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

 Cite this work as:

 Gaussian 09, Revision D.01,

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 K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,

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 V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,

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 R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,

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

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

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

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

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

 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)

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 (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)

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 (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)

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 (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)

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

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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

 113 ->155 -0.00209

 113 ->180 0.00249

 114 ->121 -0.00636

 115 ->122 -0.00310

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

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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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 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

 102 ->175 0.00170

 102 ->176 -0.00175

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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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 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)

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

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

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 (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)

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 (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.