2328222 trying DSYEV.

 RMSDP=3.09D-06 MaxDP=1.56D-04 DE=-2.43D-05 OVMax= 3.37D-04

 Cycle 8 Pass 1 IDiag 1:

 RMSU= 1.18D-06 CP: 9.85D-01 1.92D+00 8.40D-01 6.54D-01 5.51D-01

 CP: 7.74D-01 6.23D-01

 E= -1275.89280286298 Delta-E= -0.000003059754 Rises=F Damp=F

 DIIS: error= 2.84D-05 at cycle 8 NSaved= 8.

 NSaved= 8 IEnMin= 8 EnMin= -1275.89280286298 IErMin= 8 ErrMin= 2.84D-05

 ErrMax= 2.84D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.49D-07 BMatP= 3.76D-06

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

 Coeff-Com: 0.154D-02-0.221D-02 0.493D-02 0.114D-01 0.377D-01 0.127D+00

 Coeff-Com: 0.239D+00 0.581D+00

 Coeff: 0.154D-02-0.221D-02 0.493D-02 0.114D-01 0.377D-01 0.127D+00

 Coeff: 0.239D+00 0.581D+00

 Gap= 0.095 Goal= None Shift= 0.000

 RMSDP=6.20D-07 MaxDP=2.67D-05 DE=-3.06D-06 OVMax= 9.22D-05

 Cycle 9 Pass 1 IDiag 1:

 RMSU= 4.64D-07 CP: 9.85D-01 1.92D+00 8.41D-01 6.55D-01 5.50D-01

 CP: 7.72D-01 6.54D-01 7.53D-01

 E= -1275.89280295975 Delta-E= -0.000000096779 Rises=F Damp=F

 DIIS: error= 1.39D-05 at cycle 9 NSaved= 9.

 NSaved= 9 IEnMin= 9 EnMin= -1275.89280295975 IErMin= 9 ErrMin= 1.39D-05

 ErrMax= 1.39D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.67D-08 BMatP= 1.49D-07

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

 Coeff-Com: -0.826D-04 0.959D-04-0.395D-03-0.883D-03-0.552D-03 0.581D-02

 Coeff-Com: 0.242D-01 0.313D+00 0.659D+00

 Coeff: -0.826D-04 0.959D-04-0.395D-03-0.883D-03-0.552D-03 0.581D-02

 Coeff: 0.242D-01 0.313D+00 0.659D+00

 Gap= 0.095 Goal= None Shift= 0.000

 RMSDP=1.99D-07 MaxDP=7.87D-06 DE=-9.68D-08 OVMax= 2.63D-05

 Cycle 10 Pass 1 IDiag 1:

 RMSU= 1.01D-07 CP: 9.85D-01 1.92D+00 8.41D-01 6.55D-01 5.51D-01

 CP: 7.75D-01 6.48D-01 8.33D-01 7.71D-01

 E= -1275.89280297917 Delta-E= -0.000000019415 Rises=F Damp=F

 DIIS: error= 8.12D-07 at cycle 10 NSaved= 10.

 NSaved=10 IEnMin=10 EnMin= -1275.89280297917 IErMin=10 ErrMin= 8.12D-07

 ErrMax= 8.12D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.05D-10 BMatP= 2.67D-08

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

 Coeff-Com: -0.566D-04 0.713D-04-0.233D-03-0.561D-03-0.957D-03-0.481D-03

 Coeff-Com: 0.539D-02 0.110D+00 0.241D+00 0.646D+00

 Coeff: -0.566D-04 0.713D-04-0.233D-03-0.561D-03-0.957D-03-0.481D-03

 Coeff: 0.539D-02 0.110D+00 0.241D+00 0.646D+00

 Gap= 0.095 Goal= None Shift= 0.000

 RMSDP=3.64D-08 MaxDP=1.91D-06 DE=-1.94D-08 OVMax= 3.95D-06

 Cycle 11 Pass 1 IDiag 1:

 RMSU= 2.61D-08 CP: 9.85D-01 1.92D+00 8.41D-01 6.55D-01 5.51D-01

 CP: 7.76D-01 6.50D-01 8.41D-01 7.74D-01 8.75D-01

 E= -1275.89280297960 Delta-E= -0.000000000432 Rises=F Damp=F

 DIIS: error= 4.91D-07 at cycle 11 NSaved= 11.

 NSaved=11 IEnMin=11 EnMin= -1275.89280297960 IErMin=11 ErrMin= 4.91D-07

 ErrMax= 4.91D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.62D-11 BMatP= 4.05D-10

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

 Coeff-Com: -0.166D-04 0.216D-04-0.665D-04-0.185D-03-0.456D-03-0.123D-02

 Coeff-Com: -0.418D-03 0.139D-01 0.283D-01 0.309D+00 0.651D+00

 Coeff: -0.166D-04 0.216D-04-0.665D-04-0.185D-03-0.456D-03-0.123D-02

 Coeff: -0.418D-03 0.139D-01 0.283D-01 0.309D+00 0.651D+00

 Gap= 0.095 Goal= None Shift= 0.000

 RMSDP=1.09D-08 MaxDP=6.29D-07 DE=-4.32D-10 OVMax= 1.65D-06

 Cycle 12 Pass 1 IDiag 1:

 RMSU= 6.76D-09 CP: 9.85D-01 1.92D+00 8.41D-01 6.55D-01 5.51D-01

 CP: 7.76D-01 6.50D-01 8.43D-01 7.75D-01 9.24D-01

 CP: 7.81D-01

 E= -1275.89280297964 Delta-E= -0.000000000035 Rises=F Damp=F

 DIIS: error= 6.77D-08 at cycle 12 NSaved= 12.

 NSaved=12 IEnMin=12 EnMin= -1275.89280297964 IErMin=12 ErrMin= 6.77D-08

 ErrMax= 6.77D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.60D-12 BMatP= 7.62D-11

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

 Coeff-Com: -0.146D-05 0.191D-05-0.944D-05-0.360D-04-0.932D-04-0.399D-03

 Coeff-Com: -0.502D-03-0.179D-02-0.604D-02 0.582D-01 0.186D+00 0.764D+00

 Coeff: -0.146D-05 0.191D-05-0.944D-05-0.360D-04-0.932D-04-0.399D-03

 Coeff: -0.502D-03-0.179D-02-0.604D-02 0.582D-01 0.186D+00 0.764D+00

 Gap= 0.095 Goal= None Shift= 0.000

 DSYEVD-2 returned Info= 165 IAlg= 4 N= 82 NDim= 576 NE2= 2328222 trying DSYEV.

 DSYEVD-2 returned Info= 21319 IAlg= 4 N= 204 NDim= 576 NE2= 2328222 trying DSYEV.

 RMSDP=3.55D-09 MaxDP=1.43D-07 DE=-3.55D-11 OVMax= 3.88D-07

 Error on total polarization charges = 0.06478

 SCF Done: E(RB3LYP) = -1275.89280298 A.U. after 12 cycles

 NFock= 12 Conv=0.35D-08 -V/T= 1.9660

 KE= 1.320829893689D+03 PE=-8.582629289728D+03 EE= 3.220543637646D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.80

 (included in total energy above)

 Leave Link 502 at Thu Sep 19 00:36:43 2019, MaxMem= 1342177280 cpu: 591.2

 (Enter /home/blab/g09/l801.exe)

 DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

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

 HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 5 IDoV=-2 UseB2=F ITyADJ=14

 ICtDFT= 12500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

 Largest valence mixing into a core orbital is 4.89D-05

 Largest core mixing into a valence orbital is 2.00D-05

 Range of M.O.s used for correlation: 29 576

 NBasis= 576 NAE= 102 NBE= 102 NFC= 28 NFV= 0

 NROrb= 548 NOA= 74 NOB= 74 NVA= 474 NVB= 474

 \*\*\*\* Warning!!: The largest alpha MO coefficient is 0.10291871D+02

 \*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.95366482D-01

 Leave Link 801 at Thu Sep 19 00:36:43 2019, MaxMem= 1342177280 cpu: 3.2

 (Enter /home/blab/g09/l914.exe)

 RHF ground state

 MDV= 1342177280 DFT=T DoStab=F Mixed=T DoRPA=T DoScal=F NonHer=T

 Would need an additional 16054000000 words for in-memory AO integral storage.

 NEqPCM: Using non-equilibrium solvation (IEInf=1, Eps= 46.8260, EpsInf= 2.0079)

 Inv3: Mode=1 IEnd= 36540300.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 6.66D-15 for 3482.

 Iteration 1 A\*A^-1 deviation from orthogonality is 2.44D-15 for 2501 237.

 Iteration 1 A^-1\*A deviation from unit magnitude is 6.44D-15 for 3482.

 Iteration 1 A^-1\*A deviation from orthogonality is 1.54D-15 for 3481 3457.

 Making orbital integer symmetry assigments:

 Orbital symmetries:

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 40 initial guesses have been made.

 Convergence on wavefunction: 0.001000000000000

 Davidson Disk Diagonalization: ConvIn= 1.00D-03 SkipCon=T Conv= 1.00D-03.

 Max sub-space: 200 roots to seek: 40 dimension of matrix: 70152

 Iteration 1 Dimension 40 NMult 0 NNew 40

 CISAX will form 40 AO SS matrices at one time.

 NMat= 40 NSing= 40 JSym2X=-1.

 FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

 IRaf= 0 NMat= 80 IRICut= 100 DoRegI=T DoRafI=T ISym2E=-1.

 DSYEVD-2 returned Info= 81 IAlg= 4 N= 40 NDim= 40 NE2= 33554282 trying DSYEV.

 New state 1 was old state 2

 New state 2 was old state 1

 New state 3 was old state 11

 New state 4 was old state 12

 New state 5 was old state 4

 New state 6 was old state 3

 New state 7 was old state 6

 New state 9 was old state 15

 New state 10 was old state 16

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.663985328662993

 Root 2 : 2.663985328665559

 Root 3 : 3.161921232263472

 Root 4 : 3.161921232331913

 Root 5 : 3.321739587233961

 Root 6 : 3.321739587316544

 Root 7 : 3.324763706582442

 Root 8 : 3.344107054419177

 Root 9 : 3.380689725492502

 Root 10 : 3.380689725507620

 Root 11 : 3.477763551832119

 Root 12 : 3.579804705292946

 Root 13 : 3.703926005781454

 Root 14 : 3.703926005863784

 Root 15 : 3.831960892610653

 Root 16 : 3.863059664729728

 Root 17 : 3.869983055891669

 Root 18 : 3.872239951126085

 Root 19 : 4.131743429727487

 Root 20 : 4.448674145147975

 Root 21 : 4.448674145192272

 Root 22 : 4.640630455201209

 Root 23 : 4.640630455240417

 Root 24 : 4.794450565003226

 Root 25 : 4.937071827197177

 Root 26 : 5.073330591713261

 Root 27 : 5.085448430358170

 Root 28 : 5.104105650536909

 Root 29 : 5.184191791863465

 Root 30 : 5.186236698318803

 Root 31 : 5.217583639874887

 Root 32 : 5.217583639885592

 Root 33 : 5.245464172653376

 Root 34 : 5.296188503453408

 Root 35 : 5.446649860488247

 Root 36 : 5.592828024017523

 Root 37 : 5.675851281265264

 Root 38 : 5.675851281329058

 Root 39 : 6.088657400268791

 Root 40 : 7.092757303041371

 Iteration 2 Dimension 60 NMult 40 NNew 20

 CISAX will form 20 AO SS matrices at one time.

 NMat= 20 NSing= 20 JSym2X=-1.

 Root 1 not converged, maximum delta is 0.238620818276680

 Root 2 not converged, maximum delta is 0.238620818279082

 New state 3 was old state 5

 Root 3 not converged, maximum delta is 0.052765171273584

 New state 4 was old state 6

 Root 4 not converged, maximum delta is 0.052765171274785

 New state 5 was old state 3

 Root 5 not converged, maximum delta is 0.024633672788250

 New state 6 was old state 4

 Root 6 not converged, maximum delta is 0.024633672791389

 Root 7 not converged, maximum delta is 0.086418472691883

 Root 8 not converged, maximum delta is 0.068207450980671

 Root 9 not converged, maximum delta is 0.057617779241921

 Root 10 not converged, maximum delta is 0.057617779242623

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.372843423934221 Change is -0.291141904728772

 Root 2 : 2.372843423945688 Change is -0.291141904719871

 Root 3 : 3.125315843507316 Change is -0.196423743726646

 Root 4 : 3.125315843598747 Change is -0.196423743717797

 Root 5 : 3.134566786594225 Change is -0.027354445669247

 Root 6 : 3.134566786661468 Change is -0.027354445670444

 Root 7 : 3.136971061876763 Change is -0.187792644705679

 Root 8 : 3.146770784418898 Change is -0.197336270000278

 Root 9 : 3.342997786147995 Change is -0.037691939344508

 Root 10 : 3.342997786158470 Change is -0.037691939349149

 Iteration 3 Dimension 80 NMult 60 NNew 20

 CISAX will form 20 AO SS matrices at one time.

 NMat= 20 NSing= 20 JSym2X=-1.

 DSYEVD-2 returned Info= 3401 IAlg= 4 N= 80 NDim= 80 NE2= 16777141 trying DSYEV.

 Root 1 not converged, maximum delta is 0.035611807878075

 Root 2 not converged, maximum delta is 0.035611807876918

 Root 3 not converged, maximum delta is 0.020093353668920

 Root 4 not converged, maximum delta is 0.020093353672225

 New state 5 was old state 7

 Root 5 not converged, maximum delta is 0.006859712029758

 New state 6 was old state 5

 Root 6 not converged, maximum delta is 0.002569387076507

 New state 7 was old state 6

 Root 7 not converged, maximum delta is 0.002569387076599

 Root 8 not converged, maximum delta is 0.019967615245952

 Root 9 not converged, maximum delta is 0.002118926810741

 Root 10 not converged, maximum delta is 0.002118926810358

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.349250261465789 Change is -0.023593162468432

 Root 2 : 2.349250261479507 Change is -0.023593162466182

 Root 3 : 3.117731131043666 Change is -0.007584712463650

 Root 4 : 3.117731131135003 Change is -0.007584712463744

 Root 5 : 3.129152859944788 Change is -0.007818201931975

 Root 6 : 3.133887597185292 Change is -0.000679189408933

 Root 7 : 3.133887597252734 Change is -0.000679189408735

 Root 8 : 3.141009384818439 Change is -0.005761399600460

 Root 9 : 3.341651216384211 Change is -0.001346569763784

 Root 10 : 3.341651216395551 Change is -0.001346569762919

 Iteration 4 Dimension 100 NMult 80 NNew 20

 CISAX will form 20 AO SS matrices at one time.

 NMat= 20 NSing= 20 JSym2X=-1.

 Root 1 not converged, maximum delta is 0.005180359505592

 Root 2 not converged, maximum delta is 0.005180359506637

 Root 3 not converged, maximum delta is 0.007149587779682

 Root 4 not converged, maximum delta is 0.007149587779356

 Root 5 not converged, maximum delta is 0.005401861105713

 Root 6 not converged, maximum delta is 0.001087157403078

 Root 7 not converged, maximum delta is 0.001087157403096

 Root 8 not converged, maximum delta is 0.006528230995140

 Root 9 has converged.

 Root 10 has converged.

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.346487298297557 Change is -0.002762963168232

 Root 2 : 2.346487298311746 Change is -0.002762963167761

 Root 3 : 3.116694221984189 Change is -0.001036909059477

 Root 4 : 3.116694222075135 Change is -0.001036909059868

 Root 5 : 3.128087066793332 Change is -0.001065793151456

 Root 6 : 3.133866825750023 Change is -0.000020771435269

 Root 7 : 3.133866825817387 Change is -0.000020771435347

 Root 8 : 3.140360431980898 Change is -0.000648952837541

 Root 9 : 3.341579651404993 Change is -0.000071564979218

 Root 10 : 3.341579651415990 Change is -0.000071564979562

 Iteration 5 Dimension 116 NMult 100 NNew 16

 CISAX will form 16 AO SS matrices at one time.

 NMat= 16 NSing= 16 JSym2X=-1.

 DSYEVD-2 returned Info= 233 IAlg= 4 N= 116 NDim= 116 NE2= 11570442 trying DSYEV.

 Root 1 not converged, maximum delta is 0.009036848738277

 Root 2 not converged, maximum delta is 0.009036848738190

 Root 3 not converged, maximum delta is 0.001417402727120

 Root 4 not converged, maximum delta is 0.001417402726591

 Root 5 has converged.

 Root 6 not converged, maximum delta is 0.002077177007099

 Root 7 not converged, maximum delta is 0.002077177007244

 Root 8 has converged.

 Root 9 not converged, maximum delta is 0.002985094286255

 Root 10 not converged, maximum delta is 0.002985094286266

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.346292216294248 Change is -0.000195082003309

 Root 2 : 2.346292216308683 Change is -0.000195082003062

 Root 3 : 3.116624427104428 Change is -0.000069794879761

 Root 4 : 3.116624427195112 Change is -0.000069794880023

 Root 5 : 3.128013631379333 Change is -0.000073435413999

 Root 6 : 3.133866110730059 Change is -0.000000715019964

 Root 7 : 3.133866110796111 Change is -0.000000715021276

 Root 8 : 3.140305714186145 Change is -0.000054717794753

 Root 9 : 3.341579553600290 Change is -0.000000097804702

 Root 10 : 3.341579553611508 Change is -0.000000097804481

 Iteration 6 Dimension 132 NMult 116 NNew 16

 CISAX will form 16 AO SS matrices at one time.

 NMat= 16 NSing= 16 JSym2X=-1.

 Root 1 not converged, maximum delta is 0.015975915366839

 Root 2 not converged, maximum delta is 0.015975915366884

 Root 3 has converged.

 Root 4 has converged.

 Root 5 has converged.

 Root 6 has converged.

 Root 7 has converged.

 Root 8 has converged.

 Root 9 not converged, maximum delta is 0.002939489397351

 Root 10 not converged, maximum delta is 0.002939489397399

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.346287008212871 Change is -0.000005208081377

 Root 2 : 2.346287008227376 Change is -0.000005208081307

 Root 3 : 3.116620467652601 Change is -0.000003959451827

 Root 4 : 3.116620467743681 Change is -0.000003959451431

 Root 5 : 3.128013631379491 Change is 0.000000000000158

 Root 6 : 3.133866068040058 Change is -0.000000042690001

 Root 7 : 3.133866068107737 Change is -0.000000042688374

 Root 8 : 3.140305714186224 Change is 0.000000000000079

 Root 9 : 3.341577004194279 Change is -0.000002549406011

 Root 10 : 3.341577004205743 Change is -0.000002549405766

 Iteration 7 Dimension 140 NMult 132 NNew 8

 CISAX will form 8 AO SS matrices at one time.

 NMat= 8 NSing= 8 JSym2X=-1.

 Root 1 not converged, maximum delta is 0.004118490531134

 Root 2 not converged, maximum delta is 0.004118490531205

 Root 3 has converged.

 Root 4 has converged.

 Root 5 has converged.

 Root 6 has converged.

 Root 7 has converged.

 Root 8 has converged.

 Root 9 not converged, maximum delta is 0.001130105704304

 Root 10 not converged, maximum delta is 0.001130105704284

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.346286641608209 Change is -0.000000366604662

 Root 2 : 2.346286641622399 Change is -0.000000366604978

 Root 3 : 3.116620388296181 Change is -0.000000079356420

 Root 4 : 3.116620388387288 Change is -0.000000079356393

 Root 5 : 3.128013631379412 Change is -0.000000000000079

 Root 6 : 3.133866067604660 Change is -0.000000000435398

 Root 7 : 3.133866067672155 Change is -0.000000000435582

 Root 8 : 3.140305714186197 Change is -0.000000000000026

 Root 9 : 3.341576897527111 Change is -0.000000106667168

 Root 10 : 3.341576897538723 Change is -0.000000106667020

 Convergence on energies, max DE= 3.67D-07.

 Convergence on expansion vectors.

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 Excited states from <AA,BB:AA,BB> singles matrix:

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

 1PDM for each excited state written to RWF 633

 Ground to excited state transition densities written to RWF 633

 Ground to excited state transition electric dipole moments (Au):

 state X Y Z Dip. S. Osc.

 1 -0.0689 2.3473 0.0000 5.5144 0.3170

 2 2.3473 0.0689 0.0000 5.5144 0.3170

 3 -0.4699 -0.3037 0.0000 0.3131 0.0239

 4 0.3037 -0.4699 -0.0000 0.3131 0.0239

 5 0.0000 -0.0000 -0.0000 0.0000 0.0000

 6 -0.0000 -0.0000 -0.0000 0.0000 0.0000

 7 0.0000 -0.0000 -0.0000 0.0000 0.0000

 8 -0.0000 -0.0000 -0.0000 0.0000 0.0000

 9 -0.0000 0.0000 -0.0000 0.0000 0.0000

 10 0.0000 0.0000 0.0000 0.0000 0.0000

 Ground to excited state transition velocity dipole moments (Au):

 state X Y Z Dip. S. Osc.

 1 0.0069 -0.1997 -0.0000 0.0399 0.3086

 2 -0.1997 -0.0069 -0.0000 0.0399 0.3086

 3 0.0521 0.0350 -0.0000 0.0039 0.0230

 4 -0.0350 0.0521 0.0000 0.0039 0.0230

 5 -0.0000 0.0000 0.0000 0.0000 0.0000

 6 -0.0000 0.0000 0.0000 0.0000 0.0000

 7 -0.0000 -0.0000 0.0000 0.0000 0.0000

 8 0.0000 0.0000 0.0000 0.0000 0.0000

 9 0.0000 0.0000 0.0000 0.0000 0.0000

 10 -0.0000 0.0000 0.0000 0.0000 0.0000

 Ground to excited state transition magnetic dipole moments (Au):

 state X Y Z

 1 0.0000 0.0000 0.0000

 2 0.0000 -0.0000 0.0000

 3 -0.0000 0.0000 0.0000

 4 0.0000 0.0000 -0.0000

 5 -0.0000 0.0000 1.9357

 6 0.0066 -0.3708 0.0000

 7 -0.3708 -0.0066 -0.0000

 8 -0.0000 0.0000 0.0000

 9 0.5416 -0.0539 -0.0000

 10 -0.0539 -0.5416 0.0000

 Ground to excited state transition velocity quadrupole moments (Au):

 state XX YY ZZ XY XZ YZ

 1 0.0000 0.0000 -0.0000 0.0000 -0.0000 0.0000

 2 0.0000 -0.0000 -0.0000 -0.0000 0.0000 0.0000

 3 -0.0000 0.0000 -0.0000 -0.0000 -0.0000 -0.0000

 4 -0.0000 0.0000 -0.0000 -0.0000 -0.0000 -0.0000

 5 0.1998 0.1998 0.0109 -0.0000 0.0000 -0.0000

 6 0.0000 -0.0000 -0.0000 -0.0000 -0.0272 0.0066

 7 0.0000 -0.0000 0.0000 -0.0000 0.0066 0.0272

 8 0.2920 -0.2920 0.0000 0.6166 0.0000 0.0000

 9 0.0000 0.0000 0.0000 -0.0000 0.0204 0.1353

 10 0.0000 -0.0000 0.0000 0.0000 0.1353 -0.0204

 <0|del|b> \* <b|rxdel|0> + <0|del|b> \* <b|delr+rdel|0>

 Rotatory Strengths (R) in cgs (10\*\*-40 erg-esu-cm/Gauss)

 state XX YY ZZ R(velocity) E-M Angle

 1 -0.0000 0.0000 0.0000 -0.0000 90.00

 2 0.0000 -0.0000 -0.0000 -0.0000 90.00

 3 0.0000 -0.0000 -0.0000 -0.0000 90.00

 4 0.0000 -0.0000 -0.0000 -0.0000 90.00

 5 0.0000 0.0000 0.0000 0.0000 90.00

 6 -0.0000 -0.0000 -0.0000 -0.0000 90.00

 7 0.0000 0.0000 0.0000 0.0000 90.00

 8 0.0000 -0.0000 0.0000 0.0000 90.00

 9 -0.0000 0.0000 0.0000 0.0000 90.00

 10 -0.0000 0.0000 -0.0000 -0.0000 90.00

 1/2[<0|r|b>\*<b|rxdel|0> + (<0|rxdel|b>\*<b|r|0>)\*]

 Rotatory Strengths (R) in cgs (10\*\*-40 erg-esu-cm/Gauss)

 state XX YY ZZ R(length)

 1 0.0000 -0.0000 -0.0000 -0.0000

 2 -0.0000 0.0000 -0.0000 -0.0000

 3 -0.0000 0.0000 -0.0000 -0.0000

 4 -0.0000 0.0000 -0.0000 -0.0000

 5 0.0000 0.0000 0.0000 0.0000

 6 0.0000 -0.0000 0.0000 -0.0000

 7 0.0000 -0.0000 -0.0000 0.0000

 8 -0.0000 0.0000 0.0000 0.0000

 9 0.0000 0.0000 -0.0000 0.0000

 10 0.0000 0.0000 -0.0000 0.0000

 1/2[<0|del|b>\*<b|r|0> + (<0|r|b>\*<b|del|0>)\*] (Au)

 state X Y Z Dip. S. Osc.(frdel)

 1 -0.0005 -0.4686 -0.0000 0.4691 0.3128

 2 -0.4686 -0.0005 -0.0000 0.4691 0.3128

 3 -0.0245 -0.0106 -0.0000 0.0351 0.0234

 4 -0.0106 -0.0245 -0.0000 0.0351 0.0234

 5 -0.0000 -0.0000 -0.0000 0.0000 0.0000

 6 0.0000 -0.0000 -0.0000 0.0000 0.0000

 7 -0.0000 0.0000 -0.0000 0.0000 0.0000

 8 -0.0000 -0.0000 -0.0000 0.0000 0.0000

 9 -0.0000 0.0000 -0.0000 0.0000 0.0000

 10 -0.0000 0.0000 0.0000 -0.0000 -0.0000

 Excitation energies and oscillator strengths:

 Excited State 1: Singlet-EU 2.3463 eV 528.43 nm f=0.3170 <S\*\*2>=0.000

 30 ->155 0.00126

 31 ->139 -0.00101

 33 ->142 -0.00146

 34 ->155 -0.00179

 34 ->171 -0.00147

 35 ->134 -0.00161

 35 ->138 -0.00101

 35 ->182 0.00110

 36 ->145 -0.00120

 36 ->149 -0.00105

 36 ->154 -0.00111

 36 ->180 0.00119

 41 ->191 0.00101

 41 ->241 0.00107

 43 ->139 0.00107

 43 ->177 0.00101

 45 ->145 0.00118

 46 ->134 0.00131

 46 ->139 0.00166

 46 ->147 0.00142

 46 ->177 0.00132

 47 ->144 0.00126

 47 ->148 0.00148

 47 ->243 -0.00105

 48 ->137 -0.00170

 48 ->142 0.00145

 48 ->143 0.00143

 48 ->145 -0.00175

 48 ->146 -0.00177

 48 ->154 -0.00147

 48 ->190 0.00144

 49 ->149 0.00102

 49 ->153 -0.00221

 49 ->160 0.00136

 49 ->168 0.00110

 49 ->180 0.00171

 50 ->120 0.00117

 50 ->149 0.00147

 50 ->153 -0.00135

 52 ->120 0.00113

 52 ->142 0.00163

 53 ->138 0.00336

 53 ->139 0.00232

 54 ->118 0.00149

 54 ->123 0.00158

 54 ->144 0.00186

 54 ->148 0.00146

 54 ->152 -0.00134

 54 ->155 -0.00102

 54 ->171 -0.00127

 54 ->177 -0.00117

 54 ->184 -0.00106

 54 ->213 -0.00107

 57 ->117 0.00164

 57 ->120 -0.00139

 57 ->142 -0.00364

 57 ->145 -0.00157

 57 ->150 -0.00109

 58 ->145 -0.00112

 58 ->146 0.00119

 58 ->149 -0.00104

 58 ->153 0.00239

 58 ->175 -0.00117

 59 ->130 0.00119

 59 ->134 -0.00222

 59 ->135 0.00236

 59 ->141 0.00112

 59 ->144 0.00274

 59 ->148 0.00115

 59 ->151 0.00166

 59 ->155 0.00122

 59 ->162 0.00184

 59 ->163 -0.00111

 59 ->182 0.00125

 59 ->202 0.00186

 59 ->206 0.00122

 59 ->219 -0.00120

 59 ->236 0.00103

 59 ->242 0.00107

 60 ->134 0.00117

 60 ->135 0.00171

 60 ->139 -0.00260

 60 ->144 0.00251

 60 ->148 0.00164

 60 ->151 -0.00123

 60 ->155 0.00182

 60 ->170 -0.00123

 60 ->174 -0.00119

 60 ->177 -0.00129

 60 ->195 -0.00193

 60 ->202 0.00289

 60 ->206 0.00134

 60 ->237 -0.00141

 61 ->109 0.00106

 61 ->136 -0.00114

 61 ->142 0.00169

 61 ->143 -0.00164

 61 ->145 0.00324

 61 ->165 -0.00122

 62 ->112 0.00159

 62 ->118 0.00182

 62 ->123 0.00223

 62 ->134 0.00243

 62 ->155 -0.00273

 62 ->170 0.00109

 63 ->114 -0.00159

 63 ->118 -0.00123

 63 ->123 -0.00201

 63 ->134 -0.00314

 63 ->135 -0.00272

 63 ->138 0.00169

 63 ->141 -0.00121

 63 ->144 0.00134

 63 ->147 0.00131

 63 ->163 0.00134

 63 ->164 -0.00118

 63 ->171 -0.00131

 64 ->108 0.00215

 64 ->129 -0.00172

 64 ->136 -0.00354

 64 ->143 -0.00180

 64 ->145 -0.00224

 64 ->146 0.00307

 64 ->149 -0.00153

 64 ->150 0.00160

 64 ->159 0.00159

 64 ->166 0.00153

 64 ->168 -0.00171

 64 ->169 -0.00127

 64 ->176 -0.00120

 64 ->180 -0.00169

 64 ->191 0.00158

 64 ->200 -0.00112

 64 ->204 0.00166

 64 ->208 0.00110

 64 ->222 0.00107

 64 ->227 0.00123

 64 ->240 -0.00118

 65 ->117 0.00109

 65 ->120 -0.00308

 65 ->129 0.00129

 65 ->136 -0.00288

 65 ->137 -0.00112

 65 ->143 0.00101

 65 ->149 -0.00198

 65 ->154 -0.00229

 65 ->169 -0.00108

 66 ->104 -0.00243

 66 ->110 -0.00241

 66 ->124 -0.00465

 66 ->125 0.00277

 66 ->131 0.00151

 66 ->132 -0.00216

 66 ->173 -0.00250

 67 ->105 0.00517

 67 ->106 -0.00249

 67 ->107 -0.00192

 67 ->119 0.00329

 67 ->122 0.00112

 67 ->127 -0.00144

 67 ->181 -0.00122

 68 ->106 -0.00460

 68 ->107 -0.00506

 68 ->119 -0.00375

 68 ->122 0.00319

 68 ->133 -0.00153

 68 ->178 -0.00129

 68 ->183 0.00177

 69 ->120 0.00309

 69 ->129 -0.00269

 69 ->136 0.00201

 69 ->142 -0.00179

 70 ->112 -0.00174

 70 ->118 -0.00256

 70 ->123 -0.00176

 70 ->126 0.00224

 70 ->130 0.00312

 70 ->134 0.00133

 70 ->141 -0.00106

 70 ->164 -0.00114

 70 ->167 0.00141

 71 ->123 0.00191

 71 ->126 -0.00195

 71 ->135 0.00282

 71 ->155 0.00157

 72 ->109 -0.00204

 72 ->120 -0.00184

 72 ->121 -0.00116

 72 ->128 0.00116

 72 ->129 0.00251

 72 ->137 0.00175

 72 ->142 -0.00171

 72 ->154 0.00102

 72 ->169 0.00147

 72 ->180 -0.00127

 73 ->103 0.00672

 73 ->110 -0.00276

 73 ->125 -0.00162

 73 ->132 -0.00130

 73 ->158 -0.00162

 73 ->173 -0.00125

 74 ->104 -0.00304

 74 ->111 0.00413

 74 ->124 0.00116

 74 ->125 -0.00354

 74 ->131 -0.00111

 74 ->173 0.00101

 75 ->106 0.00386

 75 ->107 0.00129

 75 ->113 -0.00311

 75 ->119 -0.00364

 75 ->122 -0.00222

 76 ->105 0.00347

 76 ->106 0.00500

 76 ->107 0.00327

 76 ->113 -0.00240

 76 ->122 -0.00298

 76 ->127 -0.00191

 77 ->109 -0.00153

 77 ->116 -0.00137

 77 ->117 0.00315

 77 ->136 0.00299

 77 ->142 -0.00247

 77 ->145 -0.00194

 77 ->149 -0.00228

 77 ->150 0.00111

 77 ->165 -0.00119

 77 ->175 0.00190

 77 ->191 0.00105

 78 ->120 0.00355

 78 ->136 0.00118

 78 ->142 -0.00142

 78 ->222 0.00119

 79 ->112 0.00122

 79 ->114 -0.00169

 79 ->115 -0.00315

 79 ->123 -0.00105

 79 ->134 -0.00119

 79 ->138 -0.00250

 79 ->141 -0.00342

 79 ->144 0.00305

 79 ->148 0.00133

 79 ->152 0.00138

 79 ->155 0.00146

 79 ->167 -0.00125

 79 ->170 -0.00119

 79 ->171 0.00117

 79 ->174 0.00134

 79 ->184 0.00175

 80 ->114 0.00121

 80 ->115 0.00119

 80 ->118 -0.00119

 80 ->123 -0.00335

 80 ->126 -0.00104

 80 ->130 -0.00118

 80 ->134 -0.00107

 80 ->138 -0.00359

 80 ->148 -0.00102

 80 ->170 0.00133

 81 ->104 0.01251

 81 ->110 -0.00409

 81 ->124 -0.00192

 81 ->132 0.00168

 81 ->173 -0.00193

 82 ->109 0.00114

 82 ->117 -0.00214

 82 ->121 -0.00178

 82 ->129 -0.00151

 82 ->136 -0.00122

 82 ->142 -0.00120

 82 ->143 0.00400

 82 ->146 -0.00323

 82 ->149 0.00241

 82 ->150 -0.00195

 82 ->165 0.00130

 82 ->175 -0.00136

 82 ->176 -0.00111

 82 ->193 0.00142

 82 ->221 0.00103

 83 ->114 -0.00366

 83 ->118 0.00288

 83 ->123 0.00238

 83 ->134 -0.00291

 83 ->147 0.00149

 83 ->151 -0.00118

 83 ->152 0.00131

 83 ->155 0.00268

 83 ->167 -0.00142

 83 ->170 -0.00196

 83 ->184 0.00231

 84 ->112 0.00242

 84 ->118 -0.00332

 84 ->134 0.00320

 84 ->138 0.00128

 84 ->139 0.00120

 84 ->141 -0.00187

 84 ->144 0.00107

 84 ->147 -0.00346

 84 ->148 0.00135

 84 ->152 0.00175

 84 ->162 0.00132

 84 ->164 0.00102

 84 ->171 0.00129

 84 ->182 -0.00133

 84 ->225 -0.00101

 85 ->103 0.01523

 85 ->104 -0.00434

 85 ->111 -0.00817

 85 ->124 0.00206

 85 ->125 0.00200

 85 ->131 -0.00160

 85 ->172 -0.00194

 86 ->116 -0.00116

 86 ->120 -0.00315

 86 ->129 -0.00194

 86 ->137 0.00111

 86 ->149 0.00199

 86 ->150 0.00113

 86 ->154 0.00255

 86 ->166 0.00141

 86 ->169 0.00246

 86 ->180 -0.00133

 87 ->109 -0.00106

 87 ->117 0.00239

 87 ->120 -0.00234

 87 ->121 0.00176

 87 ->129 -0.00169

 87 ->136 0.00156

 87 ->142 0.00385

 87 ->143 -0.00124

 87 ->145 -0.00158

 87 ->146 0.00283

 87 ->149 -0.00155

 87 ->150 0.00110

 87 ->153 0.00116

 87 ->165 -0.00128

 87 ->175 0.00102

 87 ->176 0.00142

 87 ->192 -0.00116

 88 ->112 0.00726

 88 ->114 0.00459

 88 ->126 0.00214

 88 ->130 0.00149

 88 ->134 0.00255

 88 ->138 -0.00221

 88 ->139 -0.00306

 88 ->141 -0.00141

 88 ->147 0.00132

 88 ->151 0.00529

 88 ->155 0.00152

 88 ->188 -0.00156

 88 ->219 0.00138

 88 ->225 -0.00120

 88 ->226 -0.00143

 89 ->112 -0.00104

 89 ->114 -0.00206

 89 ->135 0.00245

 89 ->138 0.00126

 89 ->144 0.00294

 89 ->147 -0.00127

 89 ->151 -0.00130

 89 ->155 0.00228

 89 ->163 -0.00145

 89 ->177 -0.00153

 90 ->105 -0.00920

 90 ->106 -0.00992

 90 ->107 0.00182

 90 ->113 0.00743

 90 ->119 -0.00151

 90 ->122 -0.00126

 90 ->127 -0.00114

 90 ->133 -0.00271

 90 ->156 0.00106

 90 ->161 0.00135

 90 ->178 0.00211

 90 ->238 -0.00109

 90 ->273 -0.00114

 91 ->105 0.00910

 91 ->106 -0.00664

 91 ->107 0.00243

 91 ->113 -0.00607

 91 ->140 0.00143

 91 ->156 0.00136

 91 ->161 0.00118

 91 ->181 0.00212

 91 ->229 -0.00130

 91 ->273 -0.00117

 91 ->315 -0.00103

 92 ->120 0.00101

 92 ->121 -0.00108

 92 ->128 0.00115

 92 ->137 0.00276

 92 ->143 0.00192

 92 ->145 0.00123

 92 ->146 0.00191

 92 ->150 -0.00184

 92 ->154 0.00321

 92 ->205 0.00114

 92 ->217 0.00118

 93 ->112 0.00482

 93 ->114 0.00307

 93 ->115 -0.00122

 93 ->134 0.00180

 93 ->135 0.00309

 93 ->139 0.00688

 93 ->144 0.00288

 93 ->147 -0.00167

 93 ->151 0.00234

 93 ->174 -0.00254

 93 ->194 -0.00101

 93 ->195 -0.00174

 94 ->130 0.00112

 94 ->135 0.00196

 94 ->139 -0.00335

 94 ->141 -0.00131

 94 ->144 0.00241

 94 ->152 -0.00100

 94 ->155 0.00155

 94 ->163 -0.00133

 94 ->164 -0.00137

 94 ->170 -0.00201

 94 ->174 -0.00134

 94 ->177 -0.00228

 94 ->187 0.00231

 94 ->202 0.00130

 94 ->206 0.00103

 94 ->207 0.00134

 95 ->109 -0.00150

 95 ->116 0.00111

 95 ->117 0.00119

 95 ->129 -0.00121

 95 ->136 -0.00222

 95 ->142 -0.00337

 95 ->149 0.00210

 95 ->153 -0.00372

 95 ->159 -0.00117

 95 ->165 -0.00145

 95 ->175 0.00131

 95 ->179 -0.00101

 95 ->192 0.00145

 95 ->204 -0.00153

 95 ->217 -0.00115

 95 ->228 0.00133

 96 ->103 -0.05755

 96 ->104 -0.03487

 96 ->110 0.00351

 96 ->111 0.00345

 96 ->124 0.00221

 96 ->125 -0.00169

 96 ->132 0.00444

 96 ->158 -0.00384

 96 ->185 0.00119

 96 ->186 -0.00205

 97 ->109 0.00329

 97 ->117 0.00195

 97 ->121 -0.00125

 97 ->128 -0.00115

 97 ->129 0.00110

 97 ->137 -0.00240

 97 ->142 0.00150

 97 ->143 -0.00246

 97 ->145 -0.00385

 97 ->146 -0.00418

 97 ->149 0.00201

 97 ->154 0.00174

 97 ->159 0.00147

 97 ->160 -0.00328

 97 ->166 0.00121

 97 ->168 0.00124

 97 ->169 -0.00125

 97 ->175 -0.00119

 97 ->176 0.00340

 97 ->190 -0.00106

 97 ->192 0.00122

 97 ->208 -0.00113

 97 ->217 0.00202

 97 ->221 -0.00103

 97 ->222 -0.00150

 97 ->228 -0.00152

 98 ->103 0.17630

 98 ->104 0.15446

 98 ->110 -0.01216

 98 ->111 -0.00984

 98 ->125 -0.00266

 98 ->132 -0.00139

 98 ->308 0.00112

 99 ->106 -0.00543

 99 ->107 -0.00503

 99 ->113 -0.00454

 99 ->119 0.00372

 99 ->122 0.00393

 99 ->127 -0.00282

 99 ->133 -0.00143

 99 ->140 -0.00110

 99 ->156 0.00211

 99 ->161 0.00143

 99 ->196 0.00104

 99 ->199 0.00136

 100 ->105 0.00558

 100 ->106 -0.00494

 100 ->107 -0.01015

 100 ->113 0.00282

 100 ->119 -0.00150

 100 ->122 0.00530

 100 ->127 -0.00244

 100 ->133 -0.00369

 100 ->140 -0.00348

 100 ->156 0.00247

 100 ->161 0.00270

 100 ->178 0.00158

 100 ->183 -0.00139

 100 ->189 0.00153

 100 ->199 0.00106

 100 ->210 0.00155

 100 ->218 -0.00118

 100 ->304 0.00112

 101 ->103 0.01658

 101 ->104 0.02203

 101 ->110 -0.00966

 101 ->111 -0.00540

 101 ->124 -0.00191

 101 ->132 -0.00378

 101 ->158 0.00345

 101 ->185 -0.00149

 101 ->186 0.00175

 101 ->197 0.00109

 101 ->198 -0.00201

 101 ->300 0.00109

 102 ->103 -0.42023

 102 ->104 0.51666

 102 ->124 0.00136

 102 ->125 0.00251

 102 ->172 -0.00141

 102 ->185 -0.00349

 102 ->197 -0.00197

 102 ->198 0.00190

 102 ->223 0.00138

 102 ->224 -0.00148

 102 ->289 0.00117

 30 <-155 0.00110

 33 <-142 -0.00126

 34 <-155 -0.00153

 34 <-171 -0.00138

 35 <-134 -0.00135

 36 <-145 -0.00106

 36 <-154 -0.00101

 36 <-180 0.00108

 46 <-134 0.00112

 46 <-139 0.00140

 46 <-147 0.00119

 46 <-177 0.00116

 47 <-148 0.00118

 48 <-137 -0.00139

 48 <-142 0.00119

 48 <-143 0.00120

 48 <-145 -0.00144

 48 <-146 -0.00145

 48 <-154 -0.00124

 48 <-190 0.00117

 49 <-153 -0.00187

 49 <-160 0.00110

 49 <-180 0.00148

 50 <-149 0.00120

 50 <-153 -0.00111

 52 <-142 0.00130

 53 <-138 0.00265

 53 <-139 0.00182

 54 <-118 0.00112

 54 <-123 0.00119

 54 <-144 0.00147

 54 <-148 0.00117

 54 <-152 -0.00113

 54 <-171 -0.00106

 57 <-117 0.00120

 57 <-120 -0.00103

 57 <-142 -0.00287

 57 <-145 -0.00123

 58 <-153 0.00194

 59 <-134 -0.00176

 59 <-135 0.00188

 59 <-144 0.00217

 59 <-151 0.00139

 59 <-155 0.00102

 59 <-162 0.00151

 59 <-182 0.00108

 59 <-202 0.00156

 59 <-206 0.00104

 59 <-219 -0.00103

 60 <-135 0.00133

 60 <-139 -0.00211

 60 <-144 0.00192

 60 <-148 0.00127

 60 <-151 -0.00100

 60 <-155 0.00148

 60 <-170 -0.00102

 60 <-177 -0.00109

 60 <-195 -0.00163

 60 <-202 0.00244

 60 <-206 0.00113

 60 <-237 -0.00121

 61 <-142 0.00132

 61 <-143 -0.00128

 61 <-145 0.00251

 61 <-165 -0.00100

 62 <-112 0.00109

 62 <-118 0.00131

 62 <-123 0.00164

 62 <-134 0.00188

 62 <-155 -0.00221

 63 <-114 -0.00109

 63 <-123 -0.00147

 63 <-134 -0.00242

 63 <-135 -0.00208

 63 <-138 0.00125

 63 <-144 0.00103

 63 <-147 0.00101

 63 <-163 0.00107

 63 <-171 -0.00112

 64 <-108 0.00157

 64 <-129 -0.00128

 64 <-136 -0.00276

 64 <-143 -0.00143

 64 <-145 -0.00177

 64 <-146 0.00244

 64 <-149 -0.00120

 64 <-150 0.00130

 64 <-159 0.00130

 64 <-166 0.00123

 64 <-168 -0.00139

 64 <-169 -0.00103

 64 <-180 -0.00138

 64 <-191 0.00132

 64 <-204 0.00140

 64 <-227 0.00105

 64 <-240 -0.00100

 65 <-120 -0.00220

 65 <-136 -0.00219

 65 <-149 -0.00154

 65 <-154 -0.00181

 66 <-104 -0.00122

 66 <-110 -0.00164

 66 <-124 -0.00370

 66 <-125 0.00223

 66 <-131 0.00125

 66 <-132 -0.00168

 66 <-173 -0.00209

 67 <-105 0.00296

 67 <-106 -0.00189

 67 <-107 -0.00138

 67 <-113 -0.00107

 67 <-119 0.00224

 67 <-122 0.00108

 67 <-127 -0.00108

 67 <-181 -0.00110

 68 <-106 -0.00320

 68 <-107 -0.00355

 68 <-119 -0.00261

 68 <-122 0.00285

 68 <-133 -0.00136

 68 <-140 0.00103

 68 <-178 -0.00114

 68 <-183 0.00146

 69 <-120 0.00216

 69 <-129 -0.00191

 69 <-136 0.00149

 69 <-142 -0.00135

 70 <-112 -0.00117

 70 <-118 -0.00177

 70 <-123 -0.00119

 70 <-126 0.00158

 70 <-130 0.00221

 70 <-134 0.00103

 70 <-167 0.00112

 71 <-123 0.00132

 71 <-126 -0.00137

 71 <-135 0.00212

 71 <-155 0.00125

 72 <-109 -0.00137

 72 <-120 -0.00126

 72 <-129 0.00176

 72 <-137 0.00133

 72 <-142 -0.00129

 72 <-169 0.00117

 72 <-180 -0.00101

 73 <-103 0.00312

 73 <-110 -0.00249

 73 <-132 -0.00112

 73 <-158 -0.00120

 74 <-104 -0.00300

 74 <-111 0.00247

 74 <-125 -0.00251

 75 <-106 0.00220

 75 <-113 -0.00165

 75 <-119 -0.00239

 75 <-122 -0.00171

 76 <-105 0.00234

 76 <-106 0.00347

 76 <-107 0.00218

 76 <-113 -0.00183

 76 <-122 -0.00233

 76 <-127 -0.00128

 77 <-117 0.00209

 77 <-136 0.00216

 77 <-142 -0.00177

 77 <-145 -0.00142

 77 <-149 -0.00173

 77 <-175 0.00148

 78 <-120 0.00239

 78 <-142 -0.00105

 79 <-114 -0.00110

 79 <-115 -0.00204

 79 <-138 -0.00182

 79 <-141 -0.00247

 79 <-144 0.00221

 79 <-152 0.00106

 79 <-155 0.00115

 79 <-174 0.00105

 79 <-184 0.00138

 80 <-123 -0.00226

 80 <-138 -0.00264

 80 <-170 0.00103

 81 <-103 -0.00248

 81 <-104 0.00574

 81 <-110 -0.00304

 81 <-111 -0.00147

 81 <-124 -0.00230

 81 <-173 -0.00151

 82 <-117 -0.00139

 82 <-121 -0.00119

 82 <-129 -0.00102

 82 <-143 0.00292

 82 <-146 -0.00238

 82 <-149 0.00179

 82 <-150 -0.00147

 82 <-165 0.00103

 82 <-175 -0.00107

 82 <-193 0.00115

 83 <-114 -0.00234

 83 <-118 0.00188

 83 <-123 0.00157

 83 <-134 -0.00207

 83 <-147 0.00110

 83 <-152 0.00101

 83 <-155 0.00208

 83 <-167 -0.00111

 83 <-170 -0.00153

 83 <-184 0.00182

 84 <-112 0.00149

 84 <-118 -0.00218

 84 <-134 0.00231

 84 <-141 -0.00136

 84 <-147 -0.00256

 84 <-152 0.00131

 84 <-171 0.00103

 84 <-182 -0.00106

 85 <-103 0.00823

 85 <-104 -0.00463

 85 <-111 -0.00442

 85 <-124 0.00161

 85 <-125 0.00222

 85 <-131 -0.00141

 85 <-172 -0.00151

 86 <-120 -0.00206

 86 <-129 -0.00132

 86 <-149 0.00150

 86 <-154 0.00193

 86 <-166 0.00109

 86 <-169 0.00193

 86 <-180 -0.00105

 87 <-117 0.00154

 87 <-120 -0.00154

 87 <-121 0.00117

 87 <-129 -0.00113

 87 <-136 0.00109

 87 <-142 0.00282

 87 <-145 -0.00114

 87 <-146 0.00208

 87 <-149 -0.00114

 87 <-165 -0.00101

 87 <-176 0.00113

 88 <-112 0.00430

 88 <-114 0.00276

 88 <-126 0.00138

 88 <-134 0.00170

 88 <-138 -0.00158

 88 <-139 -0.00212

 88 <-151 0.00387

 88 <-155 0.00115

 88 <-188 -0.00123

 88 <-219 0.00113

 88 <-226 -0.00120

 89 <-114 -0.00124

 89 <-135 0.00173

 89 <-144 0.00205

 89 <-155 0.00173

 89 <-163 -0.00109

 89 <-177 -0.00118

 90 <-105 0.00153

 90 <-106 -0.00369

 90 <-107 0.00118

 90 <-113 0.00465

 90 <-133 -0.00186

 90 <-161 0.00103

 90 <-178 0.00146

 91 <-105 -0.00143

 91 <-106 -0.00165

 91 <-107 0.00161

 91 <-113 -0.00352

 91 <-119 -0.00137

 91 <-140 0.00114

 91 <-181 0.00150

 91 <-229 -0.00104

 92 <-137 0.00191

 92 <-143 0.00135

 92 <-146 0.00131

 92 <-150 -0.00133

 92 <-154 0.00229

 93 <-112 0.00267

 93 <-114 0.00173

 93 <-134 0.00113

 93 <-135 0.00208

 93 <-139 0.00468

 93 <-144 0.00198

 93 <-147 -0.00121

 93 <-151 0.00169

 93 <-174 -0.00196

 93 <-195 -0.00138

 94 <-135 0.00132

 94 <-139 -0.00228

 94 <-144 0.00165

 94 <-155 0.00112

 94 <-164 -0.00100

 94 <-170 -0.00146

 94 <-174 -0.00100

 94 <-177 -0.00173

 94 <-187 0.00185

 94 <-202 0.00103

 94 <-207 0.00107

 95 <-136 -0.00150

 95 <-142 -0.00225

 95 <-149 0.00146

 95 <-153 -0.00263

 95 <-165 -0.00112

 95 <-175 0.00102

 95 <-192 0.00116

 95 <-204 -0.00122

 95 <-228 0.00107

 96 <-103 -0.01719

 96 <-104 -0.01186

 96 <-110 0.00240

 96 <-111 0.00232

 96 <-124 0.00136

 96 <-125 -0.00106

 96 <-132 0.00291

 96 <-158 -0.00289

 96 <-186 -0.00145

 97 <-109 0.00168

 97 <-117 0.00107

 97 <-137 -0.00160

 97 <-142 0.00102

 97 <-143 -0.00156

 97 <-145 -0.00261

 97 <-146 -0.00279

 97 <-149 0.00136

 97 <-154 0.00121

 97 <-159 0.00107

 97 <-160 -0.00236

 97 <-176 0.00251

 97 <-217 0.00162

 97 <-222 -0.00121

 97 <-228 -0.00123

 98 <-103 0.03805

 98 <-104 0.03112

 98 <-110 -0.00755

 98 <-111 -0.00606

 98 <-125 -0.00172

 98 <-132 -0.00112

 98 <-308 0.00112

 99 <-105 -0.00317

 99 <-106 -0.00254

 99 <-107 -0.00248

 99 <-113 -0.00300

 99 <-119 0.00178

 99 <-122 0.00237

 99 <-127 -0.00185

 99 <-156 0.00155

 99 <-199 0.00124

 100 <-105 0.00133

 100 <-106 -0.00394

 100 <-107 -0.00505

 100 <-113 0.00206

 100 <-122 0.00287

 100 <-127 -0.00153

 100 <-133 -0.00232

 100 <-140 -0.00233

 100 <-156 0.00182

 100 <-161 0.00196

 100 <-178 0.00114

 100 <-183 -0.00102

 100 <-189 0.00112

 100 <-210 0.00129

 101 <-103 0.00164

 101 <-104 0.00423

 101 <-110 -0.00509

 101 <-111 -0.00362

 101 <-124 -0.00133

 101 <-132 -0.00230

 101 <-158 0.00249

 101 <-185 -0.00105

 101 <-186 0.00132

 101 <-198 -0.00160

 102 <-103 0.03556

 102 <-104 -0.04444

 102 <-110 0.00158

 102 <-111 -0.00145

 102 <-124 0.00130

 102 <-125 0.00197

 102 <-185 -0.00250

 102 <-197 -0.00186

 102 <-198 0.00127

 102 <-224 -0.00112

 102 <-289 0.00105

 This state for optimization and/or second-order correction.

 Total Energy, E(TD-HF/TD-KS) = -1275.80657853

 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State 2: Singlet-EU 2.3463 eV 528.43 nm f=0.3170 <S\*\*2>=0.000

 30 ->139 -0.00101

 31 ->155 -0.00126

 33 ->143 -0.00146

 34 ->134 -0.00161

 34 ->138 -0.00101

 34 ->182 0.00110

 35 ->155 -0.00179

 35 ->171 0.00147

 36 ->146 0.00120

 36 ->150 0.00105

 36 ->153 -0.00111

 36 ->179 0.00119

 41 ->190 0.00101

 41 ->240 -0.00107

 42 ->139 0.00107

 42 ->177 0.00101

 45 ->146 -0.00118

 46 ->144 0.00126

 46 ->148 -0.00148

 46 ->243 0.00105

 47 ->134 0.00131

 47 ->139 -0.00166

 47 ->147 -0.00142

 47 ->177 -0.00132

 48 ->136 0.00170

 48 ->142 -0.00143

 48 ->143 0.00145

 48 ->145 0.00177

 48 ->146 -0.00175

 48 ->153 0.00147

 48 ->191 0.00144

 49 ->150 0.00102

 49 ->154 -0.00221

 49 ->159 0.00136

 49 ->169 0.00110

 49 ->179 -0.00171

 50 ->121 0.00117

 50 ->150 0.00147

 50 ->154 -0.00135

 52 ->121 -0.00113

 52 ->143 -0.00163

 53 ->118 0.00149

 53 ->123 -0.00158

 53 ->144 0.00186

 53 ->148 -0.00146

 53 ->152 -0.00134

 53 ->155 -0.00102

 53 ->171 0.00127

 53 ->177 -0.00117

 53 ->184 -0.00106

 53 ->213 -0.00107

 54 ->138 0.00336

 54 ->139 -0.00232

 57 ->116 0.00164

 57 ->121 0.00139

 57 ->143 0.00364

 57 ->146 0.00157

 57 ->149 -0.00109

 58 ->145 -0.00119

 58 ->146 -0.00112

 58 ->150 -0.00104

 58 ->154 0.00239

 58 ->176 0.00117

 59 ->134 -0.00117

 59 ->135 0.00171

 59 ->139 -0.00260

 59 ->144 0.00251

 59 ->148 -0.00164

 59 ->151 0.00123

 59 ->155 0.00182

 59 ->170 0.00123

 59 ->174 -0.00119

 59 ->177 -0.00129

 59 ->195 0.00193

 59 ->202 -0.00289

 59 ->206 -0.00134

 59 ->237 0.00141

 60 ->130 -0.00119

 60 ->134 -0.00222

 60 ->135 -0.00236

 60 ->141 0.00112

 60 ->144 -0.00274

 60 ->148 0.00115

 60 ->151 0.00166

 60 ->155 -0.00122

 60 ->162 0.00184

 60 ->163 0.00111

 60 ->182 0.00125

 60 ->202 0.00186

 60 ->206 0.00122

 60 ->219 0.00120

 60 ->236 -0.00103

 60 ->242 -0.00107

 61 ->108 0.00106

 61 ->137 0.00114

 61 ->142 -0.00164

 61 ->143 -0.00169

 61 ->146 -0.00324

 61 ->166 0.00122

 62 ->114 0.00159

 62 ->118 -0.00123

 62 ->123 0.00201

 62 ->134 0.00314

 62 ->135 -0.00272

 62 ->138 -0.00169

 62 ->141 0.00121

 62 ->144 0.00134

 62 ->147 0.00131

 62 ->163 0.00134

 62 ->164 -0.00118

 62 ->171 0.00131

 63 ->112 0.00159

 63 ->118 -0.00182

 63 ->123 0.00223

 63 ->134 0.00243

 63 ->155 0.00273

 63 ->170 0.00109

 64 ->109 -0.00215

 64 ->128 0.00172

 64 ->137 0.00354

 64 ->142 -0.00180

 64 ->145 0.00307

 64 ->146 0.00224

 64 ->149 0.00160

 64 ->150 0.00153

 64 ->160 0.00159

 64 ->165 0.00153

 64 ->168 -0.00127

 64 ->169 0.00171

 64 ->175 0.00120

 64 ->179 -0.00169

 64 ->190 0.00158

 64 ->201 0.00112

 64 ->205 0.00166

 64 ->209 -0.00110

 64 ->221 0.00107

 64 ->228 0.00123

 64 ->241 -0.00118

 65 ->116 -0.00109

 65 ->121 -0.00308

 65 ->128 0.00129

 65 ->136 0.00112

 65 ->137 -0.00288

 65 ->142 -0.00101

 65 ->150 -0.00198

 65 ->153 0.00229

 65 ->168 0.00108

 66 ->103 -0.00243

 66 ->111 -0.00241

 66 ->124 -0.00277

 66 ->125 -0.00465

 66 ->131 0.00216

 66 ->132 0.00151

 66 ->172 0.00250

 67 ->106 -0.00460

 67 ->107 0.00506

 67 ->119 -0.00375

 67 ->122 -0.00319

 67 ->133 0.00153

 67 ->178 -0.00129

 67 ->183 -0.00177

 68 ->105 -0.00517

 68 ->106 0.00249

 68 ->107 -0.00192

 68 ->119 -0.00329

 68 ->122 0.00112

 68 ->127 0.00144

 68 ->181 0.00122

 69 ->121 -0.00309

 69 ->128 0.00269

 69 ->137 -0.00201

 69 ->143 0.00179

 70 ->123 0.00191

 70 ->126 -0.00195

 70 ->135 -0.00282

 70 ->155 -0.00157

 71 ->112 0.00174

 71 ->118 -0.00256

 71 ->123 0.00176

 71 ->126 -0.00224

 71 ->130 0.00312

 71 ->134 -0.00133

 71 ->141 0.00106

 71 ->164 -0.00114

 71 ->167 -0.00141

 72 ->108 0.00204

 72 ->120 0.00116

 72 ->121 -0.00184

 72 ->128 0.00251

 72 ->129 -0.00116

 72 ->136 -0.00175

 72 ->143 -0.00171

 72 ->153 -0.00102

 72 ->168 -0.00147

 72 ->179 0.00127

 73 ->104 0.00672

 73 ->111 0.00276

 73 ->124 -0.00162

 73 ->131 -0.00130

 73 ->157 -0.00162

 73 ->172 -0.00125

 74 ->103 -0.00304

 74 ->110 -0.00413

 74 ->124 0.00354

 74 ->125 0.00116

 74 ->132 -0.00111

 74 ->172 -0.00101

 75 ->105 0.00347

 75 ->106 0.00500

 75 ->107 -0.00327

 75 ->113 0.00240

 75 ->122 0.00298

 75 ->127 -0.00191

 76 ->106 -0.00386

 76 ->107 0.00129

 76 ->113 -0.00311

 76 ->119 0.00364

 76 ->122 -0.00222

 77 ->108 0.00153

 77 ->116 -0.00315

 77 ->117 -0.00137

 77 ->137 0.00299

 77 ->143 -0.00247

 77 ->146 -0.00194

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 83 ->152 -0.00112

 83 ->188 0.00121

 83 ->225 0.00133

 84 ->112 -0.00102

 84 ->139 0.00135

 84 ->144 -0.00157

 84 ->148 -0.00125

 84 ->152 0.00146

 84 ->182 -0.00137

 84 ->184 0.00118

 84 ->187 -0.00101

 84 ->219 -0.00117

 84 ->231 -0.00108

 85 ->103 -0.00582

 85 ->104 0.00845

 85 ->110 0.00124

 85 ->125 -0.00270

 86 ->142 -0.00122

 86 ->145 -0.00165

 86 ->153 0.00128

 86 ->159 -0.00103

 86 ->160 -0.00158

 86 ->179 -0.00164

 86 ->180 0.00110

 86 ->190 -0.00127

 87 ->143 0.00153

 87 ->145 -0.00108

 87 ->160 -0.00137

 87 ->175 0.00100

 88 ->138 0.00109

 88 ->148 0.00118

 88 ->152 -0.00174

 88 ->155 -0.00168

 88 ->170 -0.00114

 88 ->177 0.00139

 88 ->187 0.00128

 88 ->214 -0.00139

 89 ->138 0.00162

 89 ->163 -0.00106

 89 ->187 -0.00106

 89 ->220 0.00108

 89 ->226 0.00139

 90 ->106 -0.00328

 90 ->113 -0.00296

 90 ->119 -0.00358

 90 ->122 -0.00206

 90 ->140 -0.00153

 91 ->105 0.00732

 91 ->106 0.00171

 91 ->113 -0.00167

 91 ->119 -0.00226

 91 ->122 0.00190

 91 ->127 0.00132

 91 ->140 0.00109

 91 ->178 0.00106

 92 ->120 0.00148

 92 ->150 0.00117

 92 ->165 -0.00120

 92 ->190 0.00131

 92 ->192 0.00146

 93 ->118 0.00121

 93 ->123 0.00115

 93 ->135 -0.00124

 93 ->148 0.00199

 93 ->155 -0.00134

 93 ->170 -0.00106

 93 ->171 -0.00102

 93 ->187 0.00201

 93 ->194 -0.00101

 94 ->112 0.00126

 94 ->135 0.00165

 94 ->139 0.00164

 94 ->147 -0.00115

 94 ->162 -0.00196

 94 ->164 0.00131

 94 ->174 -0.00154

 94 ->195 -0.00113

 94 ->219 0.00111

 95 ->109 0.00148

 95 ->136 0.00108

 95 ->150 -0.00149

 95 ->154 0.00246

 95 ->166 0.00146

 96 ->103 0.07342

 96 ->104 -0.10507

 96 ->110 0.00615

 96 ->111 -0.01066

 96 ->124 0.00599

 96 ->125 0.00422

 96 ->132 -0.00304

 96 ->172 -0.00137

 96 ->185 0.00152

 96 ->197 0.00124

 96 ->223 0.00120

 97 ->142 0.00190

 97 ->143 -0.00126

 97 ->146 0.00139

 97 ->153 -0.00152

 97 ->160 0.00142

 97 ->168 -0.00108

 97 ->216 0.00157

 97 ->240 -0.00102

 98 ->103 0.10734

 98 ->104 -0.10094

 98 ->110 0.00203

 98 ->111 -0.00321

 98 ->124 -0.00169

 98 ->125 -0.00313

 98 ->131 0.00119

 98 ->172 -0.00124

 98 ->185 -0.00110

 99 ->105 -0.02583

 99 ->107 -0.00257

 99 ->113 -0.00650

 99 ->119 -0.00788

 99 ->122 0.00619

 99 ->127 0.00214

 99 ->140 0.00102

 99 ->161 0.00156

 99 ->178 -0.00117

 99 ->183 -0.00110

 99 ->196 0.00105

 100 ->105 -0.04669

 100 ->113 -0.00994

 100 ->119 -0.01491

 100 ->127 0.00195

 100 ->133 0.00350

 100 ->156 0.00129

 100 ->181 0.00129

 100 ->196 0.00190

 101 ->103 -0.44532

 101 ->104 0.50484

 101 ->110 -0.00741

 101 ->111 0.00989

 101 ->124 -0.00994

 101 ->125 -0.00990

 101 ->131 0.00264

 101 ->132 0.00463

 101 ->157 -0.00143

 101 ->186 0.00112

 101 ->197 -0.00144

 102 ->103 -0.04681

 102 ->104 -0.05066

 102 ->110 0.00535

 102 ->125 0.00193

 102 ->131 0.00194

 102 ->132 -0.00224

 102 ->158 0.00112

 102 ->198 -0.00112

 102 ->282 0.00118

 40 <-136 0.00106

 48 <-160 -0.00109

 53 <-148 0.00139

 54 <-138 -0.00175

 54 <-147 -0.00128

 57 <-143 -0.00161

 59 <-155 -0.00103

 61 <-136 0.00144

 61 <-143 0.00109

 63 <-135 0.00110

 63 <-138 -0.00102

 63 <-187 0.00141

 64 <-137 -0.00104

 64 <-145 -0.00128

 66 <-103 -0.00259

 66 <-104 0.00336

 66 <-111 -0.00105

 66 <-125 0.00106

 67 <-105 -0.00212

 67 <-106 0.00124

 67 <-113 0.00117

 68 <-105 -0.00299

 68 <-113 0.00289

 69 <-117 -0.00106

 69 <-129 0.00106

 69 <-160 0.00123

 70 <-118 -0.00112

 70 <-123 -0.00150

 70 <-130 -0.00101

 70 <-148 -0.00105

 70 <-177 -0.00117

 70 <-187 -0.00111

 71 <-126 0.00108

 72 <-117 0.00118

 72 <-120 -0.00138

 72 <-160 -0.00103

 73 <-103 -0.00143

 73 <-104 0.00140

 73 <-110 0.00121

 73 <-111 -0.00316

 74 <-103 0.00127

 74 <-110 0.00148

 74 <-111 -0.00133

 75 <-105 -0.00104

 75 <-106 -0.00170

 75 <-119 0.00120

 78 <-168 0.00106

 81 <-110 0.00205

 81 <-111 -0.00173

 82 <-192 -0.00103

 83 <-225 0.00106

 84 <-144 -0.00100

 84 <-152 0.00101

 84 <-182 -0.00110

 85 <-111 -0.00100

 85 <-125 -0.00163

 86 <-145 -0.00103

 86 <-160 -0.00111

 86 <-179 -0.00130

 88 <-152 -0.00111

 88 <-155 -0.00109

 88 <-214 -0.00104

 89 <-226 0.00109

 90 <-105 0.00204

 90 <-106 -0.00108

 90 <-113 -0.00142

 90 <-119 -0.00220

 90 <-122 -0.00160

 91 <-105 0.00302

 91 <-119 -0.00197

 91 <-122 0.00134

 92 <-192 0.00108

 93 <-148 0.00119

 93 <-187 0.00145

 94 <-139 0.00105

 94 <-162 -0.00133

 94 <-174 -0.00107

 95 <-154 0.00157

 96 <-103 -0.00377

 96 <-104 0.00188

 96 <-110 0.00476

 96 <-111 -0.00783

 96 <-124 0.00144

 96 <-132 -0.00179

 96 <-185 0.00168

 96 <-197 0.00166

 96 <-223 0.00106

 97 <-142 0.00106

 97 <-216 0.00116

 98 <-103 -0.00479

 98 <-104 0.00545

 98 <-110 0.00124

 98 <-111 -0.00174

 98 <-124 -0.00148

 98 <-125 -0.00246

 99 <-105 0.00531

 99 <-106 0.00415

 99 <-107 -0.00130

 99 <-113 -0.00401

 99 <-119 -0.00182

 99 <-122 0.00373

 99 <-127 0.00161

 99 <-161 0.00100

 99 <-189 0.00117

 100 <-105 0.00953

 100 <-106 -0.00235

 100 <-113 -0.00679

 100 <-119 -0.00363

 100 <-133 0.00247

 100 <-189 0.00125

 100 <-196 0.00172

 100 <-199 -0.00127

 101 <-103 0.01033

 101 <-104 -0.01113

 101 <-110 -0.00251

 101 <-111 0.00324

 101 <-124 -0.00343

 101 <-125 -0.00340

 101 <-131 0.00143

 101 <-132 0.00236

 101 <-197 -0.00198

 102 <-103 0.01230

 102 <-104 0.01543

 102 <-110 0.00345

 102 <-131 0.00131

 102 <-235 0.00103

 102 <-282 0.00109

 Excited State 4: Singlet-EU 3.1166 eV 397.82 nm f=0.0239 <S\*\*2>=0.000

 37 ->137 0.00104

 38 ->141 0.00108

 39 ->144 0.00106

 40 ->137 -0.00127

 40 ->180 -0.00109

 47 ->148 -0.00105

 48 ->128 0.00107

 48 ->159 0.00139

 48 ->169 0.00117

 49 ->142 -0.00116

 49 ->192 0.00119

 50 ->146 0.00105

 51 ->146 -0.00118

 53 ->112 0.00104

 53 ->123 0.00115

 53 ->135 -0.00126

 53 ->138 -0.00260

 53 ->147 0.00186

 53 ->152 -0.00137

 53 ->174 0.00106

 54 ->118 -0.00133

 54 ->130 0.00124

 54 ->148 -0.00188

 56 ->105 -0.00106

 57 ->121 -0.00103

 57 ->142 0.00223

 57 ->145 0.00102

 57 ->146 0.00131

 59 ->134 0.00124

 59 ->152 0.00122

 60 ->139 0.00121

 60 ->152 0.00114

 60 ->155 -0.00129

 61 ->137 0.00199

 61 ->142 -0.00149

 61 ->154 -0.00123

 61 ->192 0.00124

 61 ->193 0.00117

 62 ->114 0.00148

 62 ->126 0.00119

 62 ->135 -0.00155

 62 ->138 -0.00156

 62 ->141 0.00127

 62 ->148 0.00102

 62 ->152 0.00132

 62 ->155 0.00121

 62 ->187 0.00183

 62 ->194 0.00104

 63 ->112 -0.00123

 63 ->118 0.00117

 63 ->134 0.00106

 63 ->138 0.00124

 63 ->144 -0.00104

 64 ->136 0.00140

 64 ->143 0.00121

 64 ->145 0.00114

 64 ->146 -0.00180

 65 ->120 0.00118

 65 ->128 -0.00110

 65 ->142 -0.00105

 65 ->143 -0.00126

 65 ->159 -0.00114

 66 ->103 -0.00786

 66 ->104 -0.00624

 66 ->111 -0.00101

 66 ->124 0.00139

 66 ->125 -0.00110

 67 ->105 0.00522

 67 ->106 0.00125

 67 ->113 0.00364

 68 ->105 -0.00354

 68 ->106 0.00200

 68 ->113 -0.00145

 68 ->119 0.00127

 69 ->116 0.00178

 69 ->121 0.00134

 69 ->128 0.00161

 69 ->129 0.00117

 69 ->150 0.00107

 69 ->154 -0.00102

 69 ->159 0.00169

 69 ->191 0.00124

 70 ->118 0.00141

 70 ->126 -0.00170

 70 ->148 -0.00130

 71 ->114 0.00139

 71 ->115 -0.00161

 71 ->118 0.00186

 71 ->123 -0.00246

 71 ->126 -0.00104

 71 ->130 0.00155

 71 ->144 0.00100

 71 ->148 -0.00148

 71 ->174 0.00109

 71 ->177 0.00158

 71 ->187 -0.00144

 71 ->220 -0.00101

 71 ->225 0.00120

 71 ->231 0.00107

 72 ->116 0.00199

 72 ->121 0.00229

 72 ->128 0.00133

 72 ->143 0.00120

 72 ->159 0.00143

 72 ->180 0.00117

 72 ->191 0.00113

 73 ->103 0.00357

 73 ->104 0.00347

 73 ->110 0.00439

 73 ->111 0.00145

 73 ->125 0.00129

 74 ->103 0.00389

 74 ->104 0.00642

 74 ->110 -0.00206

 74 ->111 -0.00256

 74 ->124 0.00126

 74 ->131 0.00135

 75 ->105 -0.00428

 75 ->113 0.00208

 75 ->119 -0.00145

 75 ->122 0.00102

 75 ->133 0.00136

 76 ->106 -0.00214

 76 ->119 0.00258

 76 ->127 0.00147

 77 ->128 -0.00121

 77 ->136 -0.00117

 77 ->150 -0.00131

 77 ->232 0.00116

 78 ->120 -0.00106

 78 ->149 0.00106

 78 ->169 0.00139

 79 ->130 0.00129

 79 ->141 0.00144

 80 ->123 0.00153

 80 ->138 0.00103

 80 ->148 -0.00133

 80 ->164 0.00103

 80 ->194 -0.00121

 81 ->103 0.01006

 81 ->104 0.00856

 81 ->110 0.00139

 81 ->111 0.00241

 81 ->124 0.00103

 81 ->125 -0.00164

 82 ->121 0.00143

 82 ->129 0.00104

 82 ->136 0.00122

 82 ->142 0.00109

 82 ->143 -0.00115

 82 ->160 0.00135

 82 ->168 -0.00100

 82 ->193 -0.00138

 82 ->204 -0.00109

 82 ->221 -0.00106

 83 ->112 -0.00102

 83 ->139 -0.00135

 83 ->144 0.00157

 83 ->148 -0.00125

 83 ->152 -0.00146

 83 ->182 -0.00137

 83 ->184 -0.00118

 83 ->187 -0.00101

 83 ->219 0.00117

 83 ->231 0.00108

 84 ->114 0.00138

 84 ->118 0.00117

 84 ->126 0.00114

 84 ->138 -0.00100

 84 ->147 0.00101

 84 ->148 -0.00121

 84 ->152 -0.00112

 84 ->188 -0.00121

 84 ->225 0.00133

 85 ->103 0.00845

 85 ->104 0.00582

 85 ->111 0.00124

 85 ->124 0.00270

 86 ->143 0.00122

 86 ->146 0.00165

 86 ->154 -0.00128

 86 ->159 0.00158

 86 ->160 -0.00103

 86 ->179 0.00110

 86 ->180 0.00164

 86 ->191 0.00127

 87 ->142 -0.00153

 87 ->146 -0.00108

 87 ->159 -0.00137

 87 ->176 -0.00100

 88 ->138 0.00162

 88 ->163 0.00106

 88 ->187 -0.00106

 88 ->220 0.00108

 88 ->226 0.00139

 89 ->138 -0.00109

 89 ->148 -0.00118

 89 ->152 -0.00174

 89 ->155 -0.00168

 89 ->170 0.00114

 89 ->177 0.00139

 89 ->187 -0.00128

 89 ->214 0.00139

 90 ->105 -0.00732

 90 ->106 -0.00171

 90 ->113 -0.00167

 90 ->119 0.00226

 90 ->122 0.00190

 90 ->127 -0.00132

 90 ->140 0.00109

 90 ->178 -0.00106

 91 ->106 -0.00328

 91 ->113 0.00296

 91 ->119 -0.00358

 91 ->122 0.00206

 91 ->140 0.00153

 92 ->121 0.00148

 92 ->149 -0.00117

 92 ->166 -0.00120

 92 ->191 0.00131

 92 ->193 0.00146

 93 ->112 0.00126

 93 ->135 -0.00165

 93 ->139 -0.00164

 93 ->147 0.00115

 93 ->162 -0.00196

 93 ->164 -0.00131

 93 ->174 0.00154

 93 ->195 -0.00113

 93 ->219 -0.00111

 94 ->118 0.00121

 94 ->123 -0.00115

 94 ->135 -0.00124

 94 ->148 -0.00199

 94 ->155 -0.00134

 94 ->170 0.00106

 94 ->171 0.00102

 94 ->187 -0.00201

 94 ->194 -0.00101

 95 ->108 0.00148

 95 ->137 -0.00108

 95 ->149 -0.00149

 95 ->153 0.00246

 95 ->165 0.00146

 96 ->103 0.10507

 96 ->104 0.07342

 96 ->110 -0.01066

 96 ->111 -0.00615

 96 ->124 0.00422

 96 ->125 -0.00599

 96 ->131 -0.00304

 96 ->173 0.00137

 96 ->186 0.00152

 96 ->198 0.00124

 96 ->224 0.00120

 97 ->142 -0.00126

 97 ->143 -0.00190

 97 ->145 0.00139

 97 ->154 0.00152

 97 ->159 -0.00142

 97 ->169 0.00108

 97 ->217 -0.00157

 97 ->241 -0.00102

 98 ->103 0.10094

 98 ->104 0.10734

 98 ->110 -0.00321

 98 ->111 -0.00203

 98 ->124 -0.00313

 98 ->125 0.00169

 98 ->132 -0.00119

 98 ->173 0.00124

 98 ->186 -0.00110

 99 ->105 0.04669

 99 ->113 -0.00994

 99 ->119 0.01491

 99 ->127 -0.00195

 99 ->133 0.00350

 99 ->156 -0.00129

 99 ->181 -0.00129

 99 ->196 -0.00190

 100 ->105 -0.02583

 100 ->107 0.00257

 100 ->113 0.00650

 100 ->119 -0.00788

 100 ->122 -0.00619

 100 ->127 0.00214

 100 ->140 -0.00102

 100 ->161 -0.00156

 100 ->178 -0.00117

 100 ->183 0.00110

 100 ->196 0.00105

 101 ->103 0.50484

 101 ->104 0.44532

 101 ->110 -0.00989

 101 ->111 -0.00741

 101 ->124 0.00990

 101 ->125 -0.00994

 101 ->131 -0.00463

 101 ->132 0.00264

 101 ->158 -0.00143

 101 ->185 0.00112

 101 ->198 0.00144

 102 ->103 0.05066

 102 ->104 -0.04681

 102 ->111 -0.00535

 102 ->124 0.00193

 102 ->131 -0.00224

 102 ->132 -0.00194

 102 ->157 0.00112

 102 ->197 0.00112

 102 ->281 -0.00118

 40 <-137 -0.00106

 48 <-159 0.00109

 53 <-138 -0.00175

 53 <-147 0.00128

 54 <-148 -0.00139

 57 <-142 0.00161

 60 <-155 -0.00103

 61 <-137 0.00144

 61 <-142 -0.00109

 62 <-135 -0.00110

 62 <-138 -0.00102

 62 <-187 0.00141

 64 <-136 0.00104

 64 <-146 -0.00128

 66 <-103 -0.00336

 66 <-104 -0.00259

 66 <-110 -0.00105

 66 <-124 0.00106

 67 <-105 0.00299

 67 <-113 0.00289

 68 <-105 -0.00212

 68 <-106 0.00124

 68 <-113 -0.00117

 69 <-116 0.00106

 69 <-128 0.00106

 69 <-159 0.00123

 70 <-126 -0.00108

 71 <-118 0.00112

 71 <-123 -0.00150

 71 <-130 0.00101

 71 <-148 -0.00105

 71 <-177 0.00117

 71 <-187 -0.00111

 72 <-116 0.00118

 72 <-121 0.00138

 72 <-159 0.00103

 73 <-103 0.00140

 73 <-104 0.00143

 73 <-110 0.00316

 73 <-111 0.00121

 74 <-104 0.00127

 74 <-110 -0.00133

 74 <-111 -0.00148

 76 <-105 -0.00104

 76 <-106 -0.00170

 76 <-119 0.00120

 78 <-169 0.00106

 81 <-110 0.00173

 81 <-111 0.00205

 82 <-193 -0.00103

 83 <-144 0.00100

 83 <-152 -0.00101

 83 <-182 -0.00110

 84 <-225 0.00106

 85 <-110 0.00100

 85 <-124 0.00163

 86 <-146 0.00103

 86 <-159 0.00111

 86 <-180 0.00130

 88 <-226 0.00109

 89 <-152 -0.00111

 89 <-155 -0.00109

 89 <-214 0.00104

 90 <-105 -0.00302

 90 <-119 0.00197

 90 <-122 0.00134

 91 <-105 0.00204

 91 <-106 -0.00108

 91 <-113 0.00142

 91 <-119 -0.00220

 91 <-122 0.00160

 92 <-193 0.00108

 93 <-139 -0.00105

 93 <-162 -0.00133

 93 <-174 0.00107

 94 <-148 -0.00119

 94 <-187 -0.00145

 95 <-153 0.00157

 96 <-103 -0.00188

 96 <-104 -0.00377

 96 <-110 -0.00783

 96 <-111 -0.00476

 96 <-125 -0.00144

 96 <-131 -0.00179

 96 <-186 0.00168

 96 <-198 0.00166

 96 <-224 0.00106

 97 <-143 -0.00106

 97 <-217 -0.00116

 98 <-103 -0.00545

 98 <-104 -0.00479

 98 <-110 -0.00174

 98 <-111 -0.00124

 98 <-124 -0.00246

 98 <-125 0.00148

 99 <-105 -0.00953

 99 <-106 0.00235

 99 <-113 -0.00679

 99 <-119 0.00363

 99 <-133 0.00247

 99 <-189 0.00125

 99 <-196 -0.00172

 99 <-199 -0.00127

 100 <-105 0.00531

 100 <-106 0.00415

 100 <-107 0.00130

 100 <-113 0.00401

 100 <-119 -0.00182

 100 <-122 -0.00373

 100 <-127 0.00161

 100 <-161 -0.00100

 100 <-189 -0.00117

 101 <-103 -0.01113

 101 <-104 -0.01033

 101 <-110 -0.00324

 101 <-111 -0.00251

 101 <-124 0.00340

 101 <-125 -0.00343

 101 <-131 -0.00236

 101 <-132 0.00143

 101 <-198 0.00198

 102 <-103 -0.01543

 102 <-104 0.01230

 102 <-111 -0.00345

 102 <-132 -0.00131

 102 <-234 0.00103

 102 <-281 -0.00109

 Excited state symmetry could not be determined.

 Excited State 5: Singlet-?Sym 3.1280 eV 396.37 nm f=0.0000 <S\*\*2>=0.000

 37 ->141 0.00132

 37 ->171 0.00130

 37 ->182 0.00139

 40 ->135 0.00125

 40 ->144 -0.00110

 40 ->155 0.00127

 44 ->115 -0.00105

 44 ->155 -0.00111

 48 ->130 -0.00132

 48 ->139 0.00133

 48 ->155 -0.00185

 49 ->135 -0.00116

 50 ->118 0.00111

 51 ->135 -0.00118

 51 ->147 0.00104

 51 ->174 0.00105

 52 ->138 -0.00103

 53 ->108 -0.00107

 53 ->121 0.00166

 53 ->129 0.00106

 53 ->142 -0.00145

 53 ->146 -0.00174

 54 ->109 0.00107

 54 ->120 0.00166

 54 ->128 -0.00106

 54 ->143 0.00145

 54 ->145 -0.00174

 57 ->112 -0.00164

 57 ->123 -0.00115

 57 ->126 0.00101

 57 ->138 0.00233

 61 ->114 0.00120

 61 ->138 -0.00133

 61 ->141 0.00178

 61 ->148 0.00160

 61 ->187 0.00194

 61 ->195 -0.00115

 62 ->137 0.00146

 62 ->143 0.00181

 63 ->136 0.00146

 63 ->142 0.00181

 64 ->134 -0.00138

 64 ->138 -0.00197

 64 ->182 0.00101

 65 ->115 0.00116

 65 ->130 0.00122

 65 ->152 -0.00215

 65 ->155 -0.00143

 65 ->174 -0.00105

 65 ->236 0.00155

 66 ->113 0.00288

 67 ->103 -0.01089

 67 ->104 -0.00178

 67 ->110 -0.00130

 67 ->111 -0.00243

 68 ->103 -0.00178

 68 ->104 0.01089

 68 ->110 0.00243

 68 ->111 -0.00130

 69 ->114 -0.00172

 69 ->123 0.00238

 69 ->126 0.00206

 69 ->148 0.00278

 69 ->171 0.00144

 69 ->182 0.00128

 69 ->187 0.00165

 69 ->220 0.00111

 69 ->230 -0.00118

 69 ->256 -0.00130

 69 ->258 0.00123

 70 ->116 -0.00164

 70 ->117 0.00191

 70 ->120 -0.00220

 70 ->129 -0.00163

 70 ->142 -0.00109

 70 ->153 0.00106

 70 ->159 -0.00106

 70 ->160 -0.00138

 70 ->179 -0.00135

 70 ->190 -0.00137

 70 ->228 0.00101

 70 ->233 0.00113

 70 ->241 -0.00105

 71 ->116 -0.00191

 71 ->117 -0.00164

 71 ->121 -0.00220

 71 ->128 -0.00163

 71 ->143 -0.00109

 71 ->154 0.00106

 71 ->159 -0.00138

 71 ->160 0.00106

 71 ->180 -0.00135

 71 ->191 -0.00137

 71 ->227 0.00101

 71 ->232 0.00113

 71 ->240 -0.00105

 72 ->115 0.00175

 72 ->118 -0.00325

 72 ->130 -0.00166

 72 ->135 -0.00115

 72 ->147 0.00103

 72 ->174 -0.00123

 72 ->177 -0.00155

 72 ->194 0.00114

 72 ->225 -0.00166

 72 ->231 -0.00106

 73 ->105 -0.00708

 73 ->119 0.00253

 74 ->113 0.00300

 74 ->133 0.00123

 75 ->103 0.01025

 75 ->104 0.00313

 75 ->111 -0.00216

 75 ->124 0.00188

 76 ->103 0.00313

 76 ->104 -0.01025

 76 ->110 0.00216

 76 ->125 0.00188

 77 ->130 0.00154

 77 ->164 0.00120

 77 ->174 -0.00105

 77 ->177 0.00104

 77 ->194 -0.00115

 77 ->231 0.00120

 78 ->148 0.00132

 78 ->171 0.00128

 78 ->182 0.00168

 78 ->230 -0.00117

 79 ->168 -0.00105

 79 ->205 -0.00106

 80 ->169 -0.00105

 80 ->204 -0.00106

 81 ->105 -0.00897

 81 ->127 -0.00109

 82 ->114 -0.00149

 82 ->123 0.00117

 82 ->134 -0.00104

 82 ->148 -0.00207

 82 ->187 -0.00174

 82 ->188 0.00108

 82 ->195 0.00126

 83 ->146 -0.00151

 83 ->159 -0.00110

 83 ->160 0.00147

 83 ->180 -0.00166

 83 ->192 -0.00106

 84 ->145 -0.00151

 84 ->159 -0.00147

 84 ->160 -0.00110

 84 ->179 -0.00166

 84 ->193 0.00106

 85 ->105 -0.00736

 85 ->119 -0.00228

 85 ->127 -0.00133

 86 ->135 -0.00122

 86 ->139 0.00160

 86 ->144 -0.00230

 86 ->152 0.00182

 86 ->155 -0.00108

 86 ->177 -0.00180

 86 ->184 0.00154

 86 ->194 0.00159

 86 ->219 -0.00113

 86 ->225 -0.00120

 86 ->231 -0.00163

 86 ->261 0.00102

 87 ->112 0.00132

 87 ->148 -0.00177

 87 ->188 -0.00153

 88 ->160 0.00172

 89 ->159 -0.00172

 90 ->103 0.02639

 90 ->104 0.00757

 90 ->111 0.00303

 90 ->125 -0.00133

 90 ->131 0.00110

 91 ->103 0.00757

 91 ->104 -0.02639

 91 ->110 -0.00303

 91 ->124 0.00133

 91 ->132 0.00110

 92 ->123 0.00101

 92 ->148 0.00156

 92 ->162 0.00135

 92 ->170 -0.00108

 92 ->187 0.00223

 93 ->149 0.00108

 93 ->153 -0.00170

 93 ->165 -0.00122

 93 ->192 0.00150

 94 ->150 -0.00108

 94 ->154 0.00170

 94 ->166 0.00122

 94 ->193 -0.00150

 95 ->115 -0.00109

 95 ->135 0.00157

 95 ->139 0.00104

 95 ->164 0.00128

 95 ->174 -0.00155

 96 ->107 0.00155

 96 ->113 0.01578

 96 ->122 -0.00207

 96 ->133 -0.00316

 96 ->189 -0.00166

 96 ->238 -0.00106

 97 ->144 0.00166

 97 ->152 -0.00197

 97 ->155 -0.00161

 97 ->177 0.00148

 97 ->236 0.00102

 98 ->122 -0.00192

 99 ->103 -0.47633

 99 ->104 -0.14008

 99 ->110 0.00810

 99 ->111 0.01540

 99 ->124 -0.01120

 99 ->125 0.00433

 99 ->131 0.00456

 99 ->132 0.00137

 99 ->185 -0.00114

 99 ->198 -0.00136

 99 ->223 -0.00124

 100 ->103 -0.14008

 100 ->104 0.47633

 100 ->110 -0.01540

 100 ->111 0.00810

 100 ->124 -0.00433

 100 ->125 -0.01120

 100 ->131 -0.00137

 100 ->132 0.00456

 100 ->186 0.00114

 100 ->197 -0.00136

 100 ->224 0.00124

 101 ->105 -0.06025

 101 ->106 0.00115

 101 ->119 -0.02242

 101 ->127 0.00377

 101 ->156 0.00131

 101 ->181 0.00104

 101 ->196 0.00263

 101 ->210 -0.00132

 102 ->113 0.00427

 102 ->122 -0.00103

 102 ->133 -0.00163

 102 ->140 -0.00147

 102 ->199 0.00113

 102 ->262 0.00112

 102 ->292 -0.00119

 37 <-141 0.00108

 37 <-182 0.00115

 40 <-155 0.00108

 48 <-155 -0.00152

 53 <-121 0.00114

 53 <-142 -0.00104

 53 <-146 -0.00113

 54 <-120 0.00114

 54 <-143 0.00104

 54 <-145 -0.00113

 57 <-112 -0.00102

 57 <-138 0.00156

 61 <-141 0.00130

 61 <-148 0.00114

 61 <-187 0.00152

 62 <-137 0.00105

 62 <-143 0.00117

 63 <-136 0.00105

 63 <-142 0.00117

 64 <-138 -0.00128

 65 <-152 -0.00148

 65 <-236 0.00119

 66 <-113 0.00236

 67 <-103 -0.00358

 67 <-110 -0.00115

 67 <-111 -0.00221

 68 <-104 0.00358

 68 <-110 0.00221

 68 <-111 -0.00115

 69 <-123 0.00145

 69 <-126 0.00135

 69 <-148 0.00193

 69 <-171 0.00113

 69 <-182 0.00110

 69 <-187 0.00128

 69 <-256 -0.00106

 69 <-258 0.00103

 70 <-117 0.00113

 70 <-120 -0.00133

 70 <-129 -0.00108

 70 <-160 -0.00100

 70 <-179 -0.00107

 70 <-190 -0.00109

 71 <-116 -0.00113

 71 <-121 -0.00133

 71 <-128 -0.00108

 71 <-159 -0.00100

 71 <-180 -0.00107

 71 <-191 -0.00109

 72 <-115 0.00101

 72 <-118 -0.00194

 72 <-130 -0.00110

 72 <-177 -0.00115

 72 <-225 -0.00134

 73 <-105 -0.00449

 73 <-119 0.00172

 74 <-113 0.00167

 75 <-111 -0.00102

 76 <-110 0.00102

 78 <-182 0.00132

 81 <-105 -0.00244

 82 <-148 -0.00136

 82 <-187 -0.00128

 83 <-146 -0.00105

 83 <-180 -0.00126

 84 <-145 -0.00105

 84 <-179 -0.00126

 85 <-105 -0.00182

 86 <-139 0.00107

 86 <-144 -0.00141

 86 <-152 0.00121

 86 <-177 -0.00130

 86 <-184 0.00126

 86 <-194 0.00127

 86 <-231 -0.00132

 87 <-148 -0.00114

 87 <-188 -0.00116

 88 <-160 0.00110

 89 <-159 -0.00110

 90 <-103 0.00426

 90 <-111 0.00273

 91 <-104 -0.00426

 91 <-110 -0.00273

 92 <-187 0.00161

 93 <-153 -0.00106

 93 <-192 0.00106

 94 <-154 0.00106

 94 <-193 -0.00106

 95 <-174 -0.00107

 96 <-113 0.01001

 96 <-122 -0.00129

 96 <-133 -0.00256

 96 <-189 -0.00222

 96 <-199 0.00140

 97 <-152 -0.00118

 97 <-177 0.00105

 98 <-113 0.00160

 98 <-122 -0.00109

 99 <-103 0.01243

 99 <-104 0.00290

 99 <-110 0.00355

 99 <-111 0.00802

 99 <-124 -0.00328

 99 <-125 0.00172

 99 <-131 0.00233

 99 <-132 0.00102

 99 <-185 -0.00139

 99 <-198 -0.00181

 100 <-103 0.00290

 100 <-104 -0.01243

 100 <-110 -0.00802

 100 <-111 0.00355

 100 <-124 -0.00172

 100 <-125 -0.00328

 100 <-131 -0.00102

 100 <-132 0.00233

 100 <-186 0.00139

 100 <-197 -0.00181

 101 <-105 0.01424

 101 <-119 -0.00609

 101 <-127 0.00207

 101 <-196 0.00236

 101 <-210 -0.00133

 102 <-107 0.00370

 102 <-113 0.00191

 102 <-122 -0.00211

 102 <-262 0.00106

 Excited State 6: Singlet-EG 3.1339 eV 395.63 nm f=0.0000 <S\*\*2>=0.000

 34 ->106 0.00112

 39 ->106 -0.00106

 53 ->119 -0.00100

 54 ->106 0.00104

 54 ->122 -0.00103

 57 ->110 -0.00115

 61 ->111 0.00149

 63 ->105 0.00102

 63 ->113 -0.00160

 63 ->119 -0.00132

 65 ->103 -0.00157

 65 ->104 0.00138

 65 ->110 -0.00109

 65 ->111 0.00221

 69 ->103 0.00101

 69 ->104 -0.00171

 69 ->125 0.00119

 70 ->105 -0.00178

 70 ->119 -0.00115

 72 ->103 -0.00264

 72 ->104 0.00264

 77 ->103 0.00216

 77 ->104 -0.00138

 78 ->103 -0.00375

 78 ->104 0.00448

 78 ->110 0.00139

 78 ->111 -0.00198

 78 ->124 -0.00160

 78 ->125 -0.00207

 79 ->106 -0.00147

 80 ->105 0.00221

 82 ->103 -0.00374

 82 ->104 0.00335

 82 ->111 -0.00224

 82 ->124 -0.00159

 82 ->125 -0.00111

 83 ->105 -0.00301

 83 ->106 0.00141

 83 ->119 -0.00129

 84 ->105 0.00169

 84 ->106 0.00193

 84 ->119 0.00126

 86 ->103 0.00534

 86 ->104 -0.00467

 86 ->110 0.00102

 86 ->111 -0.00207

 87 ->103 -0.00312

 87 ->104 0.00592

 87 ->110 0.00280

 87 ->111 -0.00130

 87 ->125 -0.00193

 88 ->105 0.02664

 88 ->106 -0.00707

 88 ->119 0.00524

 88 ->127 -0.00112

 89 ->105 -0.01424

 89 ->106 -0.01204

 89 ->107 -0.00213

 89 ->119 -0.00342

 89 ->127 -0.00102

 89 ->140 -0.00249

 90 ->112 -0.00106

 92 ->103 0.00436

 92 ->104 -0.00453

 92 ->110 -0.00172

 92 ->111 0.00275

 92 ->124 0.00160

 92 ->125 0.00180

 93 ->105 0.01763

 93 ->119 0.00291

 94 ->106 -0.00731

 94 ->122 -0.00158

 94 ->140 -0.00183

 95 ->103 -0.00587

 97 ->103 0.52698

 97 ->104 -0.46910

 97 ->110 0.00739

 97 ->111 -0.01578

 97 ->124 0.00320

 97 ->125 0.00129

 97 ->131 0.00194

 97 ->132 -0.00151

 97 ->185 -0.00102

 97 ->234 -0.00163

 99 ->112 0.00179

 99 ->114 0.00132

 99 ->134 0.00125

 99 ->151 0.00178

 101 ->142 -0.00139

 88 <-106 0.00117

 89 <-106 0.00217

 89 <-122 0.00159

 97 <-103 -0.00308

 97 <-104 0.00273

 97 <-111 0.00146

 97 <-124 0.00125

 97 <-125 0.00127

 98 <-153 -0.00133

 98 <-176 0.00125

 102 <-145 -0.00124

 102 <-154 0.00129

 102 <-175 -0.00126

 102 <-176 0.00103

 Excited State 7: Singlet-EG 3.1339 eV 395.63 nm f=0.0000 <S\*\*2>=0.000

 35 ->106 0.00112

 38 ->106 0.00106

 53 ->106 0.00104

 53 ->122 0.00103

 54 ->119 0.00100

 57 ->111 -0.00115

 61 ->110 -0.00149

 62 ->105 0.00102

 62 ->113 0.00160

 62 ->119 -0.00132

 65 ->103 -0.00138

 65 ->104 -0.00157

 65 ->110 0.00221

 65 ->111 0.00109

 69 ->103 -0.00171

 69 ->104 -0.00101

 69 ->124 -0.00119

 71 ->105 -0.00178

 71 ->119 -0.00115

 72 ->103 -0.00264

 72 ->104 -0.00264

 77 ->103 0.00138

 77 ->104 0.00216

 78 ->103 0.00448

 78 ->104 0.00375

 78 ->110 0.00198

 78 ->111 0.00139

 78 ->124 0.00207

 78 ->125 -0.00160

 79 ->105 -0.00221

 80 ->106 -0.00147

 82 ->103 0.00335

 82 ->104 0.00374

 82 ->110 0.00224

 82 ->124 0.00111

 82 ->125 -0.00159

 83 ->105 0.00169

 83 ->106 0.00193

 83 ->119 0.00126

 84 ->105 0.00301

 84 ->106 -0.00141

 84 ->119 0.00129

 86 ->103 0.00467

 86 ->104 0.00534

 86 ->110 -0.00207

 86 ->111 -0.00102

 87 ->103 0.00592

 87 ->104 0.00312

 87 ->110 0.00130

 87 ->111 0.00280

 87 ->124 0.00193

 88 ->105 -0.01424

 88 ->106 -0.01204

 88 ->107 0.00213

 88 ->119 -0.00342

 88 ->127 -0.00102

 88 ->140 0.00249

 89 ->105 -0.02664

 89 ->106 0.00707

 89 ->119 -0.00524

 89 ->127 0.00112

 91 ->112 -0.00106

 92 ->103 -0.00453

 92 ->104 -0.00436

 92 ->110 -0.00275

 92 ->111 -0.00172

 92 ->124 -0.00180

 92 ->125 0.00160

 93 ->106 -0.00731

 93 ->122 0.00158

 93 ->140 0.00183

 94 ->105 -0.01763

 94 ->119 -0.00291

 95 ->104 -0.00587

 97 ->103 0.46910

 97 ->104 0.52698

 97 ->110 -0.01578

 97 ->111 -0.00739

 97 ->124 0.00129

 97 ->125 -0.00320

 97 ->131 -0.00151

 97 ->132 -0.00194

 97 ->186 -0.00102

 97 ->235 0.00163

 100 ->112 0.00179

 100 ->114 0.00132

 100 ->134 0.00125

 100 ->151 0.00178

 101 ->143 -0.00139

 88 <-106 0.00217

 88 <-122 -0.00159

 89 <-106 -0.00117

 97 <-103 -0.00273

 97 <-104 -0.00308

 97 <-110 0.00146

 97 <-124 0.00127

 97 <-125 -0.00125

 98 <-154 0.00133

 98 <-175 -0.00125

 102 <-146 0.00124

 102 <-153 0.00129

 102 <-175 -0.00103

 102 <-176 -0.00126

 Excited state symmetry could not be determined.

 Excited State 8: Singlet-?Sym 3.1403 eV 394.82 nm f=0.0000 <S\*\*2>=0.000

 36 ->155 0.00134

 37 ->135 -0.00126

 37 ->144 0.00131

 37 ->155 -0.00158

 38 ->168 -0.00102

 39 ->169 0.00102

 40 ->141 -0.00144

 40 ->171 -0.00127

 40 ->182 -0.00141

 42 ->168 0.00112

 43 ->169 0.00112

 44 ->112 -0.00103

 44 ->138 0.00115

 44 ->171 0.00113

 45 ->115 0.00107

 45 ->155 0.00116

 48 ->126 0.00123

 48 ->148 0.00196

 48 ->182 0.00135

 49 ->134 -0.00148

 49 ->138 -0.00168

 49 ->141 0.00100

 49 ->151 0.00112

 49 ->182 0.00109

 50 ->138 0.00167

 51 ->138 -0.00199

 52 ->130 0.00122

 52 ->139 -0.00104

 52 ->152 -0.00126

 53 ->121 0.00124

 53 ->129 -0.00104

 53 ->137 0.00106

 53 ->142 -0.00217

 53 ->143 0.00142

 53 ->146 -0.00155

 53 ->179 -0.00103

 54 ->120 -0.00124

 54 ->128 -0.00104

 54 ->136 -0.00106

 54 ->142 -0.00142

 54 ->143 -0.00217

 54 ->145 0.00155

 54 ->180 -0.00103

 57 ->118 0.00135

 57 ->130 -0.00149

 57 ->135 0.00127

 57 ->139 0.00130

 57 ->147 -0.00203

 57 ->152 0.00152

 57 ->174 -0.00108

 58 ->138 -0.00127

 59 ->153 -0.00138

 59 ->159 0.00114

 60 ->154 -0.00138

 60 ->160 -0.00114

 61 ->135 -0.00247

 61 ->147 0.00173

 61 ->152 0.00153

 61 ->174 0.00121

 61 ->177 -0.00109

 61 ->194 0.00142

 62 ->137 0.00179

 62 ->166 -0.00106

 62 ->191 0.00101

 62 ->192 0.00145

 62 ->193 0.00109

 63 ->136 -0.00179

 63 ->165 0.00106

 63 ->190 -0.00101

 63 ->192 -0.00109

 63 ->193 0.00145

 64 ->147 0.00127

 64 ->163 -0.00116

 64 ->194 0.00128

 65 ->114 -0.00151

 65 ->141 -0.00104

 65 ->148 -0.00100

 65 ->187 -0.00246

 65 ->220 0.00115

 65 ->230 -0.00113

 66 ->105 0.00726

 66 ->119 -0.00161

 67 ->103 -0.00392

 67 ->104 -0.00888

 67 ->110 -0.00353

 67 ->125 -0.00124

 68 ->103 0.00888

 68 ->104 -0.00392

 68 ->111 0.00353

 68 ->124 -0.00124

 69 ->115 0.00190

 69 ->118 -0.00220

 69 ->130 -0.00219

 69 ->139 0.00136

 69 ->144 -0.00115

 69 ->152 0.00114

 69 ->174 -0.00141

 69 ->177 -0.00224

 69 ->194 0.00124

 69 ->219 -0.00117

 69 ->225 -0.00144

 69 ->231 -0.00153

 69 ->261 0.00117

 70 ->117 -0.00234

 70 ->120 0.00184

 70 ->128 -0.00115

 70 ->129 0.00167

 70 ->146 -0.00113

 70 ->153 -0.00120

 70 ->160 0.00186

 70 ->180 -0.00147

 70 ->190 0.00125

 70 ->227 0.00112

 70 ->232 0.00110

 70 ->240 -0.00102

 71 ->116 -0.00234

 71 ->121 -0.00184

 71 ->128 -0.00167

 71 ->129 -0.00115

 71 ->145 -0.00113

 71 ->154 0.00120

 71 ->159 -0.00186

 71 ->179 -0.00147

 71 ->191 -0.00125

 71 ->228 0.00112

 71 ->233 0.00110

 71 ->241 -0.00102

 72 ->114 -0.00177

 72 ->123 0.00273

 72 ->126 0.00194

 72 ->148 0.00174

 72 ->170 -0.00110

 72 ->171 0.00105

 72 ->187 0.00197

 72 ->188 0.00105

 72 ->220 0.00118

 72 ->256 -0.00117

 72 ->258 0.00105

 73 ->113 -0.00550

 74 ->105 -0.00263

 74 ->119 -0.00323

 74 ->127 -0.00171

 75 ->103 0.00269

 75 ->104 0.00950

 75 ->110 -0.00187

 75 ->111 0.00101

 75 ->125 -0.00188

 75 ->131 0.00133

 76 ->103 -0.00950

 76 ->104 0.00269

 76 ->110 0.00101

 76 ->111 0.00187

 76 ->124 -0.00188

 76 ->132 -0.00133

 77 ->126 -0.00175

 77 ->141 0.00136

 77 ->148 -0.00104

 77 ->187 -0.00137

 77 ->230 0.00112

 78 ->139 0.00106

 78 ->144 -0.00133

 78 ->155 -0.00194

 78 ->184 0.00118

 79 ->120 -0.00106

 79 ->149 0.00124

 79 ->193 -0.00134

 80 ->121 0.00106

 80 ->150 -0.00124

 80 ->192 -0.00134

 81 ->113 -0.00205

 81 ->133 0.00129

 82 ->118 -0.00150

 82 ->144 0.00156

 82 ->164 0.00170

 82 ->174 -0.00117

 82 ->177 0.00102

 82 ->194 -0.00196

 82 ->219 0.00109

 82 ->231 0.00108

 83 ->145 -0.00195

 83 ->154 0.00139

 83 ->159 -0.00104

 83 ->169 -0.00149

 83 ->191 -0.00104

 83 ->241 -0.00103

 84 ->146 -0.00195

 84 ->153 -0.00139

 84 ->160 0.00104

 84 ->168 0.00149

 84 ->190 0.00104

 84 ->240 -0.00103

 85 ->122 0.00155

 85 ->133 0.00150

 86 ->148 0.00352

 86 ->171 0.00101

 86 ->182 0.00138

 86 ->187 0.00231

 86 ->214 -0.00115

 86 ->237 0.00103

 86 ->256 -0.00126

 86 ->258 0.00110

 87 ->139 -0.00146

 87 ->152 -0.00161

 87 ->174 0.00201

 87 ->177 0.00135

 87 ->225 0.00126

 88 ->153 0.00166

 88 ->159 -0.00106

 88 ->190 -0.00107

 88 ->192 -0.00153

 89 ->154 0.00166

 89 ->160 0.00106

 89 ->191 -0.00107

 89 ->193 -0.00153

 90 ->103 0.00754

 90 ->104 0.01112

 90 ->110 0.00289

 90 ->125 0.00283

 91 ->103 -0.01112

 91 ->104 0.00754

 91 ->111 -0.00289

 91 ->124 0.00283

 92 ->115 -0.00106

 92 ->118 -0.00188

 92 ->135 0.00146

 92 ->152 0.00245

 92 ->194 0.00102

 92 ->231 -0.00111

 92 ->236 -0.00130

 93 ->108 -0.00214

 93 ->120 -0.00108

 93 ->142 -0.00140

 93 ->159 -0.00109

 93 ->160 -0.00146

 93 ->204 0.00139

 94 ->109 -0.00214

 94 ->121 -0.00108

 94 ->143 -0.00140

 94 ->159 -0.00146

 94 ->160 0.00109

 94 ->205 -0.00139

 95 ->112 -0.00313

 95 ->138 0.00117

 95 ->162 0.00172

 95 ->195 0.00196

 96 ->105 -0.04204

 96 ->106 -0.00159

 96 ->119 -0.01969

 96 ->127 0.00308

 96 ->156 0.00131

 96 ->196 0.00294

 96 ->210 -0.00156

 97 ->148 -0.00141

 97 ->170 0.00154

 97 ->187 -0.00261

 97 ->214 0.00156

 98 ->105 -0.03060

 98 ->119 -0.00347

 98 ->127 0.00102

 98 ->181 0.00116

 99 ->103 -0.18201

 99 ->104 -0.46314

 99 ->110 0.01608

 99 ->111 0.00127

 99 ->124 -0.00202

 99 ->125 0.01112

 99 ->131 0.00315

 99 ->132 -0.00325

 99 ->157 0.00108

 99 ->197 0.00135

 99 ->224 -0.00133

 100 ->103 0.46314

 100 ->104 -0.18201

 100 ->110 0.00127

 100 ->111 -0.01608

 100 ->124 0.01112

 100 ->125 0.00202

 100 ->131 -0.00325

 100 ->132 -0.00315

 100 ->158 -0.00108

 100 ->198 0.00135

 100 ->223 0.00133

 101 ->107 0.00125

 101 ->113 0.01508

 101 ->122 -0.00242

 101 ->133 -0.00305

 101 ->189 -0.00108

 101 ->229 0.00119

 101 ->297 0.00121

 102 ->105 0.01005

 102 ->106 0.00523

 102 ->119 -0.00292

 102 ->127 0.00234

 102 ->156 -0.00109

 102 ->210 -0.00151

 102 ->284 -0.00113

 36 <-155 0.00114

 37 <-155 -0.00132

 40 <-141 -0.00117

 40 <-182 -0.00117

 48 <-148 0.00145

 48 <-182 0.00120

 49 <-134 -0.00104

 49 <-138 -0.00109

 50 <-138 0.00115

 51 <-138 -0.00133

 53 <-142 -0.00152

 54 <-143 -0.00152

 57 <-139 0.00104

 57 <-147 -0.00140

 57 <-152 0.00105

 59 <-153 -0.00110

 60 <-154 -0.00110

 61 <-135 -0.00179

 61 <-147 0.00119

 61 <-152 0.00110

 61 <-194 0.00106

 62 <-137 0.00128

 62 <-192 0.00110

 63 <-136 -0.00128

 63 <-193 0.00110

 65 <-187 -0.00187

 66 <-105 0.00404

 66 <-119 -0.00170

 67 <-103 -0.00128

 67 <-104 -0.00329

 67 <-110 -0.00302

 67 <-125 -0.00103

 68 <-103 0.00329

 68 <-104 -0.00128

 68 <-111 0.00302

 68 <-124 -0.00103

 69 <-115 0.00111

 69 <-118 -0.00132

 69 <-130 -0.00144

 69 <-174 -0.00103

 69 <-177 -0.00166

 69 <-194 0.00100

 69 <-225 -0.00117

 69 <-231 -0.00126

 70 <-117 -0.00138

 70 <-120 0.00111

 70 <-129 0.00111

 70 <-160 0.00135

 70 <-180 -0.00114

 71 <-116 -0.00138

 71 <-121 -0.00111

 71 <-128 -0.00111

 71 <-159 -0.00135

 71 <-179 -0.00114

 72 <-114 -0.00102

 72 <-123 0.00164

 72 <-126 0.00126

 72 <-148 0.00121

 72 <-187 0.00151

 73 <-113 -0.00378

 74 <-119 -0.00109

 74 <-127 -0.00108

 77 <-126 -0.00105

 77 <-187 -0.00102

 78 <-155 -0.00142

 79 <-193 -0.00102

 80 <-192 -0.00102

 81 <-113 -0.00180

 81 <-133 0.00107

 82 <-164 0.00113

 82 <-194 -0.00143

 83 <-145 -0.00120

 83 <-169 -0.00115

 84 <-146 -0.00120

 84 <-168 0.00115

 85 <-122 0.00124

 86 <-148 0.00234

 86 <-182 0.00117

 86 <-187 0.00174

 86 <-256 -0.00102

 87 <-152 -0.00103

 87 <-174 0.00143

 88 <-153 0.00105

 88 <-192 -0.00111

 89 <-154 0.00105

 89 <-193 -0.00111

 90 <-110 0.00220

 90 <-125 0.00178

 91 <-111 -0.00220

 91 <-124 0.00178

 92 <-152 0.00151

 93 <-204 0.00103

 94 <-205 -0.00103

 95 <-112 -0.00124

 95 <-162 0.00119

 95 <-195 0.00144

 96 <-105 0.01194

 96 <-119 -0.00582

 96 <-127 0.00187

 96 <-196 0.00257

 96 <-210 -0.00158

 97 <-187 -0.00183

 97 <-214 0.00115

 98 <-105 0.00536

 99 <-103 0.00369

 99 <-104 0.01169

 99 <-110 0.00872

 99 <-125 0.00253

 99 <-131 0.00192

 99 <-132 -0.00115

 99 <-186 -0.00131

 99 <-197 0.00127

 99 <-198 -0.00148

 99 <-224 -0.00102

 100 <-103 -0.01169

 100 <-104 0.00369

 100 <-111 -0.00872

 100 <-124 0.00253

 100 <-131 -0.00115

 100 <-132 -0.00192

 100 <-185 0.00131

 100 <-197 0.00148

 100 <-198 0.00127

 100 <-223 0.00102

 101 <-113 0.00964

 101 <-122 -0.00151

 101 <-133 -0.00232

 101 <-189 -0.00192

 101 <-199 0.00148

 102 <-105 0.00469

 102 <-106 0.00282

 102 <-119 -0.00106

 102 <-249 -0.00104

 102 <-284 -0.00121

 Excited State 9: Singlet-EG 3.3416 eV 371.03 nm f=0.0000 <S\*\*2>=0.000

 29 ->103 -0.00131

 30 ->105 0.00127

 30 ->119 0.00120

 33 ->103 0.00200

 33 ->104 -0.00152

 33 ->124 0.00125

 33 ->125 0.00100

 34 ->105 -0.00179

 34 ->119 -0.00132

 35 ->122 0.00142

 36 ->103 -0.00142

 36 ->124 -0.00147

 48 ->103 -0.00100

 49 ->103 0.00374

 49 ->104 -0.00296

 50 ->103 0.00165

 53 ->122 0.00122

 58 ->103 -0.00222

 58 ->104 0.00159

 58 ->111 0.00125

 59 ->105 0.00205

 59 ->106 0.00176

 59 ->119 0.00146

 59 ->122 0.00101

 60 ->105 0.00187

 60 ->106 -0.00194

 60 ->119 0.00132

 61 ->125 0.00170

 64 ->103 -0.00126

 64 ->104 0.00152

 64 ->110 0.00135

 64 ->111 -0.00158

 64 ->124 -0.00128

 64 ->125 -0.00178

 69 ->103 -0.00144

 69 ->111 -0.00118

 69 ->124 -0.00150

 70 ->106 0.00136

 71 ->105 -0.00232

 71 ->119 -0.00108

 71 ->122 0.00117

 72 ->103 -0.00195

 72 ->104 0.00173

 77 ->103 -0.00433

 77 ->104 0.00310

 77 ->111 0.00136

 77 ->124 -0.00172

 77 ->125 -0.00109

 79 ->113 0.00154

 79 ->119 0.00175

 79 ->122 -0.00127

 80 ->105 -0.00119

 80 ->113 -0.00119

 80 ->122 -0.00105

 82 ->104 0.00297

 82 ->110 0.00247

 82 ->124 0.00142

 82 ->125 -0.00118

 87 ->103 0.00308

 87 ->111 0.00278

 87 ->124 0.00214

 88 ->105 -0.00962

 88 ->106 -0.00542

 88 ->107 -0.00121

 88 ->119 -0.00236

 88 ->122 0.00230

 89 ->105 -0.01320

 89 ->106 0.00449

 89 ->119 -0.00304

 91 ->134 -0.00102

 92 ->103 0.01307

 92 ->104 0.01192

 92 ->110 0.00829

 92 ->111 0.00793

 92 ->124 0.00825

 92 ->125 -0.00434

 92 ->131 -0.00130

 92 ->132 0.00308

 92 ->158 -0.00141

 92 ->235 0.00127

 92 ->251 -0.00122

 92 ->252 -0.00152

 93 ->105 0.01528

 93 ->106 0.02543

 93 ->107 0.00389

 93 ->119 0.00355

 93 ->122 -0.00635

 93 ->127 0.00239

 93 ->133 0.00156

 93 ->140 -0.00144

 93 ->156 -0.00111

 93 ->161 -0.00129

 93 ->229 0.00171

 93 ->238 0.00198

 93 ->273 0.00109

 94 ->105 0.06680

 94 ->106 -0.00741

 94 ->113 0.00262

 94 ->119 0.01030

 94 ->253 0.00185

 95 ->103 0.56326

 95 ->104 -0.41951

 95 ->110 0.00308

 95 ->111 -0.01054

 95 ->124 0.00650

 95 ->125 0.00436

 95 ->132 -0.00137

 95 ->234 -0.00205

 95 ->251 0.00112

 95 ->252 -0.00166

 97 ->103 0.00246

 97 ->104 -0.00441

 98 ->137 -0.00122

 98 ->149 -0.00107

 36 <-103 -0.00115

 49 <-103 0.00140

 49 <-104 -0.00117

 59 <-105 0.00104

 60 <-105 0.00101

 87 <-103 -0.00113

 89 <-105 0.00132

 90 <-162 0.00124

 90 <-187 0.00111

 91 <-134 -0.00106

 91 <-151 0.00125

 91 <-162 0.00173

 91 <-195 0.00155

 92 <-103 -0.00452

 92 <-104 -0.00326

 92 <-124 -0.00283

 92 <-125 0.00175

 93 <-105 -0.00130

 93 <-107 -0.00125

 93 <-122 0.00298

 93 <-133 -0.00106

 93 <-140 0.00114

 94 <-105 -0.00555

 94 <-119 -0.00323

 95 <-103 -0.00572

 95 <-104 0.00429

 95 <-124 -0.00253

 95 <-125 -0.00206

 95 <-131 0.00105

 98 <-137 -0.00118

 98 <-143 -0.00144

 98 <-145 -0.00108

 98 <-146 -0.00150

 98 <-154 -0.00210

 102 <-136 -0.00119

 102 <-142 -0.00145

 102 <-145 -0.00117

 102 <-149 0.00115

 102 <-153 -0.00237

 Excited State 10: Singlet-EG 3.3416 eV 371.03 nm f=0.0000 <S\*\*2>=0.000

 29 ->104 0.00131

 31 ->105 -0.00127

 31 ->119 -0.00120

 33 ->103 0.00152

 33 ->104 0.00200

 33 ->124 0.00100

 33 ->125 -0.00125

 34 ->122 0.00142

 35 ->105 -0.00179

 35 ->119 -0.00132

 36 ->104 0.00142

 36 ->125 -0.00147

 48 ->104 -0.00100

 49 ->103 0.00296

 49 ->104 0.00374

 50 ->104 0.00165

 54 ->122 0.00122

 58 ->103 -0.00159

 58 ->104 -0.00222

 58 ->110 0.00125

 59 ->105 0.00187

 59 ->106 -0.00194

 59 ->119 0.00132

 60 ->105 -0.00205

 60 ->106 -0.00176

 60 ->119 -0.00146

 60 ->122 0.00101

 61 ->124 -0.00170

 64 ->103 0.00152

 64 ->104 0.00126

 64 ->110 0.00158

 64 ->111 0.00135

 64 ->124 0.00178

 64 ->125 -0.00128

 69 ->104 0.00144

 69 ->110 0.00118

 69 ->125 -0.00150

 70 ->105 0.00232

 70 ->119 0.00108

 70 ->122 0.00117

 71 ->106 0.00136

 72 ->103 -0.00173

 72 ->104 -0.00195

 77 ->103 -0.00310

 77 ->104 -0.00433

 77 ->110 0.00136

 77 ->124 -0.00109

 77 ->125 0.00172

 79 ->105 0.00119

 79 ->113 -0.00119

 79 ->122 -0.00105

 80 ->113 -0.00154

 80 ->119 0.00175

 80 ->122 0.00127

 82 ->103 0.00297

 82 ->111 0.00247

 82 ->124 0.00118

 82 ->125 0.00142

 87 ->104 -0.00308

 87 ->110 -0.00278

 87 ->125 0.00214

 88 ->105 -0.01320

 88 ->106 0.00449

 88 ->119 -0.00304

 89 ->105 0.00962

 89 ->106 0.00542

 89 ->107 -0.00121

 89 ->119 0.00236

 89 ->122 0.00230

 90 ->134 0.00102

 92 ->103 0.01192

 92 ->104 -0.01307

 92 ->110 -0.00793

 92 ->111 0.00829

 92 ->124 0.00434

 92 ->125 0.00825

 92 ->131 -0.00308

 92 ->132 -0.00130

 92 ->157 0.00141

 92 ->234 -0.00127

 92 ->251 0.00152

 92 ->252 -0.00122

 93 ->105 0.06680

 93 ->106 -0.00741

 93 ->113 -0.00262

 93 ->119 0.01030

 93 ->253 0.00185

 94 ->105 -0.01528

 94 ->106 -0.02543

 94 ->107 0.00389

 94 ->119 -0.00355

 94 ->122 -0.00635

 94 ->127 -0.00239

 94 ->133 0.00156

 94 ->140 -0.00144

 94 ->156 0.00111

 94 ->161 -0.00129

 94 ->229 0.00171

 94 ->238 0.00198

 94 ->273 -0.00109

 95 ->103 0.41951

 95 ->104 0.56326

 95 ->110 -0.01054

 95 ->111 -0.00308

 95 ->124 0.00436

 95 ->125 -0.00650

 95 ->131 -0.00137

 95 ->235 0.00205

 95 ->251 -0.00166

 95 ->252 -0.00112

 97 ->103 0.00441

 97 ->104 0.00246

 98 ->136 -0.00122

 98 ->150 0.00107

 36 <-104 0.00115

 49 <-103 0.00117

 49 <-104 0.00140

 59 <-105 0.00101

 60 <-105 -0.00104

 87 <-104 0.00113

 88 <-105 0.00132

 90 <-134 0.00106

 90 <-151 -0.00125

 90 <-162 -0.00173

 90 <-195 -0.00155

 91 <-162 0.00124

 91 <-187 0.00111

 92 <-103 -0.00326

 92 <-104 0.00452

 92 <-124 -0.00175

 92 <-125 -0.00283

 93 <-105 -0.00555

 93 <-119 -0.00323

 94 <-105 0.00130

 94 <-107 -0.00125

 94 <-122 0.00298

 94 <-133 -0.00106

 94 <-140 0.00114

 95 <-103 -0.00429

 95 <-104 -0.00572

 95 <-124 -0.00206

 95 <-125 0.00253

 95 <-132 -0.00105

 98 <-136 -0.00118

 98 <-142 -0.00144

 98 <-145 -0.00150

 98 <-146 0.00108

 98 <-153 -0.00210

 102 <-137 0.00119

 102 <-143 0.00145

 102 <-146 0.00117

 102 <-150 -0.00115

 102 <-154 0.00237

 SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 10 LETran= 190.

 Leave Link 914 at Thu Sep 19 00:42:44 2019, MaxMem= 1342177280 cpu: 3181.6

 (Enter /home/blab/g09/l601.exe)

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

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

 Population analysis using the SCF density.

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 Orbital symmetries:

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 The electronic state is 1-AG.

 Alpha occ. eigenvalues -- -14.32250 -14.32250 -14.32250 -14.32250 -14.30743

 Alpha occ. eigenvalues -- -14.30743 -14.30742 -14.30742 -10.24817 -10.24817

 Alpha occ. eigenvalues -- -10.24817 -10.24817 -10.24660 -10.24660 -10.24660

 Alpha occ. eigenvalues -- -10.24660 -10.19030 -10.19030 -10.19030 -10.19030

 Alpha occ. eigenvalues -- -10.17456 -10.17456 -10.17456 -10.17456 -10.16324

 Alpha occ. eigenvalues -- -10.16324 -10.16324 -10.16324 -1.00641 -0.99218

 Alpha occ. eigenvalues -- -0.99218 -0.96439 -0.94354 -0.90169 -0.90169

 Alpha occ. eigenvalues -- -0.86923 -0.79987 -0.79467 -0.79467 -0.79225

 Alpha occ. eigenvalues -- -0.75193 -0.71923 -0.71923 -0.70449 -0.69213

 Alpha occ. eigenvalues -- -0.68105 -0.68105 -0.63376 -0.61025 -0.59193

 Alpha occ. eigenvalues -- -0.57992 -0.57664 -0.56913 -0.56913 -0.55972

 Alpha occ. eigenvalues -- -0.55972 -0.54772 -0.54440 -0.53934 -0.53934

 Alpha occ. eigenvalues -- -0.51903 -0.50694 -0.50694 -0.49311 -0.48755

 Alpha occ. eigenvalues -- -0.46245 -0.44665 -0.44665 -0.44393 -0.43475

 Alpha occ. eigenvalues -- -0.43475 -0.42860 -0.42829 -0.40747 -0.40504

 Alpha occ. eigenvalues -- -0.40504 -0.40054 -0.39728 -0.39326 -0.39326

 Alpha occ. eigenvalues -- -0.39104 -0.37980 -0.37645 -0.37645 -0.37644

 Alpha occ. eigenvalues -- -0.37140 -0.36698 -0.32961 -0.32961 -0.32035

 Alpha occ. eigenvalues -- -0.32035 -0.31036 -0.28222 -0.28222 -0.26512

 Alpha occ. eigenvalues -- -0.26302 -0.25824 -0.25254 -0.25199 -0.25199

 Alpha occ. eigenvalues -- -0.24934 -0.20573

 Alpha virt. eigenvalues -- -0.11036 -0.11036 -0.04829 0.02873 0.03445

 Alpha virt. eigenvalues -- 0.04551 0.04551 0.04676 0.04676 0.05517

 Alpha virt. eigenvalues -- 0.05962 0.06957 0.07036 0.08243 0.08243

 Alpha virt. eigenvalues -- 0.09322 0.09750 0.10059 0.10059 0.10260

 Alpha virt. eigenvalues -- 0.10275 0.11310 0.11310 0.12910 0.13634

 Alpha virt. eigenvalues -- 0.13649 0.13649 0.13713 0.13998 0.13998

 Alpha virt. eigenvalues -- 0.14392 0.18353 0.20354 0.20857 0.20857

 Alpha virt. eigenvalues -- 0.20943 0.21724 0.21978 0.22082 0.22088

 Alpha virt. eigenvalues -- 0.22088 0.23045 0.23433 0.23433 0.25968

 Alpha virt. eigenvalues -- 0.27482 0.27928 0.27928 0.28743 0.29207

 Alpha virt. eigenvalues -- 0.29839 0.29839 0.30506 0.31414 0.31614

 Alpha virt. eigenvalues -- 0.31614 0.32053 0.32053 0.32177 0.32188

 Alpha virt. eigenvalues -- 0.32587 0.34813 0.35452 0.35452 0.36036

 Alpha virt. eigenvalues -- 0.37700 0.37700 0.38034 0.39064 0.39229

 Alpha virt. eigenvalues -- 0.39229 0.40223 0.40422 0.40422 0.41258

 Alpha virt. eigenvalues -- 0.41876 0.43664 0.43664 0.43931 0.44094

 Alpha virt. eigenvalues -- 0.44318 0.45605 0.46426 0.46426 0.47127

 Alpha virt. eigenvalues -- 0.48112 0.49080 0.49354 0.49354 0.49741

 Alpha virt. eigenvalues -- 0.49741 0.49774 0.51546 0.51698 0.51919

 Alpha virt. eigenvalues -- 0.51919 0.53253 0.54091 0.54091 0.54212

 Alpha virt. eigenvalues -- 0.54651 0.56594 0.56594 0.56768 0.56811

 Alpha virt. eigenvalues -- 0.57551 0.57551 0.57867 0.58548 0.58548

 Alpha virt. eigenvalues -- 0.58960 0.59001 0.59633 0.60048 0.60048

 Alpha virt. eigenvalues -- 0.60641 0.62032 0.62939 0.63511 0.63511

 Alpha virt. eigenvalues -- 0.63650 0.63650 0.63672 0.65250 0.65370

 Alpha virt. eigenvalues -- 0.65370 0.68407 0.68436 0.68859 0.69124

 Alpha virt. eigenvalues -- 0.69124 0.69440 0.69440 0.70382 0.71145

 Alpha virt. eigenvalues -- 0.71716 0.73478 0.73822 0.73822 0.75041

 Alpha virt. eigenvalues -- 0.75635 0.76198 0.76198 0.78120 0.78120

 Alpha virt. eigenvalues -- 0.79138 0.79819 0.80256 0.80968 0.80968

 Alpha virt. eigenvalues -- 0.81215 0.81747 0.81747 0.82590 0.82742

 Alpha virt. eigenvalues -- 0.85427 0.85494 0.85494 0.87110 0.88951

 Alpha virt. eigenvalues -- 0.88986 0.88986 0.89944 0.94704 0.96792

 Alpha virt. eigenvalues -- 0.96792 0.97909 0.98212 1.00221 1.00221

 Alpha virt. eigenvalues -- 1.01002 1.03639 1.03639 1.04306 1.05310

 Alpha virt. eigenvalues -- 1.05310 1.06917 1.08323 1.08965 1.08965

 Alpha virt. eigenvalues -- 1.10666 1.10819 1.13390 1.13704 1.14111

 Alpha virt. eigenvalues -- 1.14111 1.14326 1.14326 1.14431 1.14720

 Alpha virt. eigenvalues -- 1.15537 1.18358 1.19235 1.19235 1.19258

 Alpha virt. eigenvalues -- 1.21045 1.21569 1.21569 1.23578 1.23924

 Alpha virt. eigenvalues -- 1.27875 1.29036 1.29434 1.29434 1.30552

 Alpha virt. eigenvalues -- 1.36917 1.36917 1.37377 1.39087 1.39219

 Alpha virt. eigenvalues -- 1.41057 1.41057 1.41073 1.42270 1.42270

 Alpha virt. eigenvalues -- 1.44194 1.45199 1.49599 1.49954 1.49954

 Alpha virt. eigenvalues -- 1.51130 1.51145 1.51145 1.51313 1.52113

 Alpha virt. eigenvalues -- 1.52141 1.52141 1.53041 1.54269 1.54978

 Alpha virt. eigenvalues -- 1.54978 1.55490 1.56240 1.56240 1.57420

 Alpha virt. eigenvalues -- 1.58742 1.60455 1.61183 1.61183 1.62307

 Alpha virt. eigenvalues -- 1.62992 1.62992 1.63417 1.67265 1.68634

 Alpha virt. eigenvalues -- 1.68699 1.68699 1.69533 1.69533 1.70095

 Alpha virt. eigenvalues -- 1.71322 1.72274 1.72274 1.74425 1.76242

 Alpha virt. eigenvalues -- 1.76242 1.76552 1.80180 1.80323 1.80323

 Alpha virt. eigenvalues -- 1.80476 1.85189 1.86922 1.86922 1.87443

 Alpha virt. eigenvalues -- 1.88858 1.90765 1.90765 1.90827 1.92112

 Alpha virt. eigenvalues -- 1.94508 1.95617 1.96823 1.96823 1.97023

 Alpha virt. eigenvalues -- 2.01186 2.01313 2.01313 2.01395 2.02349

 Alpha virt. eigenvalues -- 2.02450 2.02878 2.02878 2.05602 2.07295

 Alpha virt. eigenvalues -- 2.08238 2.09461 2.09461 2.12898 2.12898

 Alpha virt. eigenvalues -- 2.15356 2.16203 2.16203 2.17939 2.18043

 Alpha virt. eigenvalues -- 2.20520 2.27690 2.29307 2.29483 2.29483

 Alpha virt. eigenvalues -- 2.29771 2.30040 2.33440 2.33440 2.35110

 Alpha virt. eigenvalues -- 2.35357 2.35357 2.36254 2.38025 2.38159

 Alpha virt. eigenvalues -- 2.38159 2.39486 2.39486 2.39533 2.40439

 Alpha virt. eigenvalues -- 2.44103 2.48204 2.48204 2.48239 2.48339

 Alpha virt. eigenvalues -- 2.48400 2.48400 2.49463 2.49586 2.55733

 Alpha virt. eigenvalues -- 2.56095 2.56095 2.56564 2.58269 2.58269

 Alpha virt. eigenvalues -- 2.59695 2.60721 2.60721 2.63483 2.63995

 Alpha virt. eigenvalues -- 2.64974 2.66981 2.67560 2.71131 2.71131

 Alpha virt. eigenvalues -- 2.72347 2.72882 2.72882 2.73074 2.76275

 Alpha virt. eigenvalues -- 2.76275 2.77167 2.80179 2.83534 2.84441

 Alpha virt. eigenvalues -- 2.84441 2.84908 2.85049 2.85616 2.85637

 Alpha virt. eigenvalues -- 2.85637 2.92377 2.92377 2.93634 2.94164

 Alpha virt. eigenvalues -- 2.96296 2.97536 2.97536 3.02010 3.03993

 Alpha virt. eigenvalues -- 3.05048 3.05048 3.06184 3.12973 3.12974

 Alpha virt. eigenvalues -- 3.13289 3.13840 3.13840 3.14167 3.14678

 Alpha virt. eigenvalues -- 3.14678 3.16488 3.17104 3.17104 3.18486

 Alpha virt. eigenvalues -- 3.21148 3.21148 3.21637 3.22745 3.25061

 Alpha virt. eigenvalues -- 3.27005 3.28947 3.28947 3.28989 3.30992

 Alpha virt. eigenvalues -- 3.30992 3.36909 3.38070 3.39127 3.39127

 Alpha virt. eigenvalues -- 3.39557 3.53535 3.57764 3.57764 3.70494

 Alpha virt. eigenvalues -- 3.72781 3.73082 3.73082 3.76647 3.78490

 Alpha virt. eigenvalues -- 3.78848 3.78848 3.79481 3.80978 3.81836

 Alpha virt. eigenvalues -- 3.81836 3.87103 3.87771 3.87872 3.87872

 Alpha virt. eigenvalues -- 3.91080 4.05344 4.05344 4.05938 4.06030

 Alpha virt. eigenvalues -- 4.11854 4.12881 4.12881 4.19212 4.28441

 Alpha virt. eigenvalues -- 4.35857 4.35857 4.38303 4.46515 4.51554

 Alpha virt. eigenvalues -- 4.61569 4.61569 5.00290 5.03591 5.03591

 Alpha virt. eigenvalues -- 5.12288 5.15720 5.33647 5.33647 5.50650

 Alpha virt. eigenvalues -- 7.78170 7.78170 7.89352 7.95141 8.22857

 Alpha virt. eigenvalues -- 11.19717 23.43723 23.46128 23.46128 23.47472

 Alpha virt. eigenvalues -- 23.66987 23.67576 23.67576 23.67694 23.82368

 Alpha virt. eigenvalues -- 23.83455 23.83455 23.84689 23.87337 23.88434

 Alpha virt. eigenvalues -- 23.88434 23.88609 24.11177 24.11654 24.11654

 Alpha virt. eigenvalues -- 24.12342 35.56472 35.60996 35.60996 35.62181

 Alpha virt. eigenvalues -- 35.67530 35.68773 35.68773 35.69123

 Condensed to atoms (all electrons):

 1 2 3 4 5 6

 1 C 4.621931 0.410026 -0.136670 -0.053739 0.420186 -0.001919

 2 N 0.410026 7.112585 0.388016 -0.065435 -0.097756 -0.081366

 3 C -0.136670 0.388016 4.655580 0.410576 -0.068313 0.561427

 4 C -0.053739 -0.065435 0.410576 5.046570 0.621604 -0.073233

 5 C 0.420186 -0.097756 -0.068313 0.621604 5.118940 0.004606

 6 N -0.001919 -0.081366 0.561427 -0.073233 0.004606 6.571365

 7 C -0.000844 -0.003804 -0.100180 0.003713 -0.000326 0.518840

 8 N 0.000567 -0.020650 -0.004898 -0.000131 -0.000198 -0.074413

 9 C -0.000014 0.000426 -0.000656 0.000023 -0.000004 0.000190

 10 C -0.000004 -0.000092 0.000113 0.000017 0.000000 0.003476

 11 C 0.000023 0.000246 0.003754 -0.000344 0.000011 -0.041487

 12 N 0.518840 -0.074413 0.000190 0.003476 -0.041487 -0.000156

 13 C 0.003713 -0.000131 0.000023 0.000017 -0.000344 -0.000000

 14 C -0.000326 -0.000198 -0.000004 0.000000 0.000011 -0.000000

 15 C -0.000844 0.000567 -0.000014 -0.000004 0.000023 -0.000001

 16 N -0.003804 -0.020650 0.000426 -0.000092 0.000246 -0.000006

 17 C -0.100180 -0.004898 -0.000656 0.000113 0.003754 -0.000025

 18 N -0.000018 -0.000005 -0.000001 -0.000000 -0.000000 0.000000

 19 N 0.000164 -0.003309 0.000219 0.000002 0.000003 -0.000005

 20 C -0.000059 0.000219 -0.000009 -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 -0.000002 0.000164 -0.000059 -0.000000 -0.000000 -0.000018

 24 N -0.000001 -0.000006 -0.000025 -0.000000 -0.000000 -0.000156

 25 Zn -0.015664 0.117767 -0.017413 -0.000719 -0.000395 -0.005399

 26 C 0.009801 0.008953 -0.070530 0.266014 -0.056103 0.014326

 27 H -0.048983 0.006281 0.009926 -0.043579 0.395842 -0.000011

 28 C 0.000000 0.000001 0.000001 -0.000000 0.000000 -0.000020

 29 H 0.000001 0.000075 -0.000139 -0.000152 -0.000004 0.006277

 30 C -0.000366 0.000063 0.000000 -0.000000 -0.000040 0.000000

 31 H 0.000011 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 0.000212 -0.000240 0.006145 -0.041216 -0.005306 0.000076

 35 H -0.000129 0.000425 -0.005308 -0.044172 -0.000327 0.003905

 36 H -0.000129 0.000425 -0.005308 -0.044172 -0.000327 0.003905

 37 H 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000008

 38 H 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000008

 39 H -0.000000 -0.000000 0.000001 0.000000 0.000000 -0.000010

 40 H 0.000010 0.000014 -0.000000 -0.000000 -0.000016 0.000000

 41 H 0.000010 0.000014 -0.000000 -0.000000 -0.000016 0.000000

 42 H 0.000040 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 -0.000844 0.000567 -0.000014 -0.000004 0.000023 0.518840

 2 N -0.003804 -0.020650 0.000426 -0.000092 0.000246 -0.074413

 3 C -0.100180 -0.004898 -0.000656 0.000113 0.003754 0.000190

 4 C 0.003713 -0.000131 0.000023 0.000017 -0.000344 0.003476

 5 C -0.000326 -0.000198 -0.000004 0.000000 0.000011 -0.041487

 6 N 0.518840 -0.074413 0.000190 0.003476 -0.041487 -0.000156

 7 C 4.621931 0.410026 -0.136670 -0.053739 0.420186 -0.000018

 8 N 0.410026 7.112585 0.388016 -0.065435 -0.097756 -0.000005

 9 C -0.136670 0.388016 4.655580 0.410576 -0.068313 -0.000001

 10 C -0.053739 -0.065435 0.410576 5.046570 0.621604 -0.000000

 11 C 0.420186 -0.097756 -0.068313 0.621604 5.118940 -0.000000

 12 N -0.000018 -0.000005 -0.000001 -0.000000 -0.000000 6.571365

 13 C -0.000000 0.000002 -0.000000 0.000000 -0.000000 -0.073233

 14 C -0.000000 0.000003 -0.000000 -0.000000 0.000000 0.004606

 15 C -0.000002 0.000164 -0.000059 -0.000000 -0.000000 -0.001919

 16 N 0.000164 -0.003309 0.000219 0.000002 0.000003 -0.081366

 17 C -0.000059 0.000219 -0.000009 -0.000000 -0.000000 0.561427

 18 N -0.000001 -0.000006 -0.000025 -0.000000 -0.000000 -0.000156

 19 N 0.000567 -0.020650 -0.004898 -0.000131 -0.000198 -0.000006

 20 C -0.000014 0.000426 -0.000656 0.000023 -0.000004 -0.000025

 21 C -0.000004 -0.000092 0.000113 0.000017 0.000000 -0.000000

 22 C 0.000023 0.000246 0.003754 -0.000344 0.000011 -0.000000

 23 C -0.000844 -0.003804 -0.100180 0.003713 -0.000326 -0.000001

 24 N -0.001919 -0.081366 0.561427 -0.073233 0.004606 0.000000

 25 Zn -0.015664 0.117767 -0.017413 -0.000719 -0.000395 -0.005399

 26 C -0.000366 0.000063 0.000000 -0.000000 -0.000040 -0.000020

 27 H 0.000011 0.000001 0.000000 0.000000 -0.000000 0.006277

 28 C 0.009801 0.008953 -0.070530 0.266014 -0.056103 -0.000000

 29 H -0.048983 0.006281 0.009926 -0.043579 0.395842 0.000000

 30 C 0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.014326

 31 H -0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000011

 32 C 0.000000 0.000001 0.000001 -0.000000 0.000000 0.000000

 33 H 0.000001 0.000075 -0.000139 -0.000152 -0.000004 -0.000000

 34 H 0.000040 0.000000 0.000000 0.000000 -0.000001 -0.000010

 35 H 0.000010 0.000014 -0.000000 -0.000000 -0.000016 0.000008

 36 H 0.000010 0.000014 -0.000000 -0.000000 -0.000016 0.000008

 37 H -0.000129 0.000425 -0.005308 -0.044172 -0.000327 -0.000000

 38 H -0.000129 0.000425 -0.005308 -0.044172 -0.000327 -0.000000

 39 H 0.000212 -0.000240 0.006145 -0.041216 -0.005306 -0.000000

 40 H 0.000000 0.000000 0.000000 -0.000000 0.000000 0.003905

 41 H 0.000000 0.000000 0.000000 -0.000000 0.000000 0.003905

 42 H 0.000000 -0.000000 0.000000 0.000000 0.000000 0.000076

 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 0.003713 -0.000326 -0.000844 -0.003804 -0.100180 -0.000018

 2 N -0.000131 -0.000198 0.000567 -0.020650 -0.004898 -0.000005

 3 C 0.000023 -0.000004 -0.000014 0.000426 -0.000656 -0.000001

 4 C 0.000017 0.000000 -0.000004 -0.000092 0.000113 -0.000000

 5 C -0.000344 0.000011 0.000023 0.000246 0.003754 -0.000000

 6 N -0.000000 -0.000000 -0.000001 -0.000006 -0.000025 0.000000

 7 C -0.000000 -0.000000 -0.000002 0.000164 -0.000059 -0.000001

 8 N 0.000002 0.000003 0.000164 -0.003309 0.000219 -0.000006

 9 C -0.000000 -0.000000 -0.000059 0.000219 -0.000009 -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 -0.073233 0.004606 -0.001919 -0.081366 0.561427 -0.000156

 13 C 5.046570 0.621604 -0.053739 -0.065435 0.410576 0.003476

 14 C 0.621604 5.118940 0.420186 -0.097756 -0.068313 -0.041487

 15 C -0.053739 0.420186 4.621931 0.410026 -0.136670 0.518840

 16 N -0.065435 -0.097756 0.410026 7.112585 0.388016 -0.074413

 17 C 0.410576 -0.068313 -0.136670 0.388016 4.655580 0.000190

 18 N 0.003476 -0.041487 0.518840 -0.074413 0.000190 6.571365

 19 N -0.000092 0.000246 -0.003804 -0.020650 0.000426 -0.081366

 20 C 0.000113 0.003754 -0.100180 -0.004898 -0.000656 0.561427

 21 C 0.000017 -0.000344 0.003713 -0.000131 0.000023 -0.073233

 22 C 0.000000 0.000011 -0.000326 -0.000198 -0.000004 0.004606

 23 C -0.000004 0.000023 -0.000844 0.000567 -0.000014 -0.001919

 24 N -0.000000 -0.000000 -0.000018 -0.000005 -0.000001 -0.000156

 25 Zn -0.000719 -0.000395 -0.015664 0.117767 -0.017413 -0.005399

 26 C -0.000000 0.000000 0.000000 0.000001 0.000001 -0.000000

 27 H -0.000152 -0.000004 0.000001 0.000075 -0.000139 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 0.266014 -0.056103 0.009801 0.008953 -0.070530 -0.000020

 31 H -0.043579 0.395842 -0.048983 0.006281 0.009926 0.006277

 32 C -0.000000 -0.000040 -0.000366 0.000063 0.000000 0.014326

 33 H 0.000000 -0.000000 0.000011 0.000001 0.000000 -0.000011

 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 -0.044172 -0.000327 -0.000129 0.000425 -0.005308 0.000008

 41 H -0.044172 -0.000327 -0.000129 0.000425 -0.005308 0.000008

 42 H -0.041216 -0.005306 0.000212 -0.000240 0.006145 -0.000010

 43 H -0.000000 -0.000016 0.000010 0.000014 -0.000000 0.003905

 44 H -0.000000 -0.000016 0.000010 0.000014 -0.000000 0.003905

 45 H 0.000000 -0.000001 0.000040 0.000000 0.000000 0.000076

 19 20 21 22 23 24

 1 C 0.000164 -0.000059 -0.000000 -0.000000 -0.000002 -0.000001

 2 N -0.003309 0.000219 0.000002 0.000003 0.000164 -0.000006

 3 C 0.000219 -0.000009 -0.000000 -0.000000 -0.000059 -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 -0.000005 -0.000001 -0.000000 -0.000000 -0.000018 -0.000156

 7 C 0.000567 -0.000014 -0.000004 0.000023 -0.000844 -0.001919

 8 N -0.020650 0.000426 -0.000092 0.000246 -0.003804 -0.081366

 9 C -0.004898 -0.000656 0.000113 0.003754 -0.100180 0.561427

 10 C -0.000131 0.000023 0.000017 -0.000344 0.003713 -0.073233

 11 C -0.000198 -0.000004 0.000000 0.000011 -0.000326 0.004606

 12 N -0.000006 -0.000025 -0.000000 -0.000000 -0.000001 0.000000

 13 C -0.000092 0.000113 0.000017 0.000000 -0.000004 -0.000000

 14 C 0.000246 0.003754 -0.000344 0.000011 0.000023 -0.000000

 15 C -0.003804 -0.100180 0.003713 -0.000326 -0.000844 -0.000018

 16 N -0.020650 -0.004898 -0.000131 -0.000198 0.000567 -0.000005

 17 C 0.000426 -0.000656 0.000023 -0.000004 -0.000014 -0.000001

 18 N -0.081366 0.561427 -0.073233 0.004606 -0.001919 -0.000156

 19 N 7.112585 0.388016 -0.065435 -0.097756 0.410026 -0.074413

 20 C 0.388016 4.655580 0.410576 -0.068313 -0.136670 0.000190

 21 C -0.065435 0.410576 5.046570 0.621604 -0.053739 0.003476

 22 C -0.097756 -0.068313 0.621604 5.118940 0.420186 -0.041487

 23 C 0.410026 -0.136670 -0.053739 0.420186 4.621931 0.518840

 24 N -0.074413 0.000190 0.003476 -0.041487 0.518840 6.571365

 25 Zn 0.117767 -0.017413 -0.000719 -0.000395 -0.015664 -0.005399

 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 0.000063 0.000000 -0.000000 -0.000040 -0.000366 0.014326

 29 H 0.000001 0.000000 0.000000 -0.000000 0.000011 -0.000011

 30 C 0.000001 0.000001 -0.000000 0.000000 0.000000 -0.000000

 31 H 0.000075 -0.000139 -0.000152 -0.000004 0.000001 0.000000

 32 C 0.008953 -0.070530 0.266014 -0.056103 0.009801 -0.000020

 33 H 0.006281 0.009926 -0.043579 0.395842 -0.048983 0.006277

 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 0.000014 -0.000000 -0.000000 -0.000016 0.000010 0.003905

 38 H 0.000014 -0.000000 -0.000000 -0.000016 0.000010 0.003905

 39 H 0.000000 0.000000 0.000000 -0.000001 0.000040 0.000076

 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 0.000425 -0.005308 -0.044172 -0.000327 -0.000129 0.000008

 44 H 0.000425 -0.005308 -0.044172 -0.000327 -0.000129 0.000008

 45 H -0.000240 0.006145 -0.041216 -0.005306 0.000212 -0.000010

 25 26 27 28 29 30

 1 C -0.015664 0.009801 -0.048983 0.000000 0.000001 -0.000366

 2 N 0.117767 0.008953 0.006281 0.000001 0.000075 0.000063

 3 C -0.017413 -0.070530 0.009926 0.000001 -0.000139 0.000000

 4 C -0.000719 0.266014 -0.043579 -0.000000 -0.000152 -0.000000

 5 C -0.000395 -0.056103 0.395842 0.000000 -0.000004 -0.000040

 6 N -0.005399 0.014326 -0.000011 -0.000020 0.006277 0.000000

 7 C -0.015664 -0.000366 0.000011 0.009801 -0.048983 0.000000

 8 N 0.117767 0.000063 0.000001 0.008953 0.006281 -0.000000

 9 C -0.017413 0.000000 0.000000 -0.070530 0.009926 0.000000

 10 C -0.000719 -0.000000 0.000000 0.266014 -0.043579 -0.000000

 11 C -0.000395 -0.000040 -0.000000 -0.056103 0.395842 -0.000000

 12 N -0.005399 -0.000020 0.006277 -0.000000 0.000000 0.014326

 13 C -0.000719 -0.000000 -0.000152 -0.000000 -0.000000 0.266014

 14 C -0.000395 0.000000 -0.000004 -0.000000 -0.000000 -0.056103

 15 C -0.015664 0.000000 0.000001 0.000000 -0.000000 0.009801

 16 N 0.117767 0.000001 0.000075 -0.000000 0.000000 0.008953

 17 C -0.017413 0.000001 -0.000139 0.000000 -0.000000 -0.070530

 18 N -0.005399 -0.000000 0.000000 0.000000 -0.000000 -0.000020

 19 N 0.117767 -0.000000 0.000000 0.000063 0.000001 0.000001

 20 C -0.017413 0.000000 -0.000000 0.000000 0.000000 0.000001

 21 C -0.000719 -0.000000 -0.000000 -0.000000 0.000000 -0.000000

 22 C -0.000395 -0.000000 -0.000000 -0.000040 -0.000000 0.000000

 23 C -0.015664 0.000000 -0.000000 -0.000366 0.000011 0.000000

 24 N -0.005399 0.000000 -0.000000 0.014326 -0.000011 -0.000000

 25 Zn 10.221248 0.000380 -0.000037 0.000380 -0.000037 0.000380

 26 C 0.000380 5.368877 -0.004663 -0.000000 0.000069 -0.000000

 27 H -0.000037 -0.004663 0.449569 -0.000000 -0.000000 0.000069

 28 C 0.000380 -0.000000 -0.000000 5.368877 -0.004663 0.000000

 29 H -0.000037 0.000069 -0.000000 -0.004663 0.449569 -0.000000

 30 C 0.000380 -0.000000 0.000069 0.000000 -0.000000 5.368877

 31 H -0.000037 -0.000000 -0.000000 -0.000000 0.000000 -0.004663

 32 C 0.000380 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

 33 H -0.000037 -0.000000 0.000000 0.000069 -0.000000 -0.000000

 34 H 0.000067 0.389367 0.001402 -0.000000 0.000000 -0.000000

 35 H 0.000075 0.388838 -0.000118 -0.000000 0.000038 0.000000

 36 H 0.000075 0.388838 -0.000118 -0.000000 0.000038 0.000000

 37 H 0.000075 0.000000 0.000000 0.388838 -0.000118 0.000000

 38 H 0.000075 0.000000 0.000000 0.388838 -0.000118 0.000000

 39 H 0.000067 -0.000000 0.000000 0.389367 0.001402 -0.000000

 40 H 0.000075 -0.000000 0.000038 0.000000 -0.000000 0.388838

 41 H 0.000075 -0.000000 0.000038 0.000000 -0.000000 0.388838

 42 H 0.000067 -0.000000 0.000000 -0.000000 -0.000000 0.389367

 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 0.000067 -0.000000 -0.000000 -0.000000 0.000000 -0.000000

 31 32 33 34 35 36

 1 C 0.000011 0.000000 -0.000000 0.000212 -0.000129 -0.000129

 2 N 0.000001 -0.000000 0.000000 -0.000240 0.000425 0.000425

 3 C 0.000000 0.000000 -0.000000 0.006145 -0.005308 -0.005308

 4 C 0.000000 -0.000000 -0.000000 -0.041216 -0.044172 -0.044172

 5 C -0.000000 -0.000000 -0.000000 -0.005306 -0.000327 -0.000327

 6 N -0.000000 -0.000000 0.000000 0.000076 0.003905 0.003905

 7 C -0.000000 0.000000 0.000001 0.000040 0.000010 0.000010

 8 N 0.000000 0.000001 0.000075 0.000000 0.000014 0.000014

 9 C -0.000000 0.000001 -0.000139 0.000000 -0.000000 -0.000000

 10 C -0.000000 -0.000000 -0.000152 0.000000 -0.000000 -0.000000

 11 C -0.000000 0.000000 -0.000004 -0.000001 -0.000016 -0.000016

 12 N -0.000011 0.000000 -0.000000 -0.000010 0.000008 0.000008

 13 C -0.043579 -0.000000 0.000000 0.000000 0.000000 0.000000

 14 C 0.395842 -0.000040 -0.000000 0.000000 -0.000000 -0.000000

 15 C -0.048983 -0.000366 0.000011 -0.000000 0.000000 0.000000

 16 N 0.006281 0.000063 0.000001 -0.000000 0.000000 0.000000

 17 C 0.009926 0.000000 0.000000 0.000001 -0.000000 -0.000000

 18 N 0.006277 0.014326 -0.000011 -0.000000 -0.000000 -0.000000

 19 N 0.000075 0.008953 0.006281 -0.000000 0.000000 0.000000

 20 C -0.000139 -0.070530 0.009926 0.000000 0.000000 0.000000

 21 C -0.000152 0.266014 -0.043579 0.000000 -0.000000 -0.000000

 22 C -0.000004 -0.056103 0.395842 0.000000 0.000000 0.000000

 23 C 0.000001 0.009801 -0.048983 0.000000 0.000000 0.000000

 24 N 0.000000 -0.000020 0.006277 0.000000 0.000000 0.000000

 25 Zn -0.000037 0.000380 -0.000037 0.000067 0.000075 0.000075

 26 C -0.000000 0.000000 -0.000000 0.389367 0.388838 0.388838

 27 H -0.000000 -0.000000 0.000000 0.001402 -0.000118 -0.000118

 28 C -0.000000 -0.000000 0.000069 -0.000000 -0.000000 -0.000000

 29 H 0.000000 -0.000000 -0.000000 0.000000 0.000038 0.000038

 30 C -0.004663 -0.000000 -0.000000 -0.000000 0.000000 0.000000

 31 H 0.449569 0.000069 -0.000000 0.000000 0.000000 0.000000

 32 C 0.000069 5.368877 -0.004663 -0.000000 0.000000 0.000000

 33 H -0.000000 -0.004663 0.449569 -0.000000 -0.000000 -0.000000

 34 H 0.000000 -0.000000 -0.000000 0.460336 -0.025690 -0.025690

 35 H 0.000000 0.000000 -0.000000 -0.025690 0.472337 -0.029899

 36 H 0.000000 0.000000 -0.000000 -0.025690 -0.029899 0.472337

 37 H -0.000000 -0.000000 0.000038 0.000000 0.000000 -0.000000

 38 H -0.000000 -0.000000 0.000038 0.000000 -0.000000 0.000000

 39 H -0.000000 -0.000000 0.000000 -0.000000 -0.000000 -0.000000

 40 H -0.000118 0.000000 0.000000 -0.000000 0.000000 -0.000000

 41 H -0.000118 0.000000 0.000000 -0.000000 -0.000000 0.000000

 42 H 0.001402 -0.000000 0.000000 -0.000000 0.000000 0.000000

 43 H 0.000038 0.388838 -0.000118 0.000000 0.000000 -0.000000

 44 H 0.000038 0.388838 -0.000118 0.000000 -0.000000 0.000000

 45 H 0.000000 0.389367 0.001402 0.000000 0.000000 0.000000

 37 38 39 40 41 42

 1 C 0.000000 0.000000 -0.000000 0.000010 0.000010 0.000040

 2 N 0.000000 0.000000 -0.000000 0.000014 0.000014 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 -0.000016 -0.000016 -0.000001

 6 N 0.000008 0.000008 -0.000010 0.000000 0.000000 0.000000

 7 C -0.000129 -0.000129 0.000212 0.000000 0.000000 0.000000

 8 N 0.000425 0.000425 -0.000240 0.000000 0.000000 -0.000000

 9 C -0.005308 -0.005308 0.006145 0.000000 0.000000 0.000000

 10 C -0.044172 -0.044172 -0.041216 -0.000000 -0.000000 0.000000

 11 C -0.000327 -0.000327 -0.005306 0.000000 0.000000 0.000000

 12 N -0.000000 -0.000000 -0.000000 0.003905 0.003905 0.000076

 13 C -0.000000 -0.000000 0.000000 -0.044172 -0.044172 -0.041216

 14 C 0.000000 0.000000 0.000000 -0.000327 -0.000327 -0.005306

 15 C 0.000000 0.000000 0.000000 -0.000129 -0.000129 0.000212

 16 N 0.000000 0.000000 -0.000000 0.000425 0.000425 -0.000240

 17 C 0.000000 0.000000 0.000000 -0.005308 -0.005308 0.006145

 18 N 0.000000 0.000000 0.000000 0.000008 0.000008 -0.000010

 19 N 0.000014 0.000014 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 -0.000016 -0.000016 -0.000001 -0.000000 -0.000000 0.000000

 23 C 0.000010 0.000010 0.000040 0.000000 0.000000 -0.000000

 24 N 0.003905 0.003905 0.000076 -0.000000 -0.000000 -0.000000

 25 Zn 0.000075 0.000075 0.000067 0.000075 0.000075 0.000067

 26 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

 27 H 0.000000 0.000000 0.000000 0.000038 0.000038 0.000000

 28 C 0.388838 0.388838 0.389367 0.000000 0.000000 -0.000000

 29 H -0.000118 -0.000118 0.001402 -0.000000 -0.000000 -0.000000

 30 C 0.000000 0.000000 -0.000000 0.388838 0.388838 0.389367

 31 H -0.000000 -0.000000 -0.000000 -0.000118 -0.000118 0.001402

 32 C -0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

 33 H 0.000038 0.000038 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 0.472337 -0.029899 -0.025690 0.000000 -0.000000 0.000000

 38 H -0.029899 0.472337 -0.025690 -0.000000 0.000000 0.000000

 39 H -0.025690 -0.025690 0.460336 0.000000 0.000000 0.000000

 40 H 0.000000 -0.000000 0.000000 0.472337 -0.029899 -0.025690

 41 H -0.000000 0.000000 0.000000 -0.029899 0.472337 -0.025690

 42 H 0.000000 0.000000 0.000000 -0.025690 -0.025690 0.460336

 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 -0.000016 -0.000016 -0.000001

 15 C 0.000010 0.000010 0.000040

 16 N 0.000014 0.000014 0.000000

 17 C -0.000000 -0.000000 0.000000

 18 N 0.003905 0.003905 0.000076

 19 N 0.000425 0.000425 -0.000240

 20 C -0.005308 -0.005308 0.006145

 21 C -0.044172 -0.044172 -0.041216

 22 C -0.000327 -0.000327 -0.005306

 23 C -0.000129 -0.000129 0.000212

 24 N 0.000008 0.000008 -0.000010

 25 Zn 0.000075 0.000075 0.000067

 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 0.000038 0.000038 0.000000

 32 C 0.388838 0.388838 0.389367

 33 H -0.000118 -0.000118 0.001402

 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 0.472337 -0.029899 -0.025690

 44 H -0.029899 0.472337 -0.025690

 45 H -0.025690 -0.025690 0.460336

 Mulliken charges:

 1

 1 C 0.378160

 2 N -0.673318

 3 C 0.373786

 4 C 0.014861

 5 C -0.294261

 6 N -0.410180

 7 C 0.378160

 8 N -0.673318

 9 C 0.373786

 10 C 0.014861

 11 C -0.294261

 12 N -0.410180

 13 C 0.014861

 14 C -0.294261

 15 C 0.378160

 16 N -0.673318

 17 C 0.373786

 18 N -0.410180

 19 N -0.673318

 20 C 0.373786

 21 C 0.014861

 22 C -0.294261

 23 C 0.378160

 24 N -0.410180

 25 Zn 1.463811

 26 C -0.703807

 27 H 0.228275

 28 C -0.703807

 29 H 0.228275

 30 C -0.703807

 31 H 0.228275

 32 C -0.703807

 33 H 0.228275

 34 H 0.240507

 35 H 0.240011

 36 H 0.240011

 37 H 0.240011

 38 H 0.240011

 39 H 0.240507

 40 H 0.240011

 41 H 0.240011

 42 H 0.240507

 43 H 0.240011

 44 H 0.240011

 45 H 0.240507

 Sum of Mulliken charges = -0.00000

 Mulliken charges with hydrogens summed into heavy atoms:

 1

 1 C 0.378160

 2 N -0.673318

 3 C 0.373786

 4 C 0.014861

 5 C -0.065986

 6 N -0.410180

 7 C 0.378160

 8 N -0.673318

 9 C 0.373786

 10 C 0.014861

 11 C -0.065986

 12 N -0.410180

 13 C 0.014861

 14 C -0.065986

 15 C 0.378160

 16 N -0.673318

 17 C 0.373786

 18 N -0.410180

 19 N -0.673318

 20 C 0.373786

 21 C 0.014861

 22 C -0.065986

 23 C 0.378160

 24 N -0.410180

 25 Zn 1.463811

 26 C 0.016724

 28 C 0.016724

 30 C 0.016724

 32 C 0.016724

 Electronic spatial extent (au): <R\*\*2>= 11195.1997

 Charge= -0.0000 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= -159.4449 YY= -159.4449 ZZ= -172.1721

 XY= -0.0000 XZ= -0.0000 YZ= -0.0000

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

 XX= 4.2424 YY= 4.2424 ZZ= -8.4848

 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= -6798.9436 YYYY= -6798.9436 ZZZZ= -207.2805 XXXY= 71.8537

 XXXZ= 0.0000 YYYX= -71.8537 YYYZ= 0.0000 ZZZX= -0.0000

 ZZZY= 0.0000 XXYY= -2615.8182 XXZZ= -1357.0890 YYZZ= -1357.0890

 XXYZ= 0.0000 YYXZ= -0.0000 ZZXY= 0.0000

 N-N= 2.765362955413D+03 E-N=-8.582629308128D+03 KE= 1.320829893689D+03

 Symmetry AG KE= 6.510415995449D+02

 Symmetry BG KE= 6.543085983539D+01

 Symmetry AU KE= 2.240914772315D+01

 Symmetry BU KE= 5.819482865859D+02

 Leave Link 601 at Thu Sep 19 00:42:45 2019, MaxMem= 1342177280 cpu: 7.8

 (Enter /home/blab/g09/l9999.exe)

 Test job not archived.

 1\1\ WCSS.PL-BEM-DHCP-129-94-98-136\SP\RB3LYP TD-FC\GenECP\C20H16N8Zn1

 \BLAB\19-Sep-2019\0\\#p td(root=1,nstates=10) b3lyp/genecp scrf=(solve

 nt=dmso,smd) empiricaldispersion=gd3bj IOp(9/40=3)\\ZntAz0td\\0,1\C,0,

 -2.184914,2.066138,0.\N,0,-1.862347,0.743984,0.\C,0,-2.99981,0.,0.\C,0

 ,-4.15743,0.91558,0.\C,0,-3.641934,2.17904,0.\N,0,-3.09962,-1.333079,0

 .\C,0,-2.066138,-2.184914,0.\N,0,-0.743984,-1.862347,0.\C,0,0.,-2.9998

 1,0.\C,0,-0.91558,-4.15743,0.\C,0,-2.17904,-3.641934,0.\N,0,-1.333079,

 3.09962,0.\C,0,0.91558,4.15743,0.\C,0,2.17904,3.641934,0.\C,0,2.066138

 ,2.184914,0.\N,0,0.743984,1.862347,0.\C,0,0.,2.99981,0.\N,0,3.09962,1.

 333079,0.\N,0,1.862347,-0.743984,0.\C,0,2.99981,0.,0.\C,0,4.15743,-0.9

 1558,0.\C,0,3.641934,-2.17904,0.\C,0,2.184914,-2.066138,0.\N,0,1.33307

 9,-3.09962,0.\Zn,0,0.,0.,0.\C,0,-5.580146,0.47492,0.\H,0,-4.186125,3.1

 13387,0.\C,0,-0.47492,-5.580146,0.\H,0,-3.113387,-4.186125,0.\C,0,0.47

 492,5.580146,0.\H,0,3.113387,4.186125,0.\C,0,5.580146,-0.47492,0.\H,0,

 4.186125,-3.113387,0.\H,0,-6.259862,1.328678,0.\H,0,-5.80321,-0.14056,

 0.877139\H,0,-5.80321,-0.14056,-0.877139\H,0,0.14056,-5.80321,0.877139

 \H,0,0.14056,-5.80321,-0.877139\H,0,-1.328678,-6.259862,0.\H,0,-0.1405

 6,5.80321,0.877139\H,0,-0.14056,5.80321,-0.877139\H,0,1.328678,6.25986

 2,0.\H,0,5.80321,0.14056,0.877139\H,0,5.80321,0.14056,-0.877139\H,0,6.

 259862,-1.328678,0.\\Version=ES64L-G09RevE.01\State=1-AG\HF=-1275.8928

 03\RMSD=3.547e-09\PG=C04H [O(Zn1),SGH(C20H8N8),X(H8)]\\@

 A DANDELION FROM A LOVER MEANS MORE THAN AN ORCHID FROM A FRIEND.

 Job cpu time: 0 days 1 hours 3 minutes 27.8 seconds.

 File lengths (MBytes): RWF= 1312 Int= 0 D2E= 0 Chk= 129 Scr= 1

 Normal termination of Gaussian 09 at Thu Sep 19 00:42:56 2019.