Entering Gaussian System, Link 0=g09

 Initial command:

 /apps/gaussian/g09d01/g09/l1.exe "/srv/scratch/z5105842/Gau-21419.inp" -scrdir="/srv/scratch/z5105842/"

 Entering Link 1 = /apps/gaussian/g09d01/g09/l1.exe PID= 21435.

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

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

 Cite this work as:

 Gaussian 09, Revision D.01,

 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,

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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=ZnTPP0td.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: 0.8

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

 --------

 ZnTPP0td

 --------

 Symbolic Z-matrix:

 Charge = 0 Multiplicity = 1

 C -0.68148 4.26916 0.16409

 C -1.11054 2.89013 0.0355

 N 0. 2.09053 -0.02746

 C 1.11054 2.89013 0.0355

 C 0.68148 4.26916 0.16409

 C 2.45218 2.45218 0.

 C 2.89013 1.11054 -0.0355

 N 2.09053 0. 0.02746

 C 2.89013 -1.11054 -0.0355

 C 4.26916 -0.68148 -0.16409

 C 4.26916 0.68148 -0.16409

 C -2.45218 2.45218 0.

 C -2.89013 1.11054 -0.0355

 C -4.26916 0.68148 -0.16409

 C -4.26916 -0.68148 -0.16409

 C -2.89013 -1.11054 -0.0355

 N -2.09053 0. 0.02746

 C -2.45218 -2.45218 0.

 C -1.11054 -2.89013 0.0355

 C -0.68148 -4.26916 0.16409

 C 0.68148 -4.26916 0.16409

 C 1.11054 -2.89013 0.0355

 N 0. -2.09053 -0.02746

 C 2.45218 -2.45218 0.

 C 3.50824 3.50824 0.

 C 3.62136 4.40504 -1.06967

 C 4.60749 5.38875 -1.07114

 C 5.49381 5.49381 0.

 C 5.38875 4.60749 1.07114

 C 4.40504 3.62136 1.06967

 C -5.49381 5.49381 0.

 C -4.60749 5.38875 -1.07114

 C -3.62136 4.40504 -1.06967

 C -3.50824 3.50824 0.

 C -4.40504 3.62136 1.06967

 C -5.38875 4.60749 1.07114

 C 3.50824 -3.50824 0.

 C 4.40504 -3.62136 1.06967

 C 5.38875 -4.60749 1.07114

 C 5.49381 -5.49381 0.

 C 4.60749 -5.38875 -1.07114

 C 3.62136 -4.40504 -1.06967

 C -3.50824 -3.50824 0.

 C -4.40504 -3.62136 1.06967

 C -5.38875 -4.60749 1.07114

 C -5.49381 -5.49381 0.

 C -4.60749 -5.38875 -1.07114

 C -3.62136 -4.40504 -1.06967

 H -1.33092 5.12562 0.25983

 H 1.33092 5.12562 0.25983

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 H -5.12562 1.33092 -0.25983

 H -5.12562 -1.33092 -0.25983

 H -1.33092 -5.12562 0.25983

 H 1.33092 -5.12562 0.25983

 H 2.93697 4.32321 -1.90704

 H 4.68458 6.07145 -1.91098

 H 6.26099 6.26099 0.

 H 6.07145 4.68458 1.91098

 H 4.32321 2.93697 1.90704

 H -6.26099 6.26099 0.

 H -4.68458 6.07145 -1.91098

 H -2.93697 4.32321 -1.90704

 H -4.32321 2.93697 1.90704

 H -6.07145 4.68458 1.91098

 H 4.32321 -2.93697 1.90704

 H 6.07145 -4.68458 1.91098

 H 6.26099 -6.26099 0.

 H 4.68458 -6.07145 -1.91098

 H 2.93697 -4.32321 -1.90704

 H -4.32321 -2.93697 1.90704

 H -6.07145 -4.68458 1.91098

 H -6.26099 -6.26099 0.

 H -4.68458 -6.07145 -1.91098

 H -2.93697 -4.32321 -1.90704

 Zn 0. 0. 0.

 NAtoms= 77 NQM= 77 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 12 12 12 12 12 12

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

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

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

 Atom 31 32 33 34 35 36 37 38 39 40

 IAtWgt= 12 12 12 12 12 12 12 12 12 12

 AtmWgt= 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000

 NucSpn= 0 0 0 0 0 0 0 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 0.0000000 0.0000000 0.0000000 0.0000000

 NMagM= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

 AtZNuc= 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000

 Atom 41 42 43 44 45 46 47 48 49 50

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

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

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

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

 Atom 51 52 53 54 55 56 57 58 59 60

 IAtWgt= 1 1 1 1 1 1 1 1 1 1

 AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

 NucSpn= 1 1 1 1 1 1 1 1 1 1

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

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

 NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

 AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

 Atom 61 62 63 64 65 66 67 68 69 70

 IAtWgt= 1 1 1 1 1 1 1 1 1 1

 AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

 NucSpn= 1 1 1 1 1 1 1 1 1 1

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

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

 NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

 AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

 Atom 71 72 73 74 75 76 77

 IAtWgt= 1 1 1 1 1 1 64

 AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 63.9291454

 NucSpn= 1 1 1 1 1 1 0

 AtZEff= 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

 NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 0.0000000

 AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 30.0000000

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

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

 Stoichiometry C44H28N4Zn

 Framework group D2D[O(Zn),2SGD(N2),X(C44H28)]

 Deg. of freedom 29

 Full point group D2D NOp 8

 Largest Abelian subgroup C2V NOp 4

 Largest concise Abelian subgroup C2V NOp 4

 Standard orientation:

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

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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

 1 6 0 -0.681484 4.269157 0.164086

 2 6 0 -1.110541 2.890129 0.035503

 3 7 0 0.000000 2.090529 -0.027459

 4 6 0 1.110541 2.890129 0.035503

 5 6 0 0.681484 4.269157 0.164086

 6 6 0 2.452183 2.452183 0.000000

 7 6 0 2.890129 1.110541 -0.035503

 8 7 0 2.090529 0.000000 0.027459

 9 6 0 2.890129 -1.110541 -0.035503

 10 6 0 4.269157 -0.681484 -0.164086

 11 6 0 4.269157 0.681484 -0.164086

 12 6 0 -2.452183 2.452183 0.000000

 13 6 0 -2.890129 1.110541 -0.035503

 14 6 0 -4.269157 0.681484 -0.164086

 15 6 0 -4.269157 -0.681484 -0.164086

 16 6 0 -2.890129 -1.110541 -0.035503

 17 7 0 -2.090529 0.000000 0.027459

 18 6 0 -2.452183 -2.452183 0.000000

 19 6 0 -1.110541 -2.890129 0.035503

 20 6 0 -0.681484 -4.269157 0.164086

 21 6 0 0.681484 -4.269157 0.164086

 22 6 0 1.110541 -2.890129 0.035503

 23 7 0 0.000000 -2.090529 -0.027459

 24 6 0 2.452183 -2.452183 0.000000

 25 6 0 3.508242 3.508242 0.000000

 26 6 0 3.621357 4.405038 -1.069674

 27 6 0 4.607485 5.388753 -1.071137

 28 6 0 5.493806 5.493806 0.000000

 29 6 0 5.388753 4.607485 1.071137

 30 6 0 4.405038 3.621357 1.069674

 31 6 0 -5.493806 5.493806 0.000000

 32 6 0 -4.607485 5.388753 -1.071137

 33 6 0 -3.621357 4.405038 -1.069674

 34 6 0 -3.508242 3.508242 0.000000

 35 6 0 -4.405038 3.621357 1.069674

 36 6 0 -5.388753 4.607485 1.071137

 37 6 0 3.508242 -3.508242 0.000000

 38 6 0 4.405038 -3.621357 1.069674

 39 6 0 5.388753 -4.607485 1.071137

 40 6 0 5.493806 -5.493806 0.000000

 41 6 0 4.607485 -5.388753 -1.071137

 42 6 0 3.621357 -4.405038 -1.069674

 43 6 0 -3.508242 -3.508242 0.000000

 44 6 0 -4.405038 -3.621357 1.069674

 45 6 0 -5.388753 -4.607485 1.071137

 46 6 0 -5.493806 -5.493806 0.000000

 47 6 0 -4.607485 -5.388753 -1.071137

 48 6 0 -3.621357 -4.405038 -1.069674

 49 1 0 -1.330917 5.125618 0.259828

 50 1 0 1.330917 5.125618 0.259828

 51 1 0 5.125618 -1.330917 -0.259828

 52 1 0 5.125618 1.330917 -0.259828

 53 1 0 -5.125618 1.330917 -0.259828

 54 1 0 -5.125618 -1.330917 -0.259828

 55 1 0 -1.330917 -5.125618 0.259828

 56 1 0 1.330917 -5.125618 0.259828

 57 1 0 2.936967 4.323214 -1.907040

 58 1 0 4.684584 6.071446 -1.910980

 59 1 0 6.260992 6.260992 0.000000

 60 1 0 6.071446 4.684584 1.910980

 61 1 0 4.323214 2.936967 1.907040

 62 1 0 -6.260992 6.260992 0.000000

 63 1 0 -4.684584 6.071446 -1.910980

 64 1 0 -2.936967 4.323214 -1.907040

 65 1 0 -4.323214 2.936967 1.907040

 66 1 0 -6.071446 4.684584 1.910980

 67 1 0 4.323214 -2.936967 1.907040

 68 1 0 6.071446 -4.684584 1.910980

 69 1 0 6.260992 -6.260992 0.000000

 70 1 0 4.684584 -6.071446 -1.910980

 71 1 0 2.936967 -4.323214 -1.907040

 72 1 0 -4.323214 -2.936967 1.907040

 73 1 0 -6.071446 -4.684584 1.910980

 74 1 0 -6.260992 -6.260992 0.000000

 75 1 0 -4.684584 -6.071446 -1.910980

 76 1 0 -2.936967 -4.323214 -1.907040

 77 30 0 0.000000 0.000000 0.000000

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

 Rotational constants (GHZ): 0.0582110 0.0582110 0.0300828

 Leave Link 202 at Thu Sep 5 21:44:33 2019, MaxMem= 1342177280 cpu: 0.1

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

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

 Centers: 77

 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: 49 50 51 52 53 54 55 56 57 58

 Centers: 59 60 61 62 63 64 65 66 67 68

 Centers: 69 70 71 72 73 74 75 76 1 2

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

 Centers: 15 16 18 19 20 21 22 24 25 26

 Centers: 27 28 29 30 31 32 33 34 35 36

 Centers: 37 38 39 40 41 42 43 44 45 46

 Centers: 47 48 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

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 10 6

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 11 6

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 12 6

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 15 6

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 16 6

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 17 7

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 18 6

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 22 6

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 23 7

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 49 1

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 74 1

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 75 1

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 76 1

 No pseudopotential on this center.

 77 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

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

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

 There are 272 symmetry adapted cartesian basis functions of A1 symmetry.

 There are 243 symmetry adapted cartesian basis functions of A2 symmetry.

 There are 254 symmetry adapted cartesian basis functions of B1 symmetry.

 There are 254 symmetry adapted cartesian basis functions of B2 symmetry.

 There are 256 symmetry adapted basis functions of A1 symmetry.

 There are 232 symmetry adapted basis functions of A2 symmetry.

 There are 242 symmetry adapted basis functions of B1 symmetry.

 There are 242 symmetry adapted basis functions of B2 symmetry.

 972 basis functions, 1715 primitive gaussians, 1023 cartesian basis functions

 166 alpha electrons 166 beta electrons

 nuclear repulsion energy 5738.4943932451 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= 77 NActive= 77 NUniq= 13 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= -0.2224135404 Hartrees.

 Nuclear repulsion after empirical dispersion term = 5738.2719797046 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= 77.

 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 = 77

 GePol: Total number of spheres = 77

 GePol: Number of exposed spheres = 77 (100.00%)

 GePol: Number of points = 5690

 GePol: Average weight of points = 0.11

 GePol: Minimum weight of points = 0.75D-07

 GePol: Maximum weight of points = 0.18390

 GePol: Number of points with low weight = 272

 GePol: Fraction of low-weight points (<1% of avg) = 4.78%

 GePol: Cavity surface area = 614.366 Ang\*\*2

 GePol: Cavity volume = 630.258 Ang\*\*3

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

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

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

 PCM non-electrostatic energy = -0.0025488972 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 5738.2694308075 Hartrees.

 Leave Link 301 at Thu Sep 5 21:44:33 2019, MaxMem= 1342177280 cpu: 1.2

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

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

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

 One-electron integrals computed using PRISM.

 One-electron integral symmetry used in STVInt

 8 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36757 LenP2D= 95282.

 LDataN: DoStor=T MaxTD1= 5 Len= 102

 NBasis= 972 RedAO= T EigKep= 6.36D-05 NBF= 256 232 242 242

 NBsUse= 972 1.00D-06 EigRej= -1.00D+00 NBFU= 256 232 242 242

 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= 952 960 976 976 976 MxSgAt= 77 MxSgA2= 77.

 Leave Link 302 at Thu Sep 5 21:44:35 2019, MaxMem= 1342177280 cpu: 19.9

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

 Leave Link 308 at Thu Sep 5 21:44:35 2019, MaxMem= 1342177280 cpu: 2.9

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

 DipDrv: MaxL=1.

 Leave Link 303 at Thu Sep 5 21:44:35 2019, MaxMem= 1342177280 cpu: 1.9

 (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= -1979.25549734393

 JPrj=0 DoOrth=F DoCkMO=F.

 Initial guess orbital symmetries:

 Occupied (E) (E) (A1) (B2) (B1) (E) (E) (A1) (A2) (E) (E)

 (B2) (B1) (E) (E) (A1) (A2) (E) (E) (B2) (B1)

 (E) (E) (A1) (B2) (E) (E) (A1) (A2) (E) (E) (B1)

 (B1) (E) (E) (A1) (B1) (E) (E) (A1) (B2) (E) (E)

 (A2) (A1) (E) (E) (B1) (A1) (E) (E) (B2) (B1)

 (E) (E) (A1) (B1) (E) (E) (A1) (A1) (E) (E) (B2)

 (A2) (E) (E) (B2) (B1) (E) (E) (A1) (A2) (E) (E)

 (B1) (B2) (B2) (E) (E) (A2) (A1) (B1) (E) (E)

 (E) (E) (A1) (B1) (B2) (E) (E) (B1) (A2) (A1)

 (E) (E) (A1) (E) (E) (B2) (B1) (E) (E) (A2) (B2)

 (E) (E) (A1) (A2) (E) (E) (B1) (A1) (A1) (E) (E)

 (B2) (A2) (E) (E) (B1) (E) (E) (B2) (B1) (B2)

 (E) (E) (E) (E) (A2) (A1) (A1) (E) (E) (A2) (B2)

 (E) (E) (B2) (E) (E) (B1) (A2) (A1) (E) (E) (A2)

 (E) (E) (B2) (B2) (B1) (A1) (E) (E) (B2) (A2)

 (E) (E) (A1) (E) (E) (B1) (B2)

 Virtual (E) (E) (A2) (E) (E) (B1) (B2) (A1) (E) (E) (A2)

 (A1) (E) (E) (B1) (A1) (B2) (A2) (E) (E) (A1)

 (E) (E) (B1) (B2) (E) (E) (A2) (B2) (A1) (E) (E)

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 (A2) (E) (E) (B1) (E) (E) (A1) (B2) (B1) (E) (E)

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 (E) (E) (B1) (B1) (B2) (E) (E) (A2) (A1) (E) (E)

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 (B1) (A1) (E) (E) (A2) (B2) (B1) (A1) (E) (E)

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 (B1) (E) (E) (A1) (B2) (A1) (E) (E)

 The electronic state of the initial guess is 1-A1.

 Leave Link 401 at Thu Sep 5 21:44:38 2019, MaxMem= 1342177280 cpu: 36.9

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

 Closed shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 3183261 IEndB= 3183261 NGot= 1342177280 MDV= 1340058212

 LenX= 1340058212 LenY= 1339010660

 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= 530000000 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= 97128300.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 1.04D-14 for 1411.

 Iteration 1 A\*A^-1 deviation from orthogonality is 5.32D-15 for 5415 1279.

 Iteration 1 A^-1\*A deviation from unit magnitude is 9.77D-15 for 448.

 Iteration 1 A^-1\*A deviation from orthogonality is 4.87D-12 for 3423 3413.

 E= -1977.86979971692

 DIIS: error= 9.76D-02 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -1977.86979971692 IErMin= 1 ErrMin= 9.76D-02

 ErrMax= 9.76D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.26D+00 BMatP= 1.26D+00

 IDIUse=3 WtCom= 2.43D-02 WtEn= 9.76D-01

 Coeff-Com: 0.100D+01

 Coeff-En: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.106 Goal= None Shift= 0.000

 GapD= 0.106 DampG=1.000 DampE=0.250 DampFc=0.2500 IDamp=-1.

 Damping current iteration by 2.50D-01

 RMSDP=1.86D-03 MaxDP=9.55D-02 OVMax= 1.55D-01

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 4.59D-04 CP: 9.89D-01

 E= -1978.23434090525 Delta-E= -0.364541188328 Rises=F Damp=T

 DIIS: error= 4.17D-02 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -1978.23434090525 IErMin= 2 ErrMin= 4.17D-02

 ErrMax= 4.17D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.72D-01 BMatP= 1.26D+00

 IDIUse=3 WtCom= 5.83D-01 WtEn= 4.17D-01

 Coeff-Com: -0.102D+01 0.202D+01

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

 Coeff: -0.597D+00 0.160D+01

 Gap= 0.102 Goal= None Shift= 0.000

 RMSDP=7.18D-04 MaxDP=3.82D-02 DE=-3.65D-01 OVMax= 6.21D-02

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 4.10D-04 CP: 9.71D-01 2.26D+00

 E= -1978.87163772524 Delta-E= -0.637296819993 Rises=F Damp=F

 DIIS: error= 6.88D-03 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 3 EnMin= -1978.87163772524 IErMin= 3 ErrMin= 6.88D-03

 ErrMax= 6.88D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.13D-02 BMatP= 3.72D-01

 IDIUse=3 WtCom= 9.31D-01 WtEn= 6.88D-02

 Coeff-Com: -0.858D-01 0.345D+00 0.741D+00

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

 Coeff: -0.799D-01 0.321D+00 0.759D+00

 Gap= 0.100 Goal= None Shift= 0.000

 RMSDP=2.68D-04 MaxDP=1.66D-02 DE=-6.37D-01 OVMax= 3.62D-02

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 1.82D-04 CP: 9.77D-01 1.92D+00 7.16D-01

 E= -1978.89712835253 Delta-E= -0.025490627289 Rises=F Damp=F

 DIIS: error= 3.28D-03 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -1978.89712835253 IErMin= 4 ErrMin= 3.28D-03

 ErrMax= 3.28D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.50D-03 BMatP= 3.13D-02

 IDIUse=3 WtCom= 9.67D-01 WtEn= 3.28D-02

 Coeff-Com: 0.634D-01-0.345D-01 0.417D+00 0.554D+00

 Coeff-En: 0.000D+00 0.000D+00 0.950D-01 0.905D+00

 Coeff: 0.613D-01-0.334D-01 0.406D+00 0.566D+00

 Gap= 0.099 Goal= None Shift= 0.000

 RMSDP=1.13D-04 MaxDP=6.14D-03 DE=-2.55D-02 OVMax= 1.91D-02

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 5.90D-05 CP: 9.76D-01 1.96D+00 8.06D-01 5.28D-01

 E= -1978.90379140222 Delta-E= -0.006663049687 Rises=F Damp=F

 DIIS: error= 1.92D-03 at cycle 5 NSaved= 5.

 NSaved= 5 IEnMin= 5 EnMin= -1978.90379140222 IErMin= 5 ErrMin= 1.92D-03

 ErrMax= 1.92D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-03 BMatP= 7.50D-03

 IDIUse=3 WtCom= 9.81D-01 WtEn= 1.92D-02

 Coeff-Com: 0.422D-01-0.485D-01 0.173D+00 0.343D+00 0.491D+00

 Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.680D-01 0.932D+00

 Coeff: 0.414D-01-0.476D-01 0.169D+00 0.338D+00 0.500D+00

 Gap= 0.099 Goal= None Shift= 0.000

 RMSDP=3.24D-05 MaxDP=2.21D-03 DE=-6.66D-03 OVMax= 5.25D-03

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 1.69D-05 CP: 9.76D-01 1.97D+00 8.17D-01 5.92D-01 5.83D-01

 E= -1978.90472522440 Delta-E= -0.000933822179 Rises=F Damp=F

 DIIS: error= 6.56D-04 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -1978.90472522440 IErMin= 6 ErrMin= 6.56D-04

 ErrMax= 6.56D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.82D-05 BMatP= 1.10D-03

 IDIUse=3 WtCom= 9.93D-01 WtEn= 6.56D-03

 Coeff-Com: 0.147D-01-0.196D-01 0.487D-01 0.118D+00 0.247D+00 0.591D+00

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

 Coeff: 0.146D-01-0.195D-01 0.484D-01 0.118D+00 0.245D+00 0.593D+00

 Gap= 0.099 Goal= None Shift= 0.000

 RMSDP=6.46D-06 MaxDP=3.92D-04 DE=-9.34D-04 OVMax= 1.38D-03

 Cycle 7 Pass 1 IDiag 1:

 RMSU= 3.58D-06 CP: 9.76D-01 1.97D+00 8.19D-01 5.95D-01 6.09D-01

 CP: 7.12D-01

 E= -1978.90476135642 Delta-E= -0.000036132024 Rises=F Damp=F

 DIIS: error= 7.60D-05 at cycle 7 NSaved= 7.

 NSaved= 7 IEnMin= 7 EnMin= -1978.90476135642 IErMin= 7 ErrMin= 7.60D-05

 ErrMax= 7.60D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.73D-06 BMatP= 4.82D-05

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

 Coeff-Com: 0.629D-02-0.867D-02 0.192D-01 0.502D-01 0.110D+00 0.307D+00

 Coeff-Com: 0.515D+00

 Coeff: 0.629D-02-0.867D-02 0.192D-01 0.502D-01 0.110D+00 0.307D+00

 Coeff: 0.515D+00

 Gap= 0.099 Goal= None Shift= 0.000

 RMSDP=1.70D-06 MaxDP=7.88D-05 DE=-3.61D-05 OVMax= 4.51D-04

 Cycle 8 Pass 1 IDiag 1:

 RMSU= 1.19D-06 CP: 9.76D-01 1.97D+00 8.19D-01 5.97D-01 6.13D-01

 CP: 7.19D-01 6.83D-01

 E= -1978.90476361762 Delta-E= -0.000002261199 Rises=F Damp=F

 DIIS: error= 2.12D-05 at cycle 8 NSaved= 8.

 NSaved= 8 IEnMin= 8 EnMin= -1978.90476361762 IErMin= 8 ErrMin= 2.12D-05

 ErrMax= 2.12D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.42D-07 BMatP= 2.73D-06

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

 Coeff-Com: 0.649D-03-0.956D-03 0.126D-02 0.492D-02 0.119D-01 0.498D-01

 Coeff-Com: 0.246D+00 0.686D+00

 Coeff: 0.649D-03-0.956D-03 0.126D-02 0.492D-02 0.119D-01 0.498D-01

 Coeff: 0.246D+00 0.686D+00

 Gap= 0.099 Goal= None Shift= 0.000

 RMSDP=6.23D-07 MaxDP=2.40D-05 DE=-2.26D-06 OVMax= 1.20D-04

 Cycle 9 Pass 1 IDiag 1:

 RMSU= 4.02D-07 CP: 9.76D-01 1.97D+00 8.19D-01 5.97D-01 6.15D-01

 CP: 7.22D-01 7.38D-01 6.62D-01

 E= -1978.90476381657 Delta-E= -0.000000198945 Rises=F Damp=F

 DIIS: error= 1.32D-05 at cycle 9 NSaved= 9.

 NSaved= 9 IEnMin= 9 EnMin= -1978.90476381657 IErMin= 9 ErrMin= 1.32D-05

 ErrMax= 1.32D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.21D-08 BMatP= 2.42D-07

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

 Coeff-Com: 0.502D-04-0.108D-03-0.277D-03 0.863D-04 0.595D-03 0.106D-01

 Coeff-Com: 0.105D+00 0.391D+00 0.493D+00

 Coeff: 0.502D-04-0.108D-03-0.277D-03 0.863D-04 0.595D-03 0.106D-01

 Coeff: 0.105D+00 0.391D+00 0.493D+00

 Gap= 0.099 Goal= None Shift= 0.000

 RMSDP=1.92D-07 MaxDP=9.22D-06 DE=-1.99D-07 OVMax= 3.07D-05

 Cycle 10 Pass 1 IDiag 1:

 RMSU= 8.99D-08 CP: 9.76D-01 1.97D+00 8.19D-01 5.97D-01 6.15D-01

 CP: 7.25D-01 7.48D-01 7.15D-01 6.86D-01

 E= -1978.90476384796 Delta-E= -0.000000031398 Rises=F Damp=F

 DIIS: error= 1.19D-06 at cycle 10 NSaved= 10.

 NSaved=10 IEnMin=10 EnMin= -1978.90476384796 IErMin=10 ErrMin= 1.19D-06

 ErrMax= 1.19D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.75D-10 BMatP= 3.21D-08

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

 Coeff-Com: -0.489D-04 0.598D-04-0.224D-03-0.474D-03-0.929D-03-0.611D-03

 Coeff-Com: 0.158D-01 0.887D-01 0.160D+00 0.738D+00

 Coeff: -0.489D-04 0.598D-04-0.224D-03-0.474D-03-0.929D-03-0.611D-03

 Coeff: 0.158D-01 0.887D-01 0.160D+00 0.738D+00

 Gap= 0.099 Goal= None Shift= 0.000

 RMSDP=3.57D-08 MaxDP=1.68D-06 DE=-3.14D-08 OVMax= 6.26D-06

 Cycle 11 Pass 1 IDiag 1:

 RMSU= 2.73D-08 CP: 9.76D-01 1.97D+00 8.19D-01 5.97D-01 6.15D-01

 CP: 7.25D-01 7.50D-01 7.26D-01 7.02D-01 8.81D-01

 E= -1978.90476384812 Delta-E= -0.000000000161 Rises=F Damp=F

 DIIS: error= 9.44D-07 at cycle 11 NSaved= 11.

 NSaved=11 IEnMin=11 EnMin= -1978.90476384812 IErMin=11 ErrMin= 9.44D-07

 ErrMax= 9.44D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.54D-10 BMatP= 6.75D-10

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

 Coeff-Com: -0.301D-04 0.401D-04-0.965D-04-0.269D-03-0.542D-03-0.119D-02

 Coeff-Com: -0.338D-03 0.174D-01 0.479D-01 0.432D+00 0.505D+00

 Coeff: -0.301D-04 0.401D-04-0.965D-04-0.269D-03-0.542D-03-0.119D-02

 Coeff: -0.338D-03 0.174D-01 0.479D-01 0.432D+00 0.505D+00

 Gap= 0.099 Goal= None Shift= 0.000

 RMSDP=1.48D-08 MaxDP=8.48D-07 DE=-1.61D-10 OVMax= 3.20D-06

 Cycle 12 Pass 1 IDiag 1:

 RMSU= 7.03D-09 CP: 9.76D-01 1.97D+00 8.19D-01 5.97D-01 6.15D-01

 CP: 7.25D-01 7.50D-01 7.29D-01 7.04D-01 9.29D-01

 CP: 6.54D-01

 E= -1978.90476384822 Delta-E= -0.000000000100 Rises=F Damp=F

 DIIS: error= 1.51D-07 at cycle 12 NSaved= 12.

 NSaved=12 IEnMin=12 EnMin= -1978.90476384822 IErMin=12 ErrMin= 1.51D-07

 ErrMax= 1.51D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.86D-12 BMatP= 2.54D-10

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

 Coeff-Com: -0.467D-05 0.644D-05-0.108D-04-0.471D-04-0.838D-04-0.299D-03

 Coeff-Com: -0.128D-02-0.148D-02 0.230D-02 0.616D-01 0.135D+00 0.805D+00

 Coeff: -0.467D-05 0.644D-05-0.108D-04-0.471D-04-0.838D-04-0.299D-03

 Coeff: -0.128D-02-0.148D-02 0.230D-02 0.616D-01 0.135D+00 0.805D+00

 Gap= 0.099 Goal= None Shift= 0.000

 RMSDP=2.71D-09 MaxDP=1.31D-07 DE=-1.00D-10 OVMax= 4.01D-07

 Error on total polarization charges = 0.08494

 SCF Done: E(RB3LYP) = -1978.90476385 A.U. after 12 cycles

 NFock= 12 Conv=0.27D-08 -V/T= 1.9793

 KE= 2.020706235307D+03 PE=-1.615865212455D+04 EE= 6.420771694589D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.60

 (included in total energy above)

 Leave Link 502 at Thu Sep 5 21:47:21 2019, MaxMem= 1342177280 cpu: 1883.0

 (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 4.98D-05

 Largest core mixing into a valence orbital is 2.06D-05

 Range of M.O.s used for correlation: 49 972

 NBasis= 972 NAE= 166 NBE= 166 NFC= 48 NFV= 0

 NROrb= 924 NOA= 118 NOB= 118 NVA= 806 NVB= 806

 \*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.98725075D-01

 Leave Link 801 at Thu Sep 5 21:47:22 2019, MaxMem= 1342177280 cpu: 3.9

 (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 138418000000 words for in-memory AO integral storage.

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

 Inv3: Mode=1 IEnd= 97128300.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 9.33D-15 for 423.

 Iteration 1 A\*A^-1 deviation from orthogonality is 2.84D-15 for 5688 2045.

 Iteration 1 A^-1\*A deviation from unit magnitude is 8.88D-15 for 5689.

 Iteration 1 A^-1\*A deviation from orthogonality is 2.30D-15 for 5114 1632.

 Making orbital integer symmetry assigments:

 Orbital symmetries:

 Occupied (E) (E) (B2) (A1) (E) (E) (B2) (A2) (B1) (E) (E)

 (A1) (B1) (E) (E) (A1) (B1) (E) (E) (A1) (B1)

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 (A2) (E) (E) (B2) (B1) (E) (E) (A2) (A1) (E) (E)

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 (B1) (E) (E) (A1) (B2) (A1) (E) (E)

 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: 190216

 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 1 was old state 2

 New state 2 was old state 1

 New state 3 was old state 4

 New state 4 was old state 3

 New state 5 was old state 10

 New state 6 was old state 19

 New state 7 was old state 18

 New state 8 was old state 9

 New state 9 was old state 7

 New state 10 was old state 6

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.428701294553804

 Root 2 : 2.428701294561318

 Root 3 : 3.516587131283769

 Root 4 : 3.516587131292371

 Root 5 : 3.737574948387520

 Root 6 : 3.751474798011214

 Root 7 : 3.751474798016408

 Root 8 : 3.789777221301642

 Root 9 : 3.860011255053419

 Root 10 : 3.860011255054868

 Root 11 : 3.879928141245375

 Root 12 : 3.928861122070199

 Root 13 : 3.935043775686835

 Root 14 : 3.938391550040616

 Root 15 : 3.944965103579341

 Root 16 : 3.944965103585384

 Root 17 : 3.998792379426353

 Root 18 : 4.079214263132060

 Root 19 : 4.118984688881808

 Root 20 : 4.121102407888769

 Root 21 : 4.129997545101186

 Root 22 : 4.129997545108232

 Root 23 : 4.144646121011398

 Root 24 : 4.144646121012867

 Root 25 : 4.157208570676358

 Root 26 : 4.190411636358658

 Root 27 : 4.195110218156840

 Root 28 : 4.195110218160975

 Root 29 : 4.248641871883007

 Root 30 : 4.344998820039009

 Root 31 : 4.344998820046047

 Root 32 : 4.407450143252086

 Root 33 : 4.409214275449306

 Root 34 : 4.409214275451562

 Root 35 : 4.415812279712141

 Root 36 : 4.430910757956899

 Root 37 : 4.570937252676748

 Root 38 : 4.627142328889381

 Root 39 : 4.627142328890429

 Root 40 : 4.687171051634622

 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 0.048276419240189

 Root 2 not converged, maximum delta is 0.048276419239130

 New state 3 was old state 4

 Root 3 not converged, maximum delta is 0.105237263631832

 New state 4 was old state 3

 Root 4 not converged, maximum delta is 0.105237263629962

 Root 5 not converged, maximum delta is 0.132956633013194

 New state 6 was old state 9

 Root 6 not converged, maximum delta is 0.120857581823096

 New state 7 was old state 10

 Root 7 not converged, maximum delta is 0.120857581819533

 Root 8 not converged, maximum delta is 0.183429470331180

 New state 9 was old state 6

 Root 9 not converged, maximum delta is 0.047187505572209

 New state 10 was old state 7

 Root 10 not converged, maximum delta is 0.047187505575253

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.219662329494617 Change is -0.209038965059187

 Root 2 : 2.219662329504469 Change is -0.209038965056849

 Root 3 : 3.057934722647806 Change is -0.458652408644565

 Root 4 : 3.057934722648881 Change is -0.458652408634888

 Root 5 : 3.589271617406991 Change is -0.148303330980529

 Root 6 : 3.649480729468749 Change is -0.210530525584670

 Root 7 : 3.649480729473795 Change is -0.210530525581073

 Root 8 : 3.656750818764339 Change is -0.133026402537303

 Root 9 : 3.716296741982316 Change is -0.035178056028898

 Root 10 : 3.716296741986607 Change is -0.035178056029801

 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 0.004224161675550

 Root 2 not converged, maximum delta is 0.004224161675043

 Root 3 not converged, maximum delta is 0.012616494209895

 Root 4 not converged, maximum delta is 0.012616494209733

 Root 5 not converged, maximum delta is 0.019469229625695

 New state 6 was old state 8

 Root 6 not converged, maximum delta is 0.131404927576437

 New state 7 was old state 6

 Root 7 not converged, maximum delta is 0.015169229143350

 New state 8 was old state 7

 Root 8 not converged, maximum delta is 0.015169229141824

 Root 9 not converged, maximum delta is 0.009160397667692

 Root 10 not converged, maximum delta is 0.009160397667312

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.209051626711254 Change is -0.010610702783364

 Root 2 : 2.209051626721525 Change is -0.010610702782944

 Root 3 : 3.026251031978266 Change is -0.031683690669540

 Root 4 : 3.026251031979597 Change is -0.031683690669284

 Root 5 : 3.579007642490882 Change is -0.010263974916109

 Root 6 : 3.636322320972348 Change is -0.020428497791991

 Root 7 : 3.642866428769356 Change is -0.006614300699393

 Root 8 : 3.642866428774614 Change is -0.006614300699181

 Root 9 : 3.714492876456073 Change is -0.001803865526242

 Root 10 : 3.714492876460456 Change is -0.001803865526152

 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 0.002979685217567

 Root 2 not converged, maximum delta is 0.002979685217440

 Root 3 not converged, maximum delta is 0.005551206197589

 Root 4 not converged, maximum delta is 0.005551206196308

 Root 5 not converged, maximum delta is 0.006108026759717

 Root 6 not converged, maximum delta is 0.137130930300203

 Root 7 not converged, maximum delta is 0.004614856418706

 Root 8 not converged, maximum delta is 0.004614856416389

 Root 9 not converged, maximum delta is 0.001985301489102

 Root 10 not converged, maximum delta is 0.001985301489655

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.207557240907411 Change is -0.001494385803843

 Root 2 : 2.207557240917094 Change is -0.001494385804431

 Root 3 : 3.022533831082758 Change is -0.003717200895508

 Root 4 : 3.022533831083873 Change is -0.003717200895724

 Root 5 : 3.577196714157072 Change is -0.001810928333810

 Root 6 : 3.622657187266614 Change is -0.013665133705735

 Root 7 : 3.641564982906088 Change is -0.001301445863268

 Root 8 : 3.641564982911596 Change is -0.001301445863018

 Root 9 : 3.714225483995815 Change is -0.000267392460259

 Root 10 : 3.714225484000153 Change is -0.000267392460303

 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 0.001138719065031

 Root 4 not converged, maximum delta is 0.001138719061672

 Root 5 not converged, maximum delta is 0.001888205760320

 Root 6 not converged, maximum delta is 0.032875977975611

 Root 7 has converged.

 Root 8 has converged.

 Root 9 has converged.

 Root 10 has converged.

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.207461215948761 Change is -0.000096024958650

 Root 2 : 2.207461215958519 Change is -0.000096024958575

 Root 3 : 3.022193158796154 Change is -0.000340672286604

 Root 4 : 3.022193158797704 Change is -0.000340672286168

 Root 5 : 3.576961078757767 Change is -0.000235635399306

 Root 6 : 3.620299360922235 Change is -0.002357826344378

 Root 7 : 3.641458425233346 Change is -0.000106557672742

 Root 8 : 3.641458425239081 Change is -0.000106557672515

 Root 9 : 3.714194035352776 Change is -0.000031448643039

 Root 10 : 3.714194035357092 Change is -0.000031448643061

 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 not converged, maximum delta is 0.069273011040973

 Root 4 not converged, maximum delta is 0.069273011041752

 Root 5 has converged.

 Root 6 not converged, maximum delta is 0.013795277892522

 Root 7 not converged, maximum delta is 0.001176016707628

 Root 8 not converged, maximum delta is 0.001176016707622

 Root 9 not converged, maximum delta is 0.002309641306672

 Root 10 not converged, maximum delta is 0.002309641306663

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.207459660537243 Change is -0.000001555411518

 Root 2 : 2.207459660546926 Change is -0.000001555411593

 Root 3 : 3.022172199503860 Change is -0.000020959292294

 Root 4 : 3.022172199505383 Change is -0.000020959292322

 Root 5 : 3.576933084223689 Change is -0.000027994534078

 Root 6 : 3.619781110777733 Change is -0.000518250144502

 Root 7 : 3.641456779454625 Change is -0.000001645778721

 Root 8 : 3.641456779460427 Change is -0.000001645778654

 Root 9 : 3.714193574807802 Change is -0.000000460544974

 Root 10 : 3.714193574812140 Change is -0.000000460544952

 Iteration 7 Dimension 142 NMult 128 NNew 14

 CISAX will form 14 AO SS matrices at one time.

 NMat= 14 NSing= 14 JSym2X=-1.

 Root 1 has converged.

 Root 2 has converged.

 Root 3 not converged, maximum delta is 0.069273010717385

 Root 4 not converged, maximum delta is 0.069273010718170

 Root 5 has converged.

 Root 6 not converged, maximum delta is 0.001907212971949

 Root 7 not converged, maximum delta is 0.001176016707949

 Root 8 not converged, maximum delta is 0.001176016707944

 Root 9 not converged, maximum delta is 0.002309641305933

 Root 10 not converged, maximum delta is 0.002309641305904

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.207458717972577 Change is -0.000000942564666

 Root 2 : 2.207458717982148 Change is -0.000000942564778

 Root 3 : 3.022170994057352 Change is -0.000001205446508

 Root 4 : 3.022170994058930 Change is -0.000001205446453

 Root 5 : 3.576933084223759 Change is 0.000000000000069

 Root 6 : 3.619703435680521 Change is -0.000077675097212

 Root 7 : 3.641447168529113 Change is -0.000009610925513

 Root 8 : 3.641447168534869 Change is -0.000009610925558

 Root 9 : 3.714190896727137 Change is -0.000002678080665

 Root 10 : 3.714190896731497 Change is -0.000002678080643

 Iteration 8 Dimension 156 NMult 142 NNew 14

 CISAX will form 14 AO SS matrices at one time.

 NMat= 14 NSing= 14 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 : 2.207458321695631 Change is -0.000000396276946

 Root 2 : 2.207458321705350 Change is -0.000000396276798

 Root 3 : 3.022170891506403 Change is -0.000000102550950

 Root 4 : 3.022170891508007 Change is -0.000000102550922

 Root 5 : 3.576933084223667 Change is -0.000000000000092

 Root 6 : 3.619695293052603 Change is -0.000008142627919

 Root 7 : 3.641446389572518 Change is -0.000000778956595

 Root 8 : 3.641446389578229 Change is -0.000000778956640

 Root 9 : 3.714190651491251 Change is -0.000000245235886

 Root 10 : 3.714190651495456 Change is -0.000000245236041

 Convergence achieved on expansion vectors.

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

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

 1PDM for each excited state written to RWF 633

 Ground to excited state transition densities written to RWF 633

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

 state X Y Z Dip. S. Osc.

 1 -1.0775 0.0000 0.0000 1.1609 0.0628

 2 0.0000 -1.0775 0.0000 1.1609 0.0628

 3 4.7181 0.0000 0.0000 22.2607 1.6482

 4 0.0000 -4.7181 0.0000 22.2607 1.6482

 5 0.0000 0.0000 0.0000 0.0000 0.0000

 6 0.0000 0.0000 0.0000 0.0000 0.0000

 7 -0.7214 0.0000 0.0000 0.5205 0.0464

 8 0.0000 0.7214 0.0000 0.5205 0.0464

 9 0.5065 0.0000 0.0000 0.2566 0.0233

 10 0.0000 0.5065 0.0000 0.2566 0.0233

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

 state X Y Z Dip. S. Osc.

 1 0.0834 0.0000 0.0000 0.0070 0.0572

 2 0.0000 0.0834 0.0000 0.0070 0.0572

 3 -0.5158 0.0000 0.0000 0.2660 1.5969

 4 0.0000 0.5158 0.0000 0.2660 1.5969

 5 0.0000 0.0000 0.0000 0.0000 0.0000

 6 0.0000 0.0000 0.0000 0.0000 0.0000

 7 0.0973 0.0000 0.0000 0.0095 0.0472

 8 0.0000 -0.0973 0.0000 0.0095 0.0472

 9 -0.0677 0.0000 0.0000 0.0046 0.0224

 10 0.0000 -0.0677 0.0000 0.0046 0.0224

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

 state X Y Z

 1 0.0000 -0.0326 0.0000

 2 -0.0326 0.0000 0.0000

 3 0.0000 -0.0024 0.0000

 4 0.0024 0.0000 0.0000

 5 0.0000 0.0000 -2.2513

 6 0.0000 0.0000 0.0000

 7 0.0000 0.1101 0.0000

 8 -0.1101 0.0000 0.0000

 9 0.0000 -0.3690 0.0000

 10 -0.3690 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 0.0459 0.0000

 2 0.0000 0.0000 0.0000 0.0000 0.0000 -0.0459

 3 0.0000 0.0000 0.0000 0.0000 0.0255 0.0000

 4 0.0000 0.0000 0.0000 0.0000 0.0000 0.0255

 5 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

 6 0.0000 0.0000 0.0000 -0.6486 0.0000 0.0000

 7 0.0000 0.0000 0.0000 0.0000 0.0166 0.0000

 8 0.0000 0.0000 0.0000 0.0000 0.0000 0.0166

 9 0.0000 0.0000 0.0000 0.0000 -0.0569 0.0000

 10 0.0000 0.0000 0.0000 0.0000 0.0000 0.0569

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

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

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

 1 0.0000 0.0000 0.0000 0.0000 90.00

 2 0.0000 0.0000 0.0000 0.0000 90.00

 3 0.0000 0.0000 0.0000 0.0000 90.00

 4 0.0000 0.0000 0.0000 0.0000 90.00

 5 0.0000 0.0000 0.0000 0.0000 90.00

 6 0.0000 0.0000 0.0000 0.0000 90.00

 7 0.0000 0.0000 0.0000 0.0000 90.00

 8 0.0000 0.0000 0.0000 0.0000 90.00

 9 0.0000 0.0000 0.0000 0.0000 90.00

 10 0.0000 0.0000 0.0000 0.0000 90.00

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

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

 state XX YY ZZ R(length)

 1 0.0000 0.0000 0.0000 0.0000

 2 0.0000 0.0000 0.0000 0.0000

 3 0.0000 0.0000 0.0000 0.0000

 4 0.0000 0.0000 0.0000 0.0000

 5 0.0000 0.0000 0.0000 0.0000

 6 0.0000 0.0000 0.0000 0.0000

 7 0.0000 0.0000 0.0000 0.0000

 8 0.0000 0.0000 0.0000 0.0000

 9 0.0000 0.0000 0.0000 0.0000

 10 0.0000 0.0000 0.0000 0.0000

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

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

 1 -0.0899 0.0000 0.0000 0.0899 0.0599

 2 0.0000 -0.0899 0.0000 0.0899 0.0599

 3 -2.4336 0.0000 0.0000 2.4336 1.6224

 4 0.0000 -2.4336 0.0000 2.4336 1.6224

 5 0.0000 0.0000 0.0000 0.0000 0.0000

 6 0.0000 0.0000 0.0000 0.0000 0.0000

 7 -0.0702 0.0000 0.0000 0.0702 0.0468

 8 0.0000 -0.0702 0.0000 0.0702 0.0468

 9 -0.0343 0.0000 0.0000 0.0343 0.0229

 10 0.0000 -0.0343 0.0000 0.0343 0.0229

 Excitation energies and oscillator strengths:

 Excited State 1: Singlet-E 2.2075 eV 561.66 nm f=0.0628 <S\*\*2>=0.000

 52 ->237 0.00106

 57 ->228 0.00122

 58 ->226 -0.00111

 58 ->258 0.00114

 58 ->273 -0.00108

 58 ->280 0.00108

 59 ->225 -0.00142

 59 ->232 0.00163

 59 ->268 -0.00136

 60 ->229 0.00144

 60 ->237 0.00142

 72 ->224 0.00110

 72 ->228 -0.00156

 73 ->229 0.00162

 73 ->237 0.00130

 73 ->271 -0.00119

 74 ->226 0.00132

 74 ->231 0.00125

 74 ->247 -0.00110

 74 ->258 -0.00153

 74 ->273 0.00150

 74 ->296 -0.00100

 75 ->225 -0.00121

 75 ->236 -0.00170

 75 ->317 -0.00147

 76 ->228 0.00106

 76 ->238 0.00105

 84 ->238 0.00109

 84 ->257 -0.00106

 84 ->262 0.00128

 85 ->246 -0.00102

 85 ->322 -0.00122

 86 ->322 0.00132

 86 ->325 -0.00112

 88 ->226 0.00111

 88 ->285 0.00114

 90 ->228 -0.00176

 94 ->238 0.00107

 95 ->226 -0.00115

 95 ->341 0.00148

 100 ->186 0.00116

 100 ->194 0.00122

 100 ->197 0.00104

 101 ->181 -0.00103

 101 ->228 0.00161

 103 ->226 0.00228

 103 ->341 -0.00197

 103 ->347 0.00131

 104 ->180 0.00103

 104 ->225 0.00116

 104 ->232 -0.00108

 104 ->268 0.00114

 104 ->317 -0.00103

 105 ->217 0.00129

 106 ->167 -0.00203

 106 ->249 -0.00164

 106 ->349 -0.00112

 107 ->168 -0.00241

 107 ->204 0.00205

 107 ->220 0.00108

 108 ->169 -0.00248

 108 ->200 -0.00148

 109 ->205 0.00106

 110 ->169 -0.00121

 110 ->226 0.00106

 110 ->231 0.00100

 110 ->341 -0.00102

 111 ->170 -0.00118

 111 ->198 -0.00101

 111 ->232 -0.00106

 112 ->228 -0.00151

 113 ->167 0.00215

 113 ->172 0.00109

 113 ->234 -0.00150

 113 ->249 -0.00147

 113 ->257 0.00184

 113 ->315 0.00106

 113 ->320 0.00129

 113 ->324 0.00150

 113 ->349 -0.00194

 113 ->368 0.00123

 114 ->223 -0.00189

 115 ->168 -0.00447

 115 ->204 0.00194

 115 ->220 0.00143

 116 ->169 -0.00103

 116 ->193 -0.00114

 116 ->231 -0.00122

 117 ->190 -0.00106

 118 ->191 -0.00119

 119 ->170 0.00104

 119 ->222 -0.00109

 119 ->225 -0.00108

 119 ->260 -0.00113

 120 ->169 0.00148

 120 ->231 -0.00212

 120 ->233 0.00102

 121 ->229 0.00143

 121 ->237 0.00152

 122 ->168 -0.00551

 122 ->192 -0.00107

 122 ->204 0.00245

 122 ->220 0.00113

 123 ->224 0.00123

 123 ->228 -0.00161

 123 ->249 -0.00123

 123 ->257 0.00178

 123 ->278 0.00106

 123 ->305 0.00117

 123 ->315 -0.00106

 124 ->205 0.00156

 124 ->210 0.00101

 124 ->227 0.00127

 125 ->169 -0.00659

 125 ->175 -0.00161

 125 ->193 0.00128

 125 ->200 -0.00333

 125 ->221 -0.00148

 125 ->326 -0.00102

 126 ->180 0.00111

 126 ->186 0.00105

 126 ->230 0.00102

 126 ->253 0.00106

 126 ->308 0.00123

 126 ->317 -0.00133

 126 ->406 -0.00109

 127 ->240 0.00143

 127 ->258 0.00140

 127 ->341 -0.00109

 128 ->168 -0.00529

 128 ->176 -0.00117

 128 ->204 0.00142

 128 ->220 0.00104

 129 ->228 -0.00151

 130 ->322 -0.00107

 130 ->325 0.00159

 130 ->350 -0.00103

 131 ->167 -0.00168

 131 ->172 -0.00124

 132 ->276 -0.00133

 132 ->285 -0.00160

 132 ->293 -0.00100

 132 ->341 -0.00112

 133 ->180 0.00113

 133 ->230 0.00101

 133 ->259 0.00126

 133 ->317 -0.00125

 134 ->168 -0.00159

 134 ->171 0.00115

 134 ->271 0.00100

 135 ->229 -0.00118

 136 ->197 0.00106

 136 ->236 -0.00114

 137 ->175 -0.00113

 137 ->341 -0.00116

 138 ->167 -0.00335

 138 ->219 -0.00119

 138 ->257 0.00103

 138 ->324 0.00102

 139 ->201 0.00178

 139 ->223 0.00168

 139 ->237 0.00100

 139 ->246 0.00114

 140 ->167 0.00581

 140 ->203 0.00188

 141 ->185 0.00102

 141 ->199 -0.00102

 141 ->231 -0.00195

 141 ->233 0.00113

 142 ->198 0.00133

 142 ->222 -0.00119

 142 ->253 -0.00105

 143 ->204 -0.00127

 144 ->231 -0.00156

 144 ->244 0.00104

 145 ->170 0.00134

 145 ->186 -0.00108

 145 ->198 0.00127

 145 ->210 0.00127

 145 ->253 -0.00101

 146 ->172 0.00147

 146 ->181 -0.00126

 146 ->202 0.00112

 146 ->208 -0.00115

 146 ->224 0.00109

 146 ->228 -0.00146

 146 ->234 0.00133

 146 ->238 0.00174

 146 ->249 -0.00148

 146 ->257 0.00205

 146 ->270 0.00109

 147 ->167 -0.01998

 147 ->172 0.00203

 147 ->177 0.00141

 147 ->203 -0.00207

 147 ->211 -0.00176

 147 ->219 -0.00213

 147 ->266 -0.00102

 148 ->169 0.00138

 148 ->226 -0.00164

 148 ->240 0.00113

 149 ->179 -0.00228

 149 ->180 -0.00281

 149 ->186 -0.00277

 149 ->194 -0.00201

 149 ->213 -0.00116

 149 ->225 -0.00230

 149 ->236 -0.00210

 149 ->250 0.00104

 149 ->253 -0.00119

 149 ->277 -0.00143

 149 ->309 -0.00109

 149 ->317 -0.00103

 149 ->366 0.00130

 149 ->378 -0.00121

 150 ->169 0.00265

 150 ->189 0.00126

 151 ->174 0.00402

 151 ->178 0.00320

 151 ->179 -0.01218

 151 ->180 0.00394

 151 ->190 0.00187

 151 ->197 -0.00247

 151 ->205 -0.00610

 151 ->216 -0.00251

 151 ->227 -0.00169

 151 ->274 -0.00146

 151 ->370 -0.00121

 152 ->168 0.00279

 152 ->171 -0.00339

 152 ->176 -0.00170

 152 ->183 0.00552

 152 ->201 0.00132

 152 ->204 -0.00369

 152 ->207 0.00115

 152 ->212 -0.00177

 152 ->220 -0.00180

 153 ->168 -0.00158

 153 ->171 -0.00224

 153 ->176 -0.00131

 153 ->183 -0.00371

 153 ->204 0.00178

 153 ->220 0.00107

 153 ->223 0.00111

 153 ->246 -0.00107

 153 ->248 -0.00135

 153 ->271 -0.00163

 154 ->168 0.01082

 154 ->171 0.00143

 154 ->176 -0.00193

 154 ->183 -0.00135

 154 ->204 0.00114

 155 ->167 -0.00727

 155 ->172 0.00211

 155 ->177 -0.00186

 155 ->184 0.00153

 156 ->169 0.00156

 156 ->173 0.00245

 156 ->175 0.00195

 157 ->170 -0.00203

 157 ->174 -0.00306

 157 ->179 0.00182

 158 ->168 0.01096

 158 ->171 0.00191

 158 ->176 0.00144

 158 ->183 0.00258

 158 ->220 -0.00114

 158 ->223 0.00157

 158 ->229 0.00183

 158 ->235 -0.00123

 158 ->237 -0.00104

 158 ->263 -0.00143

 158 ->271 -0.00105

 159 ->167 -0.00503

 159 ->172 0.00595

 159 ->177 0.00228

 159 ->208 -0.00128

 160 ->170 0.00311

 160 ->174 0.00178

 160 ->179 -0.01000

 160 ->180 0.00293

 160 ->190 0.00109

 160 ->205 -0.00289

 160 ->216 -0.00211

 160 ->227 -0.00137

 160 ->236 -0.00156

 160 ->283 0.00100

 161 ->169 -0.00344

 161 ->173 -0.00141

 161 ->175 0.00537

 161 ->209 -0.00104

 162 ->170 0.00486

 162 ->174 0.00125

 162 ->178 0.00310

 162 ->210 0.00123

 162 ->227 0.00182

 163 ->169 -0.01640

 163 ->173 -0.00108

 163 ->189 -0.00344

 164 ->168 -0.03390

 164 ->171 -0.00277

 164 ->176 -0.00298

 164 ->183 0.00328

 164 ->201 0.00119

 164 ->204 -0.00381

 164 ->212 -0.00121

 164 ->220 -0.00221

 165 ->167 0.39512

 165 ->172 -0.00284

 165 ->177 -0.00693

 165 ->184 -0.01146

 165 ->203 0.00319

 165 ->208 -0.00115

 165 ->211 0.00166

 165 ->219 0.00230

 165 ->249 -0.00106

 166 ->168 0.58445

 166 ->171 0.00149

 166 ->176 0.00197

 166 ->183 -0.00801

 166 ->201 -0.00175

 166 ->204 0.00739

 166 ->212 0.00305

 166 ->217 0.00176

 166 ->220 0.00549

 166 ->265 0.00194

 166 ->335 -0.00110

 166 ->345 -0.00111

 57 <-228 0.00107

 58 <-258 0.00100

 59 <-225 -0.00121

 59 <-232 0.00141

 59 <-268 -0.00118

 60 <-229 0.00122

 60 <-237 0.00122

 72 <-228 -0.00132

 73 <-229 0.00135

 73 <-237 0.00111

 73 <-271 -0.00103

 74 <-226 0.00107

 74 <-231 0.00105

 74 <-258 -0.00130

 74 <-273 0.00128

 75 <-236 -0.00142

 75 <-317 -0.00125

 84 <-262 0.00108

 85 <-322 -0.00107

 86 <-322 0.00114

 90 <-228 -0.00141

 95 <-341 0.00126

 101 <-228 0.00126

 103 <-226 0.00175

 103 <-341 -0.00167

 103 <-347 0.00112

 106 <-167 -0.00129

 106 <-249 -0.00128

 107 <-168 -0.00198

 107 <-204 0.00165

 108 <-169 -0.00192

 108 <-200 -0.00119

 112 <-228 -0.00118

 113 <-167 0.00132

 113 <-234 -0.00116

 113 <-249 -0.00121

 113 <-257 0.00146

 113 <-320 0.00106

 113 <-324 0.00123

 113 <-349 -0.00164

 113 <-368 0.00105

 114 <-223 -0.00140

 115 <-168 -0.00248

 115 <-204 0.00167

 115 <-220 0.00119

 120 <-231 -0.00161

 121 <-229 0.00108

 121 <-237 0.00118

 122 <-168 -0.00256

 122 <-204 0.00204

 123 <-228 -0.00123

 123 <-257 0.00140

 124 <-205 0.00151

 124 <-227 0.00134

 125 <-169 -0.00393

 125 <-200 -0.00247

 125 <-221 -0.00117

 126 <-308 0.00100

 126 <-317 -0.00110

 127 <-240 0.00111

 127 <-258 0.00108

 128 <-168 -0.00198

 129 <-228 -0.00116

 130 <-325 0.00132

 132 <-276 -0.00107

 132 <-285 -0.00130

 133 <-317 -0.00102

 138 <-167 -0.00180

 139 <-201 0.00117

 139 <-223 0.00118

 140 <-167 0.00318

 140 <-203 0.00168

 141 <-231 -0.00140

 144 <-231 -0.00113

 146 <-228 -0.00111

 146 <-238 0.00128

 146 <-249 -0.00113

 146 <-257 0.00157

 147 <-167 -0.01052

 147 <-184 -0.00175

 147 <-203 -0.00274

 147 <-211 -0.00160

 147 <-219 -0.00197

 148 <-226 -0.00116

 149 <-180 -0.00193

 149 <-186 -0.00175

 149 <-194 -0.00133

 149 <-225 -0.00163

 149 <-236 -0.00155

 149 <-277 -0.00115

 149 <-366 0.00107

 150 <-169 -0.00524

 150 <-189 0.00113

 150 <-200 -0.00103

 151 <-174 0.00117

 151 <-178 0.00218

 151 <-179 -0.00355

 151 <-180 0.00120

 151 <-190 0.00132

 151 <-197 -0.00180

 151 <-205 -0.00452

 151 <-216 -0.00186

 151 <-227 -0.00143

 151 <-274 -0.00123

 151 <-370 -0.00107

 152 <-171 -0.00148

 152 <-183 0.00336

 152 <-204 -0.00208

 152 <-212 -0.00103

 153 <-168 0.00300

 153 <-183 -0.00244

 153 <-271 -0.00127

 154 <-168 0.00226

 155 <-167 -0.00198

 157 <-174 -0.00125

 157 <-179 0.00150

 158 <-168 -0.00233

 158 <-183 0.00226

 158 <-229 0.00120

 158 <-263 -0.00104

 159 <-167 -0.00305

 159 <-172 0.00188

 159 <-177 0.00110

 160 <-170 0.00109

 160 <-179 -0.00418

 160 <-180 0.00120

 160 <-205 -0.00193

 160 <-216 -0.00139

 160 <-227 -0.00113

 160 <-236 -0.00114

 161 <-169 0.00128

 161 <-175 0.00248

 162 <-170 0.00148

 162 <-178 0.00206

 162 <-179 0.00337

 162 <-180 -0.00100

 162 <-227 0.00116

 163 <-189 -0.00200

 164 <-168 -0.00699

 164 <-171 -0.00108

 164 <-176 -0.00106

 164 <-183 0.00188

 164 <-204 -0.00262

 164 <-220 -0.00160

 165 <-167 0.02993

 165 <-177 -0.00206

 165 <-184 -0.00601

 165 <-203 0.00238

 165 <-211 0.00103

 165 <-219 0.00190

 166 <-168 -0.01163

 166 <-183 -0.00245

 166 <-201 -0.00106

 166 <-204 0.00415

 166 <-212 0.00220

 166 <-220 0.00316

 166 <-265 0.00163

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

 Total Energy, E(TD-HF/TD-KS) = -1978.82364124

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

 Excited State 2: Singlet-E 2.2075 eV 561.66 nm f=0.0628 <S\*\*2>=0.000

 52 ->238 -0.00106

 57 ->229 0.00122

 58 ->225 -0.00142

 58 ->232 0.00163

 58 ->268 -0.00136

 59 ->226 -0.00111

 59 ->258 0.00114

 59 ->273 -0.00108

 59 ->280 0.00108

 60 ->228 0.00144

 60 ->238 0.00142

 72 ->223 -0.00110

 72 ->229 0.00156

 73 ->228 0.00162

 73 ->238 0.00130

 73 ->272 0.00119

 74 ->225 0.00121

 74 ->236 -0.00170

 74 ->317 -0.00147

 75 ->226 -0.00132

 75 ->231 -0.00125

 75 ->247 0.00110

 75 ->258 0.00153

 75 ->273 -0.00150

 75 ->296 0.00100

 76 ->229 0.00106

 76 ->237 0.00105

 84 ->237 0.00109

 84 ->256 -0.00106

 84 ->263 0.00128

 85 ->245 0.00102

 85 ->323 0.00122

 86 ->323 -0.00132

 86 ->324 0.00112

 89 ->226 0.00111

 89 ->285 -0.00114

 90 ->229 -0.00176

 94 ->237 0.00107

 96 ->226 -0.00115

 96 ->341 -0.00148

 99 ->186 0.00116

 99 ->194 0.00122

 99 ->197 -0.00104

 101 ->182 -0.00103

 101 ->229 0.00161

 103 ->180 0.00103

 103 ->225 0.00116

 103 ->232 -0.00108

 103 ->268 0.00114

 103 ->317 0.00103

 104 ->226 0.00228

 104 ->341 0.00197

 104 ->347 -0.00131

 105 ->218 0.00129

 106 ->168 -0.00203

 106 ->248 0.00164

 106 ->350 0.00112

 107 ->167 -0.00241

 107 ->203 -0.00205

 107 ->219 -0.00108

 108 ->205 0.00106

 109 ->169 -0.00248

 109 ->200 -0.00148

 110 ->170 0.00118

 110 ->198 -0.00101

 110 ->232 -0.00106

 111 ->169 0.00121

 111 ->226 0.00106

 111 ->231 0.00100

 111 ->341 0.00102

 112 ->229 -0.00151

 113 ->168 0.00215

 113 ->171 -0.00109

 113 ->235 0.00150

 113 ->248 0.00147

 113 ->256 -0.00184

 113 ->316 -0.00106

 113 ->321 -0.00129

 113 ->325 -0.00150

 113 ->350 0.00194

 113 ->369 -0.00123

 114 ->224 -0.00189

 115 ->167 -0.00447

 115 ->203 -0.00194

 115 ->219 -0.00143

 116 ->190 -0.00106

 117 ->169 -0.00103

 117 ->193 -0.00114

 117 ->231 0.00122

 118 ->192 0.00119

 119 ->169 -0.00148

 119 ->231 -0.00212

 119 ->233 0.00102

 120 ->170 -0.00104

 120 ->222 -0.00109

 120 ->225 -0.00108

 120 ->260 -0.00113

 121 ->228 0.00143

 121 ->238 0.00152

 122 ->167 -0.00551

 122 ->191 0.00107

 122 ->203 -0.00245

 122 ->219 -0.00113

 123 ->223 0.00123

 123 ->229 -0.00161

 123 ->248 -0.00123

 123 ->256 0.00178

 123 ->279 0.00106

 123 ->304 -0.00117

 123 ->316 -0.00106

 124 ->169 -0.00659

 124 ->175 -0.00161

 124 ->193 0.00128

 124 ->200 -0.00333

 124 ->221 -0.00148

 124 ->326 -0.00102

 125 ->205 0.00156

 125 ->210 0.00101

 125 ->227 0.00127

 126 ->240 -0.00143

 126 ->258 0.00140

 126 ->341 0.00109

 127 ->180 0.00111

 127 ->186 0.00105

 127 ->230 -0.00102

 127 ->253 0.00106

 127 ->308 0.00123

 127 ->317 0.00133

 127 ->406 0.00109

 128 ->167 0.00529

 128 ->177 -0.00117

 128 ->203 0.00142

 128 ->219 0.00104

 129 ->229 -0.00151

 130 ->323 0.00107

 130 ->324 -0.00159

 130 ->349 0.00103

 131 ->168 -0.00168

 131 ->171 0.00124

 132 ->180 0.00113

 132 ->230 -0.00101

 132 ->259 -0.00126

 132 ->317 0.00125

 133 ->276 0.00133

 133 ->285 0.00160

 133 ->293 0.00100

 133 ->341 0.00112

 134 ->167 -0.00159

 134 ->172 -0.00115

 134 ->272 0.00100

 135 ->228 -0.00118

 136 ->175 0.00113

 136 ->341 0.00116

 137 ->197 -0.00106

 137 ->236 0.00114

 138 ->168 -0.00335

 138 ->220 0.00119

 138 ->256 -0.00103

 138 ->325 -0.00102

 139 ->202 0.00178

 139 ->224 0.00168

 139 ->238 0.00100

 139 ->245 0.00114

 140 ->168 0.00581

 140 ->204 -0.00188

 141 ->198 0.00133

 141 ->222 -0.00119

 141 ->253 -0.00105

 142 ->185 0.00102

 142 ->199 -0.00102

 142 ->231 -0.00195

 142 ->233 0.00113

 143 ->203 0.00127

 144 ->170 -0.00134

 144 ->186 -0.00108

 144 ->198 0.00127

 144 ->210 -0.00127

 144 ->253 -0.00101

 145 ->231 -0.00156

 145 ->244 -0.00104

 146 ->171 0.00147

 146 ->182 -0.00126

 146 ->201 0.00112

 146 ->207 -0.00115

 146 ->223 0.00109

 146 ->229 -0.00146

 146 ->235 0.00133

 146 ->237 0.00174

 146 ->248 -0.00148

 146 ->256 0.00205

 146 ->269 0.00109

 147 ->168 -0.01998

 147 ->171 -0.00203

 147 ->176 -0.00141

 147 ->204 0.00207

 147 ->212 0.00176

 147 ->220 0.00213

 147 ->265 0.00102

 148 ->179 -0.00228

 148 ->180 -0.00281

 148 ->186 -0.00277

 148 ->194 -0.00201

 148 ->213 -0.00116

 148 ->225 -0.00230

 148 ->236 0.00210

 148 ->250 0.00104

 148 ->253 -0.00119

 148 ->277 -0.00143

 148 ->309 0.00109

 148 ->317 0.00103

 148 ->366 0.00130

 148 ->378 -0.00121

 149 ->169 -0.00138

 149 ->226 -0.00164

 149 ->240 -0.00113

 150 ->174 0.00402

 150 ->178 -0.00320

 150 ->179 -0.01218

 150 ->180 0.00394

 150 ->190 -0.00187

 150 ->197 0.00247

 150 ->205 0.00610

 150 ->216 0.00251

 150 ->227 0.00169

 150 ->274 0.00146

 150 ->370 0.00121

 151 ->169 -0.00265

 151 ->189 0.00126

 152 ->167 0.00279

 152 ->172 0.00339

 152 ->177 0.00170

 152 ->184 0.00552

 152 ->202 -0.00132

 152 ->203 0.00369

 152 ->208 -0.00115

 152 ->211 0.00177

 152 ->219 0.00180

 153 ->167 -0.00158

 153 ->172 0.00224

 153 ->177 0.00131

 153 ->184 -0.00371

 153 ->203 -0.00178

 153 ->219 -0.00107

 153 ->224 -0.00111

 153 ->245 0.00107

 153 ->249 0.00135

 153 ->272 -0.00163

 154 ->167 -0.01082

 154 ->172 0.00143

 154 ->177 -0.00193

 154 ->184 0.00135

 154 ->203 0.00114

 155 ->168 0.00727

 155 ->171 0.00211

 155 ->176 -0.00186

 155 ->183 -0.00153

 156 ->170 0.00203

 156 ->174 -0.00306

 156 ->179 0.00182

 157 ->169 -0.00156

 157 ->173 0.00245

 157 ->175 -0.00195

 158 ->167 0.01096

 158 ->172 -0.00191

 158 ->177 -0.00144

 158 ->184 0.00258

 158 ->219 0.00114

 158 ->224 -0.00157

 158 ->228 -0.00183

 158 ->234 0.00123

 158 ->238 0.00104

 158 ->262 0.00143

 158 ->272 -0.00105

 159 ->168 -0.00503

 159 ->171 -0.00595

 159 ->176 -0.00228

 159 ->207 0.00128

 160 ->169 -0.00344

 160 ->173 0.00141

 160 ->175 0.00537

 160 ->209 -0.00104

 161 ->170 0.00311

 161 ->174 -0.00178

 161 ->179 0.01000

 161 ->180 -0.00293

 161 ->190 0.00109

 161 ->205 -0.00289

 161 ->216 -0.00211

 161 ->227 -0.00137

 161 ->236 -0.00156

 161 ->283 -0.00100

 162 ->169 -0.01640

 162 ->173 0.00108

 162 ->189 0.00344

 163 ->170 0.00486

 163 ->174 -0.00125

 163 ->178 0.00310

 163 ->210 0.00123

 163 ->227 0.00182

 164 ->167 0.03390

 164 ->172 -0.00277

 164 ->177 -0.00298

 164 ->184 -0.00328

 164 ->202 0.00119

 164 ->203 -0.00381

 164 ->211 -0.00121

 164 ->219 -0.00221

 165 ->168 -0.39512

 165 ->171 -0.00284

 165 ->176 -0.00693

 165 ->183 0.01146

 165 ->204 0.00319

 165 ->207 -0.00115

 165 ->212 0.00166

 165 ->220 0.00230

 165 ->248 -0.00106

 166 ->167 0.58445

 166 ->172 -0.00149

 166 ->177 -0.00197

 166 ->184 -0.00801

 166 ->202 0.00175

 166 ->203 -0.00739

 166 ->211 -0.00305

 166 ->218 -0.00176

 166 ->219 -0.00549

 166 ->266 -0.00194

 166 ->336 0.00110

 166 ->346 -0.00111

 57 <-229 0.00107

 58 <-225 -0.00121

 58 <-232 0.00141

 58 <-268 -0.00118

 59 <-258 0.00100

 60 <-228 0.00122

 60 <-238 0.00122

 72 <-229 0.00132

 73 <-228 0.00135

 73 <-238 0.00111

 73 <-272 0.00103

 74 <-236 -0.00142

 74 <-317 -0.00125

 75 <-226 -0.00107

 75 <-231 -0.00105

 75 <-258 0.00130

 75 <-273 -0.00128

 84 <-263 0.00108

 85 <-323 0.00107

 86 <-323 -0.00114

 90 <-229 -0.00141

 96 <-341 -0.00126

 101 <-229 0.00126

 104 <-226 0.00175

 104 <-341 0.00167

 104 <-347 -0.00112

 106 <-168 -0.00129

 106 <-248 0.00128

 107 <-167 -0.00198

 107 <-203 -0.00165

 109 <-169 -0.00192

 109 <-200 -0.00119

 112 <-229 -0.00118

 113 <-168 0.00132

 113 <-235 0.00116

 113 <-248 0.00121

 113 <-256 -0.00146

 113 <-321 -0.00106

 113 <-325 -0.00123

 113 <-350 0.00164

 113 <-369 -0.00105

 114 <-224 -0.00140

 115 <-167 -0.00248

 115 <-203 -0.00167

 115 <-219 -0.00119

 119 <-231 -0.00161

 121 <-228 0.00108

 121 <-238 0.00118

 122 <-167 -0.00256

 122 <-203 -0.00204

 123 <-229 -0.00123

 123 <-256 0.00140

 124 <-169 -0.00393

 124 <-200 -0.00247

 124 <-221 -0.00117

 125 <-205 0.00151

 125 <-227 0.00134

 126 <-240 -0.00111

 126 <-258 0.00108

 127 <-308 0.00100

 127 <-317 0.00110

 128 <-167 0.00198

 129 <-229 -0.00116

 130 <-324 -0.00132

 132 <-317 0.00102

 133 <-276 0.00107

 133 <-285 0.00130

 138 <-168 -0.00180

 139 <-202 0.00117

 139 <-224 0.00118

 140 <-168 0.00318

 140 <-204 -0.00168

 142 <-231 -0.00140

 145 <-231 -0.00113

 146 <-229 -0.00111

 146 <-237 0.00128

 146 <-248 -0.00113

 146 <-256 0.00157

 147 <-168 -0.01052

 147 <-183 -0.00175

 147 <-204 0.00274

 147 <-212 0.00160

 147 <-220 0.00197

 148 <-180 -0.00193

 148 <-186 -0.00175

 148 <-194 -0.00133

 148 <-225 -0.00163

 148 <-236 0.00155

 148 <-277 -0.00115

 148 <-366 0.00107

 149 <-226 -0.00116

 150 <-174 0.00117

 150 <-178 -0.00218

 150 <-179 -0.00355

 150 <-180 0.00120

 150 <-190 -0.00132

 150 <-197 0.00180

 150 <-205 0.00452

 150 <-216 0.00186

 150 <-227 0.00143

 150 <-274 0.00123

 150 <-370 0.00107

 151 <-169 0.00524

 151 <-189 0.00113

 151 <-200 0.00103

 152 <-172 0.00148

 152 <-184 0.00336

 152 <-203 0.00208

 152 <-211 0.00103

 153 <-167 0.00300

 153 <-184 -0.00244

 153 <-272 -0.00127

 154 <-167 -0.00226

 155 <-168 0.00198

 156 <-174 -0.00125

 156 <-179 0.00150

 158 <-167 -0.00233

 158 <-184 0.00226

 158 <-228 -0.00120

 158 <-262 0.00104

 159 <-168 -0.00305

 159 <-171 -0.00188

 159 <-176 -0.00110

 160 <-169 0.00128

 160 <-175 0.00248

 161 <-170 0.00109

 161 <-179 0.00418

 161 <-180 -0.00120

 161 <-205 -0.00193

 161 <-216 -0.00139

 161 <-227 -0.00113

 161 <-236 -0.00114

 162 <-189 0.00200

 163 <-170 0.00148

 163 <-178 0.00206

 163 <-179 -0.00337

 163 <-180 0.00100

 163 <-227 0.00116

 164 <-167 0.00699

 164 <-172 -0.00108

 164 <-177 -0.00106

 164 <-184 -0.00188

 164 <-203 -0.00262

 164 <-219 -0.00160

 165 <-168 -0.02993

 165 <-176 -0.00206

 165 <-183 0.00601

 165 <-204 0.00238

 165 <-212 0.00103

 165 <-220 0.00190

 166 <-167 -0.01163

 166 <-184 -0.00245

 166 <-202 0.00106

 166 <-203 -0.00415

 166 <-211 -0.00220

 166 <-219 -0.00316

 166 <-266 -0.00163

 Excited State 3: Singlet-E 3.0222 eV 410.25 nm f=1.6482 <S\*\*2>=0.000

 58 ->226 0.00132

 58 ->233 0.00111

 58 ->280 -0.00102

 59 ->222 -0.00110

 60 ->223 -0.00105

 64 ->223 -0.00110

 70 ->233 0.00106

 74 ->258 0.00127

 74 ->285 -0.00112

 75 ->222 -0.00175

 75 ->236 -0.00113

 76 ->202 -0.00128

 76 ->224 -0.00121

 76 ->245 -0.00104

 76 ->251 -0.00117

 76 ->270 -0.00107

 77 ->168 0.00160

 80 ->177 -0.00108

 81 ->170 -0.00128

 81 ->198 -0.00114

 81 ->222 0.00120

 82 ->206 -0.00123

 82 ->285 0.00103

 83 ->171 0.00134

 83 ->201 -0.00109

 84 ->208 -0.00158

 84 ->211 -0.00101

 84 ->224 0.00146

 84 ->228 -0.00106

 84 ->272 -0.00104

 84 ->336 -0.00100

 85 ->171 0.00132

 85 ->229 -0.00251

 86 ->223 -0.00175

 86 ->229 0.00106

 86 ->263 0.00103

 87 ->196 0.00111

 88 ->185 0.00105

 88 ->199 -0.00132

 88 ->206 -0.00200

 88 ->209 0.00168

 88 ->215 0.00127

 88 ->247 0.00121

 88 ->258 0.00175

 88 ->264 0.00101

 89 ->170 0.00200

 89 ->222 0.00501

 89 ->230 -0.00152

 89 ->253 -0.00102

 89 ->259 0.00116

 89 ->268 0.00111

 90 ->172 -0.00123

 90 ->218 0.00121

 90 ->224 0.00207

 90 ->228 0.00125

 90 ->272 0.00104

 91 ->178 0.00118

 91 ->179 -0.00109

 91 ->205 -0.00161

 91 ->227 0.00220

 93 ->172 -0.00151

 93 ->187 0.00119

 93 ->202 0.00237

 93 ->208 0.00339

 93 ->218 0.00137

 93 ->224 0.00490

 93 ->238 -0.00266

 93 ->262 -0.00153

 93 ->349 -0.00103

 94 ->224 -0.00102

 94 ->228 0.00104

 94 ->234 -0.00151

 94 ->238 -0.00205

 94 ->245 -0.00109

 94 ->249 -0.00112

 94 ->270 -0.00130

 94 ->272 0.00119

 95 ->185 -0.00117

 95 ->226 -0.00169

 95 ->231 -0.00139

 95 ->258 -0.00117

 96 ->180 -0.00276

 96 ->190 0.00104

 96 ->194 0.00110

 96 ->197 0.00209

 96 ->198 0.00146

 96 ->232 -0.00284

 96 ->239 0.00187

 96 ->259 0.00168

 96 ->260 0.00119

 96 ->268 0.00157

 97 ->192 -0.00200

 97 ->196 -0.00272

 97 ->223 0.00219

 97 ->237 0.00178

 97 ->263 -0.00105

 98 ->182 -0.00116

 98 ->188 0.00158

 98 ->196 -0.00110

 98 ->235 -0.00103

 99 ->199 0.00120

 99 ->206 0.00168

 99 ->209 -0.00128

 99 ->215 -0.00115

 99 ->226 -0.00283

 99 ->231 0.00176

 99 ->233 -0.00151

 99 ->247 -0.00174

 99 ->258 -0.00234

 99 ->341 0.00121

 100 ->170 -0.00102

 100 ->179 -0.00166

 100 ->180 -0.00465

 100 ->186 -0.00340

 100 ->190 0.00238

 100 ->194 0.00293

 100 ->197 0.00337

 100 ->198 0.00212

 100 ->216 0.00117

 100 ->225 -0.00279

 100 ->230 0.00163

 100 ->239 0.00105

 100 ->250 -0.00114

 100 ->253 0.00172

 100 ->261 -0.00121

 101 ->172 0.00120

 101 ->181 0.00146

 101 ->187 -0.00202

 101 ->218 -0.00153

 101 ->224 -0.00156

 101 ->245 -0.00195

 101 ->249 -0.00137

 101 ->251 -0.00123

 101 ->257 0.00144

 102 ->182 0.00176

 102 ->192 0.00345

 102 ->196 0.00479

 102 ->201 0.00103

 102 ->223 0.00186

 102 ->237 -0.00340

 102 ->248 -0.00178

 102 ->256 0.00170

 103 ->185 -0.00173

 103 ->231 0.00155

 103 ->233 -0.00174

 104 ->180 -0.00233

 104 ->186 0.00150

 104 ->222 0.00172

 104 ->225 -0.00326

 104 ->230 -0.00300

 104 ->232 0.00286

 104 ->236 0.00138

 104 ->239 -0.00274

 104 ->250 -0.00162

 104 ->260 -0.00159

 104 ->268 -0.00125

 105 ->171 0.00127

 105 ->217 -0.00260

 105 ->220 -0.00107

 105 ->223 -0.00103

 105 ->246 -0.00178

 106 ->167 0.00177

 106 ->184 0.00105

 106 ->218 0.00120

 106 ->219 0.00128

 106 ->228 0.00301

 106 ->245 0.00154

 106 ->249 0.00205

 106 ->257 -0.00115

 106 ->272 0.00173

 107 ->168 0.00509

 107 ->248 -0.00151

 108 ->169 0.00268

 108 ->200 0.00103

 108 ->233 -0.00103

 108 ->254 0.00127

 109 ->170 0.00139

 109 ->178 -0.00128

 109 ->179 0.00161

 109 ->216 -0.00138

 109 ->230 -0.00102

 109 ->236 0.00113

 109 ->255 0.00130

 110 ->169 0.00116

 110 ->175 0.00195

 110 ->199 -0.00118

 110 ->214 -0.00165

 110 ->221 0.00127

 110 ->226 0.00122

 110 ->254 0.00105

 111 ->170 0.00188

 111 ->179 -0.00137

 111 ->198 0.00169

 111 ->213 -0.00165

 111 ->216 -0.00186

 111 ->230 -0.00277

 111 ->232 0.00226

 111 ->236 0.00124

 111 ->253 -0.00112

 111 ->255 -0.00111

 111 ->260 -0.00108

 111 ->308 -0.00110

 111 ->309 0.00117

 112 ->172 -0.00197

 112 ->187 0.00173

 112 ->219 0.00219

 112 ->234 0.00116

 112 ->249 0.00184

 112 ->257 -0.00159

 113 ->167 -0.00176

 113 ->187 0.00111

 113 ->203 -0.00130

 113 ->208 -0.00140

 113 ->211 -0.00136

 113 ->218 0.00181

 113 ->224 0.00220

 113 ->228 0.00487

 113 ->249 0.00135

 113 ->251 0.00143

 113 ->257 -0.00385

 113 ->272 0.00303

 113 ->278 -0.00134

 113 ->298 0.00136

 113 ->336 0.00146

 114 ->182 -0.00110

 114 ->188 0.00273

 114 ->192 0.00206

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 Excited State 4: Singlet-E 3.0222 eV 410.25 nm f=1.6482 <S\*\*2>=0.000

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 138 <-223 -0.00395

 138 <-229 0.00352

 138 <-237 0.00118

 138 <-246 0.00101

 138 <-263 0.00119

 138 <-279 -0.00191

 138 <-294 -0.00107

 139 <-202 0.00211

 139 <-224 0.00213

 139 <-238 0.00112

 139 <-245 0.00167

 140 <-183 0.00137

 140 <-223 -0.00126

 140 <-229 0.00118

 140 <-242 -0.00115

 141 <-170 -0.00149

 141 <-213 0.00104

 141 <-216 0.00157

 141 <-230 0.00271

 141 <-232 -0.00132

 141 <-241 -0.00115

 141 <-253 -0.00113

 142 <-185 0.00110

 142 <-199 -0.00126

 142 <-206 0.00139

 142 <-226 0.00139

 142 <-231 -0.00239

 142 <-233 0.00120

 143 <-167 0.00344

 143 <-203 0.00121

 143 <-243 0.00119

 144 <-178 0.00101

 144 <-186 -0.00116

 144 <-198 0.00150

 144 <-210 -0.00152

 144 <-230 0.00181

 144 <-253 -0.00125

 145 <-200 -0.00102

 145 <-231 -0.00141

 145 <-244 -0.00109

 146 <-171 0.00209

 146 <-182 -0.00129

 146 <-207 -0.00198

 146 <-220 -0.00112

 146 <-235 0.00120

 146 <-237 0.00163

 146 <-248 -0.00268

 146 <-256 0.00303

 146 <-269 0.00149

 146 <-271 -0.00109

 146 <-297 -0.00144

 146 <-310 -0.00130

 147 <-171 -0.00207

 147 <-183 -0.00297

 147 <-204 -0.00194

 147 <-212 0.00132

 147 <-265 0.00192

 147 <-282 -0.00139

 147 <-294 -0.00109

 148 <-170 0.00109

 148 <-179 -0.00407

 148 <-180 -0.00848

 148 <-186 -0.00666

 148 <-190 0.00106

 148 <-194 -0.00456

 148 <-197 0.00105

 148 <-198 0.00176

 148 <-213 -0.00212

 148 <-222 0.00173

 148 <-225 -0.00593

 148 <-232 -0.00112

 148 <-236 0.00167

 148 <-239 0.00277

 148 <-250 0.00257

 148 <-253 -0.00217

 148 <-260 0.00175

 148 <-261 0.00116

 148 <-277 0.00183

 148 <-283 0.00107

 148 <-476 0.00129

 149 <-175 0.00109

 149 <-226 -0.00514

 149 <-231 -0.00327

 149 <-233 0.00119

 149 <-240 -0.00105

 149 <-258 -0.00136

 149 <-264 -0.00262

 149 <-273 -0.00289

 149 <-280 0.00223

 149 <-292 0.00146

 149 <-329 -0.00107

 149 <-341 0.00158

 149 <-343 0.00123

 150 <-170 -0.00121

 150 <-178 -0.00159

 150 <-179 0.00155

 150 <-205 0.00240

 150 <-255 0.00124

 150 <-283 -0.00123

 150 <-284 0.00121

 150 <-289 0.00136

 150 <-309 0.00141

 151 <-173 0.00321

 151 <-185 0.00136

 151 <-189 0.00508

 151 <-200 -0.00147

 151 <-209 0.00126

 151 <-215 -0.00109

 151 <-267 0.00188

 151 <-275 -0.00102

 151 <-302 -0.00120

 152 <-167 0.01584

 152 <-172 0.00216

 152 <-184 -0.00107

 152 <-195 0.00103

 152 <-208 -0.00135

 152 <-219 -0.00104

 152 <-238 0.00151

 152 <-245 -0.00110

 152 <-281 -0.00117

 152 <-288 -0.00101

 153 <-167 0.00355

 153 <-172 0.00326

 153 <-184 -0.00236

 153 <-187 -0.00127

 153 <-191 0.00106

 153 <-202 -0.00190

 153 <-208 -0.00139

 153 <-211 0.00123

 153 <-218 -0.00146

 153 <-228 -0.00411

 153 <-238 0.00351

 153 <-249 0.00111

 153 <-266 0.00116

 153 <-272 -0.00315

 153 <-278 0.00141

 153 <-281 0.00104

 153 <-301 -0.00111

 153 <-305 0.00148

 153 <-311 0.00115

 153 <-323 0.00128

 153 <-334 -0.00131

 154 <-177 -0.00245

 154 <-184 -0.00180

 155 <-168 0.00621

 155 <-171 0.00277

 156 <-170 0.00282

 156 <-174 -0.00112

 156 <-178 -0.00251

 156 <-197 0.00131

 156 <-205 0.00148

 157 <-169 0.00142

 157 <-173 0.00353

 157 <-189 0.00169

 157 <-200 0.00113

 158 <-172 -0.00209

 158 <-177 0.00151

 158 <-181 -0.00198

 158 <-184 0.00127

 158 <-187 -0.00156

 158 <-203 -0.00190

 158 <-218 -0.00126

 158 <-228 -0.00468

 158 <-234 0.00253

 158 <-238 0.00379

 158 <-249 0.00242

 158 <-272 -0.00528

 158 <-288 -0.00107

 158 <-334 -0.00154

 158 <-338 -0.00104

 159 <-171 -0.00323

 159 <-176 -0.00339

 159 <-196 0.00119

 159 <-204 -0.00200

 159 <-212 -0.00114

 159 <-235 -0.00130

 159 <-252 -0.00111

 159 <-271 0.00119

 159 <-335 -0.00121

 160 <-175 0.00517

 160 <-200 -0.00330

 160 <-206 0.00131

 161 <-170 0.00298

 161 <-174 0.00322

 161 <-178 -0.00332

 161 <-190 -0.00171

 161 <-194 0.00104

 161 <-205 0.00162

 161 <-227 -0.00123

 161 <-232 0.00105

 161 <-289 -0.00141

 161 <-309 -0.00121

 161 <-318 -0.00116

 162 <-169 -0.00701

 162 <-173 0.00214

 162 <-175 -0.00119

 162 <-185 0.00127

 162 <-189 0.00655

 162 <-200 0.00152

 162 <-221 0.00164

 162 <-226 0.00102

 162 <-273 -0.00114

 162 <-312 0.00116

 162 <-326 -0.00128

 163 <-170 0.00287

 163 <-178 0.00743

 163 <-179 0.00332

 163 <-180 -0.00133

 163 <-190 0.00212

 163 <-197 -0.00216

 163 <-205 -0.00309

 163 <-210 0.00241

 163 <-216 -0.00212

 163 <-227 0.00355

 163 <-274 -0.00135

 163 <-283 -0.00132

 163 <-299 -0.00118

 163 <-309 0.00109

 163 <-330 -0.00150

 163 <-332 0.00133

 164 <-172 -0.00190

 164 <-177 -0.00145

 164 <-184 0.00717

 164 <-203 -0.00134

 164 <-288 0.00110

 164 <-305 0.00187

 164 <-311 0.00153

 164 <-315 0.00217

 165 <-168 -0.08030

 165 <-171 -0.00191

 165 <-176 -0.00732

 165 <-183 0.00792

 165 <-204 0.00340

 165 <-220 0.00184

 165 <-248 -0.00156

 165 <-252 0.00127

 165 <-279 0.00134

 165 <-300 -0.00105

 165 <-325 -0.00149

 165 <-333 0.00130

 165 <-339 0.00188

 165 <-345 0.00124

 166 <-167 -0.09153

 166 <-172 0.00324

 166 <-177 0.00850

 166 <-184 0.01321

 166 <-195 0.00118

 166 <-203 -0.00191

 166 <-211 -0.00272

 166 <-219 -0.00324

 166 <-224 0.00126

 166 <-249 0.00152

 166 <-266 -0.00197

 166 <-281 0.00158

 166 <-288 0.00137

 166 <-295 0.00105

 166 <-305 0.00116

 166 <-338 0.00114

 Excited State 5: Singlet-E 3.5769 eV 346.62 nm f=0.0000 <S\*\*2>=0.000

 62 ->208 0.00108

 63 ->207 -0.00108

 64 ->206 -0.00123

 74 ->229 0.00109

 75 ->228 0.00109

 84 ->190 -0.00142

 84 ->197 -0.00188

 84 ->261 0.00134

 85 ->226 0.00149

 85 ->231 0.00136

 85 ->233 -0.00112

 86 ->226 -0.00114

 86 ->231 -0.00142

 86 ->233 0.00117

 88 ->182 0.00101

 88 ->196 0.00144

 88 ->229 0.00155

 89 ->181 -0.00101

 89 ->195 -0.00144

 89 ->228 -0.00155

 93 ->180 -0.00177

 93 ->194 0.00173

 93 ->222 0.00194

 93 ->277 0.00101

 95 ->229 0.00126

 96 ->228 -0.00126

 97 ->209 -0.00101

 99 ->207 -0.00108

 99 ->223 0.00156

 100 ->208 0.00108

 100 ->224 -0.00156

 102 ->206 -0.00157

 102 ->258 -0.00153

 102 ->401 0.00107

 103 ->223 0.00128

 103 ->229 -0.00145

 104 ->224 -0.00128

 104 ->228 0.00145

 106 ->222 -0.00163

 108 ->168 0.00201

 109 ->167 -0.00201

 110 ->168 0.00154

 111 ->167 0.00154

 113 ->186 -0.00105

 113 ->222 -0.00284

 113 ->253 0.00118

 114 ->169 0.00123

 114 ->240 0.00179

 114 ->244 -0.00112

 114 ->390 0.00106

 115 ->189 0.00126

 116 ->168 0.00253

 117 ->167 -0.00253

 119 ->167 -0.00240

 119 ->228 -0.00115

 119 ->234 0.00129

 120 ->168 -0.00240

 120 ->229 0.00115

 120 ->235 -0.00129

 121 ->240 0.00246

 121 ->244 -0.00199

 121 ->254 0.00133

 121 ->276 -0.00225

 121 ->293 -0.00123

 121 ->355 -0.00121

 121 ->390 0.00167

 121 ->441 -0.00101

 122 ->189 0.00115

 123 ->190 -0.00105

 123 ->197 -0.00145

 124 ->167 -0.01781

 124 ->177 0.00206

 124 ->184 -0.00186

 124 ->203 -0.00101

 125 ->168 0.01781

 125 ->176 0.00206

 125 ->183 0.00186

 125 ->204 -0.00101

 126 ->167 0.00202

 126 ->224 -0.00146

 126 ->234 0.00111

 126 ->278 -0.00123

 127 ->168 0.00202

 127 ->223 0.00146

 127 ->235 -0.00111

 127 ->279 0.00123

 128 ->169 0.01587

 128 ->175 0.00492

 128 ->193 -0.00118

 128 ->200 0.00173

 129 ->261 0.00140

 130 ->226 -0.00367

 130 ->264 0.00116

 130 ->292 -0.00116

 130 ->296 -0.00144

 130 ->343 -0.00193

 130 ->362 -0.00160

 130 ->387 -0.00106

 130 ->422 -0.00102

 131 ->180 -0.00122

 131 ->277 0.00149

 132 ->229 0.00158

 132 ->271 0.00106

 132 ->279 0.00118

 132 ->333 -0.00119

 132 ->335 0.00100

 132 ->389 0.00101

 133 ->228 -0.00158

 133 ->272 0.00106

 133 ->278 -0.00118

 133 ->334 0.00119

 133 ->336 -0.00100

 133 ->388 -0.00101

 134 ->206 0.00125

 134 ->226 -0.00138

 134 ->343 -0.00123

 134 ->362 -0.00116

 135 ->169 -0.00310

 135 ->240 -0.00146

 135 ->244 0.00124

 136 ->195 -0.00112

 137 ->196 0.00112

 138 ->194 0.00188

 138 ->222 -0.00119

 138 ->277 -0.00121

 141 ->168 -0.00177

 142 ->167 -0.00177

 144 ->168 0.00376

 145 ->167 0.00376

 146 ->170 0.00123

 147 ->174 0.00166

 147 ->179 -0.00264

 148 ->223 0.00179

 148 ->229 0.00112

 148 ->235 -0.00103

 149 ->224 -0.00179

 149 ->228 -0.00112

 149 ->234 0.00103

 150 ->168 -0.03062

 150 ->171 -0.00223

 150 ->183 -0.00391

 151 ->167 -0.03062

 151 ->172 0.00223

 151 ->184 -0.00391

 152 ->173 0.00288

 152 ->185 0.00154

 152 ->189 0.00733

 152 ->206 -0.00220

 152 ->273 0.00102

 153 ->173 -0.00110

 153 ->185 -0.00147

 153 ->189 -0.00740

 153 ->226 -0.00208

 154 ->169 -0.01684

 154 ->175 0.00163

 154 ->193 0.00143

 154 ->200 -0.00551

 154 ->209 -0.00102

 154 ->221 -0.00193

 155 ->170 0.00272

 156 ->168 -0.05842

 156 ->171 0.00261

 156 ->183 0.00320

 156 ->204 0.00210

 156 ->220 0.00101

 157 ->167 -0.05842

 157 ->172 -0.00261

 157 ->184 0.00320

 157 ->203 -0.00210

 157 ->219 -0.00101

 158 ->173 0.00110

 158 ->189 0.00668

 158 ->226 -0.00153

 158 ->343 -0.00124

 158 ->362 -0.00100

 159 ->179 -0.00527

 159 ->180 0.00253

 159 ->194 -0.00152

 159 ->222 0.00117

 160 ->167 0.10616

 160 ->177 -0.00190

 160 ->184 -0.00719

 160 ->195 -0.00133

 160 ->203 0.00381

 160 ->211 0.00188

 160 ->219 0.00258

 160 ->224 -0.00121

 161 ->168 -0.10616

 161 ->176 -0.00190

 161 ->183 0.00719

 161 ->196 -0.00133

 161 ->204 0.00381

 161 ->212 0.00188

 161 ->220 0.00258

 161 ->223 -0.00121

 162 ->167 -0.48132

 162 ->177 0.00904

 162 ->181 -0.00101

 162 ->184 0.01177

 162 ->202 0.00111

 162 ->203 -0.00598

 162 ->208 0.00213

 162 ->211 -0.00228

 162 ->218 -0.00138

 162 ->219 -0.00396

 162 ->249 0.00158

 162 ->315 -0.00105

 163 ->168 0.48132

 163 ->176 0.00904

 163 ->182 -0.00101

 163 ->183 -0.01177

 163 ->201 0.00111

 163 ->204 -0.00598

 163 ->207 0.00213

 163 ->212 -0.00228

 163 ->217 -0.00138

 163 ->220 -0.00396

 163 ->248 0.00158

 163 ->316 -0.00105

 164 ->169 0.05331

 164 ->175 0.00397

 164 ->193 -0.00317

 164 ->200 0.01587

 164 ->209 0.00134

 164 ->215 -0.00347

 164 ->221 0.00614

 164 ->254 -0.00153

 164 ->267 0.00145

 164 ->326 0.00197

 165 ->170 0.00245

 165 ->178 -0.00563

 165 ->205 0.00296

 165 ->210 0.00144

 165 ->227 0.00156

 165 ->289 0.00103

 165 ->309 0.00106

 165 ->492 0.00115

 166 ->189 -0.00627

 84 <-197 -0.00121

 85 <-226 0.00104

 85 <-231 0.00102

 86 <-231 -0.00101

 88 <-229 0.00102

 89 <-228 -0.00102

 93 <-180 -0.00107

 93 <-194 0.00110

 93 <-222 0.00126

 99 <-223 0.00100

 100 <-224 -0.00100

 102 <-206 -0.00101

 102 <-258 -0.00102

 113 <-222 -0.00172

 114 <-240 0.00121

 121 <-240 0.00165

 121 <-244 -0.00133

 121 <-276 -0.00167

 121 <-390 0.00133

 124 <-167 -0.00414

 124 <-184 -0.00147

 125 <-168 0.00414

 125 <-183 0.00147

 128 <-169 0.00511

 128 <-175 0.00188

 130 <-226 -0.00227

 130 <-296 -0.00105

 130 <-343 -0.00144

 130 <-362 -0.00122

 132 <-229 0.00112

 133 <-228 -0.00112

 147 <-179 0.00140

 150 <-168 -0.00453

 150 <-183 -0.00314

 151 <-167 -0.00453

 151 <-184 -0.00314

 152 <-173 0.00103

 152 <-189 0.00481

 152 <-206 -0.00133

 152 <-273 0.00103

 153 <-189 -0.00498

 154 <-169 0.00272

 154 <-175 0.00220

 154 <-200 -0.00140

 156 <-168 0.00161

 156 <-183 0.00166

 157 <-167 0.00161

 157 <-184 0.00166

 158 <-189 0.00422

 158 <-343 -0.00107

 160 <-167 -0.00529

 160 <-184 -0.00412

 161 <-168 0.00529

 161 <-183 0.00412

 162 <-167 0.00555

 162 <-172 -0.00123

 162 <-184 0.00458

 162 <-203 -0.00212

 162 <-219 -0.00188

 163 <-168 -0.00555

 163 <-171 -0.00123

 163 <-183 -0.00458

 163 <-204 -0.00212

 163 <-220 -0.00188

 164 <-169 -0.00899

 164 <-175 -0.00401

 164 <-200 0.00361

 164 <-215 -0.00107

 164 <-221 0.00224

 164 <-312 -0.00109

 164 <-326 0.00101

 165 <-178 -0.00368

 165 <-197 0.00114

 165 <-205 0.00239

 165 <-216 0.00127

 165 <-492 0.00109

 Excited State 6: Singlet-E 3.6197 eV 342.53 nm f=0.0000 <S\*\*2>=0.000

 60 ->226 0.00103

 61 ->206 -0.00166

 61 ->231 -0.00142

 61 ->247 0.00136

 61 ->258 0.00146

 61 ->280 0.00105

 61 ->422 -0.00106

 62 ->208 -0.00136

 63 ->207 -0.00136

 64 ->209 -0.00117

 64 ->215 -0.00107

 64 ->275 0.00102

 74 ->229 0.00189

 75 ->228 -0.00189

 81 ->224 0.00137

 82 ->223 0.00137

 84 ->180 -0.00158

 84 ->194 0.00156

 84 ->222 0.00374

 84 ->225 0.00102

 84 ->232 -0.00129

 84 ->268 0.00159

 84 ->277 0.00184

 85 ->240 -0.00173

 85 ->244 0.00116

 85 ->276 0.00103

 86 ->240 0.00103

 87 ->226 0.00126

 88 ->182 -0.00101

 88 ->196 -0.00123

 88 ->223 0.00307

 89 ->181 -0.00101

 89 ->195 -0.00123

 89 ->224 0.00307

 93 ->190 -0.00168

 93 ->197 -0.00211

 93 ->216 -0.00103

 93 ->230 -0.00282

 93 ->261 0.00152

 93 ->317 -0.00118

 93 ->406 -0.00104

 94 ->222 -0.00117

 95 ->235 -0.00119

 95 ->279 0.00120

 96 ->234 -0.00119

 96 ->278 0.00120

 97 ->206 -0.00141

 97 ->226 -0.00214

 97 ->258 -0.00128

 97 ->264 0.00105

 97 ->401 0.00110

 99 ->182 0.00103

 99 ->196 0.00127

 99 ->207 -0.00138

 99 ->304 -0.00107

 100 ->181 0.00103

 100 ->195 0.00127

 100 ->208 -0.00138

 100 ->305 0.00107

 102 ->209 -0.00147

 102 ->215 -0.00113

 102 ->312 0.00103

 102 ->329 -0.00106

 102 ->341 0.00171

 102 ->390 -0.00157

 103 ->246 0.00114

 103 ->279 -0.00105

 104 ->245 0.00114

 104 ->278 -0.00105

 106 ->236 0.00108

 106 ->317 0.00100

 107 ->169 0.00364

 107 ->175 0.00119

 108 ->168 0.00309

 109 ->167 0.00309

 110 ->168 0.00188

 111 ->167 -0.00188

 113 ->230 -0.00123

 113 ->236 0.00155

 113 ->255 -0.00100

 113 ->309 0.00130

 113 ->317 0.00155

 114 ->185 -0.00105

 114 ->226 -0.00191

 114 ->264 0.00107

 114 ->343 -0.00114

 115 ->169 0.00507

 115 ->175 0.00286

 115 ->200 -0.00114

 116 ->168 0.00178

 116 ->196 0.00105

 117 ->167 0.00178

 117 ->195 -0.00105

 118 ->190 0.00106

 119 ->167 0.00275

 119 ->191 0.00128

 119 ->224 0.00132

 119 ->278 0.00117

 120 ->168 -0.00275

 120 ->192 0.00128

 120 ->223 0.00132

 120 ->279 0.00117

 121 ->199 0.00131

 121 ->206 0.00163

 121 ->226 -0.00242

 121 ->231 -0.00114

 121 ->296 -0.00151

 121 ->343 -0.00232

 121 ->362 -0.00215

 121 ->387 -0.00130

 121 ->422 -0.00102

 121 ->444 -0.00100

 122 ->169 0.00533

 122 ->175 0.00277

 122 ->193 -0.00103

 122 ->200 -0.00102

 123 ->194 0.00309

 123 ->222 -0.00197

 123 ->277 -0.00209

 123 ->378 -0.00101

 124 ->167 0.01283

 124 ->172 -0.00203

 124 ->177 -0.00154

 124 ->184 0.00376

 124 ->191 -0.00104

 125 ->168 0.01283

 125 ->171 0.00203

 125 ->176 0.00154

 125 ->183 0.00376

 125 ->192 0.00104

 126 ->167 -0.00132

 126 ->202 0.00114

 126 ->224 0.00112

 126 ->228 0.00152

 126 ->334 -0.00121

 126 ->336 0.00143

 126 ->377 0.00107

 127 ->168 0.00132

 127 ->201 0.00114

 127 ->223 0.00112

 127 ->229 0.00152

 127 ->333 -0.00121

 127 ->335 0.00143

 127 ->376 0.00107

 128 ->185 0.00111

 128 ->189 0.00676

 128 ->206 -0.00112

 129 ->194 -0.00164

 129 ->198 -0.00104

 129 ->222 0.00239

 129 ->225 -0.00101

 129 ->330 -0.00127

 129 ->378 0.00107

 130 ->169 -0.00124

 130 ->175 0.00137

 130 ->215 0.00117

 130 ->240 0.00227

 130 ->244 -0.00194

 130 ->254 0.00121

 130 ->276 -0.00188

 130 ->285 0.00104

 130 ->329 -0.00160

 130 ->341 0.00138

 130 ->355 -0.00116

 130 ->390 0.00147

 130 ->421 -0.00115

 130 ->441 -0.00128

 131 ->230 -0.00165

 131 ->261 0.00143

 131 ->274 -0.00116

 131 ->284 0.00122

 131 ->289 -0.00111

 131 ->317 -0.00102

 132 ->196 -0.00129

 132 ->207 0.00118

 132 ->223 -0.00157

 132 ->229 0.00211

 132 ->304 -0.00144

 132 ->316 -0.00145

 133 ->195 -0.00129

 133 ->208 0.00118

 133 ->224 -0.00157

 133 ->228 0.00211

 133 ->305 0.00144

 133 ->315 -0.00145

 134 ->169 0.00196

 134 ->209 0.00170

 134 ->215 0.00116

 134 ->390 0.00122

 135 ->189 -0.00120

 135 ->231 -0.00167

 135 ->264 -0.00179

 135 ->273 -0.00129

 135 ->280 0.00172

 135 ->343 0.00163

 136 ->167 0.00310

 136 ->172 0.00133

 136 ->191 -0.00134

 136 ->195 -0.00163

 136 ->224 -0.00128

 136 ->228 0.00126

 137 ->168 -0.00310

 137 ->171 0.00133

 137 ->192 -0.00134

 137 ->196 -0.00163

 137 ->223 -0.00128

 137 ->229 0.00126

 138 ->170 -0.00115

 138 ->190 -0.00139

 138 ->197 -0.00223

 138 ->230 0.00169

 138 ->236 0.00164

 138 ->261 -0.00132

 138 ->317 0.00124

 138 ->374 -0.00130

 139 ->199 -0.00118

 139 ->231 -0.00125

 140 ->210 0.00109

 141 ->256 0.00110

 142 ->257 0.00110

 143 ->200 -0.00141

 144 ->204 0.00106

 145 ->203 0.00106

 146 ->198 0.00119

 146 ->260 -0.00126

 146 ->330 -0.00122

 146 ->332 -0.00108

 147 ->170 0.00326

 147 ->205 -0.00126

 148 ->263 -0.00119

 148 ->271 0.00167

 148 ->304 -0.00131

 148 ->316 -0.00136

 148 ->333 -0.00134

 148 ->350 0.00107

 148 ->369 -0.00121

 149 ->262 -0.00119

 149 ->272 -0.00167

 149 ->305 0.00131

 149 ->315 -0.00136

 149 ->334 -0.00134

 149 ->349 0.00107

 149 ->368 -0.00121

 150 ->168 0.02921

 150 ->176 0.00158

 150 ->183 -0.00537

 150 ->204 -0.00285

 150 ->207 0.00165

 150 ->212 -0.00176

 150 ->217 -0.00119

 150 ->220 -0.00284

 150 ->265 -0.00112

 150 ->282 0.00119

 151 ->167 -0.02921

 151 ->177 0.00158

 151 ->184 0.00537

 151 ->203 -0.00285

 151 ->208 0.00165

 151 ->211 -0.00176

 151 ->218 -0.00119

 151 ->219 -0.00284

 151 ->266 -0.00112

 151 ->281 0.00119

 152 ->169 -0.03991

 152 ->175 -0.00224

 152 ->193 0.00198

 152 ->200 -0.01065

 152 ->209 -0.00272

 152 ->215 0.00230

 152 ->221 -0.00432

 152 ->254 0.00106

 152 ->267 -0.00137

 152 ->326 -0.00137

 153 ->169 0.02714

 153 ->175 0.00475

 153 ->193 -0.00153

 153 ->200 0.00733

 153 ->215 -0.00172

 153 ->221 0.00340

 153 ->326 0.00178

 153 ->329 -0.00206

 153 ->341 0.00167

 154 ->189 0.00274

 154 ->206 -0.00180

 155 ->194 -0.00136

 156 ->168 -0.04750

 156 ->171 -0.00118

 156 ->176 -0.00162

 156 ->183 0.00270

 156 ->196 0.00111

 157 ->167 0.04750

 157 ->172 -0.00118

 157 ->177 -0.00162

 157 ->184 -0.00270

 157 ->195 0.00111

 158 ->169 -0.02146

 158 ->175 -0.00268

 158 ->193 0.00109

 158 ->200 -0.00574

 158 ->215 0.00188

 158 ->221 -0.00247

 158 ->254 0.00100

 158 ->267 -0.00161

 158 ->312 0.00101

 158 ->326 -0.00103

 158 ->341 0.00194

 159 ->170 0.00611

 159 ->197 0.00255

 159 ->205 0.00164

 159 ->236 -0.00140

 160 ->167 -0.16127

 160 ->172 0.00347

 160 ->177 0.00497

 160 ->184 0.00752

 160 ->203 -0.00231

 160 ->211 -0.00135

 160 ->219 -0.00245

 160 ->249 0.00102

 160 ->315 -0.00125

 161 ->168 -0.16127

 161 ->171 -0.00347

 161 ->176 -0.00497

 161 ->183 0.00752

 161 ->204 0.00231

 161 ->212 0.00135

 161 ->220 0.00245

 161 ->248 -0.00102

 161 ->316 0.00125

 162 ->167 0.46206

 162 ->172 0.00303

 162 ->177 -0.00516

 162 ->184 -0.00533

 162 ->195 -0.00120

 162 ->202 -0.00146

 162 ->203 0.00504

 162 ->208 -0.00222

 162 ->211 0.00215

 162 ->219 0.00274

 162 ->305 0.00105

 162 ->315 0.00126

 163 ->168 0.46206

 163 ->171 -0.00303

 163 ->176 0.00516

 163 ->183 -0.00533

 163 ->196 0.00120

 163 ->201 0.00146

 163 ->204 -0.00504

 163 ->207 0.00222

 163 ->212 -0.00215

 163 ->220 -0.00274

 163 ->304 0.00105

 163 ->316 -0.00126

 164 ->173 -0.00131

 164 ->185 -0.00114

 164 ->189 -0.00753

 164 ->206 0.00102

 164 ->495 -0.00142

 165 ->174 -0.00542

 165 ->179 0.01405

 165 ->180 -0.00366

 165 ->283 -0.00107

 165 ->330 -0.00111

 165 ->332 0.00129

 166 ->169 -0.10157

 166 ->200 0.00532

 166 ->215 -0.00257

 166 ->221 0.00434

 166 ->267 0.00212

 166 ->275 -0.00126

 166 ->329 -0.00126

 61 <-206 -0.00120

 61 <-231 -0.00116

 61 <-247 0.00104

 61 <-258 0.00107

 74 <-229 0.00132

 75 <-228 -0.00132

 84 <-194 0.00103

 84 <-222 0.00246

 84 <-277 0.00125

 85 <-240 -0.00120

 88 <-223 0.00205

 89 <-224 0.00205

 93 <-190 -0.00101

 93 <-197 -0.00132

 93 <-230 -0.00201

 93 <-261 0.00104

 97 <-226 -0.00142

 102 <-341 0.00127

 102 <-390 -0.00121

 107 <-169 0.00215

 108 <-168 0.00132

 109 <-167 0.00132

 113 <-236 0.00114

 113 <-317 0.00114

 114 <-226 -0.00122

 115 <-169 0.00274

 115 <-175 0.00142

 115 <-200 -0.00106

 121 <-226 -0.00155

 121 <-296 -0.00114

 121 <-343 -0.00173

 121 <-362 -0.00165

 121 <-387 -0.00102

 122 <-169 0.00250

 122 <-175 0.00127

 122 <-200 -0.00102

 123 <-194 0.00164

 123 <-222 -0.00105

 123 <-277 -0.00143

 124 <-167 0.00309

 124 <-184 0.00324

 125 <-168 0.00309

 125 <-183 0.00324

 126 <-228 0.00105

 126 <-336 0.00107

 127 <-229 0.00105

 127 <-335 0.00107

 128 <-189 0.00457

 129 <-222 0.00137

 130 <-240 0.00145

 130 <-244 -0.00124

 130 <-276 -0.00137

 130 <-329 -0.00116

 130 <-390 0.00115

 130 <-441 -0.00103

 132 <-229 0.00128

 133 <-228 0.00128

 135 <-231 -0.00105

 135 <-264 -0.00121

 135 <-280 0.00112

 135 <-343 0.00120

 138 <-197 -0.00117

 147 <-205 -0.00136

 148 <-271 0.00107

 149 <-272 -0.00107

 150 <-168 0.00526

 150 <-183 -0.00286

 150 <-204 -0.00116

 150 <-212 -0.00105

 150 <-220 -0.00149

 151 <-167 -0.00526

 151 <-184 0.00286

 151 <-203 -0.00116

 151 <-211 -0.00105

 151 <-219 -0.00149

 152 <-169 0.00368

 152 <-175 0.00202

 152 <-200 -0.00241

 152 <-209 -0.00116

 152 <-221 -0.00154

 152 <-267 -0.00100

 153 <-169 -0.00598

 153 <-175 -0.00192

 153 <-221 0.00113

 153 <-329 -0.00162

 153 <-341 0.00114

 154 <-189 0.00202

 156 <-168 0.00247

 156 <-183 0.00147

 157 <-167 -0.00247

 157 <-184 -0.00147

 158 <-169 0.00447

 158 <-175 0.00182

 158 <-267 -0.00104

 158 <-341 0.00137

 160 <-167 0.00164

 160 <-184 0.00343

 161 <-168 0.00164

 161 <-183 0.00343

 162 <-167 -0.01085

 162 <-177 0.00118

 162 <-184 -0.00352

 163 <-168 -0.01085

 163 <-176 -0.00118

 163 <-183 -0.00352

 164 <-189 -0.00578

 164 <-273 -0.00115

 164 <-296 -0.00128

 165 <-179 0.00600

 165 <-180 -0.00180

 166 <-169 0.01021

 166 <-175 0.00197

 166 <-200 0.00355

 166 <-215 -0.00151

 166 <-221 0.00208

 166 <-267 0.00143

 Excited State 7: Singlet-E 3.6414 eV 340.48 nm f=0.0464 <S\*\*2>=0.000

 50 ->230 0.00102

 52 ->223 -0.00126

 61 ->207 -0.00116

 61 ->237 0.00114

 62 ->180 -0.00127

 63 ->206 -0.00121

 74 ->240 0.00103

 84 ->181 -0.00111

 84 ->191 -0.00112

 84 ->195 -0.00146

 84 ->224 0.00143

 84 ->228 -0.00101

 85 ->279 -0.00112

 88 ->206 -0.00116

 88 ->240 0.00146

 88 ->244 -0.00121

 89 ->190 -0.00108

 89 ->194 0.00170

 89 ->197 -0.00133

 89 ->222 0.00110

 89 ->230 -0.00102

 93 ->181 -0.00134

 93 ->191 -0.00112

 93 ->195 -0.00193

 93 ->224 0.00105

 93 ->234 -0.00105

 93 ->270 -0.00135

 95 ->226 -0.00133

 96 ->180 0.00127

 96 ->194 0.00120

 97 ->207 -0.00114

 97 ->229 0.00147

 99 ->206 -0.00110

 99 ->209 -0.00145

 99 ->215 -0.00102

 99 ->390 -0.00102

 99 ->401 0.00106

 100 ->179 0.00106

 100 ->180 0.00231

 100 ->186 0.00172

 100 ->190 0.00104

 100 ->197 0.00142

 100 ->222 -0.00167

 102 ->207 -0.00144

 102 ->389 -0.00107

 103 ->226 0.00140

 103 ->231 0.00176

 107 ->168 0.00285

 110 ->231 0.00112

 113 ->224 -0.00148

 113 ->228 0.00160

 113 ->234 -0.00109

 114 ->229 0.00148

 114 ->235 -0.00111

 114 ->237 0.00103

 115 ->168 0.00705

 115 ->204 0.00103

 119 ->197 0.00108

 120 ->226 -0.00101

 120 ->231 -0.00112

 120 ->240 0.00156

 120 ->244 -0.00108

 120 ->276 -0.00141

 121 ->168 -0.00104

 121 ->229 0.00319

 121 ->235 -0.00201

 121 ->237 0.00112

 121 ->279 0.00118

 121 ->333 -0.00108

 121 ->389 0.00145

 122 ->168 0.00802

 122 ->176 0.00109

 122 ->204 0.00114

 123 ->195 -0.00110

 123 ->249 -0.00106

 124 ->178 0.00271

 124 ->179 0.00268

 124 ->180 -0.00108

 124 ->210 0.00119

 124 ->227 0.00195

 125 ->169 0.00640

 125 ->175 0.00247

 125 ->189 0.00326

 126 ->222 -0.00115

 126 ->253 0.00107

 127 ->240 0.00298

 127 ->244 -0.00232

 127 ->254 0.00107

 127 ->285 0.00105

 127 ->343 -0.00126

 128 ->168 0.01367

 128 ->176 0.00102

 128 ->183 0.00371

 128 ->316 0.00106

 129 ->228 -0.00155

 129 ->234 0.00137

 129 ->238 0.00103

 130 ->168 0.00244

 130 ->223 0.00148

 130 ->229 0.00206

 130 ->235 -0.00166

 130 ->271 0.00185

 130 ->279 0.00220

 130 ->325 0.00146

 130 ->333 -0.00118

 131 ->228 0.00120

 131 ->262 -0.00119

 132 ->169 -0.00113

 132 ->226 -0.00330

 132 ->231 -0.00140

 132 ->276 -0.00149

 132 ->293 -0.00119

 132 ->343 -0.00167

 132 ->362 -0.00143

 132 ->390 0.00140

 133 ->179 0.00105

 133 ->180 0.00199

 133 ->186 0.00151

 133 ->194 0.00172

 133 ->222 -0.00110

 133 ->225 0.00131

 133 ->253 0.00113

 133 ->261 -0.00148

 133 ->277 -0.00134

 134 ->168 -0.00270

 134 ->229 0.00117

 134 ->279 0.00115

 135 ->168 -0.00443

 135 ->192 -0.00113

 135 ->196 -0.00121

 135 ->229 -0.00158

 135 ->271 -0.00159

 135 ->304 0.00178

 136 ->180 0.00114

 136 ->186 0.00131

 136 ->194 0.00200

 136 ->225 0.00130

 137 ->169 0.00145

 137 ->226 -0.00119

 138 ->195 -0.00102

 138 ->228 -0.00111

 138 ->262 0.00116

 140 ->167 0.00110

 143 ->168 0.00183

 146 ->167 0.00111

 146 ->172 0.00108

 146 ->228 -0.00125

 146 ->234 0.00115

 147 ->167 -0.00514

 147 ->172 0.00163

 147 ->184 -0.00380

 147 ->203 0.00147

 148 ->169 0.00109

 148 ->226 -0.00356

 148 ->240 0.00202

 148 ->244 -0.00159

 148 ->247 -0.00108

 148 ->258 -0.00167

 148 ->343 -0.00112

 149 ->170 -0.00120

 149 ->179 -0.00265

 149 ->180 -0.00754

 149 ->186 -0.00613

 149 ->190 -0.00145

 149 ->194 -0.00391

 149 ->197 -0.00162

 149 ->198 0.00179

 149 ->213 -0.00169

 149 ->222 -0.00132

 149 ->225 -0.00381

 149 ->236 -0.00225

 149 ->250 0.00198

 149 ->253 -0.00242

 149 ->259 -0.00190

 149 ->260 0.00120

 149 ->366 0.00177

 149 ->371 -0.00102

 149 ->378 -0.00162

 149 ->393 0.00114

 149 ->476 -0.00112

 150 ->169 -0.00559

 150 ->175 -0.00506

 150 ->200 0.00586

 150 ->221 0.00249

 151 ->178 0.00197

 151 ->179 0.00231

 151 ->205 -0.00103

 152 ->168 -0.01431

 152 ->171 0.00177

 152 ->176 -0.00381

 152 ->183 0.00824

 152 ->188 0.00105

 152 ->204 0.00146

 152 ->207 -0.00123

 152 ->220 0.00176

 153 ->168 0.07801

 153 ->171 -0.00103

 153 ->176 0.00146

 153 ->183 -0.00925

 153 ->192 -0.00148

 153 ->201 0.00119

 153 ->212 -0.00103

 153 ->217 0.00114

 153 ->220 -0.00106

 153 ->223 0.00315

 153 ->229 0.00215

 153 ->235 -0.00150

 153 ->237 -0.00121

 153 ->246 -0.00127

 153 ->248 -0.00102

 153 ->263 -0.00181

 153 ->271 -0.00185

 153 ->287 0.00112

 153 ->304 0.00131

 154 ->168 -0.06919

 154 ->171 0.00208

 154 ->176 -0.00289

 154 ->183 0.00422

 154 ->204 0.00358

 154 ->207 -0.00141

 154 ->212 0.00132

 154 ->220 0.00170

 155 ->167 0.01143

 155 ->172 0.00104

 155 ->177 -0.00156

 155 ->184 0.00223

 156 ->169 -0.00354

 156 ->173 0.00153

 156 ->175 0.00150

 156 ->189 0.00327

 156 ->200 -0.00337

 157 ->174 -0.00309

 157 ->178 0.00155

 157 ->179 0.00304

 157 ->210 0.00101

 158 ->168 -0.06625

 158 ->176 -0.00141

 158 ->183 0.00815

 158 ->188 0.00229

 158 ->196 -0.00167

 158 ->201 0.00149

 158 ->204 0.00140

 158 ->217 0.00198

 158 ->223 0.00253

 158 ->229 0.00226

 158 ->235 -0.00209

 158 ->237 -0.00157

 158 ->246 -0.00147

 158 ->248 -0.00226

 158 ->256 0.00120

 158 ->263 -0.00249

 158 ->271 -0.00206

 158 ->350 0.00110

 159 ->167 -0.00596

 159 ->172 0.00479

 159 ->177 -0.00262

 159 ->184 -0.00108

 160 ->174 0.00103

 160 ->178 -0.00121

 160 ->197 -0.00107

 160 ->205 -0.00265

 160 ->210 -0.00123

 160 ->216 -0.00147

 160 ->227 -0.00158

 161 ->169 -0.02702

 161 ->173 -0.00284

 161 ->175 0.00243

 161 ->189 0.00500

 161 ->193 0.00155

 161 ->200 -0.00957

 161 ->215 0.00231

 161 ->221 -0.00350

 162 ->170 0.00521

 162 ->174 0.00450

 162 ->178 0.00431

 162 ->179 0.00204

 162 ->205 0.00428

 162 ->210 0.00304

 162 ->216 0.00154

 162 ->227 0.00379

 163 ->169 0.03819

 163 ->173 -0.00711

 163 ->175 0.00435

 163 ->185 -0.00262

 163 ->189 -0.01319

 163 ->193 -0.00209

 163 ->200 0.00933

 163 ->206 0.00210

 163 ->215 -0.00198

 163 ->221 0.00377

 163 ->326 0.00105

 164 ->168 0.68986

 164 ->171 -0.00337

 164 ->176 0.00698

 164 ->183 -0.01242

 164 ->196 0.00118

 164 ->201 0.00229

 164 ->204 -0.01084

 164 ->207 0.00283

 164 ->212 -0.00444

 164 ->217 -0.00211

 164 ->220 -0.00657

 164 ->223 0.00102

 164 ->248 0.00157

 164 ->265 -0.00177

 165 ->167 -0.01861

 165 ->172 0.00782

 165 ->177 -0.00221

 165 ->184 -0.01315

 165 ->191 0.00144

 165 ->202 -0.00112

 165 ->203 0.00447

 165 ->208 -0.00110

 165 ->211 0.00170

 165 ->219 0.00311

 166 ->168 0.05663

 166 ->171 -0.00690

 166 ->176 -0.02303

 166 ->183 0.00791

 166 ->204 -0.00401

 88 <-240 0.00103

 89 <-194 0.00108

 93 <-195 -0.00119

 97 <-229 0.00100

 100 <-180 0.00129

 100 <-222 -0.00105

 103 <-231 0.00119

 107 <-168 0.00109

 113 <-228 0.00105

 115 <-168 0.00267

 120 <-240 0.00104

 120 <-276 -0.00101

 121 <-229 0.00207

 121 <-235 -0.00131

 121 <-389 0.00115

 122 <-168 0.00289

 124 <-178 0.00138

 124 <-179 0.00163

 124 <-227 0.00134

 125 <-169 0.00249

 125 <-175 0.00114

 125 <-189 0.00244

 127 <-240 0.00193

 127 <-244 -0.00151

 128 <-183 0.00327

 130 <-229 0.00134

 130 <-235 -0.00103

 130 <-271 0.00120

 130 <-279 0.00155

 130 <-325 0.00109

 132 <-226 -0.00200

 132 <-276 -0.00107

 132 <-343 -0.00125

 132 <-362 -0.00106

 132 <-390 0.00108

 135 <-304 0.00122

 147 <-167 -0.00110

 147 <-184 -0.00217

 148 <-226 -0.00192

 148 <-240 0.00115

 149 <-179 -0.00129

 149 <-180 -0.00290

 149 <-186 -0.00255

 149 <-194 -0.00176

 149 <-225 -0.00205

 149 <-236 -0.00133

 149 <-250 0.00119

 149 <-253 -0.00147

 149 <-259 -0.00120

 149 <-366 0.00129

 149 <-378 -0.00120

 150 <-169 -0.00505

 150 <-175 -0.00231

 150 <-200 0.00261

 150 <-221 0.00151

 152 <-168 0.00394

 152 <-183 0.00547

 153 <-183 -0.00631

 153 <-204 0.00110

 153 <-223 0.00164

 153 <-271 -0.00125

 154 <-168 0.00422

 154 <-204 0.00157

 156 <-169 0.00183

 156 <-175 0.00133

 156 <-189 0.00186

 157 <-179 0.00160

 158 <-168 0.00115

 158 <-183 0.00510

 158 <-188 0.00113

 158 <-223 0.00117

 158 <-229 0.00129

 158 <-235 -0.00109

 158 <-248 -0.00116

 158 <-263 -0.00155

 158 <-271 -0.00114

 160 <-174 0.00101

 160 <-179 -0.00278

 160 <-205 -0.00125

 160 <-227 -0.00125

 161 <-169 0.00580

 161 <-175 0.00273

 161 <-189 0.00342

 161 <-200 -0.00244

 161 <-221 -0.00140

 162 <-179 0.00494

 162 <-180 -0.00171

 162 <-205 0.00224

 162 <-210 0.00153

 162 <-216 0.00113

 162 <-227 0.00221

 163 <-169 -0.00582

 163 <-173 -0.00148

 163 <-175 -0.00256

 163 <-185 -0.00125

 163 <-189 -0.00758

 163 <-200 0.00166

 163 <-206 0.00142

 163 <-221 0.00121

 164 <-168 -0.01331

 164 <-171 -0.00204

 164 <-176 -0.00154

 164 <-183 -0.00325

 164 <-204 -0.00403

 164 <-207 0.00116

 164 <-212 -0.00142

 164 <-217 -0.00126

 164 <-220 -0.00290

 165 <-167 0.00460

 165 <-184 -0.00579

 165 <-203 0.00187

 165 <-219 0.00130

 166 <-168 -0.01384

 166 <-176 -0.00153

 166 <-183 0.00351

 166 <-204 -0.00139

 Excited State 8: Singlet-E 3.6414 eV 340.48 nm f=0.0464 <S\*\*2>=0.000

 51 ->230 0.00102

 52 ->224 -0.00126

 61 ->208 0.00116

 61 ->238 -0.00114

 62 ->206 0.00121

 63 ->180 0.00127

 75 ->240 -0.00103

 84 ->182 0.00111

 84 ->192 0.00112

 84 ->196 0.00146

 84 ->223 -0.00143

 84 ->229 0.00101

 85 ->278 -0.00112

 88 ->190 -0.00108

 88 ->194 -0.00170

 88 ->197 -0.00133

 88 ->222 -0.00110

 88 ->230 -0.00102

 89 ->206 0.00116

 89 ->240 0.00146

 89 ->244 -0.00121

 93 ->182 -0.00134

 93 ->192 -0.00112

 93 ->196 -0.00193

 93 ->223 0.00105

 93 ->235 -0.00105

 93 ->269 -0.00135

 95 ->180 -0.00127

 95 ->194 -0.00120

 96 ->226 0.00133

 97 ->208 0.00114

 97 ->228 -0.00147

 99 ->179 -0.00106

 99 ->180 -0.00231

 99 ->186 -0.00172

 99 ->190 0.00104

 99 ->197 0.00142

 99 ->222 0.00167

 100 ->206 0.00110

 100 ->209 -0.00145

 100 ->215 -0.00102

 100 ->390 -0.00102

 100 ->401 -0.00106

 102 ->208 -0.00144

 102 ->388 -0.00107

 104 ->226 -0.00140

 104 ->231 -0.00176

 107 ->167 -0.00285

 111 ->231 -0.00112

 113 ->223 -0.00148

 113 ->229 0.00160

 113 ->235 -0.00109

 114 ->228 -0.00148

 114 ->234 0.00111

 114 ->238 -0.00103

 115 ->167 -0.00705

 115 ->203 0.00103

 119 ->226 0.00101

 119 ->231 0.00112

 119 ->240 0.00156

 119 ->244 -0.00108

 119 ->276 -0.00141

 120 ->197 0.00108

 121 ->167 -0.00104

 121 ->228 -0.00319

 121 ->234 0.00201

 121 ->238 -0.00112

 121 ->278 -0.00118

 121 ->334 0.00108

 121 ->388 -0.00145

 122 ->167 -0.00802

 122 ->177 0.00109

 122 ->203 0.00114

 123 ->196 0.00110

 123 ->248 0.00106

 124 ->169 -0.00640

 124 ->175 -0.00247

 124 ->189 0.00326

 125 ->178 -0.00271

 125 ->179 0.00268

 125 ->180 -0.00108

 125 ->210 -0.00119

 125 ->227 -0.00195

 126 ->240 0.00298

 126 ->244 -0.00232

 126 ->254 0.00107

 126 ->285 0.00105

 126 ->343 0.00126

 127 ->222 0.00115

 127 ->253 -0.00107

 128 ->167 0.01367

 128 ->177 -0.00102

 128 ->184 0.00371

 128 ->315 -0.00106

 129 ->229 0.00155

 129 ->235 -0.00137

 129 ->237 -0.00103

 130 ->167 -0.00244

 130 ->224 0.00148

 130 ->228 0.00206

 130 ->234 -0.00166

 130 ->272 -0.00185

 130 ->278 0.00220

 130 ->324 0.00146

 130 ->334 -0.00118

 131 ->229 0.00120

 131 ->263 -0.00119

 132 ->179 -0.00105

 132 ->180 -0.00199

 132 ->186 -0.00151

 132 ->194 -0.00172

 132 ->222 0.00110

 132 ->225 -0.00131

 132 ->253 -0.00113

 132 ->261 -0.00148

 132 ->277 0.00134

 133 ->169 -0.00113

 133 ->226 0.00330

 133 ->231 0.00140

 133 ->276 -0.00149

 133 ->293 -0.00119

 133 ->343 0.00167

 133 ->362 0.00143

 133 ->390 0.00140

 134 ->167 0.00270

 134 ->228 0.00117

 134 ->278 0.00115

 135 ->167 -0.00443

 135 ->191 0.00113

 135 ->195 0.00121

 135 ->228 0.00158

 135 ->272 -0.00159

 135 ->305 0.00178

 136 ->169 0.00145

 136 ->226 0.00119

 137 ->180 -0.00114

 137 ->186 -0.00131

 137 ->194 -0.00200

 137 ->225 -0.00130

 138 ->196 -0.00102

 138 ->229 -0.00111

 138 ->263 0.00116

 140 ->168 -0.00110

 143 ->167 -0.00183

 146 ->168 0.00111

 146 ->171 -0.00108

 146 ->229 0.00125

 146 ->235 -0.00115

 147 ->168 0.00514

 147 ->171 0.00163

 147 ->183 0.00380

 147 ->204 0.00147

 148 ->170 -0.00120

 148 ->179 0.00265

 148 ->180 0.00754

 148 ->186 0.00613

 148 ->190 -0.00145

 148 ->194 0.00391

 148 ->197 -0.00162

 148 ->198 -0.00179

 148 ->213 0.00169

 148 ->222 0.00132

 148 ->225 0.00381

 148 ->236 -0.00225

 148 ->250 -0.00198

 148 ->253 0.00242

 148 ->259 -0.00190

 148 ->260 -0.00120

 148 ->366 -0.00177

 148 ->371 -0.00102

 148 ->378 0.00162

 148 ->393 -0.00114

 148 ->476 -0.00112

 149 ->169 0.00109

 149 ->226 0.00356

 149 ->240 0.00202

 149 ->244 -0.00159

 149 ->247 0.00108

 149 ->258 0.00167

 149 ->343 0.00112

 150 ->178 0.00197

 150 ->179 -0.00231

 150 ->205 -0.00103

 151 ->169 -0.00559

 151 ->175 -0.00506

 151 ->200 0.00586

 151 ->221 0.00249

 152 ->167 0.01431

 152 ->172 0.00177

 152 ->177 -0.00381

 152 ->184 -0.00824

 152 ->187 0.00105

 152 ->203 0.00146

 152 ->208 -0.00123

 152 ->219 0.00176

 153 ->167 -0.07801

 153 ->172 -0.00103

 153 ->177 0.00146

 153 ->184 0.00925

 153 ->191 -0.00148

 153 ->202 0.00119

 153 ->211 -0.00103

 153 ->218 0.00114

 153 ->219 -0.00106

 153 ->224 0.00315

 153 ->228 0.00215

 153 ->234 -0.00150

 153 ->238 -0.00121

 153 ->245 -0.00127

 153 ->249 -0.00102

 153 ->262 -0.00181

 153 ->272 0.00185

 153 ->288 0.00112

 153 ->305 -0.00131

 154 ->167 -0.06919

 154 ->172 -0.00208

 154 ->177 0.00289

 154 ->184 0.00422

 154 ->203 -0.00358

 154 ->208 0.00141

 154 ->211 -0.00132

 154 ->219 -0.00170

 155 ->168 0.01143

 155 ->171 -0.00104

 155 ->176 0.00156

 155 ->183 0.00223

 156 ->174 0.00309

 156 ->178 0.00155

 156 ->179 -0.00304

 156 ->210 0.00101

 157 ->169 -0.00354

 157 ->173 -0.00153

 157 ->175 0.00150

 157 ->189 -0.00327

 157 ->200 -0.00337

 158 ->167 0.06625

 158 ->177 -0.00141

 158 ->184 -0.00815

 158 ->187 0.00229

 158 ->195 -0.00167

 158 ->202 0.00149

 158 ->203 0.00140

 158 ->218 0.00198

 158 ->224 0.00253

 158 ->228 0.00226

 158 ->234 -0.00209

 158 ->238 -0.00157

 158 ->245 -0.00147

 158 ->249 -0.00226

 158 ->257 0.00120

 158 ->262 -0.00249

 158 ->272 0.00206

 158 ->349 0.00110

 159 ->168 0.00596

 159 ->171 0.00479

 159 ->176 -0.00262

 159 ->183 0.00108

 160 ->169 0.02702

 160 ->173 -0.00284

 160 ->175 -0.00243

 160 ->189 0.00500

 160 ->193 -0.00155

 160 ->200 0.00957

 160 ->215 -0.00231

 160 ->221 0.00350

 161 ->174 0.00103

 161 ->178 0.00121

 161 ->197 0.00107

 161 ->205 0.00265

 161 ->210 0.00123

 161 ->216 0.00147

 161 ->227 0.00158

 162 ->169 -0.03819

 162 ->173 -0.00711

 162 ->175 -0.00435

 162 ->185 -0.00262

 162 ->189 -0.01319

 162 ->193 0.00209

 162 ->200 -0.00933

 162 ->206 0.00210

 162 ->215 0.00198

 162 ->221 -0.00377

 162 ->326 -0.00105

 163 ->170 -0.00521

 163 ->174 0.00450

 163 ->178 -0.00431

 163 ->179 0.00204

 163 ->205 -0.00428

 163 ->210 -0.00304

 163 ->216 -0.00154

 163 ->227 -0.00379

 164 ->167 0.68986

 164 ->172 0.00337

 164 ->177 -0.00698

 164 ->184 -0.01242

 164 ->195 -0.00118

 164 ->202 -0.00229

 164 ->203 0.01084

 164 ->208 -0.00283

 164 ->211 0.00444

 164 ->218 0.00211

 164 ->219 0.00657

 164 ->224 -0.00102

 164 ->249 -0.00157

 164 ->266 0.00177

 165 ->168 -0.01861

 165 ->171 -0.00782

 165 ->176 0.00221

 165 ->183 -0.01315

 165 ->192 -0.00144

 165 ->201 0.00112

 165 ->204 -0.00447

 165 ->207 0.00110

 165 ->212 -0.00170

 165 ->220 -0.00311

 166 ->167 -0.05663

 166 ->172 -0.00690

 166 ->177 -0.02303

 166 ->184 -0.00791

 166 ->203 -0.00401

 88 <-194 -0.00108

 89 <-240 0.00103

 93 <-196 -0.00119

 97 <-228 -0.00100

 99 <-180 -0.00129

 99 <-222 0.00105

 104 <-231 -0.00119

 107 <-167 -0.00109

 113 <-229 0.00105

 115 <-167 -0.00267

 119 <-240 0.00104

 119 <-276 -0.00101

 121 <-228 -0.00207

 121 <-234 0.00131

 121 <-388 -0.00115

 122 <-167 -0.00289

 124 <-169 -0.00249

 124 <-175 -0.00114

 124 <-189 0.00244

 125 <-178 -0.00138

 125 <-179 0.00163

 125 <-227 -0.00134

 126 <-240 0.00193

 126 <-244 -0.00151

 128 <-184 0.00327

 130 <-228 0.00134

 130 <-234 -0.00103

 130 <-272 -0.00120

 130 <-278 0.00155

 130 <-324 0.00109

 133 <-226 0.00200

 133 <-276 -0.00107

 133 <-343 0.00125

 133 <-362 0.00106

 133 <-390 0.00108

 135 <-305 0.00122

 147 <-168 0.00110

 147 <-183 0.00217

 148 <-179 0.00129

 148 <-180 0.00290

 148 <-186 0.00255

 148 <-194 0.00176

 148 <-225 0.00205

 148 <-236 -0.00133

 148 <-250 -0.00119

 148 <-253 0.00147

 148 <-259 -0.00120

 148 <-366 -0.00129

 148 <-378 0.00120

 149 <-226 0.00192

 149 <-240 0.00115

 151 <-169 -0.00505

 151 <-175 -0.00231

 151 <-200 0.00261

 151 <-221 0.00151

 152 <-167 -0.00394

 152 <-184 -0.00547

 153 <-184 0.00631

 153 <-203 0.00110

 153 <-224 0.00164

 153 <-272 0.00125

 154 <-167 0.00422

 154 <-203 -0.00157

 156 <-179 -0.00160

 157 <-169 0.00183

 157 <-175 0.00133

 157 <-189 -0.00186

 158 <-167 -0.00115

 158 <-184 -0.00510

 158 <-187 0.00113

 158 <-224 0.00117

 158 <-228 0.00129

 158 <-234 -0.00109

 158 <-249 -0.00116

 158 <-262 -0.00155

 158 <-272 0.00114

 160 <-169 -0.00580

 160 <-175 -0.00273

 160 <-189 0.00342

 160 <-200 0.00244

 160 <-221 0.00140

 161 <-174 0.00101

 161 <-179 -0.00278

 161 <-205 0.00125

 161 <-227 0.00125

 162 <-169 0.00582

 162 <-173 -0.00148

 162 <-175 0.00256

 162 <-185 -0.00125

 162 <-189 -0.00758

 162 <-200 -0.00166

 162 <-206 0.00142

 162 <-221 -0.00121

 163 <-179 0.00494

 163 <-180 -0.00171

 163 <-205 -0.00224

 163 <-210 -0.00153

 163 <-216 -0.00113

 163 <-227 -0.00221

 164 <-167 -0.01331

 164 <-172 0.00204

 164 <-177 0.00154

 164 <-184 -0.00325

 164 <-203 0.00403

 164 <-208 -0.00116

 164 <-211 0.00142

 164 <-218 0.00126

 164 <-219 0.00290

 165 <-168 0.00460

 165 <-183 -0.00579

 165 <-204 -0.00187

 165 <-220 -0.00130

 166 <-167 0.01384

 166 <-177 -0.00153

 166 <-184 -0.00351

 166 <-203 -0.00139

 Excited State 9: Singlet-E 3.7142 eV 333.81 nm f=0.0233 <S\*\*2>=0.000

 50 ->179 -0.00125

 52 ->168 0.00139

 62 ->179 0.00121

 93 ->203 0.00111

 95 ->189 0.00151

 97 ->183 0.00182

 98 ->183 0.00100

 99 ->169 0.00165

 99 ->189 0.00163

 102 ->168 -0.00167

 102 ->183 0.00225

 113 ->167 -0.00112

 124 ->180 -0.00107

 124 ->225 -0.00143

 127 ->169 -0.00111

 128 ->168 -0.00193

 130 ->168 -0.00195

 130 ->183 0.00178

 131 ->167 0.00203

 131 ->184 0.00122

 132 ->169 0.00253

 134 ->168 0.00222

 135 ->168 -0.00531

 135 ->183 -0.00589

 135 ->201 -0.00107

 135 ->204 0.00405

 135 ->220 0.00155

 135 ->397 0.00128

 136 ->179 0.00108

 138 ->167 -0.00238

 138 ->184 -0.00101

 139 ->183 0.00130

 140 ->167 -0.00144

 141 ->169 0.00243

 144 ->169 0.00232

 145 ->179 -0.00132

 147 ->167 0.00118

 148 ->169 0.03423

 148 ->175 0.00758

 148 ->189 0.00137

 148 ->193 -0.00209

 148 ->200 0.00597

 148 ->215 -0.00119

 148 ->221 0.00185

 148 ->254 -0.00115

 149 ->170 -0.00150

 149 ->174 0.00312

 149 ->178 -0.00324

 149 ->179 -0.01731

 149 ->180 0.00636

 149 ->194 0.00101

 149 ->210 -0.00204

 149 ->227 -0.00355

 151 ->180 -0.00112

 152 ->168 0.01228

 152 ->183 -0.00112

 153 ->168 0.38270

 153 ->171 0.00605

 153 ->176 0.01199

 153 ->183 -0.00975

 153 ->204 0.00133

 153 ->248 0.00109

 154 ->176 0.00130

 155 ->167 0.00562

 155 ->172 -0.00139

 157 ->170 0.00149

 158 ->168 0.59108

 158 ->171 0.00547

 158 ->176 0.01527

 158 ->182 -0.00112

 158 ->183 -0.01340

 158 ->212 -0.00159

 158 ->223 0.00102

 158 ->248 0.00171

 158 ->339 -0.00103

 159 ->167 0.00121

 159 ->172 -0.00102

 160 ->170 -0.00123

 161 ->169 0.00206

 161 ->175 -0.00142

 162 ->178 -0.00154

 162 ->180 -0.00360

 162 ->186 -0.00239

 162 ->198 0.00121

 162 ->205 0.00137

 162 ->225 -0.00188

 162 ->239 0.00102

 163 ->169 0.00424

 163 ->175 0.00158

 163 ->189 0.00165

 163 ->200 -0.00101

 164 ->168 0.01630

 164 ->183 0.00283

 164 ->223 0.00141

 165 ->167 0.02168

 165 ->172 0.00212

 165 ->177 0.00265

 166 ->168 -0.02393

 166 ->176 0.00532

 166 ->183 -0.00211

 166 ->204 -0.00119

 166 ->223 0.00181

 135 <-183 0.00116

 149 <-179 0.00274

 149 <-205 0.00152

 152 <-168 -0.00168

 153 <-168 -0.00189

 153 <-183 0.00135

 158 <-168 -0.00351

 158 <-183 0.00106

 158 <-204 -0.00161

 162 <-179 0.00133

 164 <-183 0.00126

 165 <-167 -0.00580

 165 <-228 0.00163

 165 <-272 0.00149

 166 <-168 0.00490

 166 <-229 -0.00168

 166 <-271 0.00138

 Excited State 10: Singlet-E 3.7142 eV 333.81 nm f=0.0233 <S\*\*2>=0.000

 51 ->179 -0.00125

 52 ->167 0.00139

 63 ->179 0.00121

 93 ->204 -0.00111

 96 ->189 0.00151

 97 ->184 -0.00182

 98 ->184 -0.00100

 100 ->169 -0.00165

 100 ->189 0.00163

 102 ->167 -0.00167

 102 ->184 0.00225

 113 ->168 -0.00112

 125 ->180 0.00107

 125 ->225 0.00143

 126 ->169 0.00111

 128 ->167 0.00193

 130 ->167 -0.00195

 130 ->184 0.00178

 131 ->168 0.00203

 131 ->183 0.00122

 133 ->169 -0.00253

 134 ->167 0.00222

 135 ->167 0.00531

 135 ->184 0.00589

 135 ->202 -0.00107

 135 ->203 0.00405

 135 ->219 0.00155

 135 ->398 0.00128

 137 ->179 0.00108

 138 ->168 -0.00238

 138 ->183 -0.00101

 139 ->184 -0.00130

 140 ->168 -0.00144

 142 ->169 -0.00243

 144 ->179 -0.00132

 145 ->169 -0.00232

 147 ->168 0.00118

 148 ->170 0.00150

 148 ->174 0.00312

 148 ->178 0.00324

 148 ->179 -0.01731

 148 ->180 0.00636

 148 ->194 0.00101

 148 ->210 0.00204

 148 ->227 0.00355

 149 ->169 -0.03423

 149 ->175 -0.00758

 149 ->189 0.00137

 149 ->193 0.00209

 149 ->200 -0.00597

 149 ->215 0.00119

 149 ->221 -0.00185

 149 ->254 0.00115

 150 ->180 -0.00112

 152 ->167 0.01228

 152 ->184 -0.00112

 153 ->167 0.38270

 153 ->172 -0.00605

 153 ->177 -0.01199

 153 ->184 -0.00975

 153 ->203 -0.00133

 153 ->249 -0.00109

 154 ->177 0.00130

 155 ->168 -0.00562

 155 ->171 -0.00139

 156 ->170 -0.00149

 158 ->167 0.59108

 158 ->172 -0.00547

 158 ->177 -0.01527

 158 ->181 0.00112

 158 ->184 -0.01340

 158 ->211 0.00159

 158 ->224 -0.00102

 158 ->249 -0.00171

 158 ->338 -0.00103

 159 ->168 0.00121

 159 ->171 0.00102

 160 ->169 0.00206

 160 ->175 -0.00142

 161 ->170 -0.00123

 162 ->169 0.00424

 162 ->175 0.00158

 162 ->189 -0.00165

 162 ->200 -0.00101

 163 ->178 -0.00154

 163 ->180 0.00360

 163 ->186 0.00239

 163 ->198 -0.00121

 163 ->205 0.00137

 163 ->225 0.00188

 163 ->239 -0.00102

 164 ->167 -0.01630

 164 ->184 -0.00283

 164 ->224 0.00141

 165 ->168 -0.02168

 165 ->171 0.00212

 165 ->176 0.00265

 166 ->167 -0.02393

 166 ->177 -0.00532

 166 ->184 -0.00211

 166 ->203 0.00119

 166 ->224 -0.00181

 135 <-184 -0.00116

 148 <-179 0.00274

 148 <-205 -0.00152

 152 <-167 -0.00168

 153 <-167 -0.00189

 153 <-184 0.00135

 158 <-167 -0.00351

 158 <-184 0.00106

 158 <-203 0.00161

 163 <-179 -0.00133

 164 <-184 -0.00126

 165 <-168 0.00580

 165 <-229 0.00163

 165 <-271 -0.00149

 166 <-167 0.00490

 166 <-228 0.00168

 166 <-272 0.00138

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

 Leave Link 914 at Thu Sep 5 22:07:15 2019, MaxMem= 1342177280 cpu: 14234.8

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

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

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 Population analysis using the SCF density.

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 Orbital symmetries:

 Occupied (E) (E) (B2) (A1) (E) (E) (B2) (A2) (B1) (E) (E)

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 (B2) (A1) (A1) (E) (E) (B1) (A1) (E) (E) (B2)

 (B1) (E) (E) (A1) (B2) (E) (E) (A2) (A1) (E) (E)

 (B1) (A2) (E) (E) (B2) (B1) (E) (E) (A1) (B2)

 (E) (E) (A2) (B1) (E) (E) (A1) (B1) (E) (E) (A2)

 (B1) (E) (E) (A1) (B2) (A1) (E) (E)

 The electronic state is 1-A1.

 Alpha occ. eigenvalues -- -14.30274 -14.30274 -14.30273 -14.30273 -10.20850

 Alpha occ. eigenvalues -- -10.20850 -10.20850 -10.20850 -10.20849 -10.20849

 Alpha occ. eigenvalues -- -10.20849 -10.20849 -10.19527 -10.19527 -10.19527

 Alpha occ. eigenvalues -- -10.19527 -10.18649 -10.18649 -10.18649 -10.18649

 Alpha occ. eigenvalues -- -10.17325 -10.17325 -10.17325 -10.17325 -10.17325

 Alpha occ. eigenvalues -- -10.17325 -10.17325 -10.17325 -10.17283 -10.17283

 Alpha occ. eigenvalues -- -10.17283 -10.17283 -10.17252 -10.17252 -10.17252

 Alpha occ. eigenvalues -- -10.17252 -10.17215 -10.17215 -10.17215 -10.17215

 Alpha occ. eigenvalues -- -10.16829 -10.16829 -10.16829 -10.16829 -10.16763

 Alpha occ. eigenvalues -- -10.16763 -10.16763 -10.16763 -0.96311 -0.95466

 Alpha occ. eigenvalues -- -0.95466 -0.94579 -0.86920 -0.86555 -0.86555

 Alpha occ. eigenvalues -- -0.86379 -0.82290 -0.80635 -0.80635 -0.78864

 Alpha occ. eigenvalues -- -0.76631 -0.76592 -0.76592 -0.76144 -0.74941

 Alpha occ. eigenvalues -- -0.74862 -0.74862 -0.74828 -0.74123 -0.73406

 Alpha occ. eigenvalues -- -0.73406 -0.71852 -0.70867 -0.66163 -0.66163

 Alpha occ. eigenvalues -- -0.62134 -0.61068 -0.60823 -0.60823 -0.60677

 Alpha occ. eigenvalues -- -0.59897 -0.59897 -0.59468 -0.59445 -0.58587

 Alpha occ. eigenvalues -- -0.57012 -0.56547 -0.56261 -0.56261 -0.56057

 Alpha occ. eigenvalues -- -0.55332 -0.55332 -0.54829 -0.54320 -0.52699

 Alpha occ. eigenvalues -- -0.52699 -0.52628 -0.51909 -0.51398 -0.51398

 Alpha occ. eigenvalues -- -0.49894 -0.49806 -0.49165 -0.49165 -0.46156

 Alpha occ. eigenvalues -- -0.46073 -0.45862 -0.45731 -0.45731 -0.44985

 Alpha occ. eigenvalues -- -0.44985 -0.44864 -0.44341 -0.42569 -0.42546

 Alpha occ. eigenvalues -- -0.42305 -0.42305 -0.42195 -0.42155 -0.42155

 Alpha occ. eigenvalues -- -0.42129 -0.41797 -0.41216 -0.40818 -0.40818

 Alpha occ. eigenvalues -- -0.40139 -0.40139 -0.39299 -0.39066 -0.38439

 Alpha occ. eigenvalues -- -0.38303 -0.37820 -0.37820 -0.36828 -0.36767

 Alpha occ. eigenvalues -- -0.36708 -0.36708 -0.35813 -0.35163 -0.34764

 Alpha occ. eigenvalues -- -0.34695 -0.34695 -0.34605 -0.34599 -0.34599

 Alpha occ. eigenvalues -- -0.33902 -0.31870 -0.31301 -0.31301 -0.28611

 Alpha occ. eigenvalues -- -0.28611 -0.26425 -0.26019 -0.25991 -0.25945

 Alpha occ. eigenvalues -- -0.25930 -0.25930 -0.25682 -0.25255 -0.25238

 Alpha occ. eigenvalues -- -0.25238 -0.24717 -0.24717 -0.24647 -0.20184

 Alpha occ. eigenvalues -- -0.18937

 Alpha virt. eigenvalues -- -0.09064 -0.09064 -0.03556 -0.01361 -0.01316

 Alpha virt. eigenvalues -- -0.01316 -0.01116 -0.01041 -0.01029 -0.00930

 Alpha virt. eigenvalues -- -0.00930 0.03358 0.03798 0.04518 0.04646

 Alpha virt. eigenvalues -- 0.04646 0.05596 0.05596 0.05822 0.06119

 Alpha virt. eigenvalues -- 0.07000 0.07000 0.07197 0.08446 0.08983

 Alpha virt. eigenvalues -- 0.08983 0.09147 0.09179 0.09557 0.09557

 Alpha virt. eigenvalues -- 0.10009 0.10277 0.10339 0.10376 0.11364

 Alpha virt. eigenvalues -- 0.11364 0.11918 0.11918 0.12037 0.12647

 Alpha virt. eigenvalues -- 0.13045 0.13045 0.13326 0.13423 0.13695

 Alpha virt. eigenvalues -- 0.13695 0.13809 0.14078 0.14170 0.14728

 Alpha virt. eigenvalues -- 0.15121 0.15121 0.15773 0.15773 0.16274

 Alpha virt. eigenvalues -- 0.16461 0.18510 0.18510 0.20796 0.21632

 Alpha virt. eigenvalues -- 0.22463 0.23766 0.23766 0.23814 0.23862

 Alpha virt. eigenvalues -- 0.24494 0.25350 0.25688 0.25688 0.26612

 Alpha virt. eigenvalues -- 0.26946 0.26946 0.27152 0.27581 0.28038

 Alpha virt. eigenvalues -- 0.28054 0.28054 0.28372 0.28519 0.28519

 Alpha virt. eigenvalues -- 0.28918 0.29009 0.29009 0.29010 0.29992

 Alpha virt. eigenvalues -- 0.29992 0.30039 0.30049 0.30669 0.31413

 Alpha virt. eigenvalues -- 0.31413 0.31596 0.32476 0.34392 0.35120

 Alpha virt. eigenvalues -- 0.35359 0.35359 0.35508 0.36081 0.36081

 Alpha virt. eigenvalues -- 0.36373 0.36473 0.36753 0.36753 0.36852

 Alpha virt. eigenvalues -- 0.36852 0.37487 0.37665 0.38134 0.38779

 Alpha virt. eigenvalues -- 0.38849 0.39795 0.39795 0.39797 0.39867

 Alpha virt. eigenvalues -- 0.39867 0.40128 0.40540 0.40793 0.41155

 Alpha virt. eigenvalues -- 0.41200 0.41200 0.41478 0.41535 0.41535

 Alpha virt. eigenvalues -- 0.41912 0.41955 0.41990 0.41990 0.42349

 Alpha virt. eigenvalues -- 0.42980 0.42980 0.43152 0.43431 0.43431

 Alpha virt. eigenvalues -- 0.43723 0.43879 0.44575 0.44575 0.44601

 Alpha virt. eigenvalues -- 0.44829 0.45046 0.45147 0.45219 0.45219

 Alpha virt. eigenvalues -- 0.45518 0.46539 0.46539 0.46774 0.46774

 Alpha virt. eigenvalues -- 0.46835 0.47207 0.47595 0.48416 0.48416

 Alpha virt. eigenvalues -- 0.48766 0.48766 0.49664 0.49664 0.49995

 Alpha virt. eigenvalues -- 0.49999 0.50136 0.51020 0.51114 0.51349

 Alpha virt. eigenvalues -- 0.51782 0.52598 0.52598 0.53594 0.53594

 Alpha virt. eigenvalues -- 0.53679 0.54246 0.54246 0.54286 0.54884

 Alpha virt. eigenvalues -- 0.55960 0.56631 0.57532 0.57677 0.57677

 Alpha virt. eigenvalues -- 0.57715 0.57900 0.58626 0.58626 0.59659

 Alpha virt. eigenvalues -- 0.59659 0.60331 0.60460 0.60602 0.60839

 Alpha virt. eigenvalues -- 0.60839 0.61152 0.61323 0.61323 0.61386

 Alpha virt. eigenvalues -- 0.61510 0.61516 0.61657 0.61657 0.62106

 Alpha virt. eigenvalues -- 0.62516 0.62617 0.62617 0.62762 0.63648

 Alpha virt. eigenvalues -- 0.63898 0.63898 0.64424 0.64555 0.64836

 Alpha virt. eigenvalues -- 0.64836 0.65153 0.65227 0.65335 0.65437

 Alpha virt. eigenvalues -- 0.65437 0.65564 0.66823 0.66823 0.66881

 Alpha virt. eigenvalues -- 0.67116 0.67968 0.67968 0.68150 0.69635

 Alpha virt. eigenvalues -- 0.69635 0.70395 0.70711 0.72180 0.72180

 Alpha virt. eigenvalues -- 0.72611 0.72611 0.72694 0.73045 0.73289

 Alpha virt. eigenvalues -- 0.73760 0.73787 0.73787 0.74429 0.74493

 Alpha virt. eigenvalues -- 0.75337 0.75337 0.75723 0.75848 0.75848

 Alpha virt. eigenvalues -- 0.75952 0.76469 0.76469 0.77006 0.78250

 Alpha virt. eigenvalues -- 0.78260 0.78869 0.78869 0.79700 0.79743

 Alpha virt. eigenvalues -- 0.79990 0.80537 0.80537 0.81093 0.81093

 Alpha virt. eigenvalues -- 0.81419 0.81953 0.82369 0.82664 0.82664

 Alpha virt. eigenvalues -- 0.84132 0.84615 0.85250 0.85250 0.85690

 Alpha virt. eigenvalues -- 0.85794 0.87013 0.87285 0.87285 0.87398

 Alpha virt. eigenvalues -- 0.89301 0.89301 0.89302 0.89497 0.90001

 Alpha virt. eigenvalues -- 0.90001 0.90117 0.91772 0.92560 0.92684

 Alpha virt. eigenvalues -- 0.92684 0.93361 0.93558 0.94473 0.94473

 Alpha virt. eigenvalues -- 0.94991 0.96109 0.96620 0.96788 0.96788

 Alpha virt. eigenvalues -- 0.98372 0.99146 0.99146 1.00407 1.00505

 Alpha virt. eigenvalues -- 1.01503 1.01503 1.02404 1.02469 1.02827

 Alpha virt. eigenvalues -- 1.04412 1.04412 1.05228 1.05228 1.05341

 Alpha virt. eigenvalues -- 1.05453 1.05932 1.07581 1.08591 1.09226

 Alpha virt. eigenvalues -- 1.09226 1.09719 1.11356 1.11356 1.11644

 Alpha virt. eigenvalues -- 1.12557 1.13167 1.13167 1.14992 1.14992

 Alpha virt. eigenvalues -- 1.15230 1.15462 1.15462 1.16885 1.17514

 Alpha virt. eigenvalues -- 1.17514 1.17633 1.17633 1.17867 1.18328

 Alpha virt. eigenvalues -- 1.19469 1.20497 1.20497 1.20958 1.21019

 Alpha virt. eigenvalues -- 1.21094 1.21438 1.21438 1.21749 1.21749

 Alpha virt. eigenvalues -- 1.22277 1.22828 1.22971 1.23975 1.24161

 Alpha virt. eigenvalues -- 1.24161 1.24766 1.24766 1.25277 1.25326

 Alpha virt. eigenvalues -- 1.25676 1.26445 1.27012 1.27012 1.27775

 Alpha virt. eigenvalues -- 1.28531 1.28531 1.28827 1.30246 1.31486

 Alpha virt. eigenvalues -- 1.31806 1.32636 1.32636 1.37143 1.38170

 Alpha virt. eigenvalues -- 1.38595 1.38595 1.40391 1.40391 1.41032

 Alpha virt. eigenvalues -- 1.41255 1.41741 1.43969 1.43969 1.44475

 Alpha virt. eigenvalues -- 1.45941 1.47242 1.47242 1.47706 1.47723

 Alpha virt. eigenvalues -- 1.48059 1.48534 1.48534 1.48539 1.49294

 Alpha virt. eigenvalues -- 1.49994 1.49994 1.50305 1.50690 1.52899

 Alpha virt. eigenvalues -- 1.52899 1.53718 1.54174 1.54451 1.54451

 Alpha virt. eigenvalues -- 1.55548 1.55548 1.55715 1.56727 1.56727

 Alpha virt. eigenvalues -- 1.57149 1.58563 1.59949 1.61260 1.61260

 Alpha virt. eigenvalues -- 1.61460 1.61682 1.62535 1.62535 1.64836

 Alpha virt. eigenvalues -- 1.64836 1.65259 1.67334 1.68458 1.68666

 Alpha virt. eigenvalues -- 1.68666 1.68773 1.70139 1.70207 1.70207

 Alpha virt. eigenvalues -- 1.71110 1.71110 1.71694 1.73965 1.74279

 Alpha virt. eigenvalues -- 1.74716 1.76064 1.76064 1.76158 1.76287

 Alpha virt. eigenvalues -- 1.76357 1.76357 1.77480 1.77480 1.77707

 Alpha virt. eigenvalues -- 1.79010 1.79082 1.79905 1.80586 1.80586

 Alpha virt. eigenvalues -- 1.81095 1.81289 1.81399 1.81830 1.81830

 Alpha virt. eigenvalues -- 1.83685 1.83685 1.84124 1.84128 1.84558

 Alpha virt. eigenvalues -- 1.84787 1.85072 1.85222 1.85222 1.86524

 Alpha virt. eigenvalues -- 1.87566 1.87566 1.88657 1.88870 1.88870

 Alpha virt. eigenvalues -- 1.89088 1.89660 1.89981 1.91737 1.91971

 Alpha virt. eigenvalues -- 1.91971 1.92211 1.92565 1.92713 1.92785

 Alpha virt. eigenvalues -- 1.92785 1.93158 1.93232 1.93232 1.94017

 Alpha virt. eigenvalues -- 1.94080 1.94121 1.94121 1.94591 1.96178

 Alpha virt. eigenvalues -- 1.96407 1.96407 1.96689 1.96971 1.96971

 Alpha virt. eigenvalues -- 1.98495 1.99902 1.99997 1.99997 2.00083

 Alpha virt. eigenvalues -- 2.00213 2.00556 2.00556 2.01260 2.06900

 Alpha virt. eigenvalues -- 2.07144 2.08170 2.08170 2.09100 2.09100

 Alpha virt. eigenvalues -- 2.09104 2.11700 2.13063 2.13904 2.14304

 Alpha virt. eigenvalues -- 2.14304 2.19160 2.22089 2.23720 2.24110

 Alpha virt. eigenvalues -- 2.24110 2.25803 2.25876 2.25876 2.26301

 Alpha virt. eigenvalues -- 2.26583 2.26836 2.27625 2.27625 2.27835

 Alpha virt. eigenvalues -- 2.28125 2.28341 2.28341 2.28682 2.29592

 Alpha virt. eigenvalues -- 2.29592 2.29659 2.29877 2.30520 2.30520

 Alpha virt. eigenvalues -- 2.32006 2.32115 2.32445 2.33142 2.33142

 Alpha virt. eigenvalues -- 2.33973 2.33973 2.35654 2.35762 2.36440

 Alpha virt. eigenvalues -- 2.36729 2.36729 2.36832 2.38526 2.38738

 Alpha virt. eigenvalues -- 2.39662 2.39662 2.40442 2.40442 2.40919

 Alpha virt. eigenvalues -- 2.44253 2.44865 2.44865 2.44970 2.47256

 Alpha virt. eigenvalues -- 2.47341 2.49851 2.49851 2.53871 2.54681

 Alpha virt. eigenvalues -- 2.54681 2.54903 2.55451 2.57018 2.57718

 Alpha virt. eigenvalues -- 2.57972 2.57972 2.59297 2.59374 2.59374

 Alpha virt. eigenvalues -- 2.60402 2.61072 2.61072 2.62117 2.62454

 Alpha virt. eigenvalues -- 2.62674 2.62770 2.64559 2.64559 2.65206

 Alpha virt. eigenvalues -- 2.65206 2.65617 2.65620 2.68503 2.69773

 Alpha virt. eigenvalues -- 2.70071 2.70071 2.70289 2.72767 2.72767

 Alpha virt. eigenvalues -- 2.73257 2.74889 2.74889 2.75016 2.75043

 Alpha virt. eigenvalues -- 2.77012 2.77012 2.78467 2.78610 2.79432

 Alpha virt. eigenvalues -- 2.79445 2.79445 2.80399 2.80679 2.82656

 Alpha virt. eigenvalues -- 2.82656 2.84183 2.84843 2.85481 2.85481

 Alpha virt. eigenvalues -- 2.85969 2.87050 2.89784 2.89784 2.90174

 Alpha virt. eigenvalues -- 2.90174 2.90673 2.92973 2.94116 2.95892

 Alpha virt. eigenvalues -- 2.95892 2.96850 2.98852 2.98852 2.99046

 Alpha virt. eigenvalues -- 2.99721 3.01290 3.02782 3.04316 3.04877

 Alpha virt. eigenvalues -- 3.04877 3.06540 3.07481 3.07481 3.07582

 Alpha virt. eigenvalues -- 3.08395 3.08395 3.09189 3.11350 3.11687

 Alpha virt. eigenvalues -- 3.11860 3.12217 3.12217 3.14525 3.16838

 Alpha virt. eigenvalues -- 3.16838 3.16849 3.19546 3.19619 3.19619

 Alpha virt. eigenvalues -- 3.19736 3.22486 3.25834 3.25947 3.25947

 Alpha virt. eigenvalues -- 3.26087 3.26816 3.26816 3.29255 3.29591

 Alpha virt. eigenvalues -- 3.29591 3.29856 3.29976 3.29996 3.30214

 Alpha virt. eigenvalues -- 3.30214 3.30436 3.31091 3.31193 3.31272

 Alpha virt. eigenvalues -- 3.31272 3.31847 3.32135 3.34686 3.34686

 Alpha virt. eigenvalues -- 3.34715 3.35837 3.35837 3.36785 3.38248

 Alpha virt. eigenvalues -- 3.38248 3.39729 3.40864 3.42407 3.43091

 Alpha virt. eigenvalues -- 3.43091 3.44709 3.50363 3.51898 3.51956

 Alpha virt. eigenvalues -- 3.51956 3.56786 3.58143 3.58143 3.58602

 Alpha virt. eigenvalues -- 3.58602 3.59419 3.59738 3.61534 3.62677

 Alpha virt. eigenvalues -- 3.66704 3.67307 3.67307 3.72803 3.73568

 Alpha virt. eigenvalues -- 3.75789 3.75789 3.82769 3.82769 3.82872

 Alpha virt. eigenvalues -- 3.85007 3.87457 3.87457 3.89144 3.91617

 Alpha virt. eigenvalues -- 3.93980 3.93980 3.95111 3.95447 3.96267

 Alpha virt. eigenvalues -- 3.96313 3.96313 3.96391 3.99534 4.01085

 Alpha virt. eigenvalues -- 4.01085 4.12026 4.33381 4.35441 4.40179

 Alpha virt. eigenvalues -- 4.40179 4.46726 4.49709 4.54091 4.54091

 Alpha virt. eigenvalues -- 4.61897 4.66888 4.66888 4.67840 4.78821

 Alpha virt. eigenvalues -- 4.78831 4.78831 4.78841 5.11536 5.18916

 Alpha virt. eigenvalues -- 5.18916 5.32589 7.77675 7.77675 7.88025

 Alpha virt. eigenvalues -- 7.92778 8.13982 11.12048 23.25291 23.28974

 Alpha virt. eigenvalues -- 23.28974 23.30653 23.46369 23.53063 23.53063

 Alpha virt. eigenvalues -- 23.57714 23.74795 23.75935 23.75935 23.77727

 Alpha virt. eigenvalues -- 23.81067 23.81232 23.81232 23.81492 23.85161

 Alpha virt. eigenvalues -- 23.86126 23.86126 23.86887 23.92662 23.94755

 Alpha virt. eigenvalues -- 23.94755 23.96993 23.98200 23.99159 23.99159

 Alpha virt. eigenvalues -- 23.99221 24.04793 24.04950 24.04950 24.05134

 Alpha virt. eigenvalues -- 24.08773 24.09280 24.09280 24.09729 24.13357

 Alpha virt. eigenvalues -- 24.13718 24.13718 24.14422 24.16343 24.16382

 Alpha virt. eigenvalues -- 24.16382 24.16394 35.63343 35.64463 35.66095

 Alpha virt. eigenvalues -- 35.66095

 Condensed to atoms (all electrons):

 Mulliken charges:

 1

 1 C -0.261143

 2 C 0.308669

 3 N -0.706255

 4 C 0.308669

 5 C -0.261143

 6 C -0.149008

 7 C 0.308669

 8 N -0.706255

 9 C 0.308669

 10 C -0.261143

 11 C -0.261143

 12 C -0.149008

 13 C 0.308669

 14 C -0.261143

 15 C -0.261143

 16 C 0.308669

 17 N -0.706255

 18 C -0.149008

 19 C 0.308669

 20 C -0.261143

 21 C -0.261143

 22 C 0.308669

 23 N -0.706255

 24 C -0.149008

 25 C -0.105849

 26 C -0.211897

 27 C -0.217879

 28 C -0.221701

 29 C -0.217879

 30 C -0.211897

 31 C -0.221701

 32 C -0.217879

 33 C -0.211897

 34 C -0.105849

 35 C -0.211897

 36 C -0.217879

 37 C -0.105849

 38 C -0.211897

 39 C -0.217879

 40 C -0.221701

 41 C -0.217879

 42 C -0.211897

 43 C -0.105849

 44 C -0.211897

 45 C -0.217879

 46 C -0.221701

 47 C -0.217879

 48 C -0.211897

 49 H 0.239146

 50 H 0.239146

 51 H 0.239146

 52 H 0.239146

 53 H 0.239146

 54 H 0.239146

 55 H 0.239146

 56 H 0.239146

 57 H 0.224238

 58 H 0.225860

 59 H 0.225719

 60 H 0.225860

 61 H 0.224238

 62 H 0.225719

 63 H 0.225860

 64 H 0.224238

 65 H 0.224238

 66 H 0.225860

 67 H 0.224238

 68 H 0.225860

 69 H 0.225719

 70 H 0.225860

 71 H 0.224238

 72 H 0.224238

 73 H 0.225860

 74 H 0.225719

 75 H 0.225860

 76 H 0.224238

 77 Zn 1.372414

 Sum of Mulliken charges = 0.00000

 Mulliken charges with hydrogens summed into heavy atoms:

 1

 1 C -0.021996

 2 C 0.308669

 3 N -0.706255

 4 C 0.308669

 5 C -0.021996

 6 C -0.149008

 7 C 0.308669

 8 N -0.706255

 9 C 0.308669

 10 C -0.021996

 11 C -0.021996

 12 C -0.149008

 13 C 0.308669

 14 C -0.021996

 15 C -0.021996

 16 C 0.308669

 17 N -0.706255

 18 C -0.149008

 19 C 0.308669

 20 C -0.021996

 21 C -0.021996

 22 C 0.308669

 23 N -0.706255

 24 C -0.149008

 25 C -0.105849

 26 C 0.012342

 27 C 0.007981

 28 C 0.004019

 29 C 0.007981

 30 C 0.012342

 31 C 0.004019

 32 C 0.007981

 33 C 0.012342

 34 C -0.105849

 35 C 0.012342

 36 C 0.007981

 37 C -0.105849

 38 C 0.012342

 39 C 0.007981

 40 C 0.004019

 41 C 0.007981

 42 C 0.012342

 43 C -0.105849

 44 C 0.012342

 45 C 0.007981

 46 C 0.004019

 47 C 0.007981

 48 C 0.012342

 77 Zn 1.372414

 Electronic spatial extent (au): <R\*\*2>= 33352.9763

 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= -248.6475 YY= -248.6475 ZZ= -276.6355

 XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

 XX= 9.3294 YY= 9.3294 ZZ= -18.6587

 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= 89.9106 XZZ= 0.0000 YZZ= 0.0000

 YYZ= -89.9106 XYZ= 0.0000

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

 XXXX= -21528.0535 YYYY= -21528.0535 ZZZZ= -1080.9899 XXXY= 0.0000

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

 ZZZY= 0.0000 XXYY= -5779.9006 XXZZ= -3834.9819 YYZZ= -3834.9819

 XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

 N-N= 5.738269430807D+03 E-N=-1.615865211036D+04 KE= 2.020706235307D+03

 Symmetry A1 KE= 5.778493057935D+02

 Symmetry A2 KE= 4.453814231484D+02

 Symmetry B1 KE= 4.987377531825D+02

 Symmetry B2 KE= 4.987377531825D+02

 Leave Link 601 at Thu Sep 5 22:07:21 2019, MaxMem= 1342177280 cpu: 53.3

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

 Test job not archived.

 1\1\GINC-K251\SP\RB3LYP TD-FC\GenECP\C44H28N4Zn1\Z5105842\05-Sep-2019\

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

 icaldispersion=gd3bj IOp(9/40=3)\\ZnTPP0td\\0,1\C,0,-0.681484,4.269157

 ,0.164086\C,0,-1.110541,2.890129,0.035503\N,0,0.,2.090529,-0.027459\C,

 0,1.110541,2.890129,0.035503\C,0,0.681484,4.269157,0.164086\C,0,2.4521

 83,2.452183,0.\C,0,2.890129,1.110541,-0.035503\N,0,2.090529,0.,0.02745

 9\C,0,2.890129,-1.110541,-0.035503\C,0,4.269157,-0.681484,-0.164086\C,

 0,4.269157,0.681484,-0.164086\C,0,-2.452183,2.452183,0.\C,0,-2.890129,

 1.110541,-0.035503\C,0,-4.269157,0.681484,-0.164086\C,0,-4.269157,-0.6

 81484,-0.164086\C,0,-2.890129,-1.110541,-0.035503\N,0,-2.090529,0.,0.0

 27459\C,0,-2.452183,-2.452183,0.\C,0,-1.110541,-2.890129,0.035503\C,0,

 -0.681484,-4.269157,0.164086\C,0,0.681484,-4.269157,0.164086\C,0,1.110

 541,-2.890129,0.035503\N,0,0.,-2.090529,-0.027459\C,0,2.452183,-2.4521

 83,0.\C,0,3.508242,3.508242,0.\C,0,3.621357,4.405038,-1.069674\C,0,4.6

 07485,5.388753,-1.071137\C,0,5.493806,5.493806,0.\C,0,5.388753,4.60748

 5,1.071137\C,0,4.405038,3.621357,1.069674\C,0,-5.493806,5.493806,0.\C,

 0,-4.607485,5.388753,-1.071137\C,0,-3.621357,4.405038,-1.069674\C,0,-3

 .508242,3.508242,0.\C,0,-4.405038,3.621357,1.069674\C,0,-5.388753,4.60

 7485,1.071137\C,0,3.508242,-3.508242,0.\C,0,4.405038,-3.621357,1.06967

 4\C,0,5.388753,-4.607485,1.071137\C,0,5.493806,-5.493806,0.\C,0,4.6074

 85,-5.388753,-1.071137\C,0,3.621357,-4.405038,-1.069674\C,0,-3.508242,

 -3.508242,0.\C,0,-4.405038,-3.621357,1.069674\C,0,-5.388753,-4.607485,

 1.071137\C,0,-5.493806,-5.493806,0.\C,0,-4.607485,-5.388753,-1.071137\

 C,0,-3.621357,-4.405038,-1.069674\H,0,-1.330917,5.125618,0.259828\H,0,

 1.330917,5.125618,0.259828\H,0,5.125618,-1.330917,-0.259828\H,0,5.1256

 18,1.330917,-0.259828\H,0,-5.125618,1.330917,-0.259828\H,0,-5.125618,-

 1.330917,-0.259828\H,0,-1.330917,-5.125618,0.259828\H,0,1.330917,-5.12

 5618,0.259828\H,0,2.936967,4.323214,-1.90704\H,0,4.684584,6.071446,-1.

 91098\H,0,6.260992,6.260992,0.\H,0,6.071446,4.684584,1.91098\H,0,4.323

 214,2.936967,1.90704\H,0,-6.260992,6.260992,0.\H,0,-4.684584,6.071446,

 -1.91098\H,0,-2.936967,4.323214,-1.90704\H,0,-4.323214,2.936967,1.9070

 4\H,0,-6.071446,4.684584,1.91098\H,0,4.323214,-2.936967,1.90704\H,0,6.

 071446,-4.684584,1.91098\H,0,6.260992,-6.260992,0.\H,0,4.684584,-6.071

 446,-1.91098\H,0,2.936967,-4.323214,-1.90704\H,0,-4.323214,-2.936967,1

 .90704\H,0,-6.071446,-4.684584,1.91098\H,0,-6.260992,-6.260992,0.\H,0,

 -4.684584,-6.071446,-1.91098\H,0,-2.936967,-4.323214,-1.90704\Zn,0,0.,

 0.,0.\\Version=ES64L-G09RevD.01\State=1-A1\HF=-1978.9047638\RMSD=2.710

 e-09\PG=D02D [O(Zn1),2SGD(N2),X(C44H28)]\\@

 A BIRD IN THE HAND IS SAFER THAN ONE OVERHEAD.

 -- NEWTON'S SEVENTH LAW

 Job cpu time: 0 days 4 hours 30 minutes 48.1 seconds.

 File lengths (MBytes): RWF= 3666 Int= 0 D2E= 0 Chk= 343 Scr= 2

 Normal termination of Gaussian 09 at Thu Sep 5 22:07:24 2019.