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

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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

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

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\*

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

Pseudopotential Parameters

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

Center Atomic Valence Angular Power

Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

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

1 6

No pseudopotential on this center.

2 7

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.

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

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

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

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

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

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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Virtual (EG) (EG) (BU) (BU) (EG) (EG) (AU) (AU) (AG) (BU)

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

(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:

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

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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.

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

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

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Excited State 3: Singlet-EU 3.1166 eV 397.82 nm f=0.0239 <S\*\*2>=0.000

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81 ->110 0.00241

81 ->111 -0.00139

81 ->124 -0.00164

81 ->125 -0.00103

82 ->120 0.00143

82 ->128 -0.00104

82 ->137 -0.00122

82 ->142 -0.00115

82 ->143 -0.00109

82 ->159 -0.00135

82 ->169 0.00100

82 ->192 -0.00138

82 ->205 -0.00109

82 ->222 0.00106

83 ->114 -0.00138

83 ->118 0.00117

83 ->126 -0.00114

83 ->138 0.00100

83 ->147 0.00101

83 ->148 0.00121

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.

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Population analysis using the SCF density.

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Orbital symmetries:

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

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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.