Entering Gaussian System, Link 0=g09

Initial command:

/apps/gaussian/g09d01/g09/l1.exe "/srv/scratch/z5105842/Gau-351899.inp" -scrdir="/srv/scratch/z5105842/"

Entering Link 1 = /apps/gaussian/g09d01/g09/l1.exe PID= 351915.

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

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

Cite this work as:

Gaussian 09, Revision D.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-G09RevD.01 24-Apr-2013

5-Sep-2019

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

%nprocshared=12

Will use up to 12 processors via shared memory.

%mem=10GB

%chk=ZnOMP0td.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 5 21:44:32 2019, MaxMem= 1342177280 cpu: 0.5

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

--------

ZnOMP0td

--------

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C -0.6867 4.28537 0.00348

C -1.10658 2.88798 0.00435

N 0. 2.08649 0.

C 1.10658 2.88798 -0.00435

C 0.6867 4.28537 -0.00348

C 2.43064 2.43064 -0.00727

C 2.88798 1.10658 -0.00435

N 2.08649 0. 0.

C 2.88798 -1.10658 0.00435

C 4.28537 -0.6867 0.00348

C 4.28537 0.6867 -0.00348

C -2.43064 2.43064 0.00727

C -2.88798 1.10658 0.00435

C -4.28537 0.6867 0.00348

C -4.28537 -0.6867 -0.00348

C -2.88798 -1.10658 -0.00435

N -2.08649 0. 0.

C -2.43064 -2.43064 -0.00727

C -1.10658 -2.88798 -0.00435

C -0.6867 -4.28537 -0.00348

C 0.6867 -4.28537 0.00348

C 1.10658 -2.88798 0.00435

N 0. -2.08649 0.

C 2.43064 -2.43064 0.00727

Zn 0. 0. 0.

H -3.19754 -3.19754 -0.01086

H -3.19754 3.19754 0.01086

H 3.19754 3.19754 -0.01086

H 3.19754 -3.19754 0.01086

C 1.6205 5.45326 -0.00905

H 2.28024 5.43618 -0.88272

H 2.26705 5.45596 0.87478

H 1.07892 6.40034 -0.02417

C -1.6205 5.45326 0.00905

H -2.28024 5.43618 0.88272

H -2.26705 5.45596 -0.87478

H -1.07892 6.40034 0.02417

C -5.45326 1.6205 0.00904

H -5.45596 2.26705 -0.87478

H -5.43618 2.28023 0.88272

H -6.40034 1.07892 0.02416

C -5.45326 -1.6205 -0.00904

H -5.45596 -2.26705 0.87478

H -5.43618 -2.28023 -0.88272

H -6.40034 -1.07892 -0.02416

C -1.6205 -5.45326 -0.00905

H -2.28024 -5.43618 -0.88272

H -2.26705 -5.45596 0.87478

H -1.07892 -6.40034 -0.02417

C 1.6205 -5.45326 0.00905

H 2.28024 -5.43618 0.88272

H 2.26705 -5.45596 -0.87478

H 1.07892 -6.40034 0.02417

C 5.45326 -1.6205 0.00904

H 5.45596 -2.26705 -0.87478

H 5.43618 -2.28023 0.88272

H 6.40034 -1.07892 0.02416

C 5.45326 1.6205 -0.00904

H 5.45596 2.26705 0.87478

H 5.43618 2.28023 -0.88272

H 6.40034 1.07892 -0.02416

NAtoms= 61 NQM= 61 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 12 14 12 12 12 12 14 12 12

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

NucSpn= 0 0 2 0 0 0 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 0.0000000 2.0440000 0.0000000 0.0000000 0.0000000 0.0000000 2.0440000 0.0000000 0.0000000

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

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

Atom 11 12 13 14 15 16 17 18 19 20

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

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

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

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

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

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

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

Atom 21 22 23 24 25 26 27 28 29 30

IAtWgt= 12 12 14 12 64 1 1 1 1 12

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

NucSpn= 0 0 2 0 0 1 1 1 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 2.0440000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 0.0000000 0.0000000 0.4037610 0.0000000 0.0000000 2.7928460 2.7928460 2.7928460 2.7928460 0.0000000

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

Atom 31 32 33 34 35 36 37 38 39 40

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

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

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

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

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

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

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

Atom 41 42 43 44 45 46 47 48 49 50

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

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

NucSpn= 1 0 1 1 1 0 1 1 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 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 0.0000000 2.7928460 2.7928460 2.7928460 0.0000000

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

Atom 51 52 53 54 55 56 57 58 59 60

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

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

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

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

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

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

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

Atom 61

IAtWgt= 1

AtmWgt= 1.0078250

NucSpn= 1

AtZEff= 0.0000000

NQMom= 0.0000000

NMagM= 2.7928460

AtZNuc= 1.0000000

Leave Link 101 at Thu Sep 5 21:44:33 2019, MaxMem= 1342177280 cpu: 1.3

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

Stoichiometry C28H28N4Zn

Framework group D2[O(Zn),C2'(N.N),C2"(N.N),X(C28H28)]

Deg. of freedom 44

Full point group D2 NOp 4

Largest Abelian subgroup D2 NOp 4

Largest concise Abelian subgroup D2 NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.686702 4.285372 0.003479

2 6 0 -1.106584 2.887980 0.004353

3 7 0 0.000000 2.086488 0.000000

4 6 0 1.106584 2.887980 -0.004353

5 6 0 0.686702 4.285372 -0.003479

6 6 0 2.430637 2.430637 -0.007272

7 6 0 2.887980 1.106584 -0.004353

8 7 0 2.086488 0.000000 0.000000

9 6 0 2.887980 -1.106584 0.004353

10 6 0 4.285372 -0.686702 0.003479

11 6 0 4.285372 0.686702 -0.003479

12 6 0 -2.430637 2.430637 0.007272

13 6 0 -2.887980 1.106584 0.004353

14 6 0 -4.285372 0.686702 0.003479

15 6 0 -4.285372 -0.686702 -0.003479

16 6 0 -2.887980 -1.106584 -0.004353

17 7 0 -2.086488 0.000000 0.000000

18 6 0 -2.430637 -2.430637 -0.007272

19 6 0 -1.106584 -2.887980 -0.004353

20 6 0 -0.686702 -4.285372 -0.003479

21 6 0 0.686702 -4.285372 0.003479

22 6 0 1.106584 -2.887980 0.004353

23 7 0 0.000000 -2.086488 0.000000

24 6 0 2.430637 -2.430637 0.007272

25 30 0 0.000000 0.000000 0.000000

26 1 0 -3.197535 -3.197535 -0.010861

27 1 0 -3.197535 3.197535 0.010861

28 1 0 3.197535 3.197535 -0.010861

29 1 0 3.197535 -3.197535 0.010861

30 6 0 1.620502 5.453258 -0.009045

31 1 0 2.280236 5.436177 -0.882720

32 1 0 2.267047 5.455960 0.874782

33 1 0 1.078919 6.400341 -0.024170

34 6 0 -1.620502 5.453258 0.009045

35 1 0 -2.280236 5.436177 0.882720

36 1 0 -2.267047 5.455960 -0.874782

37 1 0 -1.078919 6.400341 0.024170

38 6 0 -5.453258 1.620502 0.009044

39 1 0 -5.455955 2.267051 -0.874780

40 1 0 -5.436181 2.280232 0.882722

41 1 0 -6.400341 1.078919 0.024161

42 6 0 -5.453258 -1.620502 -0.009044

43 1 0 -5.455955 -2.267051 0.874780

44 1 0 -5.436181 -2.280232 -0.882722

45 1 0 -6.400341 -1.078919 -0.024161

46 6 0 -1.620502 -5.453258 -0.009045

47 1 0 -2.280236 -5.436177 -0.882720

48 1 0 -2.267047 -5.455960 0.874782

49 1 0 -1.078919 -6.400341 -0.024170

50 6 0 1.620502 -5.453258 0.009045

51 1 0 2.280236 -5.436177 0.882720

52 1 0 2.267047 -5.455960 -0.874782

53 1 0 1.078919 -6.400341 0.024170

54 6 0 5.453258 -1.620502 0.009044

55 1 0 5.455955 -2.267051 -0.874780

56 1 0 5.436181 -2.280232 0.882722

57 1 0 6.400341 -1.078919 0.024161

58 6 0 5.453258 1.620502 -0.009044

59 1 0 5.455955 2.267051 0.874780

60 1 0 5.436181 2.280232 -0.882722

61 1 0 6.400341 1.078919 -0.024161

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

Rotational constants (GHZ): 0.1320714 0.1320714 0.0662516

Leave Link 202 at Thu Sep 5 21:44:33 2019, MaxMem= 1342177280 cpu: 0.0

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

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

Centers: 25

S 1 1.00

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

S 1 1.00

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

S 1 1.00

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

P 1 1.00

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

P 1 1.00

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

D 3 1.00

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

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

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

D 1 1.00

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

D 1 1.00

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

\*\*\*\*

Centers: 26 27 28 29 31 32 33 35 36 37

Centers: 39 40 41 43 44 45 47 48 49 51

Centers: 52 53 55 56 57 59 60 61 1 2

Centers: 4 5 6 7 9 10 11 12 13 14

Centers: 15 16 18 19 20 21 22 24 30 34

Centers: 38 42 46 50 54 58 3 8 17 23

6-311G\*

\*\*\*\*

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

Pseudopotential Parameters

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

Center Atomic Valence Angular Power

Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

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

1 6

No pseudopotential on this center.

2 6

No pseudopotential on this center.

3 7

No pseudopotential on this center.

4 6

No pseudopotential on this center.

5 6

No pseudopotential on this center.

6 6

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 6

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 6

No pseudopotential on this center.

17 7

No pseudopotential on this center.

18 6

No pseudopotential on this center.

19 6

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 7

No pseudopotential on this center.

24 6

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 1

No pseudopotential on this center.

27 1

No pseudopotential on this center.

28 1

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 1

No pseudopotential on this center.

33 1

No pseudopotential on this center.

34 6

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 6

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 6

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.

46 6

No pseudopotential on this center.

47 1

No pseudopotential on this center.

48 1

No pseudopotential on this center.

49 1

No pseudopotential on this center.

50 6

No pseudopotential on this center.

51 1

No pseudopotential on this center.

52 1

No pseudopotential on this center.

53 1

No pseudopotential on this center.

54 6

No pseudopotential on this center.

55 1

No pseudopotential on this center.

56 1

No pseudopotential on this center.

57 1

No pseudopotential on this center.

58 6

No pseudopotential on this center.

59 1

No pseudopotential on this center.

60 1

No pseudopotential on this center.

61 1

No pseudopotential on this center.

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

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

There are 188 symmetry adapted cartesian basis functions of A symmetry.

There are 175 symmetry adapted cartesian basis functions of B1 symmetry.

There are 178 symmetry adapted cartesian basis functions of B2 symmetry.

There are 178 symmetry adapted cartesian basis functions of B3 symmetry.

There are 176 symmetry adapted basis functions of A symmetry.

There are 168 symmetry adapted basis functions of B1 symmetry.

There are 170 symmetry adapted basis functions of B2 symmetry.

There are 170 symmetry adapted basis functions of B3 symmetry.

684 basis functions, 1203 primitive gaussians, 719 cartesian basis functions

118 alpha electrons 118 beta electrons

nuclear repulsion energy 3398.3901105063 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= 61 NActive= 61 NUniq= 17 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T 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= -0.1507092807 Hartrees.

Nuclear repulsion after empirical dispersion term = 3398.2394012255 Hartrees.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 61.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: Karplus/York (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

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

GePol: Number of generator spheres = 61

GePol: Total number of spheres = 61

GePol: Number of exposed spheres = 61 (100.00%)

GePol: Number of points = 4418

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.87D-10

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 264

GePol: Fraction of low-weight points (<1% of avg) = 5.98%

GePol: Cavity surface area = 465.501 Ang\*\*2

GePol: Cavity volume = 456.370 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0007090702 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3398.2386921554 Hartrees.

Leave Link 301 at Thu Sep 5 21:44:33 2019, MaxMem= 1342177280 cpu: 1.0

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 31878 NPrTT= 143508 LenC2= 24441 LenP2D= 63346.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 684 RedAO= T EigKep= 4.39D-05 NBF= 176 168 170 170

NBsUse= 684 1.00D-06 EigRej= -1.00D+00 NBFU= 176 168 170 170

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= 706 706 706 706 706 MxSgAt= 61 MxSgA2= 61.

Leave Link 302 at Thu Sep 5 21:44:34 2019, MaxMem= 1342177280 cpu: 8.9

(Enter /apps/gaussian/g09d01/g09/l308.exe)

Leave Link 308 at Thu Sep 5 21:44:34 2019, MaxMem= 1342177280 cpu: 1.5

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

DipDrv: MaxL=1.

Leave Link 303 at Thu Sep 5 21:44:34 2019, MaxMem= 1342177280 cpu: 1.1

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

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

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

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

Petite list used in FoFCou.

Harris En= -1369.47800803946

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

Occupied (B3) (B2) (A) (A) (B1) (B1) (B2) (B3) (A) (B3)

(B2) (A) (B1) (B2) (B3) (A) (B3) (B2) (A) (A)

(B1) (B2) (B3) (B1) (A) (B3) (B2) (B1) (A) (B2)

(B3) (B1) (A) (B3) (B2) (A) (B1) (A) (B3) (B2)

(A) (B2) (B3) (B1) (A) (B1) (B2) (B3) (A) (A)

(B3) (B2) (B1) (B2) (B3) (A) (B1) (A) (B2) (B3)

(A) (B1) (B1) (B3) (B2) (A) (B1) (B3) (B2) (B3)

(B2) (A) (A) (B1) (B3) (B2) (A) (B1) (A) (B2)

(B3) (B1) (B1) (A) (B3) (B2) (A) (B2) (B3) (B1)

(A) (B2) (B3) (B3) (B2) (B1) (B1) (A) (B2) (B3)

(B2) (B3) (B1) (B1) (B1) (A) (B3) (B2) (A) (A)

(B2) (B3) (B1) (B3) (B2) (B1) (B1) (A)

Virtual (B2) (B3) (A) (B1) (B2) (B3) (A) (A) (B1) (A)

(B2) (B3) (A) (A) (B2) (B3) (B1) (B2) (B3) (A)

(B1) (B2) (B3) (A) (B1) (A) (B3) (B2) (B3) (B2)

(B1) (A) (B3) (B2) (B1) (B1) (B3) (B2) (B2) (B3)

(B1) (A) (A) (A) (A) (B1) (B3) (B2) (B1) (B3)

(B2) (B1) (B2) (B3) (A) (B1) (B3) (B2) (B1) (A)

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(B2) (A) (A) (A) (B2) (B3) (B3) (B2) (B1) (A)

(B3) (B2) (B1) (B1) (B1) (B3) (B2) (B2) (B3) (A)

(A) (B1) (A) (B3) (B2) (B1) (A) (B1) (B2) (B3)

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(A) (A) (B1) (B1) (B1) (B3) (B2) (B3) (B2) (A)

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(B1) (A) (B3) (B2) (B1) (B1) (B3) (B2) (A) (B3)

(B2) (A) (B1) (A) (B1) (A) (B3) (B2) (B1) (B1)

(B2) (B3) (A) (B1) (A) (B3) (B2) (B2) (B3) (B1)

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(B1) (A) (B3) (B2) (A) (B1) (B3) (B2) (A) (B1)

(B3) (B2) (A) (B1) (B3) (B2) (A) (B1) (B3) (B2)

(B1) (A) (A) (B3) (B2)

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

Leave Link 401 at Thu Sep 5 21:44:36 2019, MaxMem= 1342177280 cpu: 20.5

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1586253 IEndB= 1586253 NGot= 1342177280 MDV= 1341125348

LenX= 1341125348 LenY= 1340607668

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= 640000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

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

wScrn= 0.000000 ICntrl= 0 IOpCl= 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= 58556172.

Iteration 1 A\*A^-1 deviation from unit magnitude is 7.33D-15 for 1105.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.68D-15 for 4314 1332.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.99D-15 for 734.

Iteration 1 A^-1\*A deviation from orthogonality is 2.73D-14 for 4374 4230.

E= -1368.15185229101

DIIS: error= 9.52D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1368.15185229101 IErMin= 1 ErrMin= 9.52D-02

ErrMax= 9.52D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D+00 BMatP= 1.13D+00

IDIUse=3 WtCom= 4.79D-02 WtEn= 9.52D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.105 Goal= None Shift= 0.000

GapD= 0.105 DampG=1.000 DampE=0.250 DampFc=0.2500 IDamp=-1.

Damping current iteration by 2.50D-01

RMSDP=2.54D-03 MaxDP=1.27D-01 OVMax= 1.63D-01

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.26D-04 CP: 9.87D-01

E= -1368.47573586005 Delta-E= -0.323883569037 Rises=F Damp=T

DIIS: error= 4.08D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1368.47573586005 IErMin= 2 ErrMin= 4.08D-02

ErrMax= 4.08D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.08D-01 BMatP= 1.13D+00

IDIUse=3 WtCom= 5.92D-01 WtEn= 4.08D-01

Coeff-Com: -0.970D+00 0.197D+01

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

Coeff: -0.575D+00 0.157D+01

Gap= 0.108 Goal= None Shift= 0.000

RMSDP=9.17D-04 MaxDP=4.51D-02 DE=-3.24D-01 OVMax= 6.87D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.70D-04 CP: 9.64D-01 2.23D+00

E= -1369.01688442846 Delta-E= -0.541148568412 Rises=F Damp=F

DIIS: error= 9.39D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1369.01688442846 IErMin= 3 ErrMin= 9.39D-03

ErrMax= 9.39D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.19D-02 BMatP= 3.08D-01

IDIUse=3 WtCom= 9.06D-01 WtEn= 9.39D-02

Coeff-Com: -0.535D-02 0.237D+00 0.768D+00

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

Coeff: -0.485D-02 0.215D+00 0.790D+00

Gap= 0.109 Goal= None Shift= 0.000

RMSDP=3.20D-04 MaxDP=1.52D-02 DE=-5.41D-01 OVMax= 2.61D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.19D-04 CP: 9.71D-01 1.90D+00 7.84D-01

E= -1369.04463184219 Delta-E= -0.027747413728 Rises=F Damp=F

DIIS: error= 4.11D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1369.04463184219 IErMin= 4 ErrMin= 4.11D-03

ErrMax= 4.11D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.79D-03 BMatP= 3.19D-02

IDIUse=3 WtCom= 9.59D-01 WtEn= 4.11D-02

Coeff-Com: 0.944D-01-0.853D-01 0.411D+00 0.580D+00

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

Coeff: 0.905D-01-0.818D-01 0.394D+00 0.597D+00

Gap= 0.108 Goal= None Shift= 0.000

RMSDP=1.22D-04 MaxDP=3.95D-03 DE=-2.77D-02 OVMax= 1.71D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 6.05D-05 CP: 9.70D-01 1.92D+00 8.77D-01 5.65D-01

E= -1369.04838060020 Delta-E= -0.003748758013 Rises=F Damp=F

DIIS: error= 1.63D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1369.04838060020 IErMin= 5 ErrMin= 1.63D-03

ErrMax= 1.63D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.34D-04 BMatP= 4.79D-03

IDIUse=3 WtCom= 9.84D-01 WtEn= 1.63D-02

Coeff-Com: 0.554D-01-0.666D-01 0.189D+00 0.365D+00 0.457D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.615D-01 0.938D+00

Coeff: 0.545D-01-0.655D-01 0.186D+00 0.360D+00 0.465D+00

Gap= 0.108 Goal= None Shift= 0.000

RMSDP=3.91D-05 MaxDP=2.17D-03 DE=-3.75D-03 OVMax= 7.08D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.85D-05 CP: 9.70D-01 1.93D+00 8.82D-01 6.28D-01 4.85D-01

E= -1369.04901092371 Delta-E= -0.000630323511 Rises=F Damp=F

DIIS: error= 4.93D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1369.04901092371 IErMin= 6 ErrMin= 4.93D-04

ErrMax= 4.93D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.10D-05 BMatP= 7.34D-04

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.93D-03

Coeff-Com: 0.166D-01-0.223D-01 0.489D-01 0.112D+00 0.231D+00 0.613D+00

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

Coeff: 0.166D-01-0.222D-01 0.487D-01 0.112D+00 0.230D+00 0.615D+00

Gap= 0.108 Goal= None Shift= 0.000

RMSDP=6.62D-06 MaxDP=3.30D-04 DE=-6.30D-04 OVMax= 1.18D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.72D-06 CP: 9.70D-01 1.93D+00 8.81D-01 6.26D-01 5.53D-01

CP: 8.10D-01

E= -1369.04903311018 Delta-E= -0.000022186468 Rises=F Damp=F

DIIS: error= 1.39D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1369.04903311018 IErMin= 7 ErrMin= 1.39D-04

ErrMax= 1.39D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.04D-06 BMatP= 3.10D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.39D-03

Coeff-Com: 0.450D-02-0.623D-02 0.132D-01 0.351D-01 0.922D-01 0.322D+00

Coeff-Com: 0.540D+00

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

Coeff-En: 0.100D+01

Coeff: 0.449D-02-0.623D-02 0.131D-01 0.351D-01 0.921D-01 0.321D+00

Coeff: 0.540D+00

Gap= 0.108 Goal= None Shift= 0.000

DSYEVD-2 returned Info= 353 IAlg= 4 N= 176 NDim= 684 NE2= 1959951 trying DSYEV.

RMSDP=1.67D-06 MaxDP=7.12D-05 DE=-2.22D-05 OVMax= 1.16D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 8.50D-07 CP: 9.70D-01 1.93D+00 8.82D-01 6.28D-01 5.55D-01

CP: 7.96D-01 6.59D-01

E= -1369.04903471951 Delta-E= -0.000001609330 Rises=F Damp=F

DIIS: error= 1.35D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1369.04903471951 IErMin= 8 ErrMin= 1.35D-05

ErrMax= 1.35D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.50D-08 BMatP= 2.04D-06

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

Coeff-Com: 0.805D-05-0.469D-04 0.147D-03 0.157D-02 0.659D-02 0.349D-01

Coeff-Com: 0.996D-01 0.857D+00

Coeff: 0.805D-05-0.469D-04 0.147D-03 0.157D-02 0.659D-02 0.349D-01

Coeff: 0.996D-01 0.857D+00

Gap= 0.108 Goal= None Shift= 0.000

RMSDP=2.35D-07 MaxDP=9.48D-06 DE=-1.61D-06 OVMax= 3.46D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 1.82D-07 CP: 9.70D-01 1.93D+00 8.82D-01 6.28D-01 5.56D-01

CP: 8.03D-01 6.74D-01 9.93D-01

E= -1369.04903472652 Delta-E= -0.000000007014 Rises=F Damp=F

DIIS: error= 3.24D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1369.04903472652 IErMin= 9 ErrMin= 3.24D-06

ErrMax= 3.24D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.36D-09 BMatP= 1.50D-08

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

Coeff-Com: -0.189D-03 0.242D-03-0.457D-03-0.538D-03-0.112D-03 0.623D-02

Coeff-Com: 0.335D-01 0.439D+00 0.522D+00

Coeff: -0.189D-03 0.242D-03-0.457D-03-0.538D-03-0.112D-03 0.623D-02

Coeff: 0.335D-01 0.439D+00 0.522D+00

Gap= 0.108 Goal= None Shift= 0.000

RMSDP=7.67D-08 MaxDP=6.77D-06 DE=-7.01D-09 OVMax= 1.95D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 5.45D-08 CP: 9.70D-01 1.93D+00 8.82D-01 6.28D-01 5.56D-01

CP: 8.03D-01 6.76D-01 1.01D+00 7.31D-01

E= -1369.04903473108 Delta-E= -0.000000004558 Rises=F Damp=F

DIIS: error= 1.15D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1369.04903473108 IErMin=10 ErrMin= 1.15D-06

ErrMax= 1.15D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.09D-10 BMatP= 5.36D-09

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

Coeff-Com: -0.499D-04 0.647D-04-0.123D-03-0.234D-03-0.592D-03-0.104D-02

Coeff-Com: 0.312D-02 0.528D-01 0.183D+00 0.763D+00

Coeff: -0.499D-04 0.647D-04-0.123D-03-0.234D-03-0.592D-03-0.104D-02

Coeff: 0.312D-02 0.528D-01 0.183D+00 0.763D+00

Gap= 0.108 Goal= None Shift= 0.000

RMSDP=2.19D-08 MaxDP=1.16D-06 DE=-4.56D-09 OVMax= 4.52D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 1.42D-08 CP: 9.70D-01 1.93D+00 8.82D-01 6.28D-01 5.56D-01

CP: 8.03D-01 6.78D-01 1.01D+00 7.64D-01 8.10D-01

E= -1369.04903473128 Delta-E= -0.000000000198 Rises=F Damp=F

DIIS: error= 2.92D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1369.04903473128 IErMin=11 ErrMin= 2.92D-07

ErrMax= 2.92D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.49D-11 BMatP= 2.09D-10

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

Coeff-Com: -0.197D-04 0.256D-04-0.507D-04-0.115D-03-0.338D-03-0.915D-03

Coeff-Com: 0.194D-03 0.785D-02 0.724D-01 0.397D+00 0.524D+00

Coeff: -0.197D-04 0.256D-04-0.507D-04-0.115D-03-0.338D-03-0.915D-03

Coeff: 0.194D-03 0.785D-02 0.724D-01 0.397D+00 0.524D+00

Gap= 0.108 Goal= None Shift= 0.000

RMSDP=7.29D-09 MaxDP=3.52D-07 DE=-1.98D-10 OVMax= 1.03D-06

Error on total polarization charges = 0.08120

SCF Done: E(RB3LYP) = -1369.04903473 A.U. after 11 cycles

NFock= 11 Conv=0.73D-08 -V/T= 1.9687

KE= 1.413328947183D+03 PE=-1.006194432756D+04 EE= 3.881327653486D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -0.44

(included in total energy above)

Leave Link 502 at Thu Sep 5 21:45:50 2019, MaxMem= 1342177280 cpu: 841.4

(Enter /apps/gaussian/g09d01/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 4.97D-05

Largest core mixing into a valence orbital is 2.18D-05

Range of M.O.s used for correlation: 33 684

NBasis= 684 NAE= 118 NBE= 118 NFC= 32 NFV= 0

NROrb= 652 NOA= 86 NOB= 86 NVA= 566 NVB= 566

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.14491364D+02

Leave Link 801 at Thu Sep 5 21:45:50 2019, MaxMem= 1342177280 cpu: 2.4

(Enter /apps/gaussian/g09d01/g09/l914.exe)

RHF ground state

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

Would need an additional 32960200000 words for in-memory AO integral storage.

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

Inv3: Mode=1 IEnd= 58556172.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.22D-15 for 2210.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.87D-15 for 1999 736.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.44D-15 for 730.

Iteration 1 A^-1\*A deviation from orthogonality is 2.21D-15 for 3300 1106.

Making orbital integer symmetry assigments:

Orbital symmetries:

Occupied (B2) (B3) (A) (A) (A) (B2) (B3) (B1) (B3) (B2)

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(A) (B1) (B3) (B2) (A) (B1) (B3) (B2) (B1) (A)

(A) (B2) (B3)

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: 97352

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.

New state 3 was old state 5

New state 4 was old state 6

New state 5 was old state 8

New state 6 was old state 9

New state 8 was old state 14

New state 9 was old state 15

Excitation Energies [eV] at current iteration:

Root 1 : 2.532692254564365

Root 2 : 2.532692289366061

Root 3 : 3.557563882631848

Root 4 : 3.557563885508262

Root 5 : 3.587186269844151

Root 6 : 3.597933812738586

Root 7 : 3.709123509213593

Root 8 : 3.754118303905395

Root 9 : 3.754118485485762

Root 10 : 3.873763879418334

Root 11 : 3.901235424705939

Root 12 : 3.901235748416082

Root 13 : 4.020778425171322

Root 14 : 4.020778466330357

Root 15 : 4.249162827339244

Root 16 : 4.270104743395202

Root 17 : 4.603579951261548

Root 18 : 5.048205393633132

Root 19 : 5.064415987423142

Root 20 : 5.161302135954504

Root 21 : 5.214577079255498

Root 22 : 5.239687992414264

Root 23 : 5.261634975016082

Root 24 : 5.314540071701632

Root 25 : 5.326399646318252

Root 26 : 5.380547620654016

Root 27 : 5.380547938190575

Root 28 : 5.441767307459032

Root 29 : 5.479102458777920

Root 30 : 5.566328966419998

Root 31 : 5.619662306953797

Root 32 : 5.619662327425837

Root 33 : 5.670697887354311

Root 34 : 5.738695275464579

Root 35 : 5.738695284428410

Root 36 : 5.808472558844082

Root 37 : 6.411949895048318

Root 38 : 6.411950093113676

Root 39 : 6.547400591530465

Root 40 : 6.929884400880877

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 0.052967133390690

Root 2 not converged, maximum delta is 0.052967163295145

New state 3 was old state 4

Root 3 not converged, maximum delta is 0.085388566494148

New state 4 was old state 3

Root 4 not converged, maximum delta is 0.085388513896737

Root 5 not converged, maximum delta is 0.089403047099846

Root 6 not converged, maximum delta is 0.078219497892136

Root 7 not converged, maximum delta is 0.080287753175631

New state 8 was old state 10

Root 8 not converged, maximum delta is 0.030987486769644

New state 9 was old state 8

Root 9 not converged, maximum delta is 0.032901534744804

New state 10 was old state 9

Root 10 not converged, maximum delta is 0.032901534078745

Excitation Energies [eV] at current iteration:

Root 1 : 2.349906000795673 Change is -0.182786253768693

Root 2 : 2.349906037025132 Change is -0.182786252340930

Root 3 : 3.296272266401000 Change is -0.261291619107263

Root 4 : 3.296272320109367 Change is -0.261291562522481

Root 5 : 3.405566719106768 Change is -0.181619550737383

Root 6 : 3.411801052770744 Change is -0.186132759967842

Root 7 : 3.537483007318306 Change is -0.171640501895287

Root 8 : 3.592285205560568 Change is -0.281478673857766

Root 9 : 3.722490793301100 Change is -0.031627510604295

Root 10 : 3.722490981630583 Change is -0.031627503855179

Iteration 3 Dimension 80 NMult 60 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 0.006714094422837

Root 2 not converged, maximum delta is 0.006714105601835

Root 3 not converged, maximum delta is 0.255195725652019

Root 4 not converged, maximum delta is 0.255195657122843

Root 5 not converged, maximum delta is 0.006828610118223

Root 6 not converged, maximum delta is 0.005868010312855

No map to state 7

No map to state 8

New state 9 was old state 7

Root 9 not converged, maximum delta is 0.009147103149854

New state 10 was old state 8

Root 10 not converged, maximum delta is 0.019719940491642

Excitation Energies [eV] at current iteration:

Root 1 : 2.345272253131095 Change is -0.004633747664578

Root 2 : 2.345272291215498 Change is -0.004633745809634

Root 3 : 3.204306629852312 Change is -0.091965636548688

Root 4 : 3.204306697795343 Change is -0.091965622314024

Root 5 : 3.397932350922316 Change is -0.007634368184453

Root 6 : 3.406902953103322 Change is -0.004898099667423

Root 7 : 3.490511592868253

Root 8 : 3.490511748439596

Root 9 : 3.533346284177117 Change is -0.004136723141190

Root 10 : 3.581944552552538 Change is -0.010340653008029

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 0.002305016901318

Root 2 not converged, maximum delta is 0.002305027858764

Root 3 not converged, maximum delta is 0.046764695544113

Root 4 not converged, maximum delta is 0.046764946943636

Root 5 not converged, maximum delta is 0.002696472609636

Root 6 not converged, maximum delta is 0.001558331127998

New state 7 was old state 8

Root 7 not converged, maximum delta is 0.064820018646423

New state 8 was old state 7

Root 8 not converged, maximum delta is 0.064820370638415

Root 9 not converged, maximum delta is 0.003482333609812

Root 10 not converged, maximum delta is 0.001942285241154

Excitation Energies [eV] at current iteration:

Root 1 : 2.344761366221481 Change is -0.000510886909613

Root 2 : 2.344761403152326 Change is -0.000510888063171

Root 3 : 3.186445628076803 Change is -0.017861001775509

Root 4 : 3.186445650863466 Change is -0.017861046931877

Root 5 : 3.397119060234135 Change is -0.000813290688180

Root 6 : 3.406439015791479 Change is -0.000463937311842

Root 7 : 3.454397829056170 Change is -0.036113919383426

Root 8 : 3.454397936879580 Change is -0.036113655988673

Root 9 : 3.532795948854925 Change is -0.000550335322191

Root 10 : 3.580916362104827 Change is -0.001028190447711

Iteration 5 Dimension 120 NMult 100 NNew 20

CISAX will form 20 AO SS matrices at one time.

NMat= 20 NSing= 20 JSym2X=-1.

Root 1 has converged.

Root 2 has converged.

Root 3 not converged, maximum delta is 0.004561025180877

Root 4 not converged, maximum delta is 0.004561050760444

Root 5 has converged.

Root 6 has converged.

Root 7 not converged, maximum delta is 0.006104841390980

Root 8 not converged, maximum delta is 0.006104707891145

Root 9 has converged.

Root 10 has converged.

Excitation Energies [eV] at current iteration:

Root 1 : 2.344733963207801 Change is -0.000027403013680

Root 2 : 2.344734000231568 Change is -0.000027402920759

Root 3 : 3.184961338295825 Change is -0.001484289780977

Root 4 : 3.184961356739335 Change is -0.001484294124131

Root 5 : 3.397076225821392 Change is -0.000042834412743

Root 6 : 3.406416473205141 Change is -0.000022542586338

Root 7 : 3.451239695522194 Change is -0.003158133533976

Root 8 : 3.451239834118664 Change is -0.003158102760916

Root 9 : 3.532754485761267 Change is -0.000041463093658

Root 10 : 3.580767467955823 Change is -0.000148894149005

Iteration 6 Dimension 128 NMult 120 NNew 8

CISAX will form 8 AO SS matrices at one time.

NMat= 8 NSing= 8 JSym2X=-1.

Root 1 has converged.

Root 2 has converged.

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 has converged.

Root 10 has converged.

Excitation Energies [eV] at current iteration:

Root 1 : 2.344733743531031 Change is -0.000000219676770

Root 2 : 2.344733780584532 Change is -0.000000219647035

Root 3 : 3.184871251780718 Change is -0.000090086515107

Root 4 : 3.184871269566418 Change is -0.000090087172917

Root 5 : 3.397076225821416 Change is 0.000000000000024

Root 6 : 3.406416473205068 Change is -0.000000000000073

Root 7 : 3.451050357377186 Change is -0.000189338145007

Root 8 : 3.451050496013111 Change is -0.000189338105554

Root 9 : 3.532754485761267 Change is 0.000000000000000

Root 10 : 3.580767467955823 Change is 0.000000000000000

Convergence achieved 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 0.0000 -0.5981 0.0000 0.3577 0.0205

2 0.5981 0.0000 0.0000 0.3577 0.0205

3 0.0000 -3.8066 0.0000 14.4901 1.1306

4 -3.8066 0.0000 0.0000 14.4901 1.1306

5 0.0000 0.0000 0.0000 0.0000 0.0000

6 0.0000 0.0000 0.0003 0.0000 0.0000

7 -1.5788 0.0000 0.0000 2.4927 0.2108

8 0.0000 1.5788 0.0000 2.4927 0.2108

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 0.0000 0.0525 0.0000 0.0028 0.0213

2 -0.0525 0.0000 0.0000 0.0028 0.0213

3 0.0000 0.4365 0.0000 0.1905 1.0851

4 0.4365 0.0000 0.0000 0.1905 1.0851

5 0.0000 0.0000 0.0000 0.0000 0.0000

6 0.0000 0.0000 0.0000 0.0000 0.0000

7 0.1940 0.0000 0.0000 0.0376 0.1978

8 0.0000 -0.1940 0.0000 0.0376 0.1978

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 0.0005 0.0000

2 0.0005 0.0000 0.0000

3 0.0000 0.0048 0.0000

4 -0.0048 0.0000 0.0000

5 0.0000 0.0000 2.1651

6 0.0000 0.0000 0.0000

7 -0.0049 0.0000 0.0000

8 0.0000 -0.0049 0.0000

9 0.0000 0.0000 0.0000

10 0.0000 0.0000 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 0.0004 0.0000

2 0.0000 0.0000 0.0000 0.0000 0.0000 -0.0004

3 0.0000 0.0000 0.0000 0.0000 -0.0029 0.0000

4 0.0000 0.0000 0.0000 0.0000 0.0000 -0.0029

5 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

6 0.0000 0.0000 0.0000 0.7103 0.0000 0.0000

7 0.0000 0.0000 0.0000 0.0000 0.0000 -0.0014

8 0.0000 0.0000 0.0000 0.0000 0.0014 0.0000

9 0.3129 -0.3129 0.0000 0.0000 0.0000 0.0000

10 0.7322 0.7322 0.0334 0.0000 0.0000 0.0000

<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 0.0111 0.0000 0.1882 0.0665 90.00

2 0.0000 -0.0112 -0.1883 -0.0665 90.00

3 10.1025 0.0000 2.4838 4.1954 90.00

4 0.0000 -10.1006 -2.4838 -4.1948 90.00

5 -0.0006 -0.0006 0.0000 -0.0004 90.00

6 0.0642 -0.0642 0.0000 0.0000 90.00

7 0.0000 -3.4207 -1.9093 -1.7767 90.00

8 3.4197 0.0000 1.9091 1.7763 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 0.1958 0.0000 0.0653

2 -0.1959 0.0000 0.0000 -0.0653

3 0.0000 12.8475 0.0000 4.2825

4 -12.8457 0.0000 0.0000 -4.2819

5 0.0000 0.0000 -0.0004 -0.0001

6 0.0000 0.0000 0.0000 0.0000

7 -5.5013 0.0000 0.0000 -1.8338

8 0.0000 5.5000 0.0000 1.8333

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 0.0000 -0.0314 0.0000 0.0314 0.0209

2 -0.0314 0.0000 0.0000 0.0314 0.0209

3 0.0000 -1.6615 0.0000 1.6615 1.1076

4 -1.6615 0.0000 0.0000 1.6615 1.1076

5 0.0000 0.0000 0.0000 0.0000 0.0000

6 0.0000 0.0000 0.0000 0.0000 0.0000

7 -0.3063 0.0000 0.0000 0.3063 0.2042

8 0.0000 -0.3063 0.0000 0.3063 0.2042

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-B2 2.3447 eV 528.78 nm f=0.0205 <S\*\*2>=0.000

33 ->190 -0.00121

34 ->189 -0.00114

36 ->170 0.00115

37 ->169 0.00107

37 ->173 -0.00102

37 ->206 0.00122

37 ->215 0.00156

40 ->171 -0.00123

40 ->189 0.00105

42 ->162 0.00168

42 ->171 0.00163

42 ->189 -0.00111

42 ->195 0.00108

42 ->217 -0.00104

43 ->210 -0.00143

44 ->173 0.00109

45 ->123 -0.00102

45 ->164 -0.00198

45 ->170 -0.00148

45 ->174 -0.00129

45 ->178 -0.00150

45 ->193 0.00209

45 ->216 0.00100

47 ->175 0.00138

47 ->210 -0.00117

49 ->177 -0.00161

49 ->303 0.00120

54 ->175 -0.00144

54 ->176 0.00138

54 ->184 0.00166

54 ->210 0.00119

54 ->301 0.00113

55 ->162 -0.00123

55 ->165 0.00165

55 ->187 0.00168

55 ->203 -0.00113

55 ->205 0.00173

55 ->238 -0.00111

55 ->275 0.00106

55 ->290 -0.00101

56 ->185 0.00106

56 ->207 0.00114

56 ->213 0.00127

56 ->236 0.00127

56 ->304 -0.00107

57 ->151 -0.00103

57 ->169 -0.00133

57 ->173 0.00111

57 ->177 0.00150

57 ->186 0.00125

57 ->191 -0.00160

57 ->225 -0.00103

58 ->164 0.00107

58 ->213 -0.00102

58 ->236 -0.00101

60 ->163 -0.00101

60 ->206 0.00112

60 ->215 0.00123

63 ->131 -0.00118

63 ->158 0.00114

63 ->175 -0.00120

63 ->176 -0.00180

63 ->194 0.00150

63 ->227 -0.00117

63 ->299 -0.00102

64 ->167 -0.00134

64 ->171 -0.00132

64 ->217 -0.00107

64 ->263 -0.00125

65 ->177 -0.00104

66 ->164 -0.00116

66 ->193 0.00122

66 ->287 -0.00123

67 ->151 -0.00107

67 ->159 0.00148

67 ->169 0.00173

67 ->173 -0.00131

67 ->177 0.00134

67 ->192 -0.00109

68 ->156 -0.00147

68 ->158 -0.00149

68 ->176 0.00185

68 ->220 0.00101

68 ->249 0.00264

68 ->260 -0.00132

69 ->162 0.00103

69 ->171 0.00115

69 ->235 -0.00118

70 ->156 -0.00120

70 ->175 -0.00119

70 ->211 -0.00200

70 ->220 0.00112

70 ->249 0.00188

70 ->260 -0.00114

70 ->301 -0.00147

71 ->147 -0.00119

71 ->162 -0.00155

71 ->165 0.00237

71 ->189 0.00103

71 ->203 -0.00152

71 ->238 -0.00126

71 ->275 0.00149

72 ->123 -0.00134

72 ->164 -0.00219

72 ->193 0.00134

72 ->216 -0.00109

73 ->120 0.00532

73 ->140 -0.00105

73 ->149 0.00355

74 ->123 -0.00132

74 ->152 0.00115

74 ->190 0.00103

74 ->216 -0.00112

75 ->121 -0.00417

75 ->142 0.00269

75 ->146 -0.00173

76 ->148 -0.00132

77 ->123 -0.00139

77 ->136 0.00104

77 ->152 0.00206

77 ->164 0.00122

77 ->170 -0.00118

77 ->261 -0.00126

78 ->120 -0.00182

78 ->140 0.00122

80 ->165 0.00130

80 ->171 0.00112

80 ->172 0.00120

80 ->189 -0.00107

80 ->217 -0.00106

81 ->151 0.00110

81 ->177 -0.00102

81 ->186 -0.00236

81 ->191 0.00131

81 ->206 0.00111

81 ->215 0.00127

81 ->231 0.00184

81 ->237 -0.00109

81 ->250 0.00187

81 ->262 0.00246

81 ->280 0.00113

81 ->286 0.00141

81 ->295 0.00122

81 ->323 -0.00132

82 ->174 -0.00104

83 ->119 0.00346

83 ->128 0.00173

84 ->125 0.00128

85 ->121 0.00235

85 ->132 0.00232

85 ->142 0.00136

86 ->128 0.00225

86 ->141 0.00126

87 ->159 0.00110

87 ->177 0.00176

87 ->191 -0.00132

87 ->192 -0.00124

87 ->215 -0.00131

88 ->156 -0.00101

88 ->176 -0.00218

88 ->182 -0.00121

88 ->184 -0.00190

88 ->210 -0.00174

88 ->249 -0.00236

88 ->288 -0.00106

89 ->126 0.00159

89 ->147 -0.00122

89 ->217 0.00114

89 ->263 0.00108

89 ->275 -0.00130

89 ->284 0.00106

90 ->120 0.00382

90 ->129 0.00219

90 ->140 -0.00262

90 ->149 0.00459

91 ->135 -0.00109

92 ->122 0.00190

92 ->125 0.00452

92 ->138 0.00338

92 ->148 -0.00255

92 ->166 -0.00166

93 ->121 0.00597

93 ->142 -0.00395

93 ->146 0.00293

94 ->126 -0.00156

94 ->147 0.00202

94 ->189 -0.00125

95 ->131 -0.00246

95 ->156 0.00130

95 ->176 0.00185

95 ->194 -0.00150

95 ->210 0.00104

95 ->274 -0.00110

95 ->288 0.00102

96 ->144 -0.00134

96 ->190 0.00126

97 ->124 -0.00104

97 ->151 0.00115

97 ->159 0.00196

97 ->191 -0.00112

97 ->192 -0.00134

97 ->215 -0.00123

98 ->139 -0.00127

98 ->143 -0.00107

98 ->172 0.00113

98 ->204 -0.00104

98 ->217 -0.00106

99 ->221 -0.00115

100 ->120 -0.00961

100 ->129 0.00200

100 ->149 -0.00100

100 ->181 0.00100

100 ->329 0.00141

101 ->124 -0.00161

101 ->135 0.00142

101 ->151 0.00113

101 ->173 0.00122

101 ->177 0.00212

101 ->192 -0.00116

101 ->262 -0.00179

101 ->280 0.00108

102 ->143 -0.00119

102 ->147 0.00120

102 ->162 0.00102

102 ->167 0.00159

102 ->171 0.00156

102 ->187 0.00180

102 ->203 0.00103

102 ->275 -0.00104

103 ->161 0.00123

103 ->168 -0.00107

103 ->184 -0.00137

103 ->197 0.00122

103 ->211 0.00204

103 ->221 0.00126

103 ->227 0.00134

104 ->144 -0.00160

104 ->185 0.00109

104 ->193 0.00144

105 ->144 0.00112

105 ->232 -0.00101

105 ->277 -0.00108

106 ->151 0.00176

106 ->159 0.00142

106 ->169 -0.00268

106 ->177 0.00175

106 ->215 -0.00224

107 ->119 0.01928

107 ->128 -0.00361

107 ->141 -0.00259

107 ->150 0.00424

107 ->223 -0.00114

107 ->240 0.00123

108 ->211 0.00161

109 ->167 0.00103

109 ->171 0.00134

109 ->188 0.00126

109 ->189 -0.00123

109 ->195 -0.00166

109 ->217 -0.00114

109 ->243 -0.00101

109 ->275 0.00113

109 ->279 -0.00114

109 ->284 0.00160

110 ->121 0.01112

110 ->132 0.00295

110 ->239 -0.00101

110 ->242 -0.00107

110 ->285 0.00117

111 ->122 0.00316

111 ->125 0.01502

111 ->138 0.00311

111 ->148 -0.00474

111 ->153 -0.00225

111 ->166 -0.00130

111 ->179 -0.00172

111 ->183 0.00199

111 ->234 -0.00152

111 ->256 0.00172

111 ->325 -0.00114

112 ->174 -0.00137

112 ->178 -0.00120

112 ->190 -0.00156

112 ->201 -0.00149

112 ->232 0.00102

112 ->281 0.00127

112 ->287 0.00132

113 ->120 0.00189

113 ->129 -0.00471

113 ->149 -0.00444

113 ->154 -0.00209

113 ->181 0.00249

114 ->122 0.00310

114 ->125 0.00817

114 ->138 0.00112

114 ->148 -0.00501

114 ->153 -0.00283

114 ->179 -0.00169

114 ->183 0.00213

114 ->218 -0.00110

115 ->121 0.00636

116 ->120 -0.03614

116 ->129 0.00688

116 ->149 0.00423

116 ->154 0.00252

116 ->181 -0.00234

116 ->241 0.00102

117 ->120 -0.46135

117 ->129 0.01397

117 ->149 0.00606

117 ->154 0.00296

117 ->181 -0.00219

117 ->209 -0.00124

117 ->224 -0.00215

117 ->369 -0.00126

118 ->119 0.53351

118 ->128 -0.00764

118 ->141 -0.00159

118 ->150 0.00263

118 ->155 0.00110

118 ->223 -0.00187

118 ->282 -0.00131

118 ->349 -0.00114

33 <-190 -0.00106

34 <-189 -0.00102

37 <-206 0.00105

37 <-215 0.00139

40 <-171 -0.00104

42 <-162 0.00140

42 <-171 0.00138

43 <-210 -0.00128

45 <-164 -0.00165

45 <-170 -0.00121

45 <-174 -0.00107

45 <-178 -0.00127

45 <-193 0.00179

47 <-175 0.00114

47 <-210 -0.00102

49 <-177 -0.00132

49 <-303 0.00103

54 <-175 -0.00119

54 <-176 0.00111

54 <-184 0.00136

54 <-301 0.00103

55 <-165 0.00134

55 <-187 0.00141

55 <-205 0.00146

56 <-213 0.00110

56 <-236 0.00107

57 <-169 -0.00108

57 <-177 0.00118

57 <-186 0.00102

57 <-191 -0.00132

60 <-215 0.00103

63 <-176 -0.00144

63 <-194 0.00124

64 <-167 -0.00104

64 <-171 -0.00103

64 <-263 -0.00106

66 <-287 -0.00105

67 <-159 0.00113

67 <-169 0.00135

67 <-173 -0.00102

67 <-177 0.00105

68 <-156 -0.00110

68 <-158 -0.00111

68 <-176 0.00142

68 <-249 0.00222

68 <-260 -0.00112

70 <-211 -0.00166

70 <-249 0.00159

70 <-301 -0.00126

71 <-162 -0.00119

71 <-165 0.00179

71 <-203 -0.00122

71 <-238 -0.00104

71 <-275 0.00126

72 <-164 -0.00166

72 <-193 0.00108

73 <-120 0.00314

73 <-149 0.00296

75 <-121 -0.00243

75 <-142 0.00193

75 <-146 -0.00129

76 <-148 -0.00126

77 <-152 0.00145

77 <-261 -0.00105

81 <-186 -0.00180

81 <-215 0.00105

81 <-231 0.00153

81 <-250 0.00155

81 <-262 0.00206

81 <-286 0.00120

81 <-295 0.00104

81 <-323 -0.00116

83 <-119 0.00202

83 <-128 0.00142

85 <-121 0.00178

85 <-132 0.00164

86 <-128 0.00138

87 <-177 0.00131

87 <-191 -0.00101

87 <-215 -0.00105

88 <-176 -0.00162

88 <-184 -0.00146

88 <-210 -0.00141

88 <-249 -0.00194

89 <-126 0.00101

89 <-275 -0.00108

90 <-120 0.00137

90 <-129 0.00149

90 <-140 -0.00182

90 <-149 0.00360

92 <-122 0.00133

92 <-125 0.00303

92 <-138 0.00254

92 <-148 -0.00225

92 <-166 -0.00160

93 <-121 0.00316

93 <-142 -0.00270

93 <-146 0.00208

94 <-147 0.00136

95 <-131 -0.00157

95 <-176 0.00138

95 <-194 -0.00116

97 <-159 0.00136

97 <-192 -0.00102

100 <-120 -0.00338

100 <-129 0.00234

100 <-329 0.00117

101 <-177 0.00159

101 <-262 -0.00147

102 <-167 0.00113

102 <-171 0.00114

102 <-187 0.00135

103 <-184 -0.00104

103 <-211 0.00160

103 <-227 0.00110

104 <-144 -0.00106

104 <-193 0.00112

106 <-151 0.00119

106 <-169 -0.00193

106 <-177 0.00128

106 <-215 -0.00178

107 <-119 0.01029

107 <-141 -0.00224

107 <-150 0.00427

108 <-211 0.00122

109 <-195 -0.00129

109 <-284 0.00133

110 <-121 -0.00421

110 <-132 0.00116

110 <-142 0.00221

110 <-285 0.00114

111 <-122 0.00189

111 <-125 0.00308

111 <-138 0.00221

111 <-148 -0.00353

111 <-166 -0.00123

111 <-183 0.00164

111 <-234 -0.00122

111 <-256 0.00149

112 <-190 -0.00113

112 <-201 -0.00110

112 <-281 0.00103

112 <-287 0.00109

113 <-120 0.00598

113 <-129 -0.00308

113 <-149 -0.00252

113 <-154 -0.00133

113 <-181 0.00180

114 <-122 0.00125

114 <-125 0.00572

114 <-148 -0.00249

114 <-153 -0.00197

114 <-179 -0.00129

114 <-183 0.00145

115 <-121 -0.00123

116 <-120 -0.00608

116 <-129 0.00371

116 <-149 0.00261

116 <-154 0.00168

116 <-181 -0.00168

117 <-120 -0.01836

117 <-129 0.00585

117 <-149 0.00322

117 <-154 0.00171

117 <-181 -0.00163

117 <-224 -0.00186

117 <-369 -0.00135

118 <-119 0.00416

118 <-128 -0.00259

118 <-150 0.00216

118 <-223 -0.00133

118 <-247 0.00106

118 <-282 -0.00107

118 <-349 -0.00121

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

Total Energy, E(TD-HF/TD-KS) = -1368.96286735

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

Excited State 2: Singlet-B3 2.3447 eV 528.78 nm f=0.0205 <S\*\*2>=0.000

33 ->191 0.00121

35 ->189 0.00114

36 ->169 -0.00115

37 ->170 0.00107

37 ->174 0.00102

37 ->207 0.00122

37 ->216 -0.00156

39 ->171 0.00123

39 ->189 -0.00105

42 ->210 -0.00143

43 ->162 0.00168

43 ->171 0.00163

43 ->189 -0.00111

43 ->195 0.00108

43 ->217 -0.00104

44 ->174 0.00109

45 ->124 0.00102

45 ->163 0.00198

45 ->169 -0.00148

45 ->173 0.00129

45 ->177 0.00150

45 ->192 -0.00209

45 ->215 -0.00100

46 ->175 -0.00138

46 ->210 0.00117

49 ->178 -0.00161

49 ->304 -0.00120

54 ->162 -0.00123

54 ->165 -0.00165

54 ->187 -0.00168

54 ->203 0.00113

54 ->205 -0.00173

54 ->238 0.00111

54 ->275 -0.00106

54 ->290 0.00101

55 ->175 -0.00144

55 ->176 0.00138

55 ->184 0.00166

55 ->210 0.00119

55 ->301 -0.00113

56 ->186 0.00106

56 ->206 -0.00114

56 ->212 0.00127

56 ->237 0.00127

56 ->303 0.00107

57 ->152 0.00103

57 ->170 -0.00133

57 ->174 -0.00111

57 ->178 -0.00150

57 ->185 -0.00125

57 ->190 0.00160

57 ->226 0.00103

58 ->163 0.00107

58 ->212 -0.00102

58 ->237 -0.00101

60 ->164 0.00101

60 ->207 0.00112

60 ->216 -0.00123

63 ->167 -0.00134

63 ->171 0.00132

63 ->217 0.00107

63 ->263 0.00125

64 ->131 0.00118

64 ->158 -0.00114

64 ->175 0.00120

64 ->176 0.00180

64 ->194 0.00150

64 ->227 -0.00117

64 ->299 0.00102

65 ->178 0.00104

66 ->163 0.00116

66 ->192 -0.00122

66 ->286 0.00123

67 ->152 -0.00107

67 ->160 0.00148

67 ->170 -0.00173

67 ->174 -0.00131

67 ->178 0.00134

67 ->193 -0.00109

68 ->162 -0.00103

68 ->171 -0.00115

68 ->235 0.00118

69 ->156 0.00147

69 ->158 0.00149

69 ->176 -0.00185

69 ->220 0.00101

69 ->249 0.00264

69 ->260 -0.00132

70 ->147 0.00119

70 ->162 0.00155

70 ->165 0.00237

70 ->189 -0.00103

70 ->203 -0.00152

70 ->238 -0.00126

70 ->275 0.00149

71 ->156 0.00120

71 ->175 0.00119

71 ->211 -0.00200

71 ->220 0.00112

71 ->249 0.00188

71 ->260 -0.00114

71 ->301 -0.00147

72 ->124 -0.00134

72 ->163 -0.00219

72 ->192 0.00134

72 ->215 -0.00109

73 ->119 -0.00532

73 ->141 0.00105

73 ->150 -0.00355

74 ->124 0.00132

74 ->151 -0.00115

74 ->191 -0.00103

74 ->215 0.00112

75 ->148 -0.00132

76 ->121 -0.00417

76 ->142 0.00269

76 ->146 -0.00173

77 ->124 0.00139

77 ->135 -0.00104

77 ->151 -0.00206

77 ->163 -0.00122

77 ->169 -0.00118

77 ->262 0.00126

78 ->119 -0.00182

78 ->141 0.00122

79 ->165 0.00130

79 ->171 -0.00112

79 ->172 -0.00120

79 ->189 0.00107

79 ->217 0.00106

81 ->152 0.00110

81 ->178 -0.00102

81 ->185 -0.00236

81 ->190 0.00131

81 ->207 -0.00111

81 ->216 0.00127

81 ->232 0.00184

81 ->236 -0.00109

81 ->251 0.00187

81 ->261 0.00246

81 ->281 0.00113

81 ->287 0.00141

81 ->296 -0.00122

81 ->324 -0.00132

82 ->173 -0.00104

83 ->120 -0.00346

83 ->129 -0.00173

84 ->121 -0.00235

84 ->132 0.00232

84 ->142 -0.00136

85 ->125 0.00128

86 ->129 0.00225

86 ->140 0.00126

87 ->160 -0.00110

87 ->178 -0.00176

87 ->190 0.00132

87 ->193 0.00124

87 ->216 0.00131

88 ->126 -0.00159

88 ->147 0.00122

88 ->217 -0.00114

88 ->263 -0.00108

88 ->275 -0.00130

88 ->284 -0.00106

89 ->156 0.00101

89 ->176 0.00218

89 ->182 -0.00121

89 ->184 0.00190

89 ->210 0.00174

89 ->249 -0.00236

89 ->288 0.00106

90 ->119 -0.00382

90 ->128 -0.00219

90 ->141 0.00262

90 ->150 -0.00459

91 ->136 -0.00109

92 ->121 -0.00597

92 ->142 0.00395

92 ->146 -0.00293

93 ->122 -0.00190

93 ->125 0.00452

93 ->138 -0.00338

93 ->148 0.00255

93 ->166 0.00166

94 ->131 0.00246

94 ->156 -0.00130

94 ->176 -0.00185

94 ->194 -0.00150

94 ->210 -0.00104

94 ->274 0.00110

94 ->288 -0.00102

95 ->126 0.00156

95 ->147 -0.00202

95 ->189 0.00125

96 ->145 -0.00134

96 ->191 -0.00126

97 ->123 0.00104

97 ->152 -0.00115

97 ->160 -0.00196

97 ->190 0.00112

97 ->193 0.00134

97 ->216 0.00123

98 ->221 0.00115

99 ->139 0.00127

99 ->143 -0.00107

99 ->172 -0.00113

99 ->204 0.00104

99 ->217 0.00106

100 ->119 -0.00961

100 ->128 0.00200

100 ->150 -0.00100

100 ->180 -0.00100

100 ->328 0.00141

101 ->123 0.00161

101 ->136 -0.00142

101 ->152 -0.00113

101 ->174 -0.00122

101 ->178 -0.00212

101 ->193 0.00116

101 ->261 0.00179

101 ->281 -0.00108

102 ->161 0.00123

102 ->168 -0.00107

102 ->184 0.00137

102 ->197 -0.00122

102 ->211 0.00204

102 ->221 -0.00126

102 ->227 0.00134

103 ->143 -0.00119

103 ->147 -0.00120

103 ->162 -0.00102

103 ->167 0.00159

103 ->171 -0.00156

103 ->187 0.00180

103 ->203 0.00103

103 ->275 -0.00104

104 ->145 0.00160

104 ->186 0.00109

104 ->192 0.00144

105 ->145 0.00112

105 ->231 0.00101

105 ->276 0.00108

106 ->152 0.00176

106 ->160 0.00142

106 ->170 0.00268

106 ->178 0.00175

106 ->216 -0.00224

107 ->120 -0.01928

107 ->129 0.00361

107 ->140 0.00259

107 ->149 -0.00424

107 ->224 0.00114

107 ->241 -0.00123

108 ->167 0.00103

108 ->171 -0.00134

108 ->188 0.00126

108 ->189 0.00123

108 ->195 0.00166

108 ->217 0.00114

108 ->243 -0.00101

108 ->275 0.00113

108 ->279 0.00114

108 ->284 -0.00160

109 ->211 0.00161

110 ->122 0.00316

110 ->125 -0.01502

110 ->138 0.00311

110 ->148 -0.00474

110 ->153 0.00225

110 ->166 -0.00130

110 ->179 0.00172

110 ->183 0.00199

110 ->234 -0.00152

110 ->256 0.00172

110 ->325 0.00114

111 ->121 0.01112

111 ->132 -0.00295

111 ->239 0.00101

111 ->242 -0.00107

111 ->285 0.00117

112 ->173 -0.00137

112 ->177 -0.00120

112 ->191 -0.00156

112 ->200 -0.00149

112 ->231 0.00102

112 ->280 0.00127

112 ->286 0.00132

113 ->119 -0.00189

113 ->128 0.00471

113 ->150 0.00444

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43 <-171 0.00138

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69 <-260 -0.00112

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77 <-262 0.00105

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93 <-125 0.00303

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104 <-192 0.00112

106 <-152 0.00119

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Excited State 3: Singlet-B2 3.1849 eV 389.29 nm f=1.1306 <S\*\*2>=0.000

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37 ->151 -0.00109

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43 ->210 0.00113

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45 ->216 -0.00132

45 ->232 -0.00111

45 ->304 -0.00107

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49 ->169 -0.00199

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52 ->127 0.00100

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53 ->185 0.00105

54 ->131 -0.00113

54 ->156 0.00120

54 ->168 -0.00112

54 ->175 0.00165

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54 ->211 -0.00121

54 ->227 -0.00127

55 ->126 0.00140

55 ->147 -0.00247

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49 <-169 -0.00152

54 <-175 0.00127

54 <-184 -0.00133

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54 <-211 -0.00111

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67 <-250 -0.00127

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68 <-176 0.00235

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69 <-126 -0.00184

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96 <-152 0.00218

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98 <-143 -0.00181

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98 <-172 0.00320

98 <-217 -0.00125

99 <-158 -0.00267

99 <-161 -0.00197

99 <-175 0.00198

99 <-210 -0.00108

99 <-227 -0.00111

100 <-129 0.00528

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100 <-154 0.00179

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101 <-145 0.00170

101 <-159 -0.00333

101 <-169 -0.00559

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107 <-119 -0.00250

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109 <-143 -0.00220

109 <-147 0.00185

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109 <-172 -0.00611

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109 <-204 -0.00217

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110 <-214 -0.00431

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111 <-138 -0.00660

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111 <-219 -0.00175

111 <-234 0.00214

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112 <-133 -0.00205

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112 <-144 -0.00199

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112 <-170 0.00321

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112 <-180 -0.00103

112 <-185 -0.00556

112 <-198 -0.00118

112 <-201 -0.00205

112 <-207 -0.00481

112 <-216 -0.00191

112 <-226 0.00120

112 <-232 0.00212

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113 <-181 0.00275

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113 <-283 0.00154

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114 <-166 0.00492

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114 <-219 0.00116

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115 <-146 0.00178

115 <-239 -0.00146

115 <-242 -0.00151

115 <-352 0.00101

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116 <-241 0.00343

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118 <-247 0.00195

118 <-282 -0.00106

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118 <-339 -0.00109

Excited State 4: Singlet-B3 3.1849 eV 389.29 nm f=1.1306 <S\*\*2>=0.000

37 ->123 0.00121

37 ->152 -0.00109

38 ->163 -0.00111

40 ->175 -0.00141

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42 ->156 0.00118

42 ->210 -0.00113

45 ->124 0.00157

45 ->151 -0.00192

45 ->215 -0.00132

45 ->231 -0.00111

45 ->303 0.00107

48 ->178 -0.00108

49 ->152 -0.00112

49 ->170 -0.00199

50 ->200 0.00115

51 ->127 -0.00100

51 ->162 -0.00108

52 ->131 0.00102

52 ->156 -0.00105

53 ->186 -0.00105

54 ->126 -0.00140

54 ->147 0.00247

54 ->187 0.00100

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55 ->156 -0.00120

55 ->168 -0.00112

55 ->175 -0.00165

55 ->184 0.00164

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55 ->227 -0.00127

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56 ->173 0.00210

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Excited State 5: Singlet-B1 3.3971 eV 364.97 nm f=0.0000 <S\*\*2>=0.000

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67 ->171 -0.00224

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108 ->152 -0.00201

108 ->160 0.00146

108 ->170 -0.00120

108 ->185 0.00160

108 ->190 -0.00148

108 ->207 -0.00145

108 ->213 0.00111

108 ->226 0.00108

108 ->287 0.00101

109 ->151 0.00201

109 ->159 -0.00146

109 ->169 -0.00120

109 ->186 -0.00160

109 ->191 0.00148

109 ->206 -0.00145

109 ->212 -0.00111

109 ->225 -0.00108

109 ->286 -0.00101

110 ->120 0.02725

110 ->129 0.00415

110 ->140 -0.00171

111 ->119 0.02725

111 ->128 0.00415

111 ->141 -0.00171

112 ->156 -0.00150

112 ->158 -0.00202

112 ->175 0.00104

112 ->176 0.00220

112 ->184 -0.00147

112 ->210 -0.00160

112 ->222 -0.00104

112 ->288 0.00135

113 ->132 -0.01455

113 ->157 -0.00512

113 ->293 0.00169

114 ->119 -0.49673

114 ->128 0.01656

114 ->141 0.00455

114 ->150 -0.01140

114 ->155 -0.00392

114 ->240 -0.00147

114 ->282 -0.00162

115 ->120 0.49673

115 ->129 -0.01656

115 ->140 -0.00455

115 ->149 0.01140

115 ->154 -0.00392

115 ->241 0.00147

115 ->283 0.00162

116 ->121 -0.05277

116 ->142 0.01610

116 ->146 -0.01482

116 ->242 -0.00260

116 ->259 -0.00113

117 ->132 0.00609

117 ->239 0.00146

118 ->122 0.00243

118 ->138 0.00275

118 ->166 -0.00200

118 ->234 -0.00158

118 ->312 0.00116

118 ->345 -0.00116

38 <-220 0.00108

39 <-174 0.00107

40 <-173 -0.00107

41 <-175 -0.00139

50 <-227 0.00107

53 <-175 0.00101

56 <-175 0.00184

56 <-176 -0.00101

60 <-165 -0.00132

63 <-174 0.00123

64 <-173 -0.00123

66 <-168 -0.00134

66 <-194 -0.00117

66 <-220 0.00165

67 <-127 0.00113

67 <-171 -0.00143

67 <-195 0.00101

68 <-174 0.00112

68 <-185 0.00120

69 <-173 -0.00112

69 <-186 -0.00120

70 <-170 0.00139

70 <-178 0.00101

71 <-169 0.00139

71 <-177 -0.00101

72 <-184 -0.00164

73 <-132 -0.00284

74 <-161 0.00120

75 <-120 -0.00364

75 <-129 -0.00275

76 <-119 -0.00364

76 <-128 -0.00275

77 <-161 -0.00133

77 <-194 -0.00112

77 <-211 -0.00101

77 <-220 0.00152

78 <-121 -0.00441

78 <-142 -0.00107

79 <-160 0.00162

80 <-159 -0.00162

81 <-147 -0.00102

81 <-171 -0.00196

82 <-158 -0.00163

83 <-153 0.00112

90 <-132 0.00101

91 <-139 0.00153

92 <-119 -0.00203

93 <-120 0.00203

96 <-161 -0.00116

96 <-220 0.00198

96 <-227 -0.00116

96 <-289 -0.00122

97 <-143 -0.00133

98 <-159 -0.00102

98 <-191 0.00102

98 <-225 -0.00133

99 <-160 0.00102

99 <-190 -0.00102

99 <-226 0.00133

100 <-121 -0.00316

100 <-142 0.00104

101 <-203 0.00102

102 <-225 -0.00106

102 <-228 -0.00118

103 <-226 0.00106

103 <-229 0.00118

104 <-158 -0.00163

104 <-176 0.00151

104 <-222 -0.00209

104 <-233 -0.00158

104 <-255 -0.00126

104 <-294 0.00135

105 <-194 0.00145

105 <-220 -0.00165

105 <-266 -0.00122

106 <-139 -0.00103

107 <-125 -0.00165

108 <-152 -0.00104

109 <-151 0.00104

110 <-120 0.00343

110 <-129 0.00309

111 <-119 0.00343

111 <-128 0.00308

112 <-176 0.00115

112 <-210 -0.00103

112 <-288 0.00100

113 <-132 -0.00933

113 <-157 -0.00352

113 <-239 -0.00186

113 <-293 0.00114

114 <-119 0.01044

114 <-128 0.00774

114 <-150 -0.00419

114 <-155 -0.00230

114 <-223 0.00105

114 <-240 -0.00125

114 <-282 -0.00121

115 <-120 -0.01044

115 <-129 -0.00774

115 <-149 0.00419

115 <-154 -0.00230

115 <-224 -0.00105

115 <-241 0.00125

115 <-283 0.00121

116 <-121 0.01256

116 <-142 0.00242

116 <-146 -0.00527

116 <-214 0.00100

116 <-242 -0.00177

116 <-259 -0.00123

118 <-122 0.00374

118 <-138 0.00128

118 <-148 -0.00182

118 <-312 0.00110

118 <-345 -0.00108

Excited State 6: Singlet-B1 3.4064 eV 363.97 nm f=0.0000 <S\*\*2>=0.000

38 ->175 0.00215

39 ->164 0.00109

39 ->174 0.00137

39 ->207 0.00108

40 ->163 0.00109

40 ->173 0.00137

40 ->206 -0.00108

41 ->168 0.00144

41 ->220 -0.00123

41 ->227 0.00113

44 ->165 -0.00113

45 ->175 -0.00134

46 ->173 0.00114

47 ->174 0.00114

48 ->171 -0.00143

50 ->175 -0.00146

50 ->184 0.00107

53 ->220 0.00106

53 ->227 -0.00158

54 ->174 -0.00151

55 ->173 0.00151

56 ->161 -0.00144

56 ->168 -0.00173

56 ->194 -0.00130

56 ->220 0.00201

60 ->127 -0.00107

60 ->147 0.00108

60 ->171 0.00292

60 ->217 -0.00110

60 ->235 -0.00111

63 ->133 -0.00150

63 ->152 -0.00191

63 ->164 0.00120

63 ->170 -0.00148

63 ->174 -0.00129

63 ->178 -0.00138

63 ->190 -0.00112

64 ->134 -0.00150

64 ->151 -0.00191

64 ->163 0.00120

64 ->169 0.00148

64 ->173 -0.00129

64 ->177 -0.00138

64 ->191 -0.00112

65 ->126 0.00103

65 ->127 0.00120

65 ->147 -0.00154

65 ->171 -0.00167

65 ->195 0.00107

66 ->156 0.00162

66 ->158 0.00159

66 ->176 -0.00177

66 ->184 0.00168

66 ->210 0.00136

66 ->222 0.00144

66 ->233 0.00132

66 ->288 -0.00127

67 ->165 0.00273

67 ->187 -0.00257

67 ->203 -0.00135

67 ->290 0.00108

68 ->136 0.00103

68 ->160 0.00150

68 ->170 -0.00105

68 ->185 0.00197

68 ->190 -0.00148

68 ->213 0.00116

68 ->226 0.00113

68 ->229 0.00124

69 ->135 0.00103

69 ->159 0.00150

69 ->169 0.00105

69 ->186 0.00197

69 ->191 -0.00148

69 ->212 0.00116

69 ->225 0.00113

69 ->228 0.00124

70 ->174 -0.00125

70 ->292 -0.00100

71 ->173 -0.00125

71 ->291 -0.00100

72 ->137 0.00147

72 ->194 0.00172

72 ->227 -0.00175

72 ->249 0.00130

72 ->266 -0.00129

72 ->289 -0.00113

73 ->121 0.00575

73 ->142 0.00177

73 ->146 -0.00204

74 ->131 0.00136

74 ->156 -0.00114

74 ->158 -0.00153

75 ->120 -0.00484

75 ->129 -0.00415

75 ->149 0.00193

76 ->119 0.00484

76 ->128 0.00415

76 ->150 -0.00193

77 ->131 0.00183

77 ->156 -0.00168

77 ->158 0.00207

77 ->210 0.00131

77 ->222 0.00121

77 ->274 0.00142

78 ->132 0.00533

79 ->160 0.00195

79 ->170 0.00127

80 ->159 0.00195

80 ->169 -0.00127

81 ->187 -0.00116

81 ->203 0.00118

81 ->243 -0.00131

82 ->161 0.00217

82 ->260 -0.00112

83 ->138 -0.00163

84 ->119 0.00225

84 ->141 0.00120

84 ->155 -0.00110

85 ->120 0.00225

85 ->140 0.00120

85 ->154 0.00110

86 ->153 -0.00173

87 ->139 -0.00118

87 ->147 -0.00143

87 ->172 0.00121

87 ->217 0.00107

88 ->144 -0.00123

88 ->152 0.00136

89 ->145 0.00123

89 ->151 0.00136

90 ->121 0.00521

90 ->142 -0.00337

91 ->130 0.00130

91 ->143 -0.00229

91 ->167 0.00120

92 ->119 0.01434

92 ->141 -0.00241

92 ->155 -0.00112

93 ->120 0.01434

93 ->140 -0.00241

93 ->154 0.00112

94 ->135 -0.00134

94 ->145 0.00156

94 ->151 -0.00120

95 ->136 -0.00134

95 ->144 -0.00156

95 ->152 -0.00120

96 ->158 0.00204

96 ->175 0.00102

96 ->176 -0.00144

96 ->184 -0.00121

96 ->222 0.00183

96 ->233 0.00128

96 ->255 0.00113

96 ->294 -0.00180

97 ->139 0.00275

97 ->147 -0.00219

98 ->145 0.00101

98 ->151 -0.00117

98 ->159 0.00176

98 ->191 -0.00171

98 ->225 0.00168

98 ->228 0.00161

98 ->291 -0.00106

99 ->144 -0.00101

99 ->152 -0.00117

99 ->160 0.00176

99 ->190 -0.00171

99 ->226 0.00168

99 ->229 0.00161

99 ->292 -0.00106

100 ->132 0.00219

100 ->157 0.00214

101 ->126 0.00184

101 ->127 -0.00149

101 ->171 0.00126

101 ->172 -0.00110

101 ->195 -0.00147

101 ->235 -0.00102

101 ->284 0.00103

102 ->124 0.00117

102 ->159 0.00138

102 ->169 -0.00104

102 ->177 0.00178

102 ->186 0.00130

102 ->212 0.00142

102 ->225 0.00113

103 ->123 0.00117

103 ->160 0.00138

103 ->170 0.00104

103 ->178 0.00178

103 ->185 0.00130

103 ->213 0.00142

103 ->226 0.00113

104 ->161 0.00261

104 ->182 -0.00131

104 ->194 0.00223

104 ->211 0.00158

104 ->220 -0.00336

104 ->249 0.00101

104 ->266 -0.00162

104 ->289 0.00113

104 ->301 -0.00141

104 ->318 0.00151

105 ->156 -0.00142

105 ->158 -0.00154

105 ->176 0.00164

105 ->184 -0.00121

105 ->210 -0.00213

105 ->221 -0.00115

105 ->222 -0.00183

105 ->233 -0.00150

105 ->255 -0.00115

105 ->288 0.00172

106 ->130 -0.00177

106 ->167 0.00141

106 ->187 0.00208

106 ->188 -0.00136

106 ->203 0.00146

106 ->238 -0.00106

106 ->252 -0.00107

106 ->278 -0.00160

107 ->138 0.00252

108 ->152 -0.00103

108 ->160 0.00111

108 ->185 0.00114

108 ->190 -0.00113

108 ->201 -0.00119

108 ->207 -0.00204

108 ->213 0.00124

108 ->226 0.00127

108 ->236 -0.00136

108 ->277 -0.00116

108 ->287 0.00146

109 ->151 -0.00103

109 ->159 0.00111

109 ->186 0.00114

109 ->191 -0.00113

109 ->200 -0.00119

109 ->206 0.00204

109 ->212 0.00124

109 ->225 0.00127

109 ->237 -0.00136

109 ->276 -0.00116

109 ->286 0.00146

110 ->120 0.00595

110 ->129 0.00342

110 ->140 0.00227

110 ->149 -0.00266

110 ->154 0.00136

110 ->224 0.00122

110 ->283 -0.00100

111 ->119 -0.00595

111 ->128 -0.00342

111 ->141 -0.00227

111 ->150 0.00266

111 ->155 0.00136

111 ->223 -0.00122

111 ->282 0.00100

112 ->161 0.00113

112 ->194 0.00173

112 ->211 0.00187

112 ->227 -0.00141

112 ->249 0.00194

112 ->266 -0.00188

113 ->121 -0.04495

113 ->142 0.01459

113 ->146 -0.01299

113 ->214 0.00103

113 ->242 -0.00277

113 ->259 -0.00131

114 ->119 0.49751

114 ->128 -0.01485

114 ->141 -0.00392

114 ->150 0.01042

114 ->155 0.00310

114 ->240 0.00172

114 ->282 0.00155

114 ->349 0.00107

115 ->120 0.49751

115 ->129 -0.01485

115 ->140 -0.00392

115 ->149 0.01042

115 ->154 -0.00310

115 ->241 0.00172

115 ->283 0.00155

115 ->348 0.00107

116 ->132 -0.01339

116 ->157 -0.00437

116 ->293 0.00185

117 ->121 -0.03405

117 ->142 -0.00258

117 ->214 -0.00233

118 ->125 0.00448

118 ->153 -0.00226

118 ->179 -0.00116

118 ->253 0.00114

118 ->267 0.00111

118 ->341 0.00111

38 <-175 0.00171

39 <-174 0.00113

40 <-173 0.00113

41 <-168 0.00119

41 <-220 -0.00115

45 <-175 -0.00107

48 <-171 -0.00103

50 <-175 -0.00112

53 <-227 -0.00114

54 <-174 -0.00110

55 <-173 0.00110

56 <-161 -0.00100

56 <-168 -0.00130

56 <-220 0.00171

60 <-171 0.00191

63 <-152 -0.00130

63 <-170 -0.00106

64 <-151 -0.00130

64 <-169 0.00106

65 <-147 -0.00101

65 <-171 -0.00110

66 <-156 0.00109

66 <-158 0.00104

66 <-176 -0.00119

66 <-184 0.00114

66 <-222 0.00118

66 <-233 0.00107

67 <-165 0.00188

67 <-187 -0.00171

68 <-185 0.00144

68 <-190 -0.00104

68 <-229 0.00102

69 <-186 0.00144

69 <-191 -0.00104

69 <-228 0.00102

72 <-194 0.00115

72 <-227 -0.00126

72 <-266 -0.00100

73 <-121 0.00420

73 <-142 0.00111

73 <-146 -0.00152

75 <-120 -0.00294

75 <-129 -0.00312

75 <-149 0.00118

76 <-119 0.00294

76 <-128 0.00312

76 <-150 -0.00118

77 <-131 0.00103

77 <-156 -0.00101

77 <-158 0.00125

77 <-274 0.00112

78 <-132 0.00356

79 <-160 0.00121

80 <-159 0.00121

81 <-243 -0.00101

82 <-161 0.00134

86 <-153 -0.00103

91 <-143 -0.00129

92 <-119 0.00173

93 <-120 0.00173

96 <-158 0.00125

96 <-222 0.00138

96 <-233 0.00100

96 <-294 -0.00145

97 <-139 0.00149

97 <-147 -0.00119

98 <-159 0.00106

98 <-191 -0.00109

98 <-225 0.00127

98 <-228 0.00123

99 <-160 0.00106

99 <-190 -0.00109

99 <-226 0.00127

99 <-229 0.00123

100 <-132 0.00195

100 <-157 0.00145

102 <-177 0.00102

102 <-212 0.00104

103 <-178 0.00102

103 <-213 0.00104

104 <-161 0.00154

104 <-194 0.00147

104 <-211 0.00107

104 <-220 -0.00257

104 <-266 -0.00122

104 <-301 -0.00112

104 <-318 0.00123

105 <-210 -0.00142

105 <-222 -0.00138

105 <-233 -0.00111

105 <-288 0.00129

106 <-187 0.00121

106 <-278 -0.00125

107 <-138 0.00136

108 <-207 -0.00132

108 <-287 0.00110

109 <-206 0.00132

109 <-286 0.00110

110 <-120 -0.00181

110 <-129 0.00219

110 <-149 -0.00154

111 <-119 0.00181

111 <-128 -0.00219

111 <-150 0.00154

112 <-194 0.00104

112 <-211 0.00121

112 <-249 0.00139

112 <-266 -0.00135

113 <-121 0.01146

113 <-142 0.00216

113 <-146 -0.00442

113 <-214 0.00112

113 <-242 -0.00191

113 <-259 -0.00138

114 <-119 -0.01024

114 <-128 -0.00771

114 <-150 0.00259

114 <-155 0.00206

114 <-240 0.00125

114 <-282 0.00118

115 <-120 -0.01024

115 <-129 -0.00771

115 <-149 0.00259

115 <-154 -0.00206

115 <-241 0.00125

115 <-283 0.00118

116 <-132 -0.00864

116 <-157 -0.00291

116 <-239 -0.00195

116 <-293 0.00125

117 <-121 0.00386

117 <-142 -0.00256

117 <-214 -0.00128

117 <-242 0.00120

118 <-125 0.00312

118 <-300 -0.00101

118 <-341 0.00129

Excited State 7: Singlet-B3 3.4511 eV 359.27 nm f=0.2108 <S\*\*2>=0.000

35 ->127 0.00114

35 ->167 0.00125

35 ->189 0.00117

36 ->169 -0.00125

36 ->191 -0.00101

38 ->177 -0.00101

39 ->127 -0.00130

40 ->175 0.00132

41 ->225 0.00101

43 ->167 0.00133

44 ->174 0.00108

45 ->169 -0.00133

50 ->191 0.00102

51 ->127 -0.00221

51 ->162 -0.00106

51 ->189 -0.00103

52 ->227 -0.00107

53 ->191 -0.00103

55 ->168 0.00106

55 ->184 0.00102

55 ->211 -0.00127

55 ->220 -0.00114

56 ->191 0.00117

56 ->228 -0.00113

57 ->152 0.00171

57 ->170 0.00108

57 ->178 -0.00130

58 ->191 -0.00155

60 ->133 -0.00100

60 ->164 0.00175

60 ->178 -0.00124

60 ->185 -0.00147

62 ->122 -0.00105

62 ->138 -0.00108

62 ->148 0.00144

62 ->166 -0.00166

63 ->147 -0.00211

63 ->165 0.00119

63 ->187 -0.00117

63 ->195 -0.00111

64 ->161 0.00105

64 ->168 0.00101

64 ->194 0.00148

64 ->222 0.00134

65 ->207 -0.00164

66 ->135 0.00129

66 ->173 0.00200

66 ->177 0.00145

66 ->186 0.00210

67 ->133 -0.00157

67 ->152 0.00151

67 ->164 0.00194

67 ->190 -0.00234

67 ->226 -0.00108

68 ->126 -0.00201

68 ->127 0.00281

68 ->165 0.00118

68 ->167 -0.00120

68 ->171 -0.00144

68 ->172 0.00166

68 ->187 -0.00141

68 ->189 0.00225

69 ->156 0.00109

69 ->158 0.00114

69 ->175 0.00225

69 ->210 0.00145

69 ->220 -0.00119

69 ->233 0.00150

69 ->299 -0.00130

70 ->127 -0.00487

70 ->147 0.00136

70 ->162 -0.00249

70 ->167 0.00114

70 ->171 0.00116

71 ->131 -0.00135

71 ->288 0.00113

72 ->134 -0.00101

72 ->163 0.00143

72 ->177 -0.00214

72 ->191 -0.00171

72 ->192 -0.00101

72 ->215 -0.00108

73 ->119 0.00484

73 ->128 0.00182

73 ->141 0.00101

73 ->150 -0.00138

73 ->208 0.00116

74 ->124 0.00133

74 ->135 -0.00101

74 ->151 -0.00236

74 ->159 -0.00125

74 ->169 0.00149

74 ->191 0.00139

75 ->122 -0.00354

75 ->166 -0.00121

76 ->121 0.00306

76 ->132 0.00309

76 ->142 0.00140

77 ->124 0.00173

77 ->135 -0.00132

77 ->151 -0.00299

77 ->159 0.00241

77 ->163 0.00171

77 ->173 0.00131

78 ->119 0.00213

78 ->128 0.00232

78 ->150 -0.00121

79 ->127 -0.00446

79 ->130 0.00113

79 ->162 -0.00181

79 ->167 -0.00197

79 ->172 -0.00165

80 ->158 0.00255

80 ->161 0.00244

80 ->175 0.00134

80 ->176 -0.00120

80 ->211 0.00178

81 ->123 0.00147

81 ->152 -0.00198

81 ->164 0.00118

81 ->170 -0.00149

81 ->174 -0.00129

81 ->190 0.00247

81 ->193 -0.00147

81 ->207 0.00128

81 ->229 -0.00128

82 ->134 0.00155

82 ->159 0.00292

82 ->173 0.00129

82 ->177 0.00117

83 ->181 0.00105

85 ->179 0.00102

86 ->120 -0.00163

86 ->181 0.00101

87 ->136 -0.00124

87 ->170 0.00126

87 ->174 -0.00241

87 ->185 0.00189

87 ->190 -0.00105

87 ->193 0.00156

87 ->213 0.00102

88 ->127 0.00133

88 ->130 0.00123

88 ->143 -0.00102

88 ->165 -0.00173

88 ->167 0.00313

88 ->172 0.00121

88 ->189 -0.00235

88 ->203 0.00157

88 ->205 -0.00167

88 ->235 0.00103

89 ->131 -0.00217

89 ->156 0.00199

89 ->161 0.00144

89 ->168 0.00220

89 ->211 -0.00155

90 ->119 0.00566

90 ->128 -0.00212

90 ->208 0.00192

91 ->123 -0.00167

91 ->133 0.00209

91 ->144 -0.00169

91 ->178 -0.00125

91 ->193 0.00123

92 ->121 0.00240

92 ->142 -0.00199

92 ->146 0.00160

93 ->122 0.00631

93 ->125 0.00197

93 ->166 0.00283

93 ->218 -0.00118

93 ->219 -0.00159

94 ->131 0.00204

94 ->156 -0.00298

94 ->161 -0.00127

94 ->168 -0.00118

94 ->182 0.00174

94 ->194 -0.00111

94 ->211 0.00134

95 ->126 0.00269

95 ->130 0.00187

95 ->139 -0.00160

95 ->143 -0.00152

95 ->165 0.00354

95 ->167 -0.00256

95 ->171 0.00265

95 ->189 0.00109

96 ->151 0.00176

96 ->159 0.00149

96 ->163 0.00256

96 ->169 -0.00164

96 ->186 0.00118

96 ->191 -0.00183

96 ->206 -0.00193

96 ->225 0.00128

96 ->228 0.00106

96 ->291 -0.00104

97 ->123 0.00219

97 ->133 -0.00276

97 ->144 0.00236

97 ->152 -0.00136

97 ->164 -0.00107

97 ->170 0.00204

97 ->185 0.00169

98 ->161 0.00331

98 ->168 0.00122

98 ->175 0.00189

98 ->182 -0.00162

98 ->184 -0.00141

98 ->194 0.00208

98 ->220 -0.00215

98 ->222 0.00188

98 ->227 0.00107

98 ->233 0.00115

98 ->294 -0.00128

99 ->127 0.00341

99 ->130 0.00185

99 ->139 -0.00197

99 ->147 -0.00268

99 ->167 -0.00119

99 ->171 -0.00162

99 ->172 0.00254

99 ->195 -0.00121

100 ->119 0.01577

100 ->128 -0.00107

100 ->141 -0.00150

100 ->150 0.00191

100 ->208 -0.00199

100 ->240 -0.00155

100 ->297 -0.00127

101 ->133 -0.00118

101 ->144 -0.00162

101 ->160 -0.00393

101 ->170 0.00498

101 ->178 -0.00156

101 ->185 0.00104

101 ->190 0.00148

101 ->193 0.00182

101 ->201 -0.00171

101 ->207 0.00185

101 ->304 -0.00103

102 ->158 0.00329

102 ->161 -0.00130

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Excited State 8: Singlet-B2 3.4511 eV 359.27 nm f=0.2108 <S\*\*2>=0.000

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71 <-127 0.00276

71 <-162 0.00166

72 <-178 -0.00146

72 <-190 -0.00115

73 <-120 -0.00285

73 <-129 -0.00138

74 <-152 0.00143

75 <-121 0.00213

75 <-132 -0.00219

76 <-122 -0.00193

77 <-152 0.00180

77 <-160 -0.00148

77 <-164 -0.00112

78 <-120 0.00163

78 <-129 0.00170

79 <-158 -0.00157

79 <-161 0.00150

79 <-211 0.00130

80 <-127 0.00239

80 <-162 0.00111

80 <-167 -0.00128

80 <-172 0.00105

81 <-151 -0.00120

81 <-191 0.00178

81 <-192 -0.00105

82 <-160 0.00179

86 <-119 -0.00150

87 <-173 0.00156

87 <-186 -0.00127

87 <-192 -0.00107

88 <-131 0.00116

88 <-156 -0.00118

88 <-168 0.00140

88 <-211 -0.00113

89 <-165 -0.00111

89 <-167 0.00198

89 <-189 0.00163

89 <-203 0.00109

89 <-205 -0.00120

90 <-120 -0.00137

90 <-129 0.00158

90 <-209 -0.00128

91 <-134 0.00112

92 <-122 -0.00322

92 <-125 0.00150

92 <-166 -0.00202

94 <-126 -0.00134

94 <-165 0.00219

94 <-167 -0.00162

94 <-171 -0.00166

95 <-131 -0.00103

95 <-156 0.00174

95 <-182 0.00116

96 <-152 -0.00102

96 <-164 -0.00163

96 <-170 -0.00106

96 <-190 0.00129

96 <-207 -0.00136

97 <-124 -0.00105

97 <-134 0.00145

97 <-145 0.00131

97 <-169 0.00126

97 <-186 -0.00112

98 <-127 -0.00167

98 <-139 0.00108

98 <-147 0.00153

98 <-171 0.00105

98 <-172 -0.00157

99 <-161 0.00197

99 <-175 -0.00134

99 <-182 -0.00103

99 <-194 0.00141

99 <-220 -0.00164

99 <-222 -0.00141

99 <-294 0.00103

100 <-209 -0.00115

100 <-241 -0.00125

100 <-298 -0.00105

101 <-159 0.00229

101 <-169 0.00309

101 <-191 -0.00104

101 <-192 -0.00125

101 <-200 0.00114

101 <-206 0.00129

102 <-126 0.00104

102 <-127 -0.00310

102 <-139 -0.00150

102 <-143 0.00104

102 <-162 -0.00128

102 <-167 -0.00177

102 <-172 -0.00169

102 <-203 0.00114

103 <-158 -0.00188

103 <-175 -0.00117

103 <-176 0.00112

103 <-184 0.00125

103 <-220 -0.00160

103 <-221 -0.00133

103 <-227 0.00108

104 <-174 0.00155

104 <-190 -0.00190

104 <-216 -0.00173

104 <-226 0.00167

104 <-229 0.00160

105 <-144 -0.00132

105 <-174 0.00179

105 <-178 0.00178

105 <-207 -0.00137

105 <-226 0.00101

106 <-145 -0.00131

106 <-159 -0.00165

106 <-163 -0.00101

106 <-177 -0.00154

106 <-192 0.00106

106 <-200 0.00102

106 <-286 -0.00103

107 <-119 0.00256

107 <-128 0.00347

107 <-150 -0.00163

107 <-155 -0.00130

107 <-208 -0.00136

108 <-158 -0.00179

108 <-168 0.00103

108 <-176 0.00375

108 <-194 0.00150

108 <-220 -0.00114

109 <-126 -0.00211

109 <-127 0.00768

109 <-139 0.00230

109 <-143 0.00132

109 <-162 0.00226

109 <-167 0.00147

109 <-172 0.00430

109 <-187 -0.00214

109 <-195 -0.00232

109 <-204 0.00188

109 <-205 -0.00161

109 <-284 0.00166

109 <-340 -0.00129

110 <-121 -0.00583

110 <-132 -0.00404

110 <-142 -0.00101

110 <-146 0.00328

110 <-157 -0.00162

110 <-214 0.00124

110 <-239 0.00116

111 <-122 0.00157

111 <-138 0.00226

111 <-300 0.00104

112 <-123 0.00139

112 <-133 0.00110

112 <-144 0.00174

112 <-152 -0.00162

112 <-160 0.00241

112 <-170 -0.00262

112 <-178 0.00365

112 <-185 0.00503

112 <-190 -0.00104

112 <-207 0.00339

112 <-216 0.00153

112 <-287 0.00176

112 <-311 -0.00103

113 <-120 -0.00443

113 <-129 -0.01117

113 <-140 0.00161

113 <-154 -0.00274

113 <-241 0.00148

114 <-122 -0.00383

114 <-125 0.00717

114 <-138 0.00119

114 <-148 -0.00272

114 <-166 -0.00459

114 <-300 -0.00145

115 <-121 0.01084

115 <-132 -0.01003

115 <-142 0.00249

115 <-146 -0.00471

115 <-157 -0.00357

115 <-214 0.00129

115 <-239 -0.00102

116 <-120 -0.01573

116 <-129 -0.00452

116 <-140 -0.00119

116 <-149 0.00725

116 <-154 -0.00166

116 <-209 -0.00125

116 <-298 -0.00129

117 <-120 0.03991

117 <-129 -0.00672

117 <-140 -0.00248

117 <-154 -0.00179

117 <-209 -0.00104

117 <-298 0.00127

118 <-119 0.03245

118 <-128 -0.00920

118 <-141 -0.00243

118 <-150 0.00480

118 <-155 0.00284

Excited State 9: Singlet-A 3.5328 eV 350.96 nm f=0.0000 <S\*\*2>=0.000

33 ->167 -0.00152

34 ->170 -0.00135

35 ->169 -0.00135

36 ->127 0.00111

36 ->147 0.00113

36 ->189 0.00131

38 ->167 0.00119

41 ->127 -0.00159

41 ->162 -0.00102

41 ->189 -0.00121

44 ->175 -0.00102

45 ->167 0.00151

49 ->184 -0.00127

50 ->187 0.00112

51 ->169 0.00100

51 ->177 0.00119

51 ->191 0.00135

52 ->170 -0.00100

52 ->178 0.00119

52 ->190 0.00135

53 ->127 0.00245

53 ->189 0.00151

56 ->189 -0.00123

57 ->168 -0.00114

57 ->182 0.00124

57 ->211 0.00155

58 ->189 0.00125

59 ->167 -0.00108

63 ->159 -0.00116

63 ->177 -0.00170

63 ->191 0.00136

64 ->160 0.00116

64 ->178 0.00170

64 ->190 -0.00136

65 ->182 -0.00102

66 ->167 0.00205

66 ->187 0.00160

67 ->156 0.00126

67 ->176 0.00116

67 ->184 0.00160

67 ->210 -0.00139

67 ->222 0.00152

67 ->299 0.00146

68 ->177 -0.00143

68 ->186 -0.00117

68 ->191 -0.00220

68 ->228 0.00106

69 ->178 0.00143

69 ->185 0.00117

69 ->190 0.00220

69 ->229 -0.00106

70 ->186 0.00182

70 ->215 0.00103

71 ->185 -0.00182

71 ->216 -0.00103

72 ->126 -0.00121

72 ->127 0.00430

72 ->147 -0.00127

72 ->171 -0.00129

72 ->172 0.00253

72 ->263 -0.00103

73 ->125 -0.00235

74 ->165 0.00178

74 ->167 -0.00124

75 ->119 0.00189

76 ->120 0.00189

77 ->167 -0.00155

77 ->205 0.00110

78 ->122 0.00227

78 ->166 0.00126

79 ->169 0.00156

79 ->177 0.00112

80 ->170 0.00156

80 ->178 -0.00112

81 ->131 0.00138

81 ->175 0.00135

81 ->210 0.00225

81 ->233 0.00112

81 ->299 -0.00169

82 ->127 -0.00248

82 ->172 -0.00124

82 ->189 -0.00117

83 ->132 -0.00216

84 ->129 0.00182

85 ->128 -0.00182

86 ->121 -0.00259

86 ->142 -0.00101

87 ->211 0.00196

87 ->266 -0.00106

88 ->169 -0.00128

88 ->215 -0.00120

89 ->170 -0.00128

89 ->216 0.00120

90 ->125 -0.00343

92 ->120 -0.00200

92 ->140 0.00148

92 ->149 -0.00232

92 ->209 0.00115

93 ->119 0.00200

93 ->141 -0.00148

93 ->150 0.00232

93 ->208 -0.00115

94 ->160 -0.00157

94 ->170 0.00147

94 ->178 -0.00106

94 ->193 0.00101

95 ->159 0.00157

95 ->169 0.00147

95 ->177 0.00106

95 ->192 -0.00101

96 ->143 0.00138

96 ->167 0.00242

96 ->187 -0.00104

96 ->238 -0.00123

96 ->275 0.00141

97 ->211 0.00143

98 ->160 0.00105

98 ->178 0.00157

98 ->185 0.00173

98 ->190 -0.00126

99 ->159 -0.00105

99 ->177 -0.00157

99 ->186 -0.00173

99 ->191 0.00126

100 ->122 0.00596

100 ->138 -0.00123

100 ->148 0.00131

100 ->166 0.00402

101 ->161 -0.00264

101 ->168 -0.00260

101 ->179 -0.00117

101 ->182 0.00271

101 ->194 -0.00273

101 ->211 0.00207

102 ->160 -0.00155

102 ->170 0.00121

102 ->190 0.00130

102 ->207 0.00243

103 ->159 0.00155

103 ->169 0.00121

103 ->191 -0.00130

103 ->206 0.00243

104 ->127 0.00454

104 ->139 0.00130

104 ->147 -0.00155

104 ->171 -0.00186

104 ->172 0.00252

104 ->263 -0.00140

105 ->130 -0.00110

105 ->187 -0.00298

105 ->203 -0.00132

105 ->205 -0.00163

105 ->275 0.00152

105 ->278 0.00115

106 ->158 0.00193

106 ->176 -0.00253

106 ->221 0.00110

106 ->288 -0.00132

106 ->294 0.00109

107 ->132 -0.00767

107 ->157 -0.00310

108 ->124 0.00238

108 ->145 -0.00219

108 ->151 -0.00132

108 ->159 0.00103

108 ->169 0.00163

108 ->173 -0.00214

108 ->177 0.00105

108 ->186 0.00383

108 ->191 -0.00136

108 ->206 -0.00427

108 ->215 0.00139

108 ->280 0.00118

108 ->286 0.00208

108 ->310 -0.00103

109 ->123 -0.00238

109 ->144 -0.00219

109 ->152 0.00132

109 ->160 -0.00103

109 ->170 0.00163

109 ->174 0.00214

109 ->178 -0.00105

109 ->185 -0.00383

109 ->190 0.00136

109 ->207 -0.00427

109 ->216 -0.00139

109 ->281 -0.00118

109 ->287 -0.00208

109 ->311 0.00103

110 ->119 -0.01982

110 ->128 0.01057

110 ->150 -0.00283

110 ->155 -0.00254

110 ->240 -0.00101

111 ->120 -0.01982

111 ->129 0.01057

111 ->149 -0.00283

111 ->154 0.00254

111 ->241 -0.00101

112 ->126 0.00748

112 ->127 -0.02572

112 ->139 -0.00541

112 ->162 -0.00551

112 ->172 -0.00903

112 ->195 0.00405

112 ->204 -0.00380

112 ->217 -0.00139

112 ->273 -0.00158

112 ->279 0.00203

112 ->284 -0.00312

112 ->351 -0.00124

113 ->125 -0.00637

113 ->218 -0.00192

113 ->300 -0.00147

113 ->325 0.00124

114 ->120 -0.49776

114 ->129 -0.00172

114 ->140 0.00293

114 ->149 -0.00609

114 ->154 -0.00106

114 ->209 0.00229

114 ->298 0.00143

115 ->119 0.49777

115 ->128 0.00172

115 ->141 -0.00293

115 ->150 0.00609

115 ->155 -0.00106

115 ->208 -0.00229

115 ->297 -0.00143

116 ->122 0.00541

116 ->138 -0.00283

116 ->148 0.00835

116 ->166 0.00534

116 ->183 -0.00169

116 ->219 -0.00154

117 ->125 0.03514

117 ->153 -0.00340

117 ->300 -0.00191

118 ->121 0.03129

118 ->142 0.00919

118 ->146 -0.01321

118 ->242 -0.00127

33 <-167 -0.00123

34 <-170 -0.00108

35 <-169 -0.00108

36 <-189 0.00106

41 <-127 -0.00113

45 <-167 0.00117

51 <-191 0.00104

52 <-190 0.00104

53 <-127 0.00164

53 <-189 0.00115

57 <-211 0.00120

63 <-177 -0.00121

64 <-178 0.00121

66 <-167 0.00137

66 <-187 0.00114

67 <-184 0.00112

67 <-210 -0.00102

67 <-222 0.00114

67 <-299 0.00116

68 <-191 -0.00159

69 <-190 0.00159

70 <-186 0.00125

71 <-185 -0.00125

72 <-127 0.00233

72 <-172 0.00162

73 <-125 -0.00103

74 <-165 0.00115

75 <-119 0.00110

76 <-120 0.00110

78 <-122 0.00120

79 <-169 0.00100

80 <-170 0.00100

81 <-210 0.00166

81 <-299 -0.00134

82 <-127 -0.00125

83 <-132 -0.00124

87 <-211 0.00141

90 <-125 -0.00290

92 <-120 0.00282

92 <-149 -0.00144

93 <-119 -0.00282

93 <-150 0.00144

96 <-167 0.00153

96 <-275 0.00107

98 <-178 0.00100

98 <-185 0.00112

99 <-177 -0.00100

99 <-186 -0.00112

100 <-122 0.00293

100 <-166 0.00254

101 <-161 -0.00153

101 <-168 -0.00157

101 <-182 0.00179

101 <-194 -0.00185

101 <-211 0.00147

102 <-207 0.00165

103 <-206 0.00165

104 <-127 0.00203

104 <-171 -0.00112

104 <-172 0.00148

104 <-263 -0.00105

105 <-187 -0.00192

105 <-205 -0.00114

105 <-275 0.00116

106 <-158 0.00109

106 <-176 -0.00159

106 <-288 -0.00100

107 <-132 -0.00454

107 <-157 -0.00207

108 <-145 -0.00107

108 <-173 -0.00124

108 <-186 0.00231

108 <-206 -0.00280

108 <-286 0.00155

109 <-144 -0.00107

109 <-174 0.00124

109 <-185 -0.00231

109 <-207 -0.00280

109 <-287 -0.00155

110 <-119 -0.00478

110 <-128 0.00518

110 <-150 -0.00228

110 <-155 -0.00172

111 <-120 -0.00478

111 <-129 0.00518

111 <-149 -0.00228

111 <-154 0.00172

112 <-126 0.00241

112 <-127 -0.00863

112 <-139 -0.00223

112 <-162 -0.00261

112 <-172 -0.00468

112 <-195 0.00250

112 <-204 -0.00234

112 <-273 -0.00113

112 <-279 0.00150

112 <-284 -0.00230

113 <-125 0.00795

113 <-153 -0.00139

114 <-120 0.00887

114 <-129 -0.00547

114 <-149 -0.00361

114 <-154 -0.00154

114 <-209 0.00118

114 <-298 0.00132

115 <-119 -0.00887

115 <-128 0.00547

115 <-150 0.00361

115 <-155 -0.00154

115 <-208 -0.00118

115 <-297 -0.00132

116 <-122 0.00183

116 <-138 -0.00182

116 <-148 0.00425

116 <-166 0.00386

116 <-183 -0.00125

117 <-125 0.01066

117 <-153 -0.00251

117 <-300 -0.00146

118 <-121 0.00230

118 <-142 0.00509

118 <-146 -0.00660

Excited State 10: Singlet-A 3.5808 eV 346.25 nm f=0.0000 <S\*\*2>=0.000

33 ->127 -0.00122

33 ->147 -0.00106

33 ->189 -0.00148

34 ->152 0.00104

34 ->170 0.00144

34 ->190 -0.00103

35 ->151 0.00104

35 ->169 -0.00144

35 ->191 -0.00103

36 ->167 0.00204

36 ->275 0.00109

38 ->127 0.00166

38 ->189 0.00118

41 ->167 -0.00149

42 ->170 -0.00143

43 ->169 -0.00143

44 ->168 0.00101

45 ->171 0.00123

49 ->211 0.00130

50 ->127 -0.00220

50 ->189 -0.00129

51 ->191 0.00143

52 ->190 -0.00143

53 ->187 -0.00118

57 ->158 0.00130

57 ->175 0.00164

57 ->176 -0.00238

57 ->184 -0.00160

57 ->222 -0.00144

57 ->299 -0.00165

58 ->167 0.00149

58 ->275 0.00116

60 ->175 -0.00189

60 ->184 0.00107

63 ->151 -0.00117

63 ->159 0.00205

63 ->169 0.00177

63 ->177 0.00199

63 ->191 -0.00174

63 ->206 0.00155

64 ->152 -0.00117

64 ->160 0.00205

64 ->170 -0.00177

64 ->178 0.00199

64 ->190 -0.00174

64 ->207 -0.00155

65 ->158 -0.00165

65 ->176 0.00272

65 ->222 0.00106

66 ->127 -0.00226

66 ->147 0.00243

66 ->162 0.00151

66 ->171 0.00206

66 ->172 -0.00152

67 ->161 0.00215

67 ->179 0.00133

67 ->182 -0.00312

67 ->194 0.00295

67 ->211 -0.00152

67 ->227 -0.00121

67 ->249 -0.00112

67 ->260 0.00100

68 ->159 -0.00134

68 ->163 -0.00165

68 ->173 -0.00159

68 ->177 -0.00274

68 ->192 0.00106

68 ->286 0.00112

69 ->160 -0.00134

69 ->164 -0.00165

69 ->174 -0.00159

69 ->178 -0.00274

69 ->193 0.00106

69 ->287 0.00112

70 ->151 0.00177

70 ->169 -0.00117

70 ->173 -0.00114

70 ->177 0.00122

71 ->152 0.00177

71 ->170 0.00117

71 ->174 -0.00114

71 ->178 0.00122

72 ->130 0.00100

72 ->167 -0.00224

72 ->187 -0.00196

73 ->122 -0.00139

73 ->148 -0.00184

73 ->166 -0.00180

74 ->126 0.00251

74 ->127 -0.00281

74 ->147 -0.00171

74 ->171 -0.00108

74 ->172 -0.00116

75 ->119 0.00234

75 ->128 -0.00160

75 ->150 -0.00122

76 ->120 -0.00234

76 ->129 0.00160

76 ->149 0.00122

77 ->126 0.00153

77 ->147 -0.00229

77 ->171 0.00129

78 ->125 0.00217

79 ->124 0.00110

79 ->151 -0.00110

79 ->169 0.00121

80 ->123 0.00110

80 ->152 -0.00110

80 ->170 -0.00121

81 ->161 -0.00228

81 ->168 -0.00293

81 ->182 0.00223

81 ->194 -0.00250

81 ->211 0.00201

81 ->220 0.00167

81 ->249 0.00199

81 ->260 -0.00112

82 ->165 0.00172

83 ->121 0.00377

83 ->142 0.00165

84 ->120 0.00134

84 ->129 0.00292

85 ->119 0.00134

85 ->128 0.00292

86 ->132 0.00266

87 ->156 -0.00202

87 ->184 -0.00236

87 ->222 -0.00132

88 ->124 -0.00149

88 ->151 0.00208

88 ->173 0.00122

88 ->177 0.00131

88 ->191 -0.00158

88 ->200 0.00136

88 ->225 -0.00118

89 ->123 -0.00149

89 ->152 0.00208

89 ->174 0.00122

89 ->178 0.00131

89 ->190 -0.00158

89 ->201 0.00136

89 ->226 -0.00118

90 ->138 0.00384

90 ->148 -0.00317

90 ->166 -0.00244

92 ->120 -0.00192

92 ->129 0.00400

92 ->140 -0.00294

92 ->149 0.00340

93 ->119 -0.00192

93 ->128 0.00400

93 ->141 -0.00294

93 ->150 0.00340

94 ->123 0.00219

94 ->136 -0.00168

94 ->152 -0.00178

94 ->160 -0.00184

94 ->170 0.00110

94 ->174 -0.00121

94 ->178 -0.00130

94 ->190 0.00176

94 ->207 0.00111

94 ->229 -0.00108

95 ->124 0.00219

95 ->135 -0.00168

95 ->151 -0.00178

95 ->159 -0.00184

95 ->169 -0.00110

95 ->173 -0.00121

95 ->177 -0.00130

95 ->191 0.00176

95 ->206 -0.00111

95 ->228 -0.00108

96 ->139 -0.00159

96 ->147 0.00133

96 ->162 0.00197

96 ->189 0.00185

96 ->195 0.00273

96 ->217 -0.00108

96 ->284 -0.00164

97 ->131 0.00210

97 ->156 -0.00224

97 ->184 -0.00160

98 ->152 -0.00136

98 ->160 0.00119

98 ->170 -0.00233

98 ->207 -0.00180

99 ->151 -0.00136

99 ->159 0.00119

99 ->169 0.00233

99 ->206 0.00180

100 ->125 0.01064

100 ->300 -0.00110

101 ->131 0.00307

101 ->156 -0.00212

101 ->158 0.00260

101 ->175 0.00173

101 ->176 -0.00548

101 ->184 -0.00100

101 ->210 0.00205

101 ->222 -0.00178

101 ->299 -0.00201

102 ->160 -0.00168

102 ->178 -0.00206

102 ->185 -0.00236

102 ->190 0.00236

102 ->193 0.00107

102 ->226 0.00119

102 ->236 0.00132

103 ->159 -0.00168

103 ->177 -0.00206

103 ->186 -0.00236

103 ->191 0.00236

103 ->192 0.00107

103 ->225 0.00119

103 ->237 0.00132

104 ->143 -0.00130

104 ->167 -0.00260

104 ->238 0.00180

104 ->252 0.00116

104 ->275 -0.00115

105 ->126 0.00162

105 ->139 -0.00115

105 ->147 -0.00154

105 ->162 0.00131

105 ->171 -0.00334

105 ->189 0.00181

105 ->195 0.00325

105 ->273 -0.00136

105 ->279 0.00120

105 ->284 -0.00241

106 ->161 -0.00149

106 ->182 0.00149

106 ->194 -0.00283

106 ->227 0.00187

106 ->289 0.00141

107 ->121 0.00231

107 ->142 0.00178

107 ->146 -0.00543

108 ->124 0.00162

108 ->145 -0.00206

108 ->163 0.00185

108 ->169 0.00119

108 ->173 -0.00223

108 ->177 -0.00155

108 ->186 0.00101

108 ->191 -0.00392

108 ->192 -0.00207

108 ->200 -0.00113

108 ->206 -0.00328

108 ->225 -0.00126

108 ->276 0.00142

108 ->280 0.00218

108 ->286 0.00167

109 ->123 0.00162

109 ->144 0.00206

109 ->164 0.00185

109 ->170 -0.00119

109 ->174 -0.00223

109 ->178 -0.00155

109 ->185 0.00101

109 ->190 -0.00392

109 ->193 -0.00207

109 ->201 -0.00113

109 ->207 0.00328

109 ->226 -0.00126

109 ->277 0.00142

109 ->281 0.00218

109 ->287 0.00167

110 ->119 -0.01452

110 ->128 -0.00441

110 ->150 0.00590

110 ->155 0.00236

110 ->240 -0.00119

111 ->120 0.01452

111 ->129 0.00441

111 ->149 -0.00590

111 ->154 0.00236

111 ->241 0.00119

112 ->130 -0.00271

112 ->143 0.00274

112 ->165 0.00283

112 ->167 0.00232

112 ->187 -0.00542

112 ->203 -0.00328

112 ->205 -0.00242

112 ->238 -0.00111

112 ->275 0.00354

112 ->278 0.00254

112 ->340 -0.00113

113 ->122 -0.00691

113 ->138 -0.00671

113 ->148 0.01388

113 ->166 0.00217

113 ->183 -0.00252

113 ->219 -0.00158

114 ->120 0.49896

114 ->129 0.00505

114 ->140 -0.00387

114 ->149 0.01356

114 ->154 0.00174

114 ->181 -0.00136

114 ->209 -0.00213

114 ->224 0.00101

115 ->119 0.49896

115 ->128 0.00505

115 ->141 -0.00387

115 ->150 0.01356

115 ->155 -0.00174

115 ->180 0.00136

115 ->208 -0.00213

115 ->223 0.00101

116 ->125 0.01060

116 ->153 -0.00244

116 ->218 -0.00267

116 ->300 -0.00191

116 ->325 0.00145

117 ->122 0.00312

117 ->138 -0.00360

117 ->148 0.01076

117 ->166 0.00407

117 ->256 0.00173

117 ->312 0.00173

118 ->132 -0.02464

118 ->157 -0.00751

118 ->202 -0.00128

118 ->352 -0.00141

33 <-189 -0.00122

34 <-170 0.00115

35 <-169 -0.00115

36 <-167 0.00163

38 <-127 0.00120

41 <-167 -0.00116

42 <-170 -0.00109

43 <-169 -0.00109

49 <-211 0.00102

50 <-127 -0.00149

51 <-191 0.00109

52 <-190 -0.00109

57 <-175 0.00116

57 <-176 -0.00169

57 <-184 -0.00118

57 <-222 -0.00111

57 <-299 -0.00133

58 <-167 0.00103

60 <-175 -0.00135

63 <-159 0.00137

63 <-169 0.00122

63 <-177 0.00141

63 <-191 -0.00124

63 <-206 0.00116

64 <-160 0.00137

64 <-170 -0.00122

64 <-178 0.00141

64 <-190 -0.00124

64 <-207 -0.00116

65 <-158 -0.00110

65 <-176 0.00191

66 <-127 -0.00135

66 <-147 0.00153

66 <-171 0.00140

66 <-172 -0.00101

67 <-161 0.00142

67 <-182 -0.00219

67 <-194 0.00214

67 <-211 -0.00117

68 <-163 -0.00109

68 <-173 -0.00110

68 <-177 -0.00191

69 <-164 -0.00109

69 <-174 -0.00110

69 <-178 -0.00191

70 <-151 0.00107

71 <-152 0.00107

72 <-167 -0.00141

72 <-187 -0.00136

73 <-148 -0.00122

73 <-166 -0.00120

74 <-126 0.00132

74 <-127 -0.00154

77 <-147 -0.00130

81 <-161 -0.00141

81 <-168 -0.00186

81 <-182 0.00152

81 <-194 -0.00174

81 <-211 0.00140

81 <-220 0.00117

81 <-249 0.00149

82 <-165 0.00107

83 <-121 0.00137

84 <-129 0.00147

85 <-128 0.00147

86 <-132 0.00139

87 <-156 -0.00118

87 <-184 -0.00155

88 <-151 0.00118

88 <-191 -0.00104

89 <-152 0.00118

89 <-190 -0.00104

90 <-138 0.00200

90 <-148 -0.00223

90 <-166 -0.00187

92 <-120 -0.00350

92 <-129 0.00306

92 <-140 -0.00134

92 <-149 0.00222

93 <-119 -0.00350

93 <-128 0.00306

93 <-141 -0.00134

93 <-150 0.00222

94 <-123 0.00103

94 <-160 -0.00108

94 <-190 0.00118

95 <-124 0.00103

95 <-159 -0.00108

95 <-191 0.00118

96 <-162 0.00119

96 <-189 0.00125

96 <-195 0.00183

96 <-284 -0.00125

97 <-131 0.00101

97 <-156 -0.00125

97 <-184 -0.00104

98 <-170 -0.00145

98 <-207 -0.00123

99 <-169 0.00145

99 <-206 0.00123

100 <-125 0.00610

100 <-300 -0.00105

101 <-131 0.00144

101 <-156 -0.00117

101 <-158 0.00148

101 <-175 0.00101

101 <-176 -0.00344

101 <-210 0.00141

101 <-222 -0.00127

101 <-299 -0.00156

102 <-178 -0.00131

102 <-185 -0.00151

102 <-190 0.00154

103 <-177 -0.00131

103 <-186 -0.00151

103 <-191 0.00154

104 <-167 -0.00156

104 <-238 0.00130

105 <-171 -0.00206

105 <-189 0.00117

105 <-195 0.00218

105 <-273 -0.00100

105 <-284 -0.00182

106 <-194 -0.00188

106 <-227 0.00135

106 <-289 0.00107

107 <-121 0.00453

107 <-146 -0.00324

108 <-145 -0.00103

108 <-163 0.00104

108 <-173 -0.00130

108 <-191 -0.00247

108 <-192 -0.00131

108 <-206 -0.00216

108 <-276 0.00107

108 <-280 0.00166

108 <-286 0.00124

109 <-144 0.00103

109 <-164 0.00104

109 <-174 -0.00130

109 <-190 -0.00247

109 <-193 -0.00131

109 <-207 0.00216

109 <-277 0.00107

109 <-281 0.00166

109 <-287 0.00124

110 <-119 -0.00493

110 <-128 -0.00359

110 <-150 0.00303

110 <-155 0.00143

111 <-120 0.00493

111 <-129 0.00359

111 <-149 -0.00303

111 <-154 0.00143

112 <-130 -0.00101

112 <-143 0.00123

112 <-165 0.00152

112 <-167 0.00121

112 <-187 -0.00319

112 <-203 -0.00205

112 <-205 -0.00156

112 <-275 0.00259

112 <-278 0.00188

113 <-122 -0.00143

113 <-138 -0.00330

113 <-148 0.00635

113 <-166 0.00227

113 <-183 -0.00168

114 <-120 -0.01253

114 <-129 0.00621

114 <-140 -0.00118

114 <-149 0.00676

114 <-154 0.00171

114 <-181 -0.00131

114 <-209 -0.00110

115 <-119 -0.01253

115 <-128 0.00621

115 <-141 -0.00118

115 <-150 0.00676

115 <-155 -0.00171

115 <-180 0.00131

115 <-208 -0.00110

116 <-125 0.01407

116 <-153 -0.00262

116 <-218 -0.00128

116 <-300 -0.00133

117 <-148 0.00444

117 <-256 0.00107

117 <-312 0.00159

118 <-132 -0.01026

118 <-157 -0.00395

118 <-352 -0.00140

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

Leave Link 914 at Thu Sep 5 21:50:04 2019, MaxMem= 1342177280 cpu: 2978.1

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

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

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

Population analysis using the SCF density.

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

Orbital symmetries:

Occupied (B2) (B3) (A) (A) (A) (B2) (B3) (B1) (B3) (B2)

(B1) (A) (B1) (B2) (B3) (A) (B2) (B3) (A) (A)

(B1) (B3) (B2) (B1) (B1) (B1) (B3) (B2) (A) (B2)

(B3) (A) (A) (B2) (B3) (A) (B1) (A) (B3) (B2)

(A) (B2) (B3) (B1) (A) (B2) (B3) (B1) (B1) (A)

(B3) (B2) (A) (B3) (B2) (A) (B1) (A) (A) (B1)

(B3) (B2) (B3) (B2) (B1) (A) (B1) (B3) (B2) (B3)

(B2) (A) (B1) (A) (B2) (B3) (A) (B1) (B3) (B2)

(B1) (A) (A) (B3) (B2) (A) (B1) (B3) (B2) (B1)

(B1) (B3) (B2) (B2) (B3) (A) (B1) (B2) (B3) (B1)

(B1) (B2) (B3) (A) (A) (B1) (A) (B3) (B2) (B2)

(B3) (A) (B1) (B3) (B2) (B1) (B1) (A)

Virtual (B2) (B3) (A) (B1) (B2) (B3) (B1) (A) (A) (B2)

(B3) (A) (B1) (A) (B2) (B3) (B3) (B2) (B1) (B1)

(A) (B3) (B2) (A) (A) (B2) (B3) (A) (A) (B1) (B3)

(B2) (B3) (B2) (B1) (B3) (B2) (B1) (A) (B1) (B3)

(B2) (B1) (A) (B3) (B2) (A) (B1) (A) (B1) (B3)

(B2) (A) (A) (B3) (B2) (B1) (B1) (B3) (B2) (B1)

(B2) (B3) (B1) (B1) (B1) (B2) (B3) (A) (A) (A)

(B2) (B3) (B3) (B2) (B1) (A) (A) (B1) (B2) (B3)

(B3) (B2) (A) (A) (A) (A) (B3) (B2) (B2) (B3)

(B1) (B1) (B3) (B2) (A) (B3) (B2) (A) (B1) (B1)

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(A) (B3) (B2) (B1) (B1) (A) (B2) (B3) (A) (A)

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(B3) (B2) (A) (B1) (B1) (B1) (B1) (B3) (B2) (A)

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(B1) (B1) (A) (B3) (B2) (B1) (B1) (A) (B3) (B2)

(B3) (B2) (B1) (A) (A) (B1) (B2) (B3) (B1) (B3)

(B2) (B1) (A) (B3) (B2) (B1) (B1) (A) (B2) (B3)

(B3) (B2) (B1) (B1) (B3) (B2) (B1) (A) (B3) (B2)

(A) (B1) (B1) (B2) (B3) (B1) (A) (A) (B3) (B2)

(A) (A) (A) (B2) (B3) (B3) (B2) (B1) (A) (B3)

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(A) (A) (B2) (B3) (B1) (B2) (B3) (A) (B2) (B3)

(B3) (B2) (A) (A) (B1) (A) (A) (A) (B2) (B3) (A)

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(B3) (B1) (B3) (B2) (A) (B3) (B2) (B1) (B1) (A)

(B3) (B2) (A) (B1) (B3) (B2) (A) (B3) (B2) (A)

(B1) (B1) (B3) (B2) (B1) (B3) (B2) (B1) (A) (B1)

(B1) (A) (B3) (B2) (A) (B1) (A) (B1) (B3) (B2)

(B3) (B2) (B2) (B3) (B1) (A) (B1) (B3) (B2) (B1)

(B3) (B2) (A) (A) (A) (A) (B3) (B2) (A) (B1) (A)

(B3) (B2) (B1) (A) (A) (B2) (B3) (B2) (B3) (A)

(B1) (A) (B3) (B2) (B1) (B1) (B2) (B3) (A) (A)

(B1) (B1) (B3) (B2) (B3) (B2) (A) (B3) (B2) (A)

(B1) (A) (B2) (B3) (B1) (B1) (B3) (B2) (A) (B3)

(B2) (B1) (B1) (B3) (B2) (A) (B3) (B2) (B1) (A)

(A) (B1) (A) (B2) (B3) (B1) (A) (B2) (B3) (B1)

(B1) (B3) (B2) (A) (A) (B2) (B3) (B1) (B2) (B3)

(B1) (B3) (B2) (B1) (A) (A) (B1) (B2) (B3) (B1)

(B1) (B3) (B2) (B1) (B3) (B2) (B3) (B2) (A) (A)

(A) (B2) (B3) (B1) (A) (A) (A) (B2) (B3) (B1)

(B3) (B2) (B1) (A) (B2) (B3) (A) (B2) (B3) (A)

(B1) (A) (A) (B3) (B2) (B1) (B1) (B3) (B2) (B2)

(B3) (A) (A) (B1) (B3) (B2) (B1) (B1) (A) (B3)

(B2) (B1) (B3) (B2) (A) (B3) (B2) (B1) (B1) (A)

(B3) (B2) (A) (A) (B3) (B2) (B1) (B3) (B2) (B1)

(B1) (B3) (B2) (B1) (A) (A) (B2) (B3) (B1) (B3)

(B2) (B1) (B1) (A) (A) (B2) (B3) (A) (B3) (B2)

(B1) (B1) (B3) (B2) (B1) (B3) (B2) (A) (B1) (A)

(A) (A) (B2) (B3) (A) (B3) (B2) (B1) (B1) (A)

(B2) (B3) (B1) (A) (B2) (B3) (A) (B1) (B3) (B2)

(A) (B1) (B3) (B2) (A) (B1) (B3) (B2) (B1) (A)

(A) (B2) (B3)

The electronic state is 1-A.

Alpha occ. eigenvalues -- -14.29250 -14.29250 -14.29250 -14.29250 -10.19800

Alpha occ. eigenvalues -- -10.19800 -10.19800 -10.19800 -10.19799 -10.19799

Alpha occ. eigenvalues -- -10.19799 -10.19799 -10.17175 -10.17175 -10.17175

Alpha occ. eigenvalues -- -10.17175 -10.16982 -10.16982 -10.16982 -10.16982

Alpha occ. eigenvalues -- -10.16920 -10.16920 -10.16920 -10.16920 -10.15779

Alpha occ. eigenvalues -- -10.15779 -10.15779 -10.15779 -10.15779 -10.15779

Alpha occ. eigenvalues -- -10.15779 -10.15778 -0.95515 -0.94691 -0.94691

Alpha occ. eigenvalues -- -0.93860 -0.80983 -0.79473 -0.79282 -0.79282

Alpha occ. eigenvalues -- -0.78965 -0.78402 -0.78402 -0.74425 -0.73186

Alpha occ. eigenvalues -- -0.71801 -0.71801 -0.71745 -0.67319 -0.67143

Alpha occ. eigenvalues -- -0.66762 -0.66762 -0.66705 -0.63561 -0.63561

Alpha occ. eigenvalues -- -0.57786 -0.57014 -0.56102 -0.55384 -0.54936

Alpha occ. eigenvalues -- -0.54714 -0.54714 -0.53389 -0.53389 -0.53338

Alpha occ. eigenvalues -- -0.50865 -0.50750 -0.50504 -0.50504 -0.47159

Alpha occ. eigenvalues -- -0.47159 -0.46285 -0.43927 -0.43766 -0.43259

Alpha occ. eigenvalues -- -0.43259 -0.42777 -0.42723 -0.42697 -0.42697

Alpha occ. eigenvalues -- -0.42672 -0.41905 -0.40299 -0.40212 -0.40212

Alpha occ. eigenvalues -- -0.40123 -0.39903 -0.39270 -0.39270 -0.39127

Alpha occ. eigenvalues -- -0.38282 -0.38133 -0.38133 -0.37971 -0.37971

Alpha occ. eigenvalues -- -0.37662 -0.36893 -0.36830 -0.36830 -0.36449

Alpha occ. eigenvalues -- -0.35429 -0.34892 -0.34892 -0.34885 -0.34579

Alpha occ. eigenvalues -- -0.34515 -0.31515 -0.29914 -0.29914 -0.27121

Alpha occ. eigenvalues -- -0.27121 -0.24691 -0.23699 -0.22837 -0.22837

Alpha occ. eigenvalues -- -0.22639 -0.19141 -0.18643

Alpha virt. eigenvalues -- -0.07865 -0.07865 -0.01964 0.03626 0.04129

Alpha virt. eigenvalues -- 0.04129 0.04264 0.04645 0.05730 0.06092

Alpha virt. eigenvalues -- 0.06092 0.06716 0.06761 0.07359 0.07801

Alpha virt. eigenvalues -- 0.07801 0.08913 0.08913 0.10487 0.10901

Alpha virt. eigenvalues -- 0.11180 0.11745 0.11745 0.12044 0.12422

Alpha virt. eigenvalues -- 0.12492 0.12492 0.12861 0.13305 0.13533

Alpha virt. eigenvalues -- 0.13972 0.13972 0.14529 0.14529 0.15031

Alpha virt. eigenvalues -- 0.15796 0.15796 0.15902 0.16460 0.17161

Alpha virt. eigenvalues -- 0.17248 0.17248 0.17642 0.19310 0.20613

Alpha virt. eigenvalues -- 0.20613 0.20690 0.22253 0.22551 0.22630

Alpha virt. eigenvalues -- 0.22797 0.22797 0.23344 0.23787 0.23844

Alpha virt. eigenvalues -- 0.23844 0.24886 0.27222 0.27925 0.27925

Alpha virt. eigenvalues -- 0.29284 0.29763 0.29763 0.30099 0.30390

Alpha virt. eigenvalues -- 0.30855 0.31154 0.31154 0.31157 0.31919

Alpha virt. eigenvalues -- 0.32519 0.33502 0.33502 0.34348 0.34348

Alpha virt. eigenvalues -- 0.36237 0.36848 0.37764 0.38092 0.38121

Alpha virt. eigenvalues -- 0.38121 0.38228 0.38228 0.38504 0.38567

Alpha virt. eigenvalues -- 0.39077 0.39834 0.40721 0.40721 0.40953

Alpha virt. eigenvalues -- 0.40953 0.41201 0.41615 0.42893 0.42893

Alpha virt. eigenvalues -- 0.43375 0.43393 0.43393 0.43672 0.44758

Alpha virt. eigenvalues -- 0.45287 0.45392 0.45629 0.47118 0.47801

Alpha virt. eigenvalues -- 0.47801 0.47820 0.47820 0.47951 0.49023

Alpha virt. eigenvalues -- 0.49023 0.50062 0.50552 0.50552 0.50727

Alpha virt. eigenvalues -- 0.50969 0.51015 0.52613 0.52613 0.52779

Alpha virt. eigenvalues -- 0.54011 0.54156 0.54156 0.54253 0.54627

Alpha virt. eigenvalues -- 0.54731 0.54731 0.54878 0.56124 0.56124

Alpha virt. eigenvalues -- 0.56787 0.56923 0.56923 0.57592 0.57819

Alpha virt. eigenvalues -- 0.58462 0.58670 0.59189 0.59861 0.59861

Alpha virt. eigenvalues -- 0.61044 0.61422 0.61715 0.61715 0.61751

Alpha virt. eigenvalues -- 0.62084 0.62084 0.62266 0.62971 0.63352

Alpha virt. eigenvalues -- 0.63374 0.63374 0.63407 0.63407 0.63457

Alpha virt. eigenvalues -- 0.64186 0.64876 0.66169 0.66169 0.66457

Alpha virt. eigenvalues -- 0.66526 0.67271 0.67271 0.67539 0.67539

Alpha virt. eigenvalues -- 0.68139 0.68726 0.68915 0.68915 0.69131

Alpha virt. eigenvalues -- 0.70796 0.71630 0.72131 0.72131 0.73597

Alpha virt. eigenvalues -- 0.74067 0.75215 0.75215 0.75751 0.75751

Alpha virt. eigenvalues -- 0.78293 0.79885 0.80261 0.80924 0.80960

Alpha virt. eigenvalues -- 0.80960 0.84118 0.84597 0.85532 0.85702

Alpha virt. eigenvalues -- 0.85702 0.87447 0.87447 0.87934 0.88118

Alpha virt. eigenvalues -- 0.89408 0.90811 0.93123 0.93123 0.93230

Alpha virt. eigenvalues -- 0.93847 0.93847 0.94097 0.95420 0.97737

Alpha virt. eigenvalues -- 0.97737 0.99539 1.00088 1.00423 1.00919

Alpha virt. eigenvalues -- 1.00919 1.01360 1.01360 1.02063 1.03462

Alpha virt. eigenvalues -- 1.03679 1.03679 1.04441 1.04442 1.07282

Alpha virt. eigenvalues -- 1.07282 1.07341 1.08701 1.09167 1.09537

Alpha virt. eigenvalues -- 1.09537 1.10031 1.10915 1.11694 1.11944

Alpha virt. eigenvalues -- 1.11944 1.13257 1.13585 1.14327 1.16579

Alpha virt. eigenvalues -- 1.16579 1.16870 1.16870 1.20518 1.22825

Alpha virt. eigenvalues -- 1.23947 1.23947 1.25320 1.27933 1.28576

Alpha virt. eigenvalues -- 1.28576 1.29315 1.29802 1.30393 1.30605

Alpha virt. eigenvalues -- 1.30605 1.31334 1.33408 1.33408 1.34303

Alpha virt. eigenvalues -- 1.36086 1.38866 1.39663 1.40978 1.40978

Alpha virt. eigenvalues -- 1.43497 1.44330 1.45081 1.45438 1.45438

Alpha virt. eigenvalues -- 1.47714 1.47867 1.47867 1.48105 1.49881

Alpha virt. eigenvalues -- 1.49881 1.50049 1.50049 1.50224 1.50366

Alpha virt. eigenvalues -- 1.51164 1.52280 1.52751 1.52873 1.53348

Alpha virt. eigenvalues -- 1.53348 1.54396 1.54800 1.54800 1.56305

Alpha virt. eigenvalues -- 1.56663 1.57378 1.57378 1.59363 1.59363

Alpha virt. eigenvalues -- 1.60777 1.61556 1.61556 1.63539 1.64774

Alpha virt. eigenvalues -- 1.64774 1.64892 1.65617 1.65617 1.66667

Alpha virt. eigenvalues -- 1.66715 1.67522 1.68712 1.68712 1.68779

Alpha virt. eigenvalues -- 1.69142 1.69410 1.69410 1.69699 1.70335

Alpha virt. eigenvalues -- 1.70335 1.70386 1.70700 1.72089 1.74071

Alpha virt. eigenvalues -- 1.74071 1.75018 1.75307 1.75307 1.77535

Alpha virt. eigenvalues -- 1.78255 1.78679 1.79459 1.81653 1.85832

Alpha virt. eigenvalues -- 1.85832 1.86709 1.89049 1.89231 1.89678

Alpha virt. eigenvalues -- 1.90054 1.90054 1.92349 1.92349 1.93095

Alpha virt. eigenvalues -- 1.93095 1.94564 1.95567 1.96831 1.97026

Alpha virt. eigenvalues -- 1.97026 1.98022 1.99068 1.99068 1.99562

Alpha virt. eigenvalues -- 2.00780 2.00916 2.01329 2.01490 2.01490

Alpha virt. eigenvalues -- 2.01935 2.06465 2.06715 2.08150 2.08150

Alpha virt. eigenvalues -- 2.08885 2.15776 2.15804 2.15915 2.15915

Alpha virt. eigenvalues -- 2.17059 2.17059 2.18997 2.23545 2.24116

Alpha virt. eigenvalues -- 2.27284 2.27284 2.29391 2.31988 2.32585

Alpha virt. eigenvalues -- 2.32585 2.32590 2.33212 2.33344 2.35994

Alpha virt. eigenvalues -- 2.36881 2.36881 2.37282 2.37282 2.40749

Alpha virt. eigenvalues -- 2.40808 2.40808 2.41596 2.43107 2.43220

Alpha virt. eigenvalues -- 2.43489 2.43489 2.44174 2.44945 2.45037

Alpha virt. eigenvalues -- 2.45037 2.45721 2.46058 2.46058 2.46750

Alpha virt. eigenvalues -- 2.47712 2.48039 2.48039 2.50795 2.51187

Alpha virt. eigenvalues -- 2.51187 2.51868 2.53393 2.54822 2.55053

Alpha virt. eigenvalues -- 2.55477 2.56206 2.56206 2.59195 2.61629

Alpha virt. eigenvalues -- 2.63259 2.63259 2.63350 2.65172 2.65536

Alpha virt. eigenvalues -- 2.65536 2.67921 2.69190 2.69922 2.69922

Alpha virt. eigenvalues -- 2.70642 2.71087 2.71087 2.72269 2.74867

Alpha virt. eigenvalues -- 2.74867 2.77428 2.78435 2.81160 2.82405

Alpha virt. eigenvalues -- 2.83251 2.83251 2.84715 2.86638 2.87860

Alpha virt. eigenvalues -- 2.87860 2.88846 2.89838 2.89838 2.94243

Alpha virt. eigenvalues -- 2.94243 2.97054 2.97700 2.99985 3.01976

Alpha virt. eigenvalues -- 3.01976 3.02183 3.06473 3.06658 3.07039

Alpha virt. eigenvalues -- 3.09204 3.09204 3.11932 3.12730 3.12730

Alpha virt. eigenvalues -- 3.13209 3.15204 3.15781 3.15781 3.15833

Alpha virt. eigenvalues -- 3.16009 3.16009 3.16172 3.17283 3.22371

Alpha virt. eigenvalues -- 3.22842 3.22931 3.22931 3.24752 3.25068

Alpha virt. eigenvalues -- 3.25421 3.25421 3.26977 3.26977 3.27679

Alpha virt. eigenvalues -- 3.27833 3.28748 3.29305 3.29305 3.31235

Alpha virt. eigenvalues -- 3.31838 3.32481 3.33922 3.33922 3.34679

Alpha virt. eigenvalues -- 3.37452 3.37452 3.37557 3.46845 3.46845

Alpha virt. eigenvalues -- 3.46884 3.47769 3.61812 3.62012 3.62012

Alpha virt. eigenvalues -- 3.63770 3.74957 3.75954 3.75954 3.77287

Alpha virt. eigenvalues -- 3.86732 3.86732 3.88218 3.91608 3.95409

Alpha virt. eigenvalues -- 3.95409 3.99361 3.99652 4.08528 4.12381

Alpha virt. eigenvalues -- 4.12381 4.18279 4.21640 4.21640 4.23367

Alpha virt. eigenvalues -- 4.25832 4.36102 4.46261 4.54142 4.54142

Alpha virt. eigenvalues -- 4.66943 4.73360 4.73360 4.77149 5.15220

Alpha virt. eigenvalues -- 5.22076 5.22076 5.30356 7.78011 7.78011

Alpha virt. eigenvalues -- 7.88983 7.93101 8.15982 11.12096 23.38542

Alpha virt. eigenvalues -- 23.47726 23.47726 23.52820 23.62525 23.62525

Alpha virt. eigenvalues -- 23.62725 23.63406 23.66872 23.67675 23.67675

Alpha virt. eigenvalues -- 23.70843 23.72173 23.77011 23.77011 23.79254

Alpha virt. eigenvalues -- 23.95622 23.96483 23.96483 23.97705 24.08529

Alpha virt. eigenvalues -- 24.09409 24.09409 24.10207 24.12173 24.12395

Alpha virt. eigenvalues -- 24.12395 24.12718 35.64441 35.65437 35.66397

Alpha virt. eigenvalues -- 35.66397

Condensed to atoms (all electrons):

Mulliken charges:

1

1 C 0.006672

2 C 0.276269

3 N -0.697377

4 C 0.276269

5 C 0.006672

6 C -0.425441

7 C 0.276269

8 N -0.697377

9 C 0.276269

10 C 0.006671

11 C 0.006671

12 C -0.425441

13 C 0.276269

14 C 0.006671

15 C 0.006671

16 C 0.276269

17 N -0.697377

18 C -0.425441

19 C 0.276269

20 C 0.006672

21 C 0.006672

22 C 0.276269

23 N -0.697377

24 C -0.425441

25 Zn 1.361180

26 H 0.244710

27 H 0.244710

28 H 0.244710

29 H 0.244710

30 C -0.726610

31 H 0.236472

32 H 0.236561

33 H 0.239544

34 C -0.726610

35 H 0.236472

36 H 0.236561

37 H 0.239544

38 C -0.726610

39 H 0.236561

40 H 0.236472

41 H 0.239544

42 C -0.726610

43 H 0.236561

44 H 0.236472

45 H 0.239544

46 C -0.726610

47 H 0.236472

48 H 0.236561

49 H 0.239544

50 C -0.726610

51 H 0.236472

52 H 0.236561

53 H 0.239544

54 C -0.726610

55 H 0.236561

56 H 0.236472

57 H 0.239544

58 C -0.726610

59 H 0.236561

60 H 0.236472

61 H 0.239544

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 C 0.006672

2 C 0.276269

3 N -0.697377

4 C 0.276269

5 C 0.006672

6 C -0.180730

7 C 0.276269

8 N -0.697377

9 C 0.276269

10 C 0.006671

11 C 0.006671

12 C -0.180730

13 C 0.276269

14 C 0.006671

15 C 0.006671

16 C 0.276269

17 N -0.697377

18 C -0.180730

19 C 0.276269

20 C 0.006672

21 C 0.006672

22 C 0.276269

23 N -0.697377

24 C -0.180730

25 Zn 1.361180

30 C -0.014034

34 C -0.014034

38 C -0.014034

42 C -0.014034

46 C -0.014034

50 C -0.014034

54 C -0.014034

58 C -0.014034

Electronic spatial extent (au): <R\*\*2>= 15795.5437

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= -167.2257 YY= -167.2257 ZZ= -206.1359

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XX= 12.9700 YY= 12.9701 ZZ= -25.9401

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= -0.3915

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

XXXX= -9868.7583 YYYY= -9868.7580 ZZZZ= -282.1399 XXXY= 0.0000

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

ZZZY= 0.0000 XXYY= -3327.6502 XXZZ= -1931.9130 YYZZ= -1931.9130

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 3.398238692155D+03 E-N=-1.006194433801D+04 KE= 1.413328947183D+03

Symmetry A KE= 4.179144016593D+02

Symmetry B1 KE= 3.015778955926D+02

Symmetry B2 KE= 3.469183250365D+02

Symmetry B3 KE= 3.469183248945D+02

Leave Link 601 at Thu Sep 5 21:50:06 2019, MaxMem= 1342177280 cpu: 16.4

(Enter /apps/gaussian/g09d01/g09/l9999.exe)

Test job not archived.

1\1\GINC-K005\SP\RB3LYP TD-FC\GenECP\C28H28N4Zn1\Z5105842\05-Sep-2019\

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

icaldispersion=gd3bj IOp(9/40=3)\\ZnOMP0td\\0,1\C,0,-0.686702,4.285372

,0.003479\C,0,-1.106584,2.88798,0.004353\N,0,0.,2.086488,0.\C,0,1.1065

84,2.88798,-0.004353\C,0,0.686702,4.285372,-0.003479\C,0,2.430637,2.43

0637,-0.007272\C,0,2.88798,1.106584,-0.004353\N,0,2.086488,0.,0.\C,0,2

.88798,-1.106584,0.004353\C,0,4.285372,-0.686702,0.003479\C,0,4.285372

,0.686702,-0.003479\C,0,-2.430637,2.430637,0.007272\C,0,-2.88798,1.106

584,0.004353\C,0,-4.285372,0.686702,0.003479\C,0,-4.285372,-0.686702,-

0.003479\C,0,-2.88798,-1.106584,-0.004353\N,0,-2.086488,0.,0.\C,0,-2.4

30637,-2.430637,-0.007272\C,0,-1.106584,-2.88798,-0.004353\C,0,-0.6867

02,-4.285372,-0.003479\C,0,0.686702,-4.285372,0.003479\C,0,1.106584,-2

.88798,0.004353\N,0,0.,-2.086488,0.\C,0,2.430637,-2.430637,0.007272\Zn

,0,0.,0.,0.\H,0,-3.197535,-3.197535,-0.010861\H,0,-3.197535,3.197535,0

.010861\H,0,3.197535,3.197535,-0.010861\H,0,3.197535,-3.197535,0.01086

1\C,0,1.620502,5.453258,-0.009045\H,0,2.280236,5.436177,-0.88272\H,0,2

.267047,5.45596,0.874782\H,0,1.078919,6.400341,-0.02417\C,0,-1.620502,

5.453258,0.009045\H,0,-2.280236,5.436177,0.88272\H,0,-2.267047,5.45596

,-0.874782\H,0,-1.078919,6.400341,0.02417\C,0,-5.453258,1.620502,0.009

044\H,0,-5.455955,2.267051,-0.87478\H,0,-5.436181,2.280232,0.882722\H,

0,-6.400341,1.078919,0.024161\C,0,-5.453258,-1.620502,-0.009044\H,0,-5

.455955,-2.267051,0.87478\H,0,-5.436181,-2.280232,-0.882722\H,0,-6.400

341,-1.078919,-0.024161\C,0,-1.620502,-5.453258,-0.009045\H,0,-2.28023

6,-5.436177,-0.88272\H,0,-2.267047,-5.45596,0.874782\H,0,-1.078919,-6.

400341,-0.02417\C,0,1.620502,-5.453258,0.009045\H,0,2.280236,-5.436177

,0.88272\H,0,2.267047,-5.45596,-0.874782\H,0,1.078919,-6.400341,0.0241

7\C,0,5.453258,-1.620502,0.009044\H,0,5.455955,-2.267051,-0.87478\H,0,

5.436181,-2.280232,0.882722\H,0,6.400341,-1.078919,0.024161\C,0,5.4532

58,1.620502,-0.009044\H,0,5.455955,2.267051,0.87478\H,0,5.436181,2.280

232,-0.882722\H,0,6.400341,1.078919,-0.024161\\Version=ES64L-G09RevD.0

1\State=1-A\HF=-1369.0490347\RMSD=7.285e-09\PG=D02 [O(Zn1),C2'(N1.N1),

C2"(N1.N1),X(C28H28)]\\@

Everywhere is walking distance if you have the time.

-- Steven Wright

Job cpu time: 0 days 1 hours 4 minutes 37.8 seconds.

File lengths (MBytes): RWF= 2017 Int= 0 D2E= 0 Chk= 173 Scr= 2

Normal termination of Gaussian 09 at Thu Sep 5 21:50:08 2019.