Entering Gaussian System, Link 0=g09

 Input=ZnNPC0td.com

 Output=ZnNPC0td.log

 Initial command:

 /home/blab/g09/l1.exe "/home/blab/g09/scratch/Gau-46585.inp" -scrdir="/home/blab/g09/scratch/"

 Entering Link 1 = /home/blab/g09/l1.exe PID= 46593.

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

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 Cite this work as:

 Gaussian 09, Revision E.01,

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

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

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

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

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

 19-Sep-2019

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

 %nprocshared=9

 Will use up to 9 processors via shared memory.

 %mem=10GB

 %chk=ZnNPC0td.chk

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

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

 ldispersion=gd3bj IOp(9/40=3)

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

 1/38=1/1;

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

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

 4//1;

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

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

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

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

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

 Leave Link 1 at Thu Sep 19 00:35:28 2019, MaxMem= 1342177280 cpu: 40.7

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

 --------

 ZnNPC0td

 --------

 Symbolic Z-matrix:

 Charge = 0 Multiplicity = 1

 C 1.12208 2.79302 0.17278

 N 0. 2.02036 0.25982

 C -1.12208 2.79302 0.17278

 C -0.71452 4.19463 0.05147

 C 0.71452 4.19463 0.05147

 N -2.38951 2.38951 0.15461

 C -2.79302 1.12208 0.1728

 N -2.02036 0. 0.25983

 C -2.79302 -1.12208 0.1728

 C -4.19464 -0.71452 0.05153

 C -4.19464 0.71452 0.05153

 N 2.38951 2.38951 0.15461

 C 4.19464 0.71452 0.05153

 C 4.19464 -0.71452 0.05153

 C 2.79302 -1.12208 0.1728

 N 2.02036 0. 0.25983

 C 2.79302 1.12208 0.1728

 N 2.38951 -2.38951 0.15461

 N 0. -2.02036 0.25982

 C 1.12208 -2.79302 0.17278

 C 0.71452 -4.19463 0.05147

 C -0.71452 -4.19463 0.05147

 C -1.12208 -2.79302 0.17278

 N -2.38951 -2.38951 0.15461

 Zn 0. 0. 0.77753

 C 5.36349 1.42745 -0.05462

 C 6.58861 0.72073 -0.15638

 C 6.58861 -0.72073 -0.15638

 C 5.36349 -1.42745 -0.05462

 C -1.42745 -5.36348 -0.05471

 C -0.72073 -6.5886 -0.1565

 C 0.72073 -6.5886 -0.1565

 C 1.42745 -5.36348 -0.05471

 C -5.36349 1.42745 -0.05462

 C -6.58861 0.72073 -0.15638

 C -6.58861 -0.72073 -0.15638

 C -5.36349 -1.42745 -0.05462

 C 1.42745 5.36348 -0.05471

 C 0.72073 6.5886 -0.1565

 C -0.72073 6.5886 -0.1565

 C -1.42745 5.36348 -0.05471

 C 1.40241 -7.83042 -0.25896

 C 0.70807 -9.01151 -0.35678

 C -0.70807 -9.01151 -0.35678

 C -1.40241 -7.83042 -0.25896

 C 7.83043 -1.40241 -0.2588

 C 9.01152 -0.70807 -0.35659

 C 9.01152 0.70807 -0.35659

 C 7.83043 1.40241 -0.2588

 C -1.40241 7.83042 -0.25896

 C -0.70807 9.01151 -0.35678

 C 0.70807 9.01151 -0.35678

 C 1.40241 7.83042 -0.25896

 C -7.83043 -1.40241 -0.2588

 C -9.01152 -0.70807 -0.35659

 C -9.01152 0.70807 -0.35659

 C -7.83043 1.40241 -0.2588

 H 5.36498 2.51242 -0.05821

 H 5.36498 -2.51242 -0.05821

 H -2.51242 -5.36498 -0.0583

 H 2.51242 -5.36498 -0.0583

 H -5.36498 2.51242 -0.05821

 H -5.36498 -2.51242 -0.05821

 H 2.51242 5.36498 -0.0583

 H -2.51242 5.36498 -0.0583

 H 2.48784 -7.82854 -0.25881

 H 1.24326 -9.95179 -0.43509

 H -1.24326 -9.95179 -0.43509

 H -2.48784 -7.82854 -0.25881

 H 7.82856 -2.48784 -0.25866

 H 9.95181 -1.24326 -0.43487

 H 9.95181 1.24326 -0.43487

 H 7.82856 2.48784 -0.25866

 H -2.48784 7.82854 -0.25881

 H -1.24326 9.95179 -0.43509

 H 1.24326 9.95179 -0.43509

 H 2.48784 7.82854 -0.25881

 H -7.82856 -2.48784 -0.25866

 H -9.95181 -1.24326 -0.43487

 H -9.95181 1.24326 -0.43487

 H -7.82856 2.48784 -0.25866

 NAtoms= 81 NQM= 81 NQMF= 0 NMMI= 0 NMMIF= 0

 NMic= 0 NMicF= 0.

 Isotopes and Nuclear Properties:

 (Nuclear quadrupole moments (NQMom) in fm\*\*2, nuclear magnetic moments (NMagM)

 in nuclear magnetons)

 Atom 1 2 3 4 5 6 7 8 9 10

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

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

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

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

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

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

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

 Atom 11 12 13 14 15 16 17 18 19 20

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

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

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

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

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

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

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

 Atom 21 22 23 24 25 26 27 28 29 30

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

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

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

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

 AtZNuc= 6.0000000 6.0000000 6.0000000 7.0000000 30.0000000 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 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 51 52 53 54 55 56 57 58 59 60

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

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

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

 AtZNuc= 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 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 78 79 80

 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 81

 IAtWgt= 1

 AtmWgt= 1.0078250

 NucSpn= 1

 AtZEff= 0.0000000

 NQMom= 0.0000000

 NMagM= 2.7928460

 AtZNuc= 1.0000000

 Leave Link 101 at Thu Sep 19 00:35:28 2019, MaxMem= 1342177280 cpu: 0.7

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

 Stoichiometry C48H24N8Zn

 Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C48H24N4)]

 Deg. of freedom 61

 Full point group C2V NOp 4

 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 1.122077 2.793021 0.172784

 2 7 0 0.000000 2.020361 0.259821

 3 6 0 -1.122077 2.793021 0.172784

 4 6 0 -0.714524 4.194635 0.051468

 5 6 0 0.714524 4.194635 0.051468

 6 7 0 -2.389506 2.389505 0.154613

 7 6 0 -2.793023 1.122077 0.172801

 8 7 0 -2.020362 0.000000 0.259826

 9 6 0 -2.793023 -1.122077 0.172801

 10 6 0 -4.194641 -0.714524 0.051526

 11 6 0 -4.194641 0.714524 0.051526

 12 7 0 2.389506 2.389505 0.154613

 13 6 0 4.194641 0.714524 0.051526

 14 6 0 4.194641 -0.714524 0.051526

 15 6 0 2.793023 -1.122077 0.172801

 16 7 0 2.020362 -0.000000 0.259826

 17 6 0 2.793023 1.122077 0.172801

 18 7 0 2.389506 -2.389505 0.154613

 19 7 0 -0.000000 -2.020361 0.259821

 20 6 0 1.122077 -2.793021 0.172784

 21 6 0 0.714524 -4.194635 0.051468

 22 6 0 -0.714524 -4.194635 0.051468

 23 6 0 -1.122077 -2.793021 0.172784

 24 7 0 -2.389506 -2.389505 0.154613

 25 30 0 0.000000 0.000000 0.777528

 26 6 0 5.363492 1.427454 -0.054616

 27 6 0 6.588610 0.720730 -0.156377

 28 6 0 6.588610 -0.720730 -0.156377

 29 6 0 5.363492 -1.427454 -0.054616

 30 6 0 -1.427454 -5.363483 -0.054708

 31 6 0 -0.720730 -6.588598 -0.156501

 32 6 0 0.720730 -6.588598 -0.156501

 33 6 0 1.427454 -5.363483 -0.054708

 34 6 0 -5.363492 1.427454 -0.054616

 35 6 0 -6.588610 0.720730 -0.156377

 36 6 0 -6.588610 -0.720730 -0.156377

 37 6 0 -5.363492 -1.427454 -0.054616

 38 6 0 1.427454 5.363483 -0.054708

 39 6 0 0.720730 6.588598 -0.156501

 40 6 0 -0.720730 6.588598 -0.156501

 41 6 0 -1.427454 5.363483 -0.054708

 42 6 0 1.402412 -7.830417 -0.258961

 43 6 0 0.708074 -9.011507 -0.356784

 44 6 0 -0.708074 -9.011507 -0.356784

 45 6 0 -1.402412 -7.830417 -0.258961

 46 6 0 7.830431 -1.402412 -0.258803

 47 6 0 9.011524 -0.708074 -0.356593

 48 6 0 9.011524 0.708074 -0.356593

 49 6 0 7.830431 1.402412 -0.258803

 50 6 0 -1.402412 7.830417 -0.258961

 51 6 0 -0.708074 9.011507 -0.356784

 52 6 0 0.708074 9.011507 -0.356784

 53 6 0 1.402412 7.830417 -0.258961

 54 6 0 -7.830431 -1.402412 -0.258803

 55 6 0 -9.011524 -0.708074 -0.356593

 56 6 0 -9.011524 0.708074 -0.356593

 57 6 0 -7.830431 1.402412 -0.258803

 58 1 0 5.364985 2.512421 -0.058211

 59 1 0 5.364985 -2.512421 -0.058211

 60 1 0 -2.512421 -5.364975 -0.058303

 61 1 0 2.512421 -5.364975 -0.058303

 62 1 0 -5.364985 2.512421 -0.058211

 63 1 0 -5.364985 -2.512421 -0.058211

 64 1 0 2.512421 5.364975 -0.058303

 65 1 0 -2.512421 5.364975 -0.058303

 66 1 0 2.487843 -7.828541 -0.258814

 67 1 0 1.243262 -9.951788 -0.435088

 68 1 0 -1.243262 -9.951788 -0.435088

 69 1 0 -2.487843 -7.828541 -0.258814

 70 1 0 7.828556 -2.487843 -0.258655

 71 1 0 9.951808 -1.243262 -0.434870

 72 1 0 9.951808 1.243262 -0.434870

 73 1 0 7.828556 2.487843 -0.258655

 74 1 0 -2.487843 7.828541 -0.258814

 75 1 0 -1.243262 9.951788 -0.435088

 76 1 0 1.243262 9.951788 -0.435088

 77 1 0 2.487843 7.828541 -0.258814

 78 1 0 -7.828556 -2.487843 -0.258655

 79 1 0 -9.951808 -1.243262 -0.434870

 80 1 0 -9.951808 1.243262 -0.434870

 81 1 0 -7.828556 2.487843 -0.258655

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

 Rotational constants (GHZ): 0.0383619 0.0383618 0.0192836

 Leave Link 202 at Thu Sep 19 00:35:28 2019, MaxMem= 1342177280 cpu: 0.1

 (Enter /home/blab/g09/l301.exe)

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

 Centers: 25

 S 1 1.00

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

 S 1 1.00

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

 S 1 1.00

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

 P 1 1.00

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

 P 1 1.00

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

 D 3 1.00

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

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

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

 D 1 1.00

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

 D 1 1.00

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

 \*\*\*\*

 Centers: 58 59 60 61 62 63 64 65 66 67

 Centers: 68 69 70 71 72 73 74 75 76 77

 Centers: 78 79 80 81 1 3 4 5 7 9

 Centers: 10 11 13 14 15 17 20 21 22 23

 Centers: 26 27 28 29 30 31 32 33 34 35

 Centers: 36 37 38 39 40 41 42 43 44 45

 Centers: 46 47 48 49 50 51 52 53 54 55

 Centers: 56 57 2 6 8 12 16 18 19 24

 6-311G\*

 \*\*\*\*

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

 Pseudopotential Parameters

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

 Center Atomic Valence Angular Power

 Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

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

 1 6

 No pseudopotential on this center.

 2 7

 No pseudopotential on this center.

 3 6

 No pseudopotential on this center.

 4 6

 No pseudopotential on this center.

 5 6

 No pseudopotential on this center.

 6 7

 No pseudopotential on this center.

 7 6

 No pseudopotential on this center.

 8 7

 No pseudopotential on this center.

 9 6

 No pseudopotential on this center.

 10 6

 No pseudopotential on this center.

 11 6

 No pseudopotential on this center.

 12 7

 No pseudopotential on this center.

 13 6

 No pseudopotential on this center.

 14 6

 No pseudopotential on this center.

 15 6

 No pseudopotential on this center.

 16 7

 No pseudopotential on this center.

 17 6

 No pseudopotential on this center.

 18 7

 No pseudopotential on this center.

 19 7

 No pseudopotential on this center.

 20 6

 No pseudopotential on this center.

 21 6

 No pseudopotential on this center.

 22 6

 No pseudopotential on this center.

 23 6

 No pseudopotential on this center.

 24 7

 No pseudopotential on this center.

 25 30 12

 F and up

 1 386.7379660 -18.00000000 0.00000000

 2 72.8587359 -124.35274030 0.00000000

 2 15.9066170 -30.66018220 0.00000000

 2 4.3502340 -10.63589890 0.00000000

 2 1.2842199 -0.76836230 0.00000000

 S - F

 0 19.0867858 3.00000000 0.00000000

 1 5.0231080 22.52342250 0.00000000

 2 1.2701744 48.44659420 0.00000000

 2 1.0671287 -44.55601190 0.00000000

 2 0.9264190 12.99839580 0.00000000

 P - F

 0 43.4927750 5.00000000 0.00000000

 1 20.8692669 20.74355890 0.00000000

 2 21.7118378 90.30271580 0.00000000

 2 6.3616915 74.66103160 0.00000000

 2 1.2291195 9.88944240 0.00000000

 D - F

 2 13.5851800 -4.84903590 0.00000000

 2 9.8373050 3.69133790 0.00000000

 2 0.8373113 -0.50373190 0.00000000

 26 6

 No pseudopotential on this center.

 27 6

 No pseudopotential on this center.

 28 6

 No pseudopotential on this center.

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 80 1

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 81 1

 No pseudopotential on this center.

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

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

 There are 307 symmetry adapted cartesian basis functions of A1 symmetry.

 There are 278 symmetry adapted cartesian basis functions of A2 symmetry.

 There are 289 symmetry adapted cartesian basis functions of B1 symmetry.

 There are 289 symmetry adapted cartesian basis functions of B2 symmetry.

 There are 289 symmetry adapted basis functions of A1 symmetry.

 There are 265 symmetry adapted basis functions of A2 symmetry.

 There are 275 symmetry adapted basis functions of B1 symmetry.

 There are 275 symmetry adapted basis functions of B2 symmetry.

 1104 basis functions, 1951 primitive gaussians, 1163 cartesian basis functions

 190 alpha electrons 190 beta electrons

 nuclear repulsion energy 6888.8260724835 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= 81 NActive= 81 NUniq= 22 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= -0.2360382768 Hartrees.

 Nuclear repulsion after empirical dispersion term = 6888.5900342067 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= 81.

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

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

 Polarization charges: spherical gaussians, with

 point-specific exponents (IZeta= 3).

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

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

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

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

 GePol: Number of generator spheres = 81

 GePol: Total number of spheres = 81

 GePol: Number of exposed spheres = 81 (100.00%)

 GePol: Number of points = 6354

 GePol: Average weight of points = 0.11

 GePol: Minimum weight of points = 0.19D-08

 GePol: Maximum weight of points = 0.18390

 GePol: Number of points with low weight = 244

 GePol: Fraction of low-weight points (<1% of avg) = 3.84%

 GePol: Cavity surface area = 671.282 Ang\*\*2

 GePol: Cavity volume = 693.864 Ang\*\*3

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

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

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

 PCM non-electrostatic energy = -0.0172173388 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 6888.5728168679 Hartrees.

 Leave Link 301 at Thu Sep 19 00:35:28 2019, MaxMem= 1342177280 cpu: 1.2

 (Enter /home/blab/g09/l302.exe)

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

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

 One-electron integrals computed using PRISM.

 One-electron integral symmetry used in STVInt

 4 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36709 LenP2D= 95142.

 LDataN: DoStor=T MaxTD1= 5 Len= 102

 NBasis= 1104 RedAO= T EigKep= 2.88D-05 NBF= 289 265 275 275

 NBsUse= 1104 1.00D-06 EigRej= -1.00D+00 NBFU= 289 265 275 275

 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= 1060 1060 1060 1060 1060 MxSgAt= 81 MxSgA2= 81.

 Leave Link 302 at Thu Sep 19 00:35:30 2019, MaxMem= 1342177280 cpu: 13.9

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

 Leave Link 308 at Thu Sep 19 00:35:30 2019, MaxMem= 1342177280 cpu: 2.6

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

 DipDrv: MaxL=1.

 Leave Link 303 at Thu Sep 19 00:35:30 2019, MaxMem= 1342177280 cpu: 1.6

 (Enter /home/blab/g09/l401.exe)

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

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

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

 ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2348.40225961047

 JPrj=0 DoOrth=F DoCkMO=F.

 Initial guess orbital symmetries:

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

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

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

 Leave Link 401 at Thu Sep 19 00:35:34 2019, MaxMem= 1342177280 cpu: 33.9

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

 Closed shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 4099732 IEndB= 4099732 NGot= 1342177280 MDV= 1339447921

 LenX= 1339447921 LenY= 1338094189

 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= 420000000 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= 121119948.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 1.18D-14 for 6350.

 Iteration 1 A\*A^-1 deviation from orthogonality is 5.94D-15 for 6344 5465.

 Iteration 1 A^-1\*A deviation from unit magnitude is 1.13D-14 for 6350.

 Iteration 1 A^-1\*A deviation from orthogonality is 4.32D-09 for 2962 2960.

 Iteration 2 A\*A^-1 deviation from unit magnitude is 2.44D-15 for 56.

 Iteration 2 A\*A^-1 deviation from orthogonality is 3.67D-15 for 2903 323.

 Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 2869.

 Iteration 2 A^-1\*A deviation from orthogonality is 3.63D-16 for 4661 4616.

 E= -2347.08035811961

 DIIS: error= 8.83D-02 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -2347.08035811961 IErMin= 1 ErrMin= 8.83D-02

 ErrMax= 8.83D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D+00 BMatP= 1.37D+00

 IDIUse=3 WtCom= 1.17D-01 WtEn= 8.83D-01

 Coeff-Com: 0.100D+01

 Coeff-En: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.095 Goal= None Shift= 0.000

 GapD= 0.095 DampG=0.500 DampE=0.250 DampFc=0.1250 IDamp=-1.

 Damping current iteration by 1.25D-01

 RMSDP=2.16D-03 MaxDP=8.86D-02 OVMax= 1.93D-01

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 2.70D-04 CP: 9.98D-01

 E= -2347.30172924527 Delta-E= -0.221371125661 Rises=F Damp=T

 DIIS: error= 6.32D-02 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -2347.30172924527 IErMin= 2 ErrMin= 6.32D-02

 ErrMax= 6.32D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.10D-01 BMatP= 1.37D+00

 IDIUse=3 WtCom= 3.68D-01 WtEn= 6.32D-01

 Coeff-Com: -0.303D+01 0.403D+01

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

 Coeff: -0.111D+01 0.211D+01

 Gap= 0.073 Goal= None Shift= 0.000

 RMSDP=1.30D-03 MaxDP=5.68D-02 DE=-2.21D-01 OVMax= 7.81D-02

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 7.89D-04 CP: 9.81D-01 3.00D+00

 E= -2347.98333086242 Delta-E= -0.681601617152 Rises=F Damp=F

 DIIS: error= 4.02D-02 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 3 EnMin= -2347.98333086242 IErMin= 3 ErrMin= 4.02D-02

 ErrMax= 4.02D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.17D-01 BMatP= 8.10D-01

 IDIUse=3 WtCom= 5.98D-01 WtEn= 4.02D-01

 Coeff-Com: 0.196D+01-0.204D+01 0.108D+01

 Coeff-En: 0.265D-01 0.000D+00 0.974D+00

 Coeff: 0.118D+01-0.122D+01 0.103D+01

 Gap= 0.072 Goal= None Shift= 0.000

 RMSDP=6.42D-04 MaxDP=2.78D-02 DE=-6.82D-01 OVMax= 5.31D-02

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 3.73D-04 CP: 9.83D-01 3.00D+00 3.38D-01

 E= -2348.13271975824 Delta-E= -0.149388895821 Rises=F Damp=F

 DIIS: error= 1.59D-02 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -2348.13271975824 IErMin= 4 ErrMin= 1.59D-02

 ErrMax= 1.59D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.90D-02 BMatP= 2.17D-01

 IDIUse=3 WtCom= 8.41D-01 WtEn= 1.59D-01

 Coeff-Com: -0.217D+00 0.282D+00 0.263D+00 0.672D+00

 Coeff-En: 0.000D+00 0.000D+00 0.889D-01 0.911D+00

 Coeff: -0.183D+00 0.237D+00 0.235D+00 0.710D+00

 Gap= 0.070 Goal= None Shift= 0.000

 RMSDP=1.84D-04 MaxDP=9.58D-03 DE=-1.49D-01 OVMax= 2.28D-02

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 4.81D-05 CP: 9.83D-01 3.00D+00 5.17D-01 7.12D-01

 E= -2348.16291566022 Delta-E= -0.030195901973 Rises=F Damp=F

 DIIS: error= 1.64D-03 at cycle 5 NSaved= 5.

 NSaved= 5 IEnMin= 5 EnMin= -2348.16291566022 IErMin= 5 ErrMin= 1.64D-03

 ErrMax= 1.64D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.88D-03 BMatP= 3.90D-02

 IDIUse=3 WtCom= 9.84D-01 WtEn= 1.64D-02

 Coeff-Com: -0.173D+00 0.203D+00 0.100D+00 0.419D+00 0.451D+00

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

 Coeff: -0.170D+00 0.200D+00 0.984D-01 0.412D+00 0.460D+00

 Gap= 0.069 Goal= None Shift= 0.000

 RMSDP=2.97D-05 MaxDP=2.47D-03 DE=-3.02D-02 OVMax= 5.34D-03

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 1.60D-05 CP: 9.83D-01 3.00D+00 5.03D-01 7.40D-01 5.85D-01

 E= -2348.16448453667 Delta-E= -0.001568876454 Rises=F Damp=F

 DIIS: error= 3.94D-04 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -2348.16448453667 IErMin= 6 ErrMin= 3.94D-04

 ErrMax= 3.94D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.69D-05 BMatP= 1.88D-03

 IDIUse=3 WtCom= 9.96D-01 WtEn= 3.94D-03

 Coeff-Com: -0.953D-01 0.110D+00 0.281D-01 0.170D+00 0.234D+00 0.554D+00

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

 Coeff: -0.949D-01 0.109D+00 0.280D-01 0.169D+00 0.233D+00 0.556D+00

 Gap= 0.069 Goal= None Shift= 0.000

 RMSDP=8.44D-06 MaxDP=6.06D-04 DE=-1.57D-03 OVMax= 1.70D-03

 Cycle 7 Pass 1 IDiag 1:

 RMSU= 4.99D-06 CP: 9.83D-01 3.00D+00 5.05D-01 7.44D-01 6.03D-01

 CP: 5.96D-01

 E= -2348.16452705325 Delta-E= -0.000042516576 Rises=F Damp=F

 DIIS: error= 1.30D-04 at cycle 7 NSaved= 7.

 NSaved= 7 IEnMin= 7 EnMin= -2348.16452705325 IErMin= 7 ErrMin= 1.30D-04

 ErrMax= 1.30D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.72D-06 BMatP= 5.69D-05

 IDIUse=3 WtCom= 9.99D-01 WtEn= 1.30D-03

 Coeff-Com: -0.452D-01 0.516D-01 0.794D-02 0.653D-01 0.942D-01 0.342D+00

 Coeff-Com: 0.484D+00

 Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.116D+00

 Coeff-En: 0.884D+00

 Coeff: -0.451D-01 0.515D-01 0.793D-02 0.652D-01 0.941D-01 0.342D+00

 Coeff: 0.484D+00

 Gap= 0.069 Goal= None Shift= 0.000

 RMSDP=2.53D-06 MaxDP=1.76D-04 DE=-4.25D-05 OVMax= 4.98D-04

 Cycle 8 Pass 1 IDiag 1:

 RMSU= 1.58D-06 CP: 9.83D-01 3.00D+00 5.06D-01 7.43D-01 6.07D-01

 CP: 6.72D-01 6.96D-01

 E= -2348.16453509518 Delta-E= -0.000008041932 Rises=F Damp=F

 DIIS: error= 1.67D-05 at cycle 8 NSaved= 8.

 NSaved= 8 IEnMin= 8 EnMin= -2348.16453509518 IErMin= 8 ErrMin= 1.67D-05

 ErrMax= 1.67D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.20D-07 BMatP= 8.72D-06

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

 Coeff-Com: -0.977D-02 0.111D-01 0.849D-03 0.110D-01 0.143D-01 0.988D-01

 Coeff-Com: 0.202D+00 0.672D+00

 Coeff: -0.977D-02 0.111D-01 0.849D-03 0.110D-01 0.143D-01 0.988D-01

 Coeff: 0.202D+00 0.672D+00

 Gap= 0.069 Goal= None Shift= 0.000

 RMSDP=9.77D-07 MaxDP=4.33D-05 DE=-8.04D-06 OVMax= 1.37D-04

 Cycle 9 Pass 1 IDiag 1:

 RMSU= 7.71D-07 CP: 9.83D-01 3.00D+00 5.05D-01 7.44D-01 6.10D-01

 CP: 6.90D-01 7.35D-01 9.62D-01

 E= -2348.16453531474 Delta-E= -0.000000219559 Rises=F Damp=F

 DIIS: error= 1.42D-05 at cycle 9 NSaved= 9.

 NSaved= 9 IEnMin= 9 EnMin= -2348.16453531474 IErMin= 9 ErrMin= 1.42D-05

 ErrMax= 1.42D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.79D-08 BMatP= 3.20D-07

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

 Coeff-Com: 0.548D-03-0.696D-03-0.552D-03-0.248D-02-0.480D-02 0.128D-01

 Coeff-Com: 0.503D-01 0.408D+00 0.537D+00

 Coeff: 0.548D-03-0.696D-03-0.552D-03-0.248D-02-0.480D-02 0.128D-01

 Coeff: 0.503D-01 0.408D+00 0.537D+00

 Gap= 0.069 Goal= None Shift= 0.000

 RMSDP=4.43D-07 MaxDP=2.22D-05 DE=-2.20D-07 OVMax= 9.35D-05

 Cycle 10 Pass 1 IDiag 1:

 RMSU= 1.74D-07 CP: 9.83D-01 3.00D+00 5.05D-01 7.44D-01 6.09D-01

 CP: 6.89D-01 7.39D-01 9.75D-01 5.71D-01

 E= -2348.16453540874 Delta-E= -0.000000093998 Rises=F Damp=F

 DIIS: error= 2.50D-06 at cycle 10 NSaved= 10.

 NSaved=10 IEnMin=10 EnMin= -2348.16453540874 IErMin=10 ErrMin= 2.50D-06

 ErrMax= 2.50D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.74D-09 BMatP= 9.79D-08

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

 Coeff-Com: 0.743D-03-0.874D-03-0.184D-03-0.129D-02-0.217D-02 0.174D-02

 Coeff-Com: 0.999D-02 0.118D+00 0.211D+00 0.664D+00

 Coeff: 0.743D-03-0.874D-03-0.184D-03-0.129D-02-0.217D-02 0.174D-02

 Coeff: 0.999D-02 0.118D+00 0.211D+00 0.664D+00

 Gap= 0.069 Goal= None Shift= 0.000

 RMSDP=7.26D-08 MaxDP=2.74D-06 DE=-9.40D-08 OVMax= 1.27D-05

 Cycle 11 Pass 1 IDiag 1:

 RMSU= 5.29D-08 CP: 9.83D-01 3.00D+00 5.05D-01 7.44D-01 6.09D-01

 CP: 6.90D-01 7.36D-01 9.75D-01 6.04D-01 1.01D+00

 E= -2348.16453541089 Delta-E= -0.000000002157 Rises=F Damp=F

 DIIS: error= 1.23D-06 at cycle 11 NSaved= 11.

 NSaved=11 IEnMin=11 EnMin= -2348.16453541089 IErMin=11 ErrMin= 1.23D-06

 ErrMax= 1.23D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.22D-10 BMatP= 2.74D-09

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

 Coeff-Com: 0.306D-03-0.354D-03-0.263D-04-0.346D-03-0.503D-03-0.125D-03

 Coeff-Com: -0.256D-04 0.141D-01 0.506D-01 0.382D+00 0.554D+00

 Coeff: 0.306D-03-0.354D-03-0.263D-04-0.346D-03-0.503D-03-0.125D-03

 Coeff: -0.256D-04 0.141D-01 0.506D-01 0.382D+00 0.554D+00

 Gap= 0.069 Goal= None Shift= 0.000

 RMSDP=2.35D-08 MaxDP=1.37D-06 DE=-2.16D-09 OVMax= 6.21D-06

 Cycle 12 Pass 1 IDiag 1:

 RMSU= 1.55D-08 CP: 9.83D-01 3.00D+00 5.05D-01 7.44D-01 6.09D-01

 CP: 6.90D-01 7.36D-01 9.75D-01 6.06D-01 1.04D+00

 CP: 7.30D-01

 E= -2348.16453541161 Delta-E= -0.000000000713 Rises=F Damp=F

 DIIS: error= 2.54D-07 at cycle 12 NSaved= 12.

 NSaved=12 IEnMin=12 EnMin= -2348.16453541161 IErMin=12 ErrMin= 2.54D-07

 ErrMax= 2.54D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.40D-11 BMatP= 7.22D-10

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

 Coeff-Com: -0.487D-05 0.662D-05-0.738D-06 0.889D-05 0.259D-04-0.142D-03

 Coeff-Com: -0.473D-03-0.530D-02-0.459D-02 0.249D-01 0.135D+00 0.850D+00

 Coeff: -0.487D-05 0.662D-05-0.738D-06 0.889D-05 0.259D-04-0.142D-03

 Coeff: -0.473D-03-0.530D-02-0.459D-02 0.249D-01 0.135D+00 0.850D+00

 Gap= 0.069 Goal= None Shift= 0.000

 RMSDP=5.06D-09 MaxDP=2.91D-07 DE=-7.13D-10 OVMax= 2.38D-06

 Error on total polarization charges = 0.08885

 SCF Done: E(RB3LYP) = -2348.16453541 A.U. after 12 cycles

 NFock= 12 Conv=0.51D-08 -V/T= 1.9830

 KE= 2.388757903125D+03 PE=-1.931954529452D+04 EE= 7.694050039119D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -10.80

 (included in total energy above)

 Leave Link 502 at Thu Sep 19 00:40:06 2019, MaxMem= 1342177280 cpu: 2417.0

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

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

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

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

 ICtDFT= 12500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

 Largest valence mixing into a core orbital is 5.13D-05

 Largest core mixing into a valence orbital is 2.24D-05

 Range of M.O.s used for correlation: 57 1104

 NBasis= 1104 NAE= 190 NBE= 190 NFC= 56 NFV= 0

 NROrb= 1048 NOA= 134 NOB= 134 NVA= 914 NVB= 914

 \*\*\*\* Warning!!: The largest alpha MO coefficient is 0.15994799D+02

 \*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.69234720D-01

 Leave Link 801 at Thu Sep 19 00:40:06 2019, MaxMem= 1342177280 cpu: 3.9

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

 RHF ground state

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

 Would need an additional 231192000000 words for in-memory AO integral storage.

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

 Inv3: Mode=1 IEnd= 121119948.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 7.33D-15 for 6348.

 Iteration 1 A\*A^-1 deviation from orthogonality is 5.02D-15 for 4265 379.

 Iteration 1 A^-1\*A deviation from unit magnitude is 7.55D-15 for 6348.

 Iteration 1 A^-1\*A deviation from orthogonality is 3.13D-15 for 6335 6248.

 Making orbital integer symmetry assigments:

 Orbital symmetries:

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

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 40 initial guesses have been made.

 Convergence on wavefunction: 0.001000000000000

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

 Max sub-space: 200 roots to seek: 40 dimension of matrix: 244952

 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 7 was old state 10

 New state 8 was old state 7

 New state 9 was old state 8

 New state 10 was old state 9

 Excitation Energies [eV] at current iteration:

 Root 1 : 1.943051546683700

 Root 2 : 1.943055320519200

 Root 3 : 2.736598400401995

 Root 4 : 2.772943270884025

 Root 5 : 2.867223450914185

 Root 6 : 2.867225370550662

 Root 7 : 2.991796752107804

 Root 8 : 3.055239833564313

 Root 9 : 3.055245148774546

 Root 10 : 3.056556117199539

 Root 11 : 3.104471657304943

 Root 12 : 3.247907863832520

 Root 13 : 3.304933937768626

 Root 14 : 3.491693863444175

 Root 15 : 3.491699577243956

 Root 16 : 3.527361860761860

 Root 17 : 3.553659270509933

 Root 18 : 3.617180360676686

 Root 19 : 3.617181517526131

 Root 20 : 3.666595002635897

 Root 21 : 3.666601977120606

 Root 22 : 3.700397585098805

 Root 23 : 3.703969086296245

 Root 24 : 3.703974113449681

 Root 25 : 3.736489734107086

 Root 26 : 3.736496294571364

 Root 27 : 3.754790435636865

 Root 28 : 4.215469423501908

 Root 29 : 4.215471274786450

 Root 30 : 4.281019398764232

 Root 31 : 4.355113040810998

 Root 32 : 4.355113383692190

 Root 33 : 4.389230804297181

 Root 34 : 4.457617634344838

 Root 35 : 4.515027889178764

 Root 36 : 4.515030817714573

 Root 37 : 4.640211500441041

 Root 38 : 4.824650613895065

 Root 39 : 4.824650772552491

 Root 40 : 4.848061906815394

 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 0.066080023930176

 Root 2 not converged, maximum delta is 0.066079727307505

 Root 3 not converged, maximum delta is 0.129873438619475

 Root 4 not converged, maximum delta is 0.158219266232764

 Root 5 not converged, maximum delta is 0.160903960049107

 Root 6 not converged, maximum delta is 0.160901474502347

 Root 7 not converged, maximum delta is 0.163467617984334

 Root 8 not converged, maximum delta is 0.147394711864075

 Root 9 not converged, maximum delta is 0.147391959594933

 Root 10 not converged, maximum delta is 0.024266740533376

 Excitation Energies [eV] at current iteration:

 Root 1 : 1.714804414040503 Change is -0.228247132643197

 Root 2 : 1.714808528695980 Change is -0.228246791823220

 Root 3 : 2.604237121644787 Change is -0.132361278757208

 Root 4 : 2.680085399542716 Change is -0.092857871341309

 Root 5 : 2.792529374941301 Change is -0.074694075972884

 Root 6 : 2.792530431758894 Change is -0.074694938791768

 Root 7 : 2.928339101348816 Change is -0.063457650758988

 Root 8 : 2.951247620601564 Change is -0.103992212962750

 Root 9 : 2.951253416499021 Change is -0.103991732275525

 Root 10 : 2.960735456301635 Change is -0.095820660897905

 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 0.017222359775264

 Root 2 not converged, maximum delta is 0.017222364992204

 Root 3 not converged, maximum delta is 0.015420478438914

 Root 4 not converged, maximum delta is 0.014715445203377

 Root 5 not converged, maximum delta is 0.013251843379326

 Root 6 not converged, maximum delta is 0.013251571731948

 Root 7 not converged, maximum delta is 0.018850723136580

 Root 8 not converged, maximum delta is 0.012738652614395

 Root 9 not converged, maximum delta is 0.012738347198479

 Root 10 not converged, maximum delta is 0.064464343196782

 Excitation Energies [eV] at current iteration:

 Root 1 : 1.699293194192441 Change is -0.015511219848062

 Root 2 : 1.699297365655489 Change is -0.015511163040491

 Root 3 : 2.595276090303587 Change is -0.008961031341200

 Root 4 : 2.674553765688627 Change is -0.005531633854089

 Root 5 : 2.784663141806842 Change is -0.007866233134459

 Root 6 : 2.784664117139980 Change is -0.007866314618914

 Root 7 : 2.925091455350907 Change is -0.003247645997909

 Root 8 : 2.943631872837604 Change is -0.007615747763960

 Root 9 : 2.943637656479526 Change is -0.007615760019495

 Root 10 : 2.950108028111722 Change is -0.010627428189913

 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 0.003267466085234

 Root 2 not converged, maximum delta is 0.003267432286005

 Root 3 not converged, maximum delta is 0.002745291546361

 Root 4 not converged, maximum delta is 0.001960189738076

 Root 5 not converged, maximum delta is 0.003092799698849

 Root 6 not converged, maximum delta is 0.003092847835402

 Root 7 not converged, maximum delta is 0.002104616316496

 Root 8 not converged, maximum delta is 0.004450137830676

 Root 9 not converged, maximum delta is 0.004450167111436

 Root 10 not converged, maximum delta is 0.031286557939196

 Excitation Energies [eV] at current iteration:

 Root 1 : 1.697430121526239 Change is -0.001863072666202

 Root 2 : 1.697434298988322 Change is -0.001863066667167

 Root 3 : 2.594453220741411 Change is -0.000822869562176

 Root 4 : 2.673889746396525 Change is -0.000664019292102

 Root 5 : 2.783779198966307 Change is -0.000883942840535

 Root 6 : 2.783780163670490 Change is -0.000883953469490

 Root 7 : 2.924695192845736 Change is -0.000396262505172

 Root 8 : 2.942497937793928 Change is -0.001133935043676

 Root 9 : 2.942503719180477 Change is -0.001133937299048

 Root 10 : 2.948164526612305 Change is -0.001943501499418

 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 not converged, maximum delta is 0.001012220318404

 Root 2 not converged, maximum delta is 0.001012220134025

 Root 3 has converged.

 Root 4 has converged.

 Root 5 has converged.

 Root 6 has converged.

 Root 7 not converged, maximum delta is 0.001041565979628

 Root 8 has converged.

 Root 9 has converged.

 Root 10 not converged, maximum delta is 0.006205087158221

 Excitation Energies [eV] at current iteration:

 Root 1 : 1.697273075160572 Change is -0.000157046365667

 Root 2 : 1.697277252019953 Change is -0.000157046968369

 Root 3 : 2.594346103236862 Change is -0.000107117504549

 Root 4 : 2.673821590020446 Change is -0.000068156376079

 Root 5 : 2.783647432501460 Change is -0.000131766464847

 Root 6 : 2.783648395977138 Change is -0.000131767693353

 Root 7 : 2.924650212847788 Change is -0.000044979997948

 Root 8 : 2.942376135791093 Change is -0.000121802002835

 Root 9 : 2.942381917937528 Change is -0.000121801242949

 Root 10 : 2.947851391327532 Change is -0.000313135284772

 Iteration 6 Dimension 128 NMult 120 NNew 8

 CISAX will form 8 AO SS matrices at one time.

 NMat= 8 NSing= 8 JSym2X=-1.

 Root 1 has converged.

 Root 2 has converged.

 Root 3 has converged.

 Root 4 has converged.

 Root 5 has converged.

 Root 6 has converged.

 Root 7 has converged.

 Root 8 has converged.

 Root 9 has converged.

 Root 10 not converged, maximum delta is 0.002182743731251

 Excitation Energies [eV] at current iteration:

 Root 1 : 1.697264113629540 Change is -0.000008961531032

 Root 2 : 1.697268290518676 Change is -0.000008961501277

 Root 3 : 2.594345864507389 Change is -0.000000238729473

 Root 4 : 2.673818728898377 Change is -0.000002861122069

 Root 5 : 2.783647289609131 Change is -0.000000142892329

 Root 6 : 2.783648253154466 Change is -0.000000142822672

 Root 7 : 2.924647035409499 Change is -0.000003177438288

 Root 8 : 2.942374013358126 Change is -0.000002122432967

 Root 9 : 2.942379795485822 Change is -0.000002122451706

 Root 10 : 2.947779455231056 Change is -0.000071936096477

 Iteration 7 Dimension 130 NMult 128 NNew 2

 CISAX will form 2 AO SS matrices at one time.

 NMat= 2 NSing= 2 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 not converged, maximum delta is 0.001175435727393

 Excitation Energies [eV] at current iteration:

 Root 1 : 1.697264113629685 Change is 0.000000000000145

 Root 2 : 1.697268290518676 Change is 0.000000000000000

 Root 3 : 2.594345864507357 Change is -0.000000000000032

 Root 4 : 2.673818728898500 Change is 0.000000000000123

 Root 5 : 2.783647289609013 Change is -0.000000000000118

 Root 6 : 2.783648253154407 Change is -0.000000000000059

 Root 7 : 2.924647035409527 Change is 0.000000000000028

 Root 8 : 2.942374013358070 Change is -0.000000000000056

 Root 9 : 2.942379795485849 Change is 0.000000000000028

 Root 10 : 2.947771061565974 Change is -0.000008393665081

 Convergence on energies, max DE= 8.39D-06.

 Convergence on expansion vectors.

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

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

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

 1PDM for each excited state written to RWF 633

 Ground to excited state transition densities written to RWF 633

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

 state X Y Z Dip. S. Osc.

 1 0.0000 4.5574 -0.0000 20.7701 0.8637

 2 4.5574 -0.0000 0.0000 20.7700 0.8637

 3 0.0000 -0.0000 0.0000 0.0000 0.0000

 4 0.0000 -0.0000 -0.0000 0.0000 0.0000

 5 0.0000 0.7786 0.0000 0.6062 0.0413

 6 0.7786 -0.0000 0.0000 0.6062 0.0413

 7 -0.0000 -0.0000 -0.0000 0.0000 0.0000

 8 0.0000 -2.1345 -0.0000 4.5563 0.3284

 9 2.1345 0.0000 0.0000 4.5563 0.3284

 10 0.0000 0.0000 -0.0001 0.0000 0.0000

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

 state X Y Z Dip. S. Osc.

 1 -0.0000 -0.2851 -0.0000 0.0813 0.8690

 2 -0.2851 0.0000 -0.0000 0.0813 0.8690

 3 -0.0000 -0.0000 0.0000 0.0000 0.0000

 4 -0.0000 0.0000 -0.0000 0.0000 0.0000

 5 -0.0000 -0.0709 -0.0000 0.0050 0.0327

 6 -0.0709 0.0000 -0.0000 0.0050 0.0327

 7 0.0000 0.0000 0.0000 0.0000 0.0000

 8 -0.0000 0.2243 0.0000 0.0503 0.3101

 9 -0.2243 -0.0000 0.0000 0.0503 0.3101

 10 -0.0000 -0.0000 0.0000 0.0000 0.0000

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

 state X Y Z

 1 0.1347 -0.0000 -0.0000

 2 -0.0000 -0.1347 -0.0000

 3 0.0000 -0.0000 0.0002

 4 -0.0000 0.0000 0.6281

 5 0.0934 -0.0000 0.0000

 6 -0.0000 -0.0934 -0.0000

 7 -0.0000 0.0000 1.0221

 8 -0.1395 -0.0000 -0.0000

 9 0.0000 -0.1395 0.0000

 10 0.0000 -0.0000 -0.0000

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

 state XX YY ZZ XY XZ YZ

 1 0.0000 -0.0000 -0.0000 0.0000 0.0000 0.0746

 2 -0.0000 0.0000 -0.0000 0.0000 0.0746 -0.0000

 3 0.0000 -0.0000 0.0000 0.8095 0.0000 0.0000

 4 0.0000 0.0000 0.0000 -0.0004 0.0000 0.0000

 5 0.0000 0.0000 0.0000 0.0000 0.0000 0.0355

 6 0.0000 0.0000 -0.0000 -0.0000 0.0355 -0.0000

 7 0.0000 -0.0000 0.0000 -0.0002 -0.0000 -0.0000

 8 0.0000 -0.0000 -0.0000 -0.0000 0.0000 -0.1337

 9 -0.0000 0.0000 -0.0000 -0.0000 0.1336 0.0000

 10 2.7241 -2.7245 0.0000 -0.0000 0.0000 0.0000

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

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

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

 1 0.0000 -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 -0.0000 -1.2995 0.0000 1.2995 0.8663

 2 -1.2995 -0.0000 -0.0000 1.2995 0.8663

 3 -0.0000 0.0000 0.0000 0.0000 0.0000

 4 -0.0000 -0.0000 0.0000 0.0000 0.0000

 5 -0.0000 -0.0552 -0.0000 0.0552 0.0368

 6 -0.0552 -0.0000 -0.0000 0.0552 0.0368

 7 -0.0000 -0.0000 -0.0000 0.0000 0.0000

 8 -0.0000 -0.4787 -0.0000 0.4787 0.3191

 9 -0.4787 -0.0000 0.0000 0.4787 0.3191

 10 -0.0000 -0.0000 -0.0000 0.0000 0.0000

 Excitation energies and oscillator strengths:

 Excited State 1: Singlet-B2 1.6973 eV 730.49 nm f=0.8637 <S\*\*2>=0.000

 63 -> 282 -0.00120

 68 -> 261 0.00101

 77 -> 245 -0.00105

 87 -> 252 0.00164

 93 -> 254 0.00113

 93 -> 261 0.00146

 94 -> 252 0.00125

 96 -> 257 -0.00106

 96 -> 265 -0.00102

 99 -> 225 -0.00104

 101 -> 265 0.00196

 101 -> 277 -0.00126

 101 -> 345 -0.00123

 106 -> 257 0.00103

 107 -> 243 -0.00133

 107 -> 252 0.00246

 107 -> 266 -0.00188

 107 -> 275 -0.00143

 108 -> 242 -0.00232

 108 -> 251 -0.00105

 108 -> 256 -0.00159

 108 -> 260 -0.00107

 108 -> 290 -0.00187

 108 -> 361 -0.00201

 108 -> 393 0.00163

 109 -> 254 -0.00120

 110 -> 290 -0.00152

 111 -> 238 0.00131

 111 -> 243 -0.00131

 111 -> 250 0.00144

 112 -> 253 -0.00146

 112 -> 273 0.00113

 112 -> 386 0.00101

 113 -> 210 -0.00116

 113 -> 213 -0.00139

 113 -> 215 0.00101

 113 -> 250 0.00129

 115 -> 261 0.00138

 116 -> 212 -0.00154

 117 -> 208 -0.00148

 117 -> 239 -0.00166

 117 -> 245 -0.00284

 117 -> 257 -0.00229

 117 -> 265 -0.00196

 117 -> 277 0.00114

 117 -> 291 -0.00100

 117 -> 345 -0.00116

 117 -> 404 0.00103

 118 -> 212 0.00138

 118 -> 222 -0.00123

 118 -> 236 -0.00115

 119 -> 242 0.00130

 119 -> 282 0.00116

 120 -> 218 -0.00245

 120 -> 243 0.00106

 120 -> 250 0.00190

 121 -> 208 0.00127

 121 -> 245 0.00273

 121 -> 253 -0.00135

 121 -> 262 -0.00210

 121 -> 345 0.00108

 122 -> 196 0.00223

 122 -> 203 0.00133

 122 -> 221 0.00281

 122 -> 234 -0.00282

 122 -> 295 -0.00155

 123 -> 217 0.00219

 123 -> 235 -0.00110

 123 -> 253 -0.00109

 124 -> 214 0.00288

 124 -> 219 0.00222

 124 -> 230 0.00164

 125 -> 250 -0.00114

 126 -> 208 -0.00136

 126 -> 217 -0.00264

 126 -> 228 0.00121

 127 -> 254 -0.00149

 128 -> 193 0.00121

 128 -> 194 -0.00108

 128 -> 201 -0.00160

 128 -> 205 -0.00130

 128 -> 207 0.00129

 128 -> 250 0.00143

 129 -> 197 0.00142

 129 -> 206 0.00135

 129 -> 214 -0.00137

 129 -> 251 0.00103

 130 -> 197 -0.00283

 130 -> 206 -0.00274

 130 -> 231 -0.00175

 131 -> 193 0.00242

 131 -> 194 -0.00207

 131 -> 201 -0.00260

 131 -> 202 -0.00195

 131 -> 205 -0.00163

 131 -> 207 0.00253

 131 -> 215 0.00164

 131 -> 229 0.00183

 131 -> 232 0.00170

 131 -> 317 0.00105

 131 -> 344 0.00118

 132 -> 217 -0.00132

 132 -> 239 -0.00210

 132 -> 253 -0.00125

 133 -> 212 0.00195

 133 -> 244 0.00115

 134 -> 244 -0.00107

 134 -> 258 0.00147

 134 -> 261 -0.00178

 135 -> 210 -0.00168

 135 -> 213 -0.00192

 135 -> 218 0.00146

 135 -> 243 -0.00112

 135 -> 259 0.00113

 136 -> 242 0.00155

 137 -> 212 -0.00189

 137 -> 244 0.00122

 138 -> 210 0.00148

 138 -> 243 -0.00126

 138 -> 250 -0.00276

 138 -> 259 0.00115

 138 -> 271 0.00126

 138 -> 279 -0.00108

 139 -> 214 0.00117

 139 -> 224 -0.00105

 139 -> 237 -0.00161

 139 -> 241 0.00167

 139 -> 282 -0.00140

 140 -> 223 -0.00156

 140 -> 228 0.00135

 140 -> 253 0.00154

 140 -> 265 0.00149

 141 -> 192 -0.00738

 141 -> 199 -0.00214

 141 -> 221 0.00121

 141 -> 295 -0.00153

 142 -> 223 -0.00157

 142 -> 228 0.00108

 142 -> 239 -0.00124

 142 -> 253 0.00118

 143 -> 219 0.00149

 143 -> 224 0.00231

 143 -> 230 -0.00130

 143 -> 241 -0.00115

 143 -> 303 0.00112

 144 -> 210 0.00116

 144 -> 250 -0.00204

 144 -> 259 0.00130

 145 -> 228 -0.00146

 145 -> 239 0.00110

 145 -> 253 0.00295

 145 -> 262 0.00138

 145 -> 265 0.00288

 146 -> 234 0.00129

 146 -> 300 0.00131

 147 -> 206 -0.00117

 147 -> 231 -0.00118

 148 -> 193 0.00187

 148 -> 205 -0.00175

 148 -> 207 0.00196

 148 -> 229 0.00104

 148 -> 298 -0.00143

 148 -> 299 -0.00139

 150 -> 191 0.00703

 150 -> 195 -0.00102

 150 -> 200 0.00279

 150 -> 233 -0.00183

 150 -> 296 0.00125

 151 -> 192 -0.00806

 151 -> 199 -0.00157

 151 -> 203 -0.00121

 151 -> 221 0.00149

 151 -> 300 -0.00126

 152 -> 212 -0.00156

 152 -> 236 -0.00157

 152 -> 240 0.00191

 152 -> 254 0.00145

 152 -> 264 0.00117

 153 -> 263 0.00122

 153 -> 272 -0.00113

 153 -> 282 0.00235

 154 -> 205 -0.00144

 154 -> 210 -0.00167

 154 -> 213 -0.00121

 154 -> 215 -0.00146

 154 -> 238 -0.00278

 154 -> 243 -0.00253

 154 -> 279 -0.00105

 155 -> 212 0.00104

 155 -> 236 0.00169

 155 -> 244 0.00123

 155 -> 258 -0.00102

 155 -> 261 0.00208

 155 -> 274 -0.00110

 155 -> 292 -0.00105

 155 -> 318 0.00119

 156 -> 228 0.00136

 156 -> 253 -0.00193

 157 -> 243 0.00105

 157 -> 250 0.00225

 157 -> 259 -0.00175

 157 -> 278 0.00118

 157 -> 285 0.00102

 158 -> 219 0.00101

 158 -> 224 0.00126

 158 -> 230 -0.00148

 158 -> 237 -0.00138

 158 -> 241 0.00129

 158 -> 269 0.00137

 158 -> 282 0.00110

 159 -> 223 -0.00102

 159 -> 235 0.00108

 159 -> 239 0.00164

 159 -> 253 0.00208

 159 -> 257 0.00121

 159 -> 265 0.00207

 160 -> 197 -0.00456

 160 -> 198 0.00114

 160 -> 226 0.00101

 160 -> 315 -0.00160

 161 -> 193 0.00345

 161 -> 194 0.00368

 161 -> 202 -0.00262

 161 -> 207 0.00172

 161 -> 314 -0.00144

 162 -> 214 0.00100

 162 -> 242 -0.00116

 162 -> 282 0.00141

 162 -> 290 -0.00134

 163 -> 201 0.00204

 163 -> 205 0.00273

 163 -> 210 0.00203

 163 -> 215 0.00302

 163 -> 225 -0.00281

 163 -> 229 -0.00139

 163 -> 232 0.00175

 163 -> 243 0.00282

 163 -> 266 -0.00133

 164 -> 212 -0.00103

 164 -> 222 -0.00235

 164 -> 227 -0.00242

 165 -> 209 -0.00172

 165 -> 212 0.00123

 165 -> 216 0.00189

 165 -> 222 0.00220

 165 -> 227 0.00135

 165 -> 261 0.00181

 165 -> 264 0.00110

 165 -> 283 -0.00104

 166 -> 192 -0.00739

 166 -> 196 -0.00156

 166 -> 234 -0.00164

 167 -> 198 0.00128

 167 -> 206 -0.00120

 167 -> 214 -0.00106

 167 -> 242 -0.00352

 167 -> 256 -0.00174

 167 -> 263 -0.00134

 167 -> 272 0.00119

 167 -> 282 -0.00111

 167 -> 290 -0.00257

 167 -> 306 -0.00101

 167 -> 361 0.00124

 168 -> 193 0.00120

 168 -> 194 0.00166

 168 -> 201 0.00355

 168 -> 205 0.00428

 168 -> 213 -0.00119

 168 -> 215 0.00397

 168 -> 218 -0.00271

 168 -> 225 0.00205

 168 -> 238 -0.00156

 168 -> 243 0.00327

 168 -> 252 -0.00225

 168 -> 259 0.00136

 168 -> 266 -0.00117

 168 -> 271 0.00238

 168 -> 275 -0.00152

 168 -> 285 -0.00127

 168 -> 287 0.00112

 169 -> 192 -0.00847

 169 -> 196 0.00110

 169 -> 199 -0.00482

 169 -> 203 -0.00128

 169 -> 221 0.00246

 169 -> 248 0.00104

 169 -> 324 -0.00121

 170 -> 193 -0.00195

 170 -> 194 -0.00639

 170 -> 201 -0.00350

 170 -> 202 0.00116

 170 -> 207 0.00281

 170 -> 215 0.00226

 170 -> 229 0.00113

 170 -> 232 0.00115

 170 -> 255 -0.00191

 170 -> 317 -0.00101

 170 -> 347 -0.00107

 171 -> 197 -0.00104

 171 -> 198 0.00417

 171 -> 206 -0.00317

 171 -> 226 0.00185

 171 -> 231 -0.00205

 171 -> 247 0.00188

 171 -> 315 -0.00159

 172 -> 209 -0.00113

 172 -> 240 0.00107

 172 -> 244 -0.00284

 172 -> 254 -0.00117

 172 -> 261 -0.00215

 172 -> 264 0.00110

 172 -> 295 -0.00112

 173 -> 191 0.00695

 173 -> 195 0.00559

 173 -> 204 0.00467

 173 -> 249 0.00140

 173 -> 321 -0.00201

 174 -> 191 0.00418

 174 -> 195 0.00199

 174 -> 204 0.00375

 174 -> 220 -0.00338

 174 -> 249 -0.00149

 174 -> 321 0.00131

 174 -> 325 -0.00121

 175 -> 193 0.00189

 175 -> 194 0.00151

 175 -> 205 0.00345

 175 -> 207 0.00534

 175 -> 229 -0.00145

 175 -> 232 -0.00128

 176 -> 197 0.00647

 176 -> 198 -0.00296

 176 -> 206 0.00476

 176 -> 226 -0.00263

 176 -> 246 0.00230

 176 -> 322 -0.00119

 176 -> 335 0.00164

 177 -> 201 -0.00208

 177 -> 205 -0.00285

 177 -> 207 0.00118

 177 -> 215 -0.00340

 177 -> 218 0.00179

 177 -> 238 -0.00242

 177 -> 250 -0.00202

 177 -> 252 -0.00673

 177 -> 259 0.00129

 177 -> 266 0.00122

 177 -> 275 0.00133

 177 -> 278 -0.00126

 177 -> 285 -0.00125

 177 -> 287 -0.00100

 177 -> 297 0.00101

 177 -> 302 -0.00159

 178 -> 237 0.00129

 178 -> 242 0.00372

 178 -> 251 -0.00198

 178 -> 256 0.00170

 178 -> 263 0.00117

 178 -> 272 -0.00149

 178 -> 290 0.00252

 178 -> 303 -0.00121

 178 -> 306 0.00104

 178 -> 323 0.00110

 179 -> 192 0.00117

 179 -> 209 0.00255

 179 -> 212 0.00133

 179 -> 216 0.00208

 179 -> 244 0.00523

 179 -> 248 0.00119

 179 -> 254 0.00265

 179 -> 258 0.00413

 179 -> 264 -0.00179

 179 -> 268 -0.00139

 179 -> 274 0.00273

 179 -> 283 0.00195

 179 -> 292 -0.00124

 179 -> 304 -0.00116

 179 -> 312 0.00166

 179 -> 324 -0.00136

 179 -> 385 0.00105

 179 -> 398 0.00119

 179 -> 403 0.00106

 180 -> 191 -0.00163

 180 -> 208 -0.00100

 180 -> 223 0.00119

 180 -> 235 0.00101

 180 -> 239 -0.00279

 180 -> 245 -0.00274

 180 -> 249 0.00108

 180 -> 262 0.00217

 180 -> 265 -0.00411

 180 -> 267 0.00113

 180 -> 273 0.00170

 180 -> 277 0.00143

 180 -> 296 -0.00166

 181 -> 192 0.07325

 181 -> 196 0.00230

 181 -> 199 0.01131

 181 -> 203 0.00516

 181 -> 221 -0.00294

 181 -> 234 -0.00351

 181 -> 248 -0.00192

 182 -> 192 -0.07515

 182 -> 196 -0.01268

 182 -> 199 -0.00585

 182 -> 203 -0.00114

 182 -> 221 0.00112

 183 -> 197 0.00908

 183 -> 198 0.00575

 183 -> 206 -0.00263

 183 -> 226 0.00358

 183 -> 231 -0.00388

 183 -> 246 -0.00113

 183 -> 247 0.00155

 184 -> 193 -0.00416

 184 -> 201 -0.00546

 184 -> 202 -0.00309

 184 -> 205 -0.00226

 184 -> 207 0.00231

 184 -> 215 0.00162

 184 -> 229 0.00210

 184 -> 232 0.00192

 184 -> 255 -0.00168

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 185 -> 191 -0.01741

 185 -> 195 -0.01202

 185 -> 200 0.00486

 185 -> 350 0.00203

 186 -> 199 0.00887

 186 -> 221 -0.00451

 186 -> 222 -0.00102

 186 -> 234 -0.00171

 186 -> 248 -0.00142

 186 -> 359 0.00105

 187 -> 193 -0.00701

 187 -> 194 0.00215

 187 -> 202 0.00425

 187 -> 205 -0.00284

 187 -> 207 -0.01050

 187 -> 229 0.00188

 187 -> 232 0.00170

 188 -> 197 -0.02774

 188 -> 198 0.01427

 188 -> 206 -0.00167

 188 -> 226 0.00360

 188 -> 354 0.00194

 188 -> 364 -0.00168

 189 -> 191 0.00669

 189 -> 195 -0.00116

 189 -> 200 0.01299

 189 -> 204 0.00550

 189 -> 220 -0.00515

 189 -> 223 -0.00123

 189 -> 350 0.00161

 190 -> 191 0.70276

 190 -> 195 -0.02340

 190 -> 200 -0.00536

 190 -> 204 -0.00471

 190 -> 233 0.00257

 190 -> 375 0.00190

 190 -> 378 -0.00104

 190 -> 390 -0.00131

 190 -> 424 0.00112

 63 <- 282 -0.00106

 87 <- 252 0.00151

 93 <- 254 0.00102

 93 <- 261 0.00131

 94 <- 252 0.00110

 101 <- 265 0.00174

 101 <- 277 -0.00115

 101 <- 345 -0.00110

 107 <- 243 -0.00115

 107 <- 252 0.00220

 107 <- 266 -0.00166

 107 <- 275 -0.00127

 108 <- 242 -0.00192

 108 <- 256 -0.00129

 108 <- 290 -0.00162

 108 <- 361 -0.00179

 108 <- 393 0.00145

 110 <- 290 -0.00129

 111 <- 238 0.00107

 111 <- 243 -0.00110

 111 <- 250 0.00115

 112 <- 253 -0.00119

 113 <- 213 -0.00108

 113 <- 250 0.00107

 115 <- 261 0.00116

 116 <- 212 -0.00121

 117 <- 208 -0.00118

 117 <- 239 -0.00136

 117 <- 245 -0.00238

 117 <- 257 -0.00192

 117 <- 265 -0.00168

 117 <- 277 0.00101

 117 <- 345 -0.00101

 118 <- 212 0.00108

 119 <- 242 0.00108

 119 <- 282 0.00104

 120 <- 218 -0.00195

 120 <- 250 0.00160

 121 <- 208 0.00104

 121 <- 245 0.00227

 121 <- 253 -0.00118

 121 <- 262 -0.00184

 122 <- 196 0.00161

 122 <- 203 0.00100

 122 <- 221 0.00226

 122 <- 234 -0.00242

 122 <- 295 -0.00137

 123 <- 217 0.00167

 124 <- 214 0.00219

 124 <- 219 0.00170

 124 <- 230 0.00128

 126 <- 208 -0.00102

 126 <- 217 -0.00202

 127 <- 254 -0.00121

 128 <- 201 -0.00119

 128 <- 207 0.00106

 128 <- 250 0.00114

 129 <- 214 -0.00104

 130 <- 197 -0.00176

 130 <- 206 -0.00186

 130 <- 231 -0.00129

 131 <- 193 0.00168

 131 <- 194 -0.00159

 131 <- 201 -0.00195

 131 <- 202 -0.00145

 131 <- 205 -0.00120

 131 <- 207 0.00206

 131 <- 215 0.00123

 131 <- 229 0.00170

 131 <- 232 0.00158

 132 <- 217 -0.00100

 132 <- 239 -0.00165

 132 <- 253 -0.00101

 133 <- 212 0.00147

 134 <- 258 0.00120

 134 <- 261 -0.00148

 135 <- 210 -0.00126

 135 <- 213 -0.00144

 135 <- 218 0.00109

 136 <- 242 0.00125

 137 <- 212 -0.00141

 138 <- 210 0.00112

 138 <- 243 -0.00104

 138 <- 250 -0.00224

 138 <- 271 0.00106

 139 <- 237 -0.00127

 139 <- 241 0.00132

 139 <- 282 -0.00121

 140 <- 223 -0.00119

 140 <- 228 0.00103

 140 <- 253 0.00125

 140 <- 265 0.00122

 141 <- 192 -0.00401

 141 <- 199 -0.00154

 141 <- 221 0.00136

 141 <- 295 -0.00125

 142 <- 223 -0.00119

 143 <- 219 0.00112

 143 <- 224 0.00176

 144 <- 250 -0.00164

 144 <- 259 0.00105

 145 <- 228 -0.00113

 145 <- 253 0.00240

 145 <- 262 0.00117

 145 <- 265 0.00235

 146 <- 234 0.00110

 146 <- 300 0.00110

 148 <- 193 0.00123

 148 <- 205 -0.00116

 148 <- 207 0.00151

 148 <- 298 -0.00116

 148 <- 299 -0.00115

 150 <- 191 0.00509

 150 <- 200 0.00175

 150 <- 233 -0.00186

 151 <- 192 -0.00431

 151 <- 199 -0.00121

 151 <- 221 0.00163

 152 <- 212 -0.00113

 152 <- 236 -0.00118

 152 <- 240 0.00147

 152 <- 254 0.00114

 153 <- 263 0.00100

 153 <- 282 0.00194

 154 <- 210 -0.00119

 154 <- 215 -0.00104

 154 <- 238 -0.00211

 154 <- 243 -0.00200

 155 <- 236 0.00127

 155 <- 261 0.00170

 156 <- 253 -0.00153

 157 <- 250 0.00177

 157 <- 259 -0.00141

 158 <- 230 -0.00109

 158 <- 237 -0.00104

 158 <- 269 0.00109

 159 <- 239 0.00126

 159 <- 253 0.00166

 159 <- 265 0.00164

 160 <- 197 -0.00132

 160 <- 315 -0.00128

 161 <- 193 0.00153

 161 <- 194 0.00160

 161 <- 202 -0.00148

 161 <- 314 -0.00113

 162 <- 282 0.00113

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 163 <- 201 0.00135

 163 <- 205 0.00186

 163 <- 210 0.00142

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 163 <- 225 -0.00205

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 163 <- 232 0.00129

 163 <- 243 0.00217

 163 <- 266 -0.00107

 164 <- 222 -0.00170

 164 <- 227 -0.00177

 165 <- 209 -0.00118

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 165 <- 222 0.00159

 165 <- 261 0.00145

 166 <- 192 -0.00515

 166 <- 234 -0.00143

 167 <- 198 0.00109

 167 <- 242 -0.00269

 167 <- 256 -0.00134

 167 <- 263 -0.00110

 167 <- 290 -0.00211

 167 <- 361 0.00106

 168 <- 201 0.00237

 168 <- 205 0.00285

 168 <- 215 0.00274

 168 <- 218 -0.00189

 168 <- 225 0.00148

 168 <- 238 -0.00116

 168 <- 243 0.00246

 168 <- 252 -0.00174

 168 <- 259 0.00105

 168 <- 271 0.00189

 168 <- 275 -0.00122

 168 <- 285 -0.00101

 169 <- 192 -0.00403

 169 <- 196 0.00135

 169 <- 199 -0.00379

 169 <- 221 0.00237

 169 <- 324 -0.00101

 170 <- 194 -0.00372

 170 <- 201 -0.00253

 170 <- 207 0.00284

 170 <- 215 0.00165

 170 <- 255 -0.00152

 171 <- 197 0.00119

 171 <- 198 0.00359

 171 <- 206 -0.00141

 171 <- 226 0.00184

 171 <- 231 -0.00120

 171 <- 247 0.00129

 171 <- 315 -0.00114

 172 <- 244 -0.00214

 172 <- 261 -0.00165

 173 <- 191 0.00391

 173 <- 195 0.00306

 173 <- 204 0.00322

 173 <- 220 -0.00113

 173 <- 321 -0.00169

 174 <- 191 0.00298

 174 <- 195 0.00206

 174 <- 204 0.00293

 174 <- 220 -0.00169

 174 <- 249 -0.00100

 174 <- 321 0.00104

 174 <- 325 -0.00103

 175 <- 202 0.00124

 175 <- 205 0.00264

 175 <- 207 0.00272

 175 <- 229 -0.00107

 176 <- 198 -0.00256

 176 <- 206 0.00167

 176 <- 226 -0.00172

 176 <- 246 0.00164

 176 <- 335 0.00134

 177 <- 201 -0.00129

 177 <- 205 -0.00169

 177 <- 215 -0.00231

 177 <- 218 0.00119

 177 <- 238 -0.00177

 177 <- 250 -0.00146

 177 <- 252 -0.00511

 177 <- 259 0.00101

 177 <- 275 0.00106

 177 <- 285 -0.00101

 177 <- 302 -0.00130

 178 <- 242 0.00277

 178 <- 251 -0.00148

 178 <- 256 0.00131

 178 <- 272 -0.00117

 178 <- 290 0.00201

 179 <- 209 0.00163

 179 <- 216 0.00138

 179 <- 244 0.00384

 179 <- 254 0.00205

 179 <- 258 0.00309

 179 <- 264 -0.00134

 179 <- 268 -0.00111

 179 <- 274 0.00212

 179 <- 283 0.00153

 179 <- 312 0.00133

 179 <- 324 -0.00111

 179 <- 398 0.00101

 180 <- 239 -0.00204

 180 <- 245 -0.00204

 180 <- 262 0.00170

 180 <- 265 -0.00318

 180 <- 273 0.00133

 180 <- 277 0.00113

 180 <- 296 -0.00135

 181 <- 192 0.03478

 181 <- 196 0.00230

 181 <- 199 0.00905

 181 <- 203 0.00404

 181 <- 221 -0.00274

 181 <- 234 -0.00329

 181 <- 248 -0.00186

 182 <- 192 -0.03529

 182 <- 196 -0.00568

 182 <- 199 -0.00475

 182 <- 221 0.00121

 183 <- 197 0.00475

 183 <- 198 0.00496

 183 <- 206 -0.00196

 183 <- 226 0.00335

 183 <- 231 -0.00315

 183 <- 246 -0.00110

 183 <- 247 0.00127

 184 <- 201 -0.00316

 184 <- 202 -0.00210

 184 <- 205 -0.00124

 184 <- 207 0.00167

 184 <- 215 0.00106

 184 <- 229 0.00146

 184 <- 232 0.00135

 184 <- 255 -0.00121

 185 <- 191 -0.01624

 185 <- 195 -0.00614

 185 <- 220 0.00143

 185 <- 350 0.00172

 186 <- 192 0.00155

 186 <- 199 0.00594

 186 <- 221 -0.00342

 186 <- 234 -0.00157

 186 <- 248 -0.00119

 187 <- 194 0.00327

 187 <- 202 0.00219

 187 <- 205 -0.00178

 187 <- 207 -0.00607

 187 <- 229 0.00129

 187 <- 232 0.00117

 188 <- 197 -0.00664

 188 <- 198 0.00750

 188 <- 226 0.00241

 188 <- 354 0.00147

 188 <- 364 -0.00146

 189 <- 191 0.00607

 189 <- 195 0.00327

 189 <- 200 0.00560

 189 <- 204 0.00281

 189 <- 220 -0.00264

 189 <- 350 0.00121

 190 <- 191 -0.07645

 190 <- 195 -0.00646

 190 <- 200 -0.00739

 190 <- 204 -0.00223

 190 <- 233 0.00112

 190 <- 375 0.00161

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

 Total Energy, E(TD-HF/TD-KS) = -2348.10216210

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

 Excited State 2: Singlet-B1 1.6973 eV 730.49 nm f=0.8637 <S\*\*2>=0.000

 62 -> 282 0.00120

 68 -> 262 -0.00101

 77 -> 244 0.00105

 86 -> 252 -0.00164

 93 -> 253 0.00113

 93 -> 262 0.00146

 95 -> 252 0.00125

 96 -> 258 0.00106

 96 -> 264 -0.00102

 98 -> 225 -0.00104

 101 -> 264 -0.00196

 101 -> 276 0.00126

 101 -> 346 0.00123

 106 -> 258 0.00103

 107 -> 242 -0.00232

 107 -> 251 0.00105

 107 -> 256 -0.00159

 107 -> 260 0.00107

 107 -> 290 -0.00187

 107 -> 361 0.00201

 107 -> 393 -0.00163

 108 -> 243 -0.00133

 108 -> 252 -0.00246

 108 -> 266 -0.00188

 108 -> 275 -0.00143

 109 -> 253 0.00120

 110 -> 238 -0.00131

 110 -> 243 -0.00131

 110 -> 250 0.00144

 111 -> 290 -0.00152

 112 -> 254 0.00146

 112 -> 274 0.00113

 112 -> 385 0.00101

 114 -> 210 -0.00116

 114 -> 213 0.00139

 114 -> 215 0.00101

 114 -> 250 0.00129

 115 -> 262 0.00138

 116 -> 211 0.00154

 117 -> 209 0.00148

 117 -> 240 -0.00166

 117 -> 244 0.00284

 117 -> 258 0.00229

 117 -> 264 -0.00196

 117 -> 276 0.00114

 117 -> 292 -0.00100

 117 -> 346 -0.00116

 117 -> 403 0.00103

 118 -> 211 0.00138

 118 -> 223 -0.00123

 118 -> 235 -0.00115

 119 -> 218 -0.00245

 119 -> 243 0.00106

 119 -> 250 0.00190

 120 -> 242 0.00130

 120 -> 282 0.00116

 121 -> 209 -0.00127

 121 -> 244 -0.00273

 121 -> 254 -0.00135

 121 -> 261 -0.00210

 121 -> 346 0.00108

 122 -> 195 -0.00223

 122 -> 204 -0.00133

 122 -> 220 -0.00281

 122 -> 233 0.00282

 122 -> 296 -0.00155

 123 -> 216 -0.00219

 123 -> 236 0.00110

 123 -> 254 0.00109

 124 -> 250 0.00114

 125 -> 214 -0.00288

 125 -> 219 0.00222

 125 -> 230 0.00164

 126 -> 209 0.00136

 126 -> 216 -0.00264

 126 -> 227 0.00121

 127 -> 253 0.00149

 128 -> 197 0.00142

 128 -> 206 0.00135

 128 -> 214 -0.00137

 128 -> 251 -0.00103

 129 -> 193 -0.00121

 129 -> 194 -0.00108

 129 -> 201 -0.00161

 129 -> 205 -0.00130

 129 -> 207 -0.00129

 129 -> 250 0.00143

 130 -> 193 0.00242

 130 -> 194 0.00207

 130 -> 201 0.00260

 130 -> 202 -0.00195

 130 -> 205 0.00163

 130 -> 207 0.00253

 130 -> 215 -0.00164

 130 -> 229 -0.00183

 130 -> 232 -0.00170

 130 -> 317 -0.00105

 130 -> 344 -0.00118

 131 -> 197 0.00283

 131 -> 206 0.00274

 131 -> 231 0.00175

 132 -> 216 0.00132

 132 -> 240 0.00210

 132 -> 254 0.00125

 133 -> 211 -0.00195

 133 -> 245 0.00115

 134 -> 245 0.00107

 134 -> 257 -0.00147

 134 -> 262 -0.00178

 135 -> 242 0.00155

 136 -> 210 -0.00168

 136 -> 213 0.00192

 136 -> 218 0.00146

 136 -> 243 -0.00112

 136 -> 259 -0.00113

 137 -> 211 -0.00189

 137 -> 245 -0.00122

 138 -> 214 0.00117

 138 -> 224 -0.00105

 138 -> 237 -0.00161

 138 -> 241 -0.00167

 138 -> 282 -0.00140

 139 -> 210 0.00148

 139 -> 243 -0.00126

 139 -> 250 -0.00276

 139 -> 259 -0.00115

 139 -> 271 0.00126

 139 -> 279 0.00108

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 140 -> 254 0.00154

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 141 -> 191 -0.00738

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 141 -> 220 0.00121

 141 -> 296 0.00153

 142 -> 222 0.00157

 142 -> 227 -0.00108

 142 -> 240 0.00124

 142 -> 254 -0.00118

 143 -> 210 0.00116

 143 -> 250 -0.00204

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 144 -> 219 -0.00149

 144 -> 224 0.00231

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 145 -> 254 0.00295

 145 -> 261 0.00138

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 146 -> 233 -0.00129

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 147 -> 193 0.00187

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 147 -> 207 0.00196

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 153 -> 243 0.00253

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 Excited State 3: Singlet-A2 2.5943 eV 477.90 nm f=0.0000 <S\*\*2>=0.000

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 171 <- 199 0.00225

 171 <- 203 0.00325

 171 <- 221 -0.00105

 173 <- 193 -0.00287

 173 <- 202 0.00341

 173 <- 207 0.00429

 173 <- 298 0.00121

 174 <- 194 -0.00332

 174 <- 201 -0.00383

 174 <- 205 0.00335

 174 <- 299 -0.00101

 175 <- 191 -0.00506

 175 <- 195 0.00157

 175 <- 200 -0.00215

 175 <- 204 0.00380

 176 <- 192 -0.00509

 176 <- 196 0.00160

 176 <- 199 -0.00214

 176 <- 203 0.00378

 177 <- 191 -0.00102

 177 <- 265 0.00126

 178 <- 264 -0.00126

 179 <- 251 0.00100

 179 <- 260 0.00121

 180 <- 250 0.00152

 181 <- 197 -0.00127

 181 <- 206 -0.00463

 181 <- 231 -0.00323

 182 <- 197 0.00814

 182 <- 231 -0.00177

 183 <- 196 -0.00105

 183 <- 199 0.00612

 183 <- 203 0.00209

 183 <- 221 -0.00187

 183 <- 234 -0.00292

 184 <- 195 -0.00103

 184 <- 200 0.00610

 184 <- 204 0.00209

 184 <- 220 -0.00186

 184 <- 233 -0.00293

 185 <- 193 0.00304

 185 <- 202 0.00236

 185 <- 207 -0.00352

 186 <- 198 0.00782

 186 <- 226 0.00404

 187 <- 191 0.00549

 187 <- 195 -0.00723

 187 <- 204 -0.00123

 187 <- 220 0.00140

 187 <- 233 -0.00127

 188 <- 192 0.00549

 188 <- 196 -0.00722

 188 <- 203 -0.00123

 188 <- 221 0.00141

 188 <- 234 -0.00128

 189 <- 194 -0.00885

 189 <- 205 0.00165

 190 <- 193 -0.01383

 190 <- 202 0.00442

 190 <- 207 -0.00236

 190 <- 347 0.00111

 190 <- 381 -0.00123

 Excited State 4: Singlet-A2 2.6738 eV 463.70 nm f=0.0000 <S\*\*2>=0.000

 84 -> 238 -0.00101

 93 -> 282 0.00113

 97 -> 219 0.00121

 98 -> 216 -0.00117

 99 -> 217 0.00117

 100 -> 214 0.00128

 109 -> 241 -0.00107

 112 -> 238 0.00128

 117 -> 218 -0.00103

 117 -> 266 -0.00104

 118 -> 214 -0.00122

 119 -> 240 -0.00113

 120 -> 239 -0.00112

 121 -> 250 -0.00101

 121 -> 278 -0.00105

 123 -> 213 0.00115

 123 -> 225 -0.00139

 124 -> 212 0.00109

 124 -> 222 0.00115

 125 -> 211 -0.00109

 125 -> 223 -0.00115

 126 -> 210 -0.00169

 126 -> 218 -0.00145

 127 -> 251 -0.00127

 127 -> 260 0.00100

 128 -> 191 -0.00143

 129 -> 192 -0.00142

 130 -> 192 0.00277

 131 -> 191 -0.00279

 132 -> 297 -0.00133

 132 -> 316 -0.00119

 133 -> 251 0.00113

 134 -> 256 -0.00120

 141 -> 197 0.00151

 142 -> 285 -0.00109

 143 -> 283 0.00124

 144 -> 284 0.00124

 147 -> 192 0.00423

 147 -> 196 0.00154

 148 -> 191 -0.00425

 148 -> 195 -0.00155

 150 -> 193 0.00301

 150 -> 207 -0.00467

 151 -> 197 0.00380

 152 -> 251 0.00133

 155 -> 357 -0.00124

 156 -> 259 -0.00191

 156 -> 279 -0.00128

 156 -> 285 0.00151

 157 -> 253 -0.00137

 157 -> 273 -0.00174

 157 -> 284 -0.00129

 158 -> 254 -0.00137

 158 -> 274 0.00174

 158 -> 283 -0.00129

 159 -> 250 -0.00109

 159 -> 266 -0.00150

 159 -> 271 -0.00116

 159 -> 278 -0.00184

 159 -> 334 -0.00122

 160 -> 196 -0.00484

 160 -> 199 -0.00362

 160 -> 203 -0.00445

 160 -> 221 0.00174

 161 -> 195 -0.00483

 161 -> 200 -0.00364

 161 -> 204 -0.00445

 161 -> 220 0.00172

 164 -> 260 0.00134

 164 -> 369 -0.00101

 165 -> 282 -0.00103

 166 -> 198 0.00486

 167 -> 196 -0.00187

 167 -> 244 0.00142

 167 -> 258 0.00115

 168 -> 195 -0.00187

 168 -> 245 -0.00142

 168 -> 257 -0.00114

 169 -> 197 -0.00158

 169 -> 206 0.00225

 170 -> 191 -0.00502

 170 -> 195 0.00714

 170 -> 200 -0.00247

 170 -> 204 0.00413

 170 -> 220 -0.00143

 171 -> 192 0.00503

 171 -> 196 -0.00714

 171 -> 199 0.00245

 171 -> 203 -0.00415

 171 -> 221 0.00143

 173 -> 194 -0.00834

 173 -> 201 -0.00726

 173 -> 205 0.00539

 173 -> 299 -0.00160

 174 -> 193 -0.00449

 174 -> 202 0.00779

 174 -> 207 0.00223

 174 -> 298 0.00154

 175 -> 191 -0.00305

 175 -> 195 -0.00290

 175 -> 200 -0.00366

 175 -> 204 0.00482

 176 -> 192 0.00304

 176 -> 196 0.00288

 176 -> 199 0.00366

 176 -> 203 -0.00484

 177 -> 195 -0.00101

 178 -> 196 -0.00101

 179 -> 197 0.00107

 179 -> 242 -0.00194

 179 -> 256 -0.00154

 181 -> 198 0.00482

 181 -> 226 0.00178

 182 -> 198 0.01036

 182 -> 226 0.00433

 183 -> 192 -0.02319

 183 -> 196 -0.00660

 183 -> 199 0.00963

 183 -> 203 0.00255

 183 -> 221 -0.00249

 183 -> 234 -0.00321

 184 -> 191 0.02325

 184 -> 195 0.00666

 184 -> 200 -0.00963

 184 -> 204 -0.00254

 184 -> 220 0.00251

 184 -> 233 0.00322

 185 -> 194 0.03040

 185 -> 201 0.00614

 185 -> 205 -0.00267

 185 -> 317 0.00109

 186 -> 197 0.01812

 186 -> 206 -0.00375

 186 -> 231 -0.00412

 187 -> 191 0.03932

 187 -> 200 0.00422

 187 -> 204 -0.00481

 188 -> 192 -0.03941

 188 -> 199 -0.00420

 188 -> 203 0.00483

 189 -> 193 -0.01426

 189 -> 202 0.00731

 189 -> 298 0.00119

 189 -> 314 0.00109

 189 -> 381 -0.00104

 190 -> 194 0.70223

 190 -> 201 0.01704

 190 -> 229 -0.00206

 190 -> 232 -0.00171

 190 -> 344 0.00124

 126 <- 210 -0.00109

 130 <- 192 0.00150

 131 <- 191 -0.00152

 132 <- 297 -0.00103

 147 <- 192 0.00270

 148 <- 191 -0.00272

 150 <- 207 -0.00274

 151 <- 197 0.00254

 156 <- 259 -0.00136

 156 <- 285 0.00107

 157 <- 273 -0.00127

 158 <- 274 0.00127

 159 <- 266 -0.00106

 159 <- 278 -0.00130

 160 <- 192 -0.00185

 160 <- 199 -0.00273

 160 <- 203 -0.00177

 160 <- 221 0.00122

 161 <- 191 -0.00187

 161 <- 200 -0.00274

 161 <- 204 -0.00177

 161 <- 220 0.00121

 166 <- 198 0.00352

 169 <- 206 0.00256

 170 <- 191 -0.00140

 170 <- 195 0.00105

 170 <- 200 -0.00142

 170 <- 204 0.00118

 170 <- 220 -0.00163

 171 <- 192 0.00142

 171 <- 196 -0.00105

 171 <- 199 0.00142

 171 <- 203 -0.00119

 171 <- 221 0.00164

 173 <- 194 -0.00330

 173 <- 201 -0.00318

 173 <- 205 0.00309

 173 <- 229 -0.00111

 173 <- 299 -0.00115

 174 <- 193 -0.00327

 174 <- 202 0.00420

 174 <- 207 0.00227

 174 <- 298 0.00109

 175 <- 191 -0.00108

 175 <- 195 0.00262

 175 <- 200 -0.00166

 175 <- 204 0.00402

 176 <- 192 0.00115

 176 <- 196 -0.00260

 176 <- 199 0.00165

 176 <- 203 -0.00404

 179 <- 242 -0.00119

 179 <- 256 -0.00102

 181 <- 198 0.00302

 181 <- 226 0.00151

 182 <- 198 0.00582

 182 <- 226 0.00288

 183 <- 196 -0.00153

 183 <- 199 0.00505

 183 <- 203 0.00188

 183 <- 221 -0.00119

 183 <- 234 -0.00250

 184 <- 195 0.00150

 184 <- 200 -0.00504

 184 <- 204 -0.00187

 184 <- 220 0.00120

 184 <- 233 0.00250

 185 <- 194 0.00416

 185 <- 201 -0.00119

 186 <- 197 0.00441

 186 <- 206 -0.00328

 186 <- 231 -0.00294

 187 <- 191 0.00291

 187 <- 195 -0.00777

 187 <- 204 -0.00144

 188 <- 192 -0.00291

 188 <- 196 0.00778

 188 <- 203 0.00145

 189 <- 193 -0.00851

 189 <- 207 0.00175

 190 <- 194 -0.01140

 190 <- 201 -0.00223

 190 <- 205 0.00212

 190 <- 377 0.00106

 Excited State 5: Singlet-B2 2.7836 eV 445.40 nm f=0.0413 <S\*\*2>=0.000

 93 -> 261 0.00100

 97 -> 216 -0.00103

 98 -> 214 -0.00133

 98 -> 219 0.00105

 100 -> 216 0.00101

 108 -> 242 -0.00152

 111 -> 218 0.00104

 119 -> 241 0.00115

 120 -> 238 -0.00105

 121 -> 265 -0.00122

 122 -> 192 -0.00256

 123 -> 223 -0.00109

 125 -> 210 -0.00149

 125 -> 218 -0.00107

 125 -> 225 -0.00129

 126 -> 208 -0.00120

 126 -> 217 -0.00133

 126 -> 223 -0.00104

 127 -> 258 -0.00116

 131 -> 194 -0.00130

 131 -> 207 0.00149

 132 -> 265 0.00102

 138 -> 297 -0.00106

 141 -> 196 0.00108

 142 -> 284 -0.00116

 144 -> 278 0.00102

 144 -> 285 0.00105

 146 -> 192 0.00391

 147 -> 197 0.00187

 148 -> 207 0.00192

 150 -> 191 0.00525

 150 -> 195 0.00473

 150 -> 200 0.00213

 150 -> 204 0.00299

 150 -> 220 -0.00216

 151 -> 192 0.00290

 151 -> 196 0.00148

 151 -> 199 -0.00193

 151 -> 203 -0.00109

 152 -> 240 0.00119

 152 -> 244 -0.00115

 153 -> 224 -0.00103

 153 -> 251 0.00107

 153 -> 327 0.00104

 153 -> 357 -0.00115

 156 -> 253 0.00104

 156 -> 273 0.00174

 156 -> 284 0.00121

 157 -> 259 0.00150

 157 -> 266 -0.00142

 157 -> 271 -0.00106

 157 -> 278 -0.00151

 157 -> 279 0.00128

 157 -> 285 -0.00133

 157 -> 334 -0.00107

 159 -> 253 -0.00103

 159 -> 273 -0.00158

 159 -> 284 -0.00122

 160 -> 197 0.00279

 160 -> 198 0.00472

 160 -> 206 -0.00151

 160 -> 226 0.00105

 161 -> 193 -0.00475

 161 -> 194 -0.00544

 161 -> 201 -0.00196

 161 -> 205 0.00241

 161 -> 207 0.00490

 163 -> 205 0.00109

 166 -> 192 -0.00361

 166 -> 199 -0.00443

 166 -> 203 -0.00143

 166 -> 221 0.00110

 167 -> 256 0.00108

 167 -> 260 -0.00137

 168 -> 193 -0.00131

 168 -> 194 -0.00167

 168 -> 205 0.00199

 168 -> 215 0.00100

 169 -> 192 0.00102

 169 -> 199 0.00189

 170 -> 193 0.00700

 170 -> 194 0.00719

 170 -> 201 0.00268

 170 -> 202 -0.00360

 170 -> 205 -0.00381

 170 -> 207 -0.00281

 170 -> 215 0.00126

 170 -> 229 0.00113

 171 -> 206 0.00108

 172 -> 264 0.00118

 173 -> 191 0.00700

 173 -> 195 -0.00601

 173 -> 200 0.00258

 173 -> 204 -0.00815

 173 -> 220 0.00158

 173 -> 296 0.00119

 174 -> 191 0.00929

 174 -> 195 -0.00206

 174 -> 200 0.00436

 174 -> 204 -0.00660

 175 -> 193 -0.00117

 175 -> 194 -0.00353

 175 -> 201 0.00508

 175 -> 202 -0.00692

 175 -> 205 -0.00235

 175 -> 298 -0.00113

 175 -> 299 0.00113

 176 -> 197 0.00139

 176 -> 198 -0.00224

 176 -> 226 -0.00138

 176 -> 247 0.00101

 177 -> 194 -0.00133

 177 -> 252 -0.00167

 179 -> 192 0.00226

 180 -> 191 -0.00221

 181 -> 192 0.04493

 181 -> 196 0.00276

 181 -> 234 0.00157

 182 -> 192 -0.01323

 182 -> 196 0.00420

 182 -> 199 -0.01121

 182 -> 203 -0.00220

 182 -> 221 0.00437

 182 -> 222 0.00106

 182 -> 234 0.00154

 183 -> 197 -0.01638

 183 -> 198 -0.01049

 183 -> 206 0.00281

 183 -> 226 -0.00368

 183 -> 231 0.00319

 184 -> 193 0.00143

 184 -> 201 -0.00161

 184 -> 202 -0.00171

 185 -> 191 -0.02380

 185 -> 195 0.02641

 185 -> 204 0.00720

 186 -> 192 0.03137

 186 -> 196 0.00567

 186 -> 199 -0.00766

 186 -> 203 -0.00335

 186 -> 221 0.00118

 186 -> 234 0.00317

 187 -> 193 -0.01036

 187 -> 194 -0.00136

 187 -> 201 -0.00526

 187 -> 202 0.00891

 187 -> 205 0.00302

 187 -> 207 -0.00252

 187 -> 317 -0.00121

 188 -> 197 -0.00964

 188 -> 198 0.00768

 188 -> 206 0.00125

 188 -> 226 0.00130

 188 -> 231 0.00124

 189 -> 191 0.10132

 189 -> 195 -0.01006

 189 -> 200 0.01021

 189 -> 204 -0.00412

 189 -> 220 -0.00111

 190 -> 191 0.01640

 190 -> 195 0.69508

 190 -> 200 -0.00661

 190 -> 204 0.01150

 190 -> 220 0.00281

 108 <- 242 -0.00112

 122 <- 192 -0.00139

 146 <- 192 0.00235

 147 <- 197 0.00135

 148 <- 207 0.00115

 150 <- 191 0.00382

 150 <- 200 0.00123

 150 <- 220 -0.00114

 151 <- 192 0.00191

 151 <- 196 0.00104

 151 <- 199 -0.00110

 156 <- 273 0.00126

 157 <- 259 0.00105

 157 <- 266 -0.00100

 157 <- 278 -0.00105

 159 <- 273 -0.00114

 160 <- 197 0.00190

 160 <- 198 0.00284

 160 <- 206 -0.00101

 161 <- 207 0.00265

 166 <- 192 -0.00284

 166 <- 199 -0.00303

 166 <- 203 -0.00109

 169 <- 192 0.00197

 169 <- 199 0.00159

 169 <- 203 0.00100

 169 <- 221 0.00113

 170 <- 202 -0.00114

 170 <- 205 -0.00138

 170 <- 207 -0.00162

 171 <- 197 0.00123

 171 <- 198 -0.00118

 171 <- 206 0.00195

 173 <- 195 -0.00243

 173 <- 204 -0.00378

 173 <- 220 0.00148

 174 <- 191 0.00223

 174 <- 195 -0.00229

 174 <- 200 0.00153

 174 <- 204 -0.00394

 175 <- 193 0.00281

 175 <- 194 0.00246

 175 <- 201 0.00308

 175 <- 202 -0.00379

 175 <- 205 -0.00222

 176 <- 197 -0.00130

 181 <- 192 0.00380

 181 <- 199 -0.00107

 181 <- 234 0.00136

 182 <- 192 -0.00489

 182 <- 196 0.00101

 182 <- 199 -0.00553

 182 <- 203 -0.00136

 182 <- 221 0.00227

 182 <- 234 0.00120

 183 <- 197 -0.00327

 183 <- 198 -0.00582

 183 <- 206 0.00296

 183 <- 226 -0.00258

 183 <- 231 0.00236

 185 <- 191 -0.00156

 185 <- 195 0.00315

 185 <- 200 0.00141

 185 <- 220 -0.00118

 186 <- 199 -0.00418

 186 <- 203 -0.00210

 186 <- 234 0.00241

 187 <- 193 -0.00785

 187 <- 194 -0.00749

 187 <- 205 0.00109

 188 <- 198 0.00154

 189 <- 191 0.00541

 189 <- 195 -0.00711

 190 <- 191 -0.00522

 190 <- 195 -0.01113

 190 <- 204 -0.00326

 Excited State 6: Singlet-B1 2.7836 eV 445.40 nm f=0.0413 <S\*\*2>=0.000

 93 -> 262 0.00100

 97 -> 217 0.00103

 99 -> 214 0.00133

 99 -> 219 0.00105

 100 -> 217 0.00101

 107 -> 242 -0.00152

 110 -> 218 0.00104

 119 -> 238 0.00105

 120 -> 241 -0.00115

 121 -> 264 -0.00122

 122 -> 191 0.00256

 123 -> 222 0.00109

 124 -> 210 0.00149

 124 -> 218 0.00107

 124 -> 225 -0.00129

 126 -> 209 0.00120

 126 -> 216 -0.00133

 126 -> 222 -0.00104

 127 -> 257 -0.00116

 130 -> 194 0.00130

 130 -> 207 0.00149

 132 -> 264 -0.00102

 139 -> 297 0.00106

 141 -> 195 0.00108

 142 -> 283 0.00116

 143 -> 278 0.00102

 143 -> 285 -0.00105

 146 -> 191 -0.00391

 147 -> 207 0.00192

 148 -> 197 -0.00187

 150 -> 192 -0.00525

 150 -> 196 -0.00473

 150 -> 199 -0.00213

 150 -> 203 -0.00299

 150 -> 221 0.00216

 151 -> 191 0.00290

 151 -> 195 0.00148

 151 -> 200 -0.00193

 151 -> 204 -0.00109

 152 -> 239 -0.00119

 152 -> 245 -0.00115

 154 -> 224 0.00103

 154 -> 251 0.00107

 154 -> 327 0.00104

 154 -> 357 0.00115

 156 -> 254 -0.00104

 156 -> 274 0.00174

 156 -> 283 -0.00121

 158 -> 259 -0.00150

 158 -> 266 -0.00142

 158 -> 271 -0.00106

 158 -> 278 -0.00151

 158 -> 279 -0.00128

 158 -> 285 0.00133

 158 -> 334 -0.00107

 159 -> 254 -0.00103

 159 -> 274 0.00158

 159 -> 283 -0.00122

 160 -> 193 0.00475

 160 -> 194 -0.00544

 160 -> 201 -0.00196

 160 -> 205 0.00241

 160 -> 207 -0.00490

 161 -> 197 0.00279

 161 -> 198 -0.00472

 161 -> 206 -0.00151

 161 -> 226 -0.00105

 162 -> 205 0.00109

 166 -> 191 0.00361

 166 -> 200 0.00443

 166 -> 204 0.00143

 166 -> 220 -0.00110

 167 -> 193 0.00131

 167 -> 194 -0.00167

 167 -> 205 0.00199

 167 -> 215 0.00100

 168 -> 256 0.00108

 168 -> 260 0.00137

 169 -> 191 0.00102

 169 -> 200 0.00189

 170 -> 206 -0.00108

 171 -> 193 0.00700

 171 -> 194 -0.00719

 171 -> 201 -0.00268

 171 -> 202 -0.00360

 171 -> 205 0.00381

 171 -> 207 -0.00281

 171 -> 215 -0.00126

 171 -> 229 -0.00113

 172 -> 265 -0.00118

 173 -> 192 0.00700

 173 -> 196 -0.00601

 173 -> 199 0.00258

 173 -> 203 -0.00815

 173 -> 221 0.00158

 173 -> 295 -0.00119

 174 -> 192 -0.00929

 174 -> 196 0.00206

 174 -> 199 -0.00436

 174 -> 203 0.00660

 175 -> 197 -0.00139

 175 -> 198 -0.00224

 175 -> 226 -0.00138

 175 -> 247 -0.00101

 176 -> 193 -0.00117

 176 -> 194 0.00353

 176 -> 201 -0.00508

 176 -> 202 -0.00692

 176 -> 205 0.00235

 176 -> 298 -0.00113

 176 -> 299 -0.00113

 178 -> 194 -0.00133

 178 -> 252 0.00167

 179 -> 191 0.00226

 180 -> 192 0.00221

 181 -> 191 -0.04493

 181 -> 195 -0.00276

 181 -> 233 -0.00157

 182 -> 191 0.01323

 182 -> 195 -0.00420

 182 -> 200 0.01121

 182 -> 204 0.00220

 182 -> 220 -0.00437

 182 -> 223 -0.00106

 182 -> 233 -0.00154

 183 -> 193 0.00143

 183 -> 201 0.00161

 183 -> 202 -0.00171

 184 -> 197 0.01638

 184 -> 198 -0.01049

 184 -> 206 -0.00281

 184 -> 226 -0.00368

 184 -> 231 -0.00319

 185 -> 192 -0.02380

 185 -> 196 0.02641

 185 -> 203 0.00720

 186 -> 191 0.03137

 186 -> 195 0.00567

 186 -> 200 -0.00766

 186 -> 204 -0.00335

 186 -> 220 0.00118

 186 -> 233 0.00317

 187 -> 197 0.00964

 187 -> 198 0.00768

 187 -> 206 -0.00125

 187 -> 226 0.00130

 187 -> 231 -0.00124

 188 -> 193 -0.01036

 188 -> 194 0.00136

 188 -> 201 0.00526

 188 -> 202 0.00891

 188 -> 205 -0.00302

 188 -> 207 -0.00252

 188 -> 317 0.00121

 189 -> 192 -0.10132

 189 -> 196 0.01006

 189 -> 199 -0.01021

 189 -> 203 0.00412

 189 -> 221 0.00111

 190 -> 192 0.01640

 190 -> 196 0.69508

 190 -> 199 -0.00661

 190 -> 203 0.01150

 190 -> 221 0.00281

 107 <- 242 -0.00112

 122 <- 191 0.00139

 146 <- 191 -0.00235

 147 <- 207 0.00115

 148 <- 197 -0.00135

 150 <- 192 -0.00382

 150 <- 199 -0.00123

 150 <- 221 0.00114

 151 <- 191 0.00191

 151 <- 195 0.00104

 151 <- 200 -0.00110

 156 <- 274 0.00126

 158 <- 259 -0.00105

 158 <- 266 -0.00100

 158 <- 278 -0.00105

 159 <- 274 0.00114

 160 <- 207 -0.00265

 161 <- 197 0.00190

 161 <- 198 -0.00284

 161 <- 206 -0.00101

 166 <- 191 0.00284

 166 <- 200 0.00303

 166 <- 204 0.00109

 169 <- 191 0.00197

 169 <- 200 0.00159

 169 <- 204 0.00100

 169 <- 220 0.00113

 170 <- 197 -0.00123

 170 <- 198 -0.00118

 170 <- 206 -0.00195

 171 <- 202 -0.00114

 171 <- 205 0.00138

 171 <- 207 -0.00162

 173 <- 196 -0.00243

 173 <- 203 -0.00378

 173 <- 221 0.00148

 174 <- 192 -0.00223

 174 <- 196 0.00229

 174 <- 199 -0.00153

 174 <- 203 0.00394

 175 <- 197 0.00130

 176 <- 193 0.00281

 176 <- 194 -0.00246

 176 <- 201 -0.00308

 176 <- 202 -0.00379

 176 <- 205 0.00221

 181 <- 191 -0.00380

 181 <- 200 0.00107

 181 <- 233 -0.00136

 182 <- 191 0.00489

 182 <- 195 -0.00101

 182 <- 200 0.00553

 182 <- 204 0.00136

 182 <- 220 -0.00227

 182 <- 233 -0.00120

 184 <- 197 0.00327

 184 <- 198 -0.00582

 184 <- 206 -0.00296

 184 <- 226 -0.00258

 184 <- 231 -0.00236

 185 <- 192 -0.00156

 185 <- 196 0.00315

 185 <- 199 0.00141

 185 <- 221 -0.00118

 186 <- 200 -0.00418

 186 <- 204 -0.00210

 186 <- 233 0.00241

 187 <- 198 0.00154

 188 <- 193 -0.00785

 188 <- 194 0.00749

 188 <- 205 -0.00109

 189 <- 192 -0.00541

 189 <- 196 0.00711

 190 <- 192 -0.00522

 190 <- 196 -0.01113

 190 <- 203 -0.00326

 Excited State 7: Singlet-A2 2.9246 eV 423.93 nm f=0.0000 <S\*\*2>=0.000

 126 -> 210 0.00113

 130 -> 192 -0.00119

 131 -> 191 0.00120

 132 -> 297 0.00111

 141 -> 197 -0.00110

 146 -> 198 -0.00115

 147 -> 192 -0.00219

 147 -> 196 -0.00112

 147 -> 199 0.00107

 148 -> 191 0.00219

 148 -> 195 0.00112

 148 -> 200 -0.00107

 150 -> 193 -0.00248

 150 -> 202 0.00155

 151 -> 197 -0.00441

 156 -> 279 0.00104

 157 -> 273 0.00121

 158 -> 274 -0.00120

 159 -> 278 0.00117

 160 -> 192 -0.00546

 160 -> 203 0.00145

 161 -> 191 -0.00544

 161 -> 204 0.00146

 166 -> 198 -0.00193

 167 -> 192 -0.00160

 168 -> 191 -0.00160

 169 -> 197 -0.00567

 169 -> 206 -0.00405

 170 -> 191 0.00922

 170 -> 200 0.00176

 170 -> 204 -0.00125

 170 -> 220 0.00168

 171 -> 192 -0.00920

 171 -> 199 -0.00175

 171 -> 203 0.00125

 171 -> 221 -0.00168

 173 -> 194 0.00540

 173 -> 201 0.00386

 173 -> 205 -0.00324

 173 -> 229 0.00108

 173 -> 299 0.00103

 174 -> 193 0.00144

 174 -> 202 -0.00220

 174 -> 207 -0.00666

 174 -> 298 -0.00111

 175 -> 191 -0.02945

 175 -> 195 -0.00610

 175 -> 200 -0.00192

 175 -> 204 -0.00554

 175 -> 220 0.00183

 176 -> 192 0.02943

 176 -> 196 0.00610

 176 -> 199 0.00191

 176 -> 203 0.00553

 176 -> 221 -0.00183

 177 -> 191 -0.00914

 178 -> 192 -0.00911

 179 -> 197 -0.00219

 181 -> 198 -0.00600

 181 -> 226 -0.00193

 182 -> 198 -0.00440

 182 -> 226 -0.00230

 183 -> 192 -0.00816

 183 -> 196 0.00199

 183 -> 199 -0.00749

 183 -> 203 -0.00263

 183 -> 221 0.00142

 183 -> 234 0.00276

 184 -> 191 0.00819

 184 -> 195 -0.00198

 184 -> 200 0.00748

 184 -> 204 0.00263

 184 -> 220 -0.00142

 184 -> 233 -0.00277

 185 -> 201 0.00100

 185 -> 205 -0.00143

 186 -> 197 -0.00482

 186 -> 206 0.00534

 186 -> 231 0.00358

 187 -> 191 0.49657

 187 -> 195 0.00642

 187 -> 200 0.01085

 187 -> 204 0.00233

 187 -> 220 -0.00350

 188 -> 192 -0.49619

 188 -> 196 -0.00642

 188 -> 199 -0.01086

 188 -> 203 -0.00234

 188 -> 221 0.00350

 189 -> 193 -0.02646

 189 -> 202 0.00879

 189 -> 207 -0.01200

 190 -> 194 -0.05663

 190 -> 201 0.00189

 190 -> 205 -0.00319

 147 <- 192 -0.00122

 148 <- 191 0.00123

 151 <- 197 -0.00213

 169 <- 206 -0.00118

 170 <- 191 0.00214

 170 <- 220 0.00103

 171 <- 192 -0.00215

 171 <- 221 -0.00103

 173 <- 194 0.00193

 173 <- 201 0.00217

 173 <- 205 -0.00214

 174 <- 193 0.00170

 174 <- 202 -0.00281

 174 <- 207 -0.00152

 175 <- 195 -0.00114

 175 <- 204 -0.00270

 176 <- 196 0.00113

 176 <- 203 0.00271

 181 <- 198 -0.00277

 181 <- 226 -0.00148

 182 <- 198 -0.00160

 182 <- 226 -0.00115

 183 <- 192 0.00312

 183 <- 196 0.00143

 183 <- 199 -0.00261

 183 <- 234 0.00139

 184 <- 191 -0.00312

 184 <- 195 -0.00142

 184 <- 200 0.00261

 184 <- 233 -0.00139

 185 <- 194 -0.00350

 185 <- 201 0.00110

 186 <- 197 -0.00394

 186 <- 206 0.00101

 186 <- 231 0.00159

 187 <- 191 -0.00346

 187 <- 195 0.00501

 188 <- 192 0.00346

 188 <- 196 -0.00500

 189 <- 193 0.00612

 190 <- 194 0.00607

 190 <- 201 0.00121

 Excited State 8: Singlet-B2 2.9424 eV 421.37 nm f=0.3284 <S\*\*2>=0.000

 107 -> 252 0.00101

 112 -> 239 -0.00101

 113 -> 210 0.00100

 113 -> 213 0.00108

 116 -> 212 0.00141

 118 -> 212 -0.00121

 118 -> 216 0.00104

 119 -> 241 -0.00124

 120 -> 213 -0.00110

 120 -> 238 0.00117

 122 -> 192 -0.00170

 123 -> 217 -0.00133

 123 -> 228 0.00127

 124 -> 214 -0.00206

 124 -> 219 -0.00151

 124 -> 230 -0.00108

 124 -> 251 0.00108

 125 -> 210 0.00128

 126 -> 208 0.00150

 126 -> 217 0.00208

 131 -> 193 0.00192

 132 -> 239 0.00131

 132 -> 257 -0.00124

 133 -> 212 -0.00122

 134 -> 212 -0.00111

 137 -> 212 0.00107

 138 -> 210 -0.00108

 138 -> 297 0.00109

 139 -> 237 0.00112

 139 -> 241 -0.00119

 139 -> 251 0.00101

 140 -> 223 0.00128

 140 -> 239 0.00142

 141 -> 192 -0.00237

 141 -> 196 0.00184

 141 -> 203 0.00102

 142 -> 223 0.00119

 142 -> 239 0.00116

 143 -> 219 -0.00155

 143 -> 224 -0.00174

 143 -> 251 -0.00115

 147 -> 197 -0.00117

 147 -> 198 -0.00111

 148 -> 194 0.00108

 148 -> 207 0.00102

 148 -> 299 0.00101

 150 -> 191 -0.00232

 150 -> 195 -0.00249

 150 -> 204 -0.00114

 151 -> 192 -0.00444

 152 -> 236 0.00113

 152 -> 254 0.00153

 154 -> 225 0.00106

 154 -> 232 -0.00125

 154 -> 250 0.00140

 154 -> 286 -0.00125

 154 -> 287 -0.00100

 154 -> 297 0.00110

 155 -> 227 0.00161

 155 -> 236 -0.00101

 156 -> 235 -0.00120

 156 -> 257 -0.00107

 156 -> 273 -0.00102

 158 -> 230 0.00127

 158 -> 237 0.00137

 158 -> 256 0.00107

 158 -> 260 0.00135

 159 -> 273 0.00113

 160 -> 197 -0.00452

 161 -> 193 -0.00229

 161 -> 194 0.00543

 161 -> 201 0.00174

 161 -> 205 -0.00208

 163 -> 210 -0.00109

 163 -> 218 -0.00121

 163 -> 225 0.00190

 164 -> 222 0.00179

 164 -> 227 0.00124

 165 -> 209 0.00117

 165 -> 216 -0.00116

 165 -> 222 -0.00131

 166 -> 196 -0.00376

 166 -> 199 0.00137

 166 -> 203 -0.00158

 166 -> 221 0.00135

 168 -> 205 -0.00108

 168 -> 218 0.00131

 169 -> 192 -0.00165

 169 -> 196 -0.00283

 169 -> 203 -0.00258

 170 -> 194 -0.00111

 170 -> 207 0.00513

 171 -> 197 -0.00556

 171 -> 206 -0.00364

 172 -> 264 -0.00186

 173 -> 195 0.00365

 173 -> 200 -0.00185

 173 -> 204 0.00340

 173 -> 220 -0.00252

 173 -> 233 0.00155

 174 -> 191 0.01919

 174 -> 195 0.00358

 174 -> 200 0.00407

 174 -> 204 0.00575

 174 -> 220 -0.00176

 174 -> 321 -0.00142

 175 -> 193 -0.00324

 175 -> 194 -0.00183

 175 -> 201 -0.00318

 175 -> 202 0.00251

 175 -> 205 0.00225

 175 -> 207 0.00266

 175 -> 229 -0.00139

 175 -> 232 -0.00118

 176 -> 197 0.00533

 176 -> 198 -0.00361

 176 -> 206 -0.00136

 176 -> 315 0.00117

 176 -> 322 0.00102

 177 -> 218 0.00100

 177 -> 238 0.00114

 177 -> 252 0.00113

 178 -> 214 -0.00126

 179 -> 192 -0.00283

 179 -> 254 -0.00112

 180 -> 191 -0.00975

 180 -> 200 -0.00116

 180 -> 217 0.00121

 180 -> 239 0.00106

 181 -> 192 0.01920

 181 -> 196 -0.00953

 181 -> 199 0.00264

 181 -> 221 0.00146

 181 -> 234 -0.00313

 182 -> 192 -0.00970

 182 -> 196 -0.02566

 182 -> 199 0.00261

 182 -> 203 -0.00156

 182 -> 221 -0.00179

 183 -> 197 0.00756

 183 -> 198 0.00620

 183 -> 206 -0.00178

 183 -> 226 0.00258

 183 -> 231 -0.00248

 184 -> 193 -0.02640

 184 -> 194 0.02764

 184 -> 201 0.00118

 184 -> 205 -0.00174

 184 -> 207 0.00348

 185 -> 191 0.00756

 185 -> 195 0.00458

 185 -> 200 -0.00897

 185 -> 204 -0.00138

 185 -> 220 0.00225

 185 -> 233 -0.00131

 185 -> 249 -0.00111

 186 -> 192 -0.05410

 186 -> 196 0.02158

 186 -> 199 0.00529

 186 -> 203 0.00388

 186 -> 221 -0.00257

 186 -> 234 -0.00119

 187 -> 193 -0.01898

 187 -> 194 -0.00264

 187 -> 202 0.00493

 187 -> 207 -0.00742

 187 -> 229 0.00131

 187 -> 232 0.00117

 187 -> 255 0.00123

 188 -> 197 0.02853

 188 -> 198 -0.00787

 188 -> 231 0.00113

 188 -> 247 -0.00148

 188 -> 354 -0.00130

 189 -> 191 0.69391

 189 -> 195 0.01073

 189 -> 200 0.00356

 189 -> 220 -0.00302

 189 -> 249 -0.00126

 189 -> 350 -0.00107

 190 -> 191 -0.01397

 190 -> 195 -0.09951

 190 -> 200 -0.00635

 190 -> 220 0.00139

 190 -> 233 0.00105

 124 <- 214 -0.00128

 126 <- 217 0.00130

 131 <- 193 0.00110

 141 <- 192 -0.00142

 141 <- 196 0.00121

 143 <- 224 -0.00109

 150 <- 191 -0.00260

 150 <- 195 -0.00126

 151 <- 192 -0.00245

 152 <- 254 0.00104

 160 <- 197 -0.00208

 161 <- 193 -0.00189

 161 <- 194 0.00273

 161 <- 201 0.00116

 161 <- 205 -0.00123

 163 <- 225 0.00108

 164 <- 222 0.00102

 166 <- 196 -0.00214

 166 <- 199 0.00103

 166 <- 203 -0.00101

 169 <- 192 -0.00170

 169 <- 196 -0.00150

 169 <- 203 -0.00151

 170 <- 207 0.00212

 171 <- 206 -0.00116

 172 <- 264 -0.00122

 173 <- 191 0.00118

 173 <- 195 0.00183

 173 <- 204 0.00227

 174 <- 191 -0.00303

 174 <- 204 0.00243

 174 <- 220 -0.00119

 174 <- 321 -0.00107

 175 <- 193 -0.00189

 175 <- 201 -0.00172

 175 <- 202 0.00225

 175 <- 205 0.00125

 176 <- 197 0.00313

 176 <- 198 -0.00114

 181 <- 196 -0.00242

 181 <- 199 0.00125

 181 <- 234 -0.00207

 182 <- 192 0.00140

 182 <- 196 -0.00698

 182 <- 199 0.00115

 182 <- 221 -0.00118

 183 <- 197 0.00309

 183 <- 198 0.00249

 183 <- 226 0.00141

 183 <- 231 -0.00151

 184 <- 193 -0.00675

 184 <- 194 0.00659

 184 <- 207 0.00134

 185 <- 191 -0.00150

 185 <- 195 -0.00262

 185 <- 200 -0.00152

 186 <- 192 -0.00435

 186 <- 196 0.00552

 186 <- 199 0.00245

 186 <- 203 0.00172

 186 <- 221 -0.00125

 187 <- 193 0.00486

 187 <- 194 0.00387

 188 <- 197 -0.00392

 188 <- 198 0.00118

 188 <- 206 -0.00156

 188 <- 226 0.00148

 189 <- 191 -0.00910

 189 <- 195 0.00254

 189 <- 200 0.00109

 189 <- 220 -0.00182

 190 <- 191 0.00974

 190 <- 195 0.00865

 190 <- 200 -0.00563

 190 <- 220 0.00284

 Excited State 9: Singlet-B1 2.9424 eV 421.37 nm f=0.3284 <S\*\*2>=0.000

 108 -> 252 0.00101

 112 -> 240 -0.00101

 114 -> 210 -0.00100

 114 -> 213 0.00108

 116 -> 211 0.00141

 118 -> 211 0.00121

 118 -> 217 -0.00104

 119 -> 213 -0.00110

 119 -> 238 0.00117

 120 -> 241 -0.00124

 122 -> 191 -0.00170

 123 -> 216 -0.00133

 123 -> 227 0.00127

 124 -> 210 0.00128

 125 -> 214 -0.00206

 125 -> 219 0.00151

 125 -> 230 0.00108

 125 -> 251 -0.00108

 126 -> 209 0.00150

 126 -> 216 -0.00208

 130 -> 193 -0.00192

 132 -> 240 0.00131

 132 -> 258 0.00124

 133 -> 211 -0.00122

 134 -> 211 0.00111

 137 -> 211 -0.00107

 138 -> 237 -0.00112

 138 -> 241 -0.00119

 138 -> 251 0.00101

 139 -> 210 0.00108

 139 -> 297 0.00109

 140 -> 222 -0.00128

 140 -> 240 -0.00142

 141 -> 191 0.00237

 141 -> 195 -0.00184

 141 -> 204 -0.00102

 142 -> 222 0.00119

 142 -> 240 0.00116

 144 -> 219 -0.00155

 144 -> 224 0.00174

 144 -> 251 -0.00115

 147 -> 194 0.00108

 147 -> 207 -0.00102

 147 -> 299 0.00101

 148 -> 197 -0.00117

 148 -> 198 0.00111

 150 -> 192 -0.00232

 150 -> 196 -0.00249

 150 -> 203 -0.00114

 151 -> 191 0.00444

 152 -> 235 0.00113

 152 -> 253 0.00153

 153 -> 225 -0.00106

 153 -> 232 -0.00125

 153 -> 250 0.00140

 153 -> 286 0.00125

 153 -> 287 -0.00100

 153 -> 297 -0.00110

 155 -> 228 -0.00161

 155 -> 235 0.00101

 156 -> 236 -0.00120

 156 -> 258 0.00107

 156 -> 274 0.00102

 157 -> 230 0.00127

 157 -> 237 -0.00137

 157 -> 256 -0.00107

 157 -> 260 0.00135

 159 -> 274 0.00113

 160 -> 193 -0.00229

 160 -> 194 -0.00543

 160 -> 201 -0.00174

 160 -> 205 0.00208

 161 -> 197 0.00452

 162 -> 210 0.00109

 162 -> 218 0.00121

 162 -> 225 0.00190

 164 -> 223 0.00179

 164 -> 228 0.00124

 165 -> 208 0.00117

 165 -> 217 0.00116

 165 -> 223 0.00131

 166 -> 195 -0.00376

 166 -> 200 0.00137

 166 -> 204 -0.00158

 166 -> 220 0.00135

 167 -> 205 0.00108

 167 -> 218 -0.00131

 169 -> 191 0.00165

 169 -> 195 0.00283

 169 -> 204 0.00258

 170 -> 197 -0.00556

 170 -> 206 -0.00364

 171 -> 194 -0.00111

 171 -> 207 -0.00513

 172 -> 265 -0.00186

 173 -> 196 -0.00365

 173 -> 199 0.00185

 173 -> 203 -0.00340

 173 -> 221 0.00252

 173 -> 234 -0.00155

 174 -> 192 0.01919

 174 -> 196 0.00358

 174 -> 199 0.00407

 174 -> 203 0.00575

 174 -> 221 -0.00176

 174 -> 320 -0.00142

 175 -> 197 0.00533

 175 -> 198 0.00361

 175 -> 206 -0.00136

 175 -> 315 0.00117

 175 -> 322 -0.00102

 176 -> 193 0.00324

 176 -> 194 -0.00183

 176 -> 201 -0.00318

 176 -> 202 -0.00252

 176 -> 205 0.00225

 176 -> 207 -0.00266

 176 -> 229 -0.00139

 176 -> 232 -0.00118

 177 -> 214 0.00126

 178 -> 218 -0.00100

 178 -> 238 0.00114

 178 -> 252 0.00113

 179 -> 191 0.00283

 179 -> 253 0.00112

 180 -> 192 -0.00975

 180 -> 199 -0.00116

 180 -> 216 0.00121

 180 -> 240 0.00106

 181 -> 191 0.01920

 181 -> 195 -0.00953

 181 -> 200 0.00264

 181 -> 220 0.00146

 181 -> 233 -0.00313

 182 -> 191 -0.00970

 182 -> 195 -0.02566

 182 -> 200 0.00261

 182 -> 204 -0.00156

 182 -> 220 -0.00179

 183 -> 193 0.02640

 183 -> 194 0.02764

 183 -> 201 0.00118

 183 -> 205 -0.00174

 183 -> 207 -0.00348

 184 -> 197 0.00756

 184 -> 198 -0.00620

 184 -> 206 -0.00178

 184 -> 226 -0.00258

 184 -> 231 -0.00248

 185 -> 192 -0.00756

 185 -> 196 -0.00458

 185 -> 199 0.00897

 185 -> 203 0.00138

 185 -> 221 -0.00225

 185 -> 234 0.00131

 185 -> 248 0.00111

 186 -> 191 0.05410

 186 -> 195 -0.02158

 186 -> 200 -0.00529

 186 -> 204 -0.00388

 186 -> 220 0.00257

 186 -> 233 0.00119

 187 -> 197 0.02853

 187 -> 198 0.00787

 187 -> 231 0.00113

 187 -> 247 -0.00148

 187 -> 354 0.00130

 188 -> 193 0.01898

 188 -> 194 -0.00264

 188 -> 202 -0.00493

 188 -> 207 0.00742

 188 -> 229 0.00131

 188 -> 232 0.00117

 188 -> 255 0.00123

 189 -> 192 0.69391

 189 -> 196 0.01073

 189 -> 199 0.00356

 189 -> 221 -0.00302

 189 -> 248 -0.00126

 189 -> 349 -0.00107

 190 -> 192 0.01397

 190 -> 196 0.09951

 190 -> 199 0.00635

 190 -> 221 -0.00139

 190 -> 234 -0.00105

 125 <- 214 -0.00128

 126 <- 216 -0.00130

 130 <- 193 -0.00110

 141 <- 191 0.00142

 141 <- 195 -0.00121

 144 <- 224 0.00109

 150 <- 192 -0.00260

 150 <- 196 -0.00126

 151 <- 191 0.00245

 152 <- 253 0.00104

 160 <- 193 -0.00189

 160 <- 194 -0.00273

 160 <- 201 -0.00116

 160 <- 205 0.00123

 161 <- 197 0.00208

 162 <- 225 0.00108

 164 <- 223 0.00102

 166 <- 195 -0.00214

 166 <- 200 0.00103

 166 <- 204 -0.00101

 169 <- 191 0.00170

 169 <- 195 0.00150

 169 <- 204 0.00151

 170 <- 206 -0.00116

 171 <- 207 -0.00212

 172 <- 265 -0.00122

 173 <- 192 -0.00118

 173 <- 196 -0.00183

 173 <- 203 -0.00227

 174 <- 192 -0.00303

 174 <- 203 0.00243

 174 <- 221 -0.00119

 174 <- 320 -0.00107

 175 <- 197 0.00313

 175 <- 198 0.00114

 176 <- 193 0.00189

 176 <- 201 -0.00172

 176 <- 202 -0.00225

 176 <- 205 0.00125

 181 <- 195 -0.00242

 181 <- 200 0.00125

 181 <- 233 -0.00207

 182 <- 191 0.00140

 182 <- 195 -0.00698

 182 <- 200 0.00115

 182 <- 220 -0.00118

 183 <- 193 0.00675

 183 <- 194 0.00659

 183 <- 207 -0.00134

 184 <- 197 0.00309

 184 <- 198 -0.00249

 184 <- 226 -0.00141

 184 <- 231 -0.00151

 185 <- 192 0.00150

 185 <- 196 0.00262

 185 <- 199 0.00152

 186 <- 191 0.00435

 186 <- 195 -0.00552

 186 <- 200 -0.00245

 186 <- 204 -0.00172

 186 <- 220 0.00125

 187 <- 197 -0.00392

 187 <- 198 -0.00118

 187 <- 206 -0.00156

 187 <- 226 -0.00148

 188 <- 193 -0.00486

 188 <- 194 0.00387

 189 <- 192 -0.00910

 189 <- 196 0.00254

 189 <- 199 0.00109

 189 <- 221 -0.00182

 190 <- 192 -0.00974

 190 <- 196 -0.00865

 190 <- 199 0.00563

 190 <- 221 -0.00284

 Excited State 10: Singlet-A1 2.9478 eV 420.60 nm f=0.0000 <S\*\*2>=0.000

 97 -> 225 0.00107

 101 -> 260 0.00102

 109 -> 238 0.00116

 113 -> 212 0.00122

 114 -> 211 0.00122

 116 -> 213 0.00146

 118 -> 218 0.00149

 122 -> 193 -0.00392

 122 -> 202 0.00195

 122 -> 207 -0.00102

 123 -> 219 -0.00154

 123 -> 230 -0.00122

 124 -> 217 -0.00157

 125 -> 216 0.00157

 126 -> 214 0.00232

 128 -> 192 0.00153

 128 -> 196 -0.00115

 129 -> 191 0.00153

 129 -> 195 -0.00116

 130 -> 191 -0.00286

 130 -> 195 0.00234

 130 -> 204 0.00114

 131 -> 192 0.00286

 131 -> 196 -0.00234

 131 -> 203 -0.00114

 132 -> 241 0.00153

 132 -> 260 0.00115

 133 -> 213 -0.00123

 134 -> 210 -0.00121

 135 -> 288 -0.00115

 136 -> 289 0.00115

 137 -> 287 0.00116

 138 -> 240 -0.00103

 139 -> 239 -0.00103

 140 -> 224 -0.00148

 140 -> 237 -0.00148

 141 -> 194 0.00316

 141 -> 205 -0.00220

 142 -> 219 -0.00161

 142 -> 251 -0.00139

 143 -> 217 -0.00102

 143 -> 223 0.00121

 144 -> 216 -0.00102

 144 -> 222 0.00121

 145 -> 224 0.00129

 146 -> 207 0.00270

 147 -> 191 -0.00162

 147 -> 204 -0.00110

 147 -> 220 0.00143

 148 -> 192 0.00161

 148 -> 203 0.00111

 148 -> 221 -0.00143

 150 -> 198 0.00131

 151 -> 194 0.00147

 152 -> 225 0.00101

 152 -> 286 -0.00127

 153 -> 228 0.00127

 153 -> 253 -0.00109

 154 -> 227 -0.00127

 154 -> 254 0.00109

 155 -> 229 -0.00113

 155 -> 232 0.00120

 155 -> 250 -0.00148

 156 -> 230 0.00127

 156 -> 260 0.00145

 157 -> 258 0.00116

 158 -> 257 -0.00116

 159 -> 237 0.00119

 159 -> 256 0.00118

 160 -> 195 0.00232

 160 -> 200 0.00134

 160 -> 204 0.00156

 160 -> 220 -0.00246

 160 -> 233 0.00146

 161 -> 196 0.00232

 161 -> 199 0.00134

 161 -> 203 0.00156

 161 -> 221 -0.00246

 161 -> 234 0.00146

 162 -> 208 -0.00107

 162 -> 223 -0.00124

 162 -> 228 -0.00101

 163 -> 209 0.00107

 163 -> 222 -0.00124

 163 -> 227 -0.00101

 164 -> 225 -0.00209

 165 -> 210 -0.00116

 165 -> 215 -0.00104

 165 -> 218 -0.00131

 165 -> 250 -0.00114

 166 -> 193 0.00105

 166 -> 207 -0.00530

 169 -> 194 -0.00273

 169 -> 201 -0.00192

 169 -> 229 -0.00179

 169 -> 232 -0.00163

 169 -> 255 -0.00137

 170 -> 192 0.00554

 170 -> 196 0.00151

 170 -> 203 0.00179

 171 -> 191 -0.00555

 171 -> 195 -0.00151

 171 -> 204 -0.00178

 172 -> 238 0.00104

 172 -> 252 0.00221

 173 -> 197 -0.00438

 173 -> 206 -0.00506

 173 -> 231 -0.00167

 173 -> 247 0.00136

 173 -> 315 0.00119

 174 -> 198 0.00493

 174 -> 322 -0.00117

 175 -> 192 0.01292

 175 -> 199 0.00641

 175 -> 203 0.00163

 176 -> 191 -0.01291

 176 -> 200 -0.00640

 176 -> 204 -0.00163

 177 -> 192 0.00418

 177 -> 199 0.00144

 177 -> 244 0.00124

 177 -> 288 -0.00104

 178 -> 191 0.00418

 178 -> 200 0.00144

 178 -> 245 -0.00124

 178 -> 289 0.00104

 179 -> 194 0.00219

 179 -> 201 0.00323

 179 -> 205 0.00484

 179 -> 215 0.00432

 179 -> 218 -0.00171

 179 -> 243 0.00276

 179 -> 271 0.00118

 179 -> 287 0.00105

 179 -> 293 0.00127

 179 -> 334 -0.00112

 179 -> 414 -0.00161

 180 -> 251 -0.00167

 180 -> 294 -0.00162

 180 -> 310 -0.00120

 181 -> 193 0.01602

 182 -> 193 0.02005

 182 -> 202 0.00334

 182 -> 207 -0.00658

 183 -> 191 0.02882

 183 -> 195 -0.02528

 183 -> 200 -0.00126

 183 -> 204 -0.00116

 183 -> 220 0.00270

 183 -> 233 -0.00194

 184 -> 192 -0.02881

 184 -> 196 0.02533

 184 -> 199 0.00127

 184 -> 203 0.00116

 184 -> 221 -0.00269

 184 -> 234 0.00194

 185 -> 197 0.03663

 185 -> 206 0.00520

 185 -> 231 0.00227

 185 -> 247 -0.00188

 186 -> 194 0.03015

 186 -> 205 -0.00124

 186 -> 229 0.00232

 186 -> 232 0.00204

 186 -> 255 0.00140

 187 -> 192 -0.48622

 187 -> 196 -0.00965

 187 -> 199 -0.00361

 187 -> 234 0.00195

 187 -> 248 0.00203

 188 -> 191 0.48642

 188 -> 195 0.00969

 188 -> 200 0.00361

 188 -> 233 -0.00195

 188 -> 249 -0.00203

 189 -> 198 -0.00499

 189 -> 246 -0.00133

 189 -> 354 -0.00122

 190 -> 197 0.14216

 190 -> 206 0.00444

 190 -> 231 -0.00124

 122 <- 193 -0.00233

 122 <- 202 0.00129

 126 <- 214 0.00143

 130 <- 191 -0.00158

 130 <- 195 0.00156

 131 <- 192 0.00158

 131 <- 196 -0.00156

 132 <- 241 0.00102

 141 <- 194 0.00226

 141 <- 205 -0.00153

 146 <- 207 0.00131

 151 <- 194 0.00115

 155 <- 250 -0.00100

 160 <- 191 -0.00105

 160 <- 195 0.00214

 160 <- 204 0.00121

 161 <- 192 -0.00105

 161 <- 196 0.00214

 161 <- 203 0.00121

 164 <- 225 -0.00119

 166 <- 193 0.00173

 166 <- 207 -0.00239

 169 <- 194 -0.00115

 169 <- 201 -0.00102

 170 <- 192 0.00148

 170 <- 221 -0.00132

 171 <- 191 -0.00149

 171 <- 220 0.00132

 172 <- 252 0.00137

 173 <- 197 0.00118

 173 <- 247 0.00111

 174 <- 198 0.00126

 174 <- 226 0.00101

 174 <- 246 -0.00102

 175 <- 192 -0.00265

 176 <- 191 0.00265

 179 <- 201 0.00123

 179 <- 205 0.00184

 179 <- 215 0.00200

 179 <- 243 0.00151

 179 <- 414 -0.00122

 180 <- 294 -0.00110

 181 <- 193 0.00120

 181 <- 202 0.00133

 181 <- 207 -0.00205

 182 <- 193 0.00707

 182 <- 207 -0.00169

 183 <- 191 0.00185

 183 <- 195 -0.00628

 183 <- 200 -0.00118

 183 <- 220 0.00155

 184 <- 192 -0.00185

 184 <- 196 0.00629

 184 <- 199 0.00118

 184 <- 221 -0.00155

 185 <- 231 0.00125

 186 <- 194 0.00708

 186 <- 229 0.00114

 186 <- 232 0.00100

 187 <- 192 0.00517

 187 <- 199 -0.00141

 187 <- 221 0.00123

 187 <- 234 0.00129

 187 <- 248 0.00111

 188 <- 191 -0.00517

 188 <- 200 0.00140

 188 <- 220 -0.00122

 188 <- 233 -0.00129

 188 <- 249 -0.00111

 189 <- 198 0.00233

 189 <- 226 0.00215

 189 <- 246 -0.00118

 190 <- 197 0.01404

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

 Leave Link 914 at Thu Sep 19 01:06:09 2019, MaxMem= 1342177280 cpu: 14038.2

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

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

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 Population analysis using the SCF density.

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 Orbital symmetries:

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 The electronic state is 1-A1.

 Alpha occ. eigenvalues -- -14.31952 -14.31952 -14.31952 -14.31951 -14.31593

 Alpha occ. eigenvalues -- -14.31593 -14.31593 -14.31593 -10.24966 -10.24966

 Alpha occ. eigenvalues -- -10.24966 -10.24966 -10.24965 -10.24965 -10.24965

 Alpha occ. eigenvalues -- -10.24964 -10.19130 -10.19130 -10.19130 -10.19130

 Alpha occ. eigenvalues -- -10.19092 -10.19092 -10.19092 -10.19092 -10.18504

 Alpha occ. eigenvalues -- -10.18504 -10.18504 -10.18504 -10.18477 -10.18477

 Alpha occ. eigenvalues -- -10.18477 -10.18477 -10.18429 -10.18429 -10.18429

 Alpha occ. eigenvalues -- -10.18429 -10.18415 -10.18414 -10.18414 -10.18414

 Alpha occ. eigenvalues -- -10.17668 -10.17668 -10.17668 -10.17668 -10.17666

 Alpha occ. eigenvalues -- -10.17666 -10.17666 -10.17666 -10.17583 -10.17583

 Alpha occ. eigenvalues -- -10.17583 -10.17583 -10.17542 -10.17542 -10.17542

 Alpha occ. eigenvalues -- -10.17542 -1.00782 -0.99415 -0.99415 -0.96684

 Alpha occ. eigenvalues -- -0.94560 -0.90529 -0.90529 -0.88380 -0.88056

 Alpha occ. eigenvalues -- -0.88008 -0.88008 -0.86908 -0.82949 -0.82802

 Alpha occ. eigenvalues -- -0.82802 -0.82712 -0.79056 -0.78476 -0.78476

 Alpha occ. eigenvalues -- -0.78342 -0.75595 -0.75545 -0.75440 -0.75440

 Alpha occ. eigenvalues -- -0.75240 -0.73603 -0.73603 -0.72875 -0.70742

 Alpha occ. eigenvalues -- -0.69231 -0.69231 -0.65905 -0.65664 -0.65095

 Alpha occ. eigenvalues -- -0.65095 -0.63009 -0.62801 -0.60969 -0.60969

 Alpha occ. eigenvalues -- -0.60501 -0.60271 -0.60222 -0.60222 -0.60109

 Alpha occ. eigenvalues -- -0.60108 -0.58376 -0.57186 -0.56970 -0.56970

 Alpha occ. eigenvalues -- -0.56221 -0.54677 -0.54677 -0.54199 -0.53733

 Alpha occ. eigenvalues -- -0.53733 -0.53309 -0.51703 -0.51703 -0.51691

 Alpha occ. eigenvalues -- -0.51643 -0.51579 -0.51188 -0.50811 -0.50811

 Alpha occ. eigenvalues -- -0.49408 -0.46379 -0.45691 -0.45645 -0.45645

 Alpha occ. eigenvalues -- -0.45530 -0.45449 -0.44974 -0.44974 -0.44882

 Alpha occ. eigenvalues -- -0.44882 -0.44278 -0.44032 -0.43837 -0.43509

 Alpha occ. eigenvalues -- -0.43509 -0.43275 -0.42923 -0.42923 -0.42468

 Alpha occ. eigenvalues -- -0.42422 -0.42183 -0.42040 -0.42040 -0.41381

 Alpha occ. eigenvalues -- -0.39669 -0.39583 -0.39583 -0.39050 -0.38771

 Alpha occ. eigenvalues -- -0.38521 -0.37821 -0.37395 -0.37395 -0.36702

 Alpha occ. eigenvalues -- -0.35654 -0.35480 -0.35480 -0.35235 -0.34229

 Alpha occ. eigenvalues -- -0.34229 -0.34046 -0.34046 -0.33963 -0.33609

 Alpha occ. eigenvalues -- -0.33157 -0.32875 -0.32875 -0.32051 -0.31505

 Alpha occ. eigenvalues -- -0.31505 -0.30909 -0.30424 -0.29627 -0.29206

 Alpha occ. eigenvalues -- -0.29206 -0.28196 -0.28196 -0.26968 -0.26570

 Alpha occ. eigenvalues -- -0.25412 -0.25220 -0.24982 -0.24982 -0.24823

 Alpha occ. eigenvalues -- -0.24780 -0.22789 -0.22789 -0.22680 -0.17259

 Alpha virt. eigenvalues -- -0.10335 -0.10335 -0.06198 -0.05881 -0.05506

 Alpha virt. eigenvalues -- -0.05506 -0.04516 -0.00082 0.00025 0.00025

 Alpha virt. eigenvalues -- 0.00680 0.00732 0.01363 0.01363 0.02042

 Alpha virt. eigenvalues -- 0.02994 0.04955 0.04980 0.04980 0.05953

 Alpha virt. eigenvalues -- 0.06294 0.06294 0.06301 0.06376 0.07025

 Alpha virt. eigenvalues -- 0.07353 0.07353 0.07740 0.08364 0.09334

 Alpha virt. eigenvalues -- 0.09334 0.09718 0.09718 0.10551 0.10952

 Alpha virt. eigenvalues -- 0.11328 0.11682 0.11682 0.12262 0.12352

 Alpha virt. eigenvalues -- 0.12355 0.12601 0.13069 0.13069 0.13392

 Alpha virt. eigenvalues -- 0.13392 0.14410 0.14682 0.16454 0.16454

 Alpha virt. eigenvalues -- 0.17927 0.18286 0.18313 0.18651 0.18651

 Alpha virt. eigenvalues -- 0.18820 0.19051 0.19058 0.19058 0.19759

 Alpha virt. eigenvalues -- 0.20597 0.21435 0.22204 0.22204 0.22388

 Alpha virt. eigenvalues -- 0.23080 0.23162 0.23162 0.24334 0.24549

 Alpha virt. eigenvalues -- 0.25424 0.25424 0.26175 0.26237 0.26237

 Alpha virt. eigenvalues -- 0.26979 0.27821 0.27821 0.27854 0.28013

 Alpha virt. eigenvalues -- 0.28067 0.28128 0.28537 0.28537 0.28855

 Alpha virt. eigenvalues -- 0.29185 0.29185 0.29733 0.30535 0.30761

 Alpha virt. eigenvalues -- 0.30761 0.30867 0.31152 0.31152 0.31203

 Alpha virt. eigenvalues -- 0.31904 0.31918 0.32779 0.32779 0.33328

 Alpha virt. eigenvalues -- 0.34653 0.34653 0.35032 0.35185 0.35847

 Alpha virt. eigenvalues -- 0.35847 0.36149 0.36591 0.36882 0.37212

 Alpha virt. eigenvalues -- 0.37212 0.37355 0.37606 0.38057 0.38057

 Alpha virt. eigenvalues -- 0.38142 0.38361 0.38532 0.38532 0.39024

 Alpha virt. eigenvalues -- 0.39234 0.39281 0.39281 0.39744 0.39946

 Alpha virt. eigenvalues -- 0.40197 0.40245 0.40295 0.40295 0.40866

 Alpha virt. eigenvalues -- 0.40866 0.41140 0.41265 0.41700 0.41700

 Alpha virt. eigenvalues -- 0.42016 0.42680 0.42880 0.42880 0.43099

 Alpha virt. eigenvalues -- 0.43221 0.43221 0.43299 0.43427 0.43529

 Alpha virt. eigenvalues -- 0.43671 0.43671 0.43681 0.44063 0.44091

 Alpha virt. eigenvalues -- 0.44506 0.44506 0.44734 0.44882 0.45099

 Alpha virt. eigenvalues -- 0.45099 0.45373 0.46204 0.46231 0.46231

 Alpha virt. eigenvalues -- 0.46468 0.46468 0.46675 0.46706 0.47134

 Alpha virt. eigenvalues -- 0.47134 0.47315 0.47571 0.47645 0.47645

 Alpha virt. eigenvalues -- 0.48204 0.48468 0.48795 0.48968 0.49341

 Alpha virt. eigenvalues -- 0.49341 0.49721 0.50425 0.50782 0.50871

 Alpha virt. eigenvalues -- 0.50871 0.51116 0.51562 0.51562 0.52239

 Alpha virt. eigenvalues -- 0.52240 0.53216 0.53384 0.53384 0.53425

 Alpha virt. eigenvalues -- 0.53759 0.53866 0.54683 0.54977 0.55679

 Alpha virt. eigenvalues -- 0.55679 0.56454 0.56454 0.56915 0.58116

 Alpha virt. eigenvalues -- 0.58116 0.58914 0.58967 0.59474 0.60241

 Alpha virt. eigenvalues -- 0.60241 0.60730 0.60884 0.60884 0.61229

 Alpha virt. eigenvalues -- 0.61334 0.61727 0.61838 0.61838 0.62251

 Alpha virt. eigenvalues -- 0.62395 0.62688 0.62688 0.62979 0.63021

 Alpha virt. eigenvalues -- 0.63223 0.63223 0.63522 0.63598 0.64371

 Alpha virt. eigenvalues -- 0.64452 0.64515 0.64515 0.65608 0.65608

 Alpha virt. eigenvalues -- 0.65894 0.66329 0.67393 0.67648 0.67648

 Alpha virt. eigenvalues -- 0.68147 0.68260 0.68463 0.68570 0.68570

 Alpha virt. eigenvalues -- 0.68987 0.69378 0.69378 0.69455 0.70002

 Alpha virt. eigenvalues -- 0.70002 0.70672 0.70672 0.70991 0.72359

 Alpha virt. eigenvalues -- 0.72959 0.72960 0.73181 0.73293 0.73407

 Alpha virt. eigenvalues -- 0.73407 0.74017 0.74674 0.74837 0.75421

 Alpha virt. eigenvalues -- 0.75421 0.76028 0.76435 0.76536 0.76710

 Alpha virt. eigenvalues -- 0.76710 0.78410 0.78639 0.78720 0.78997

 Alpha virt. eigenvalues -- 0.78997 0.79490 0.79490 0.79851 0.80257

 Alpha virt. eigenvalues -- 0.80432 0.80432 0.80546 0.80661 0.81394

 Alpha virt. eigenvalues -- 0.81625 0.81625 0.82108 0.82368 0.82600

 Alpha virt. eigenvalues -- 0.82914 0.82914 0.84192 0.84302 0.84302

 Alpha virt. eigenvalues -- 0.85017 0.85171 0.85385 0.85385 0.85827

 Alpha virt. eigenvalues -- 0.86155 0.87762 0.87785 0.88041 0.88041

 Alpha virt. eigenvalues -- 0.88664 0.88664 0.89966 0.91836 0.91836

 Alpha virt. eigenvalues -- 0.92146 0.92862 0.92862 0.93573 0.94542

 Alpha virt. eigenvalues -- 0.94847 0.94847 0.95988 0.96024 0.96396

 Alpha virt. eigenvalues -- 0.97156 0.97311 0.97311 0.97544 0.97750

 Alpha virt. eigenvalues -- 0.97836 0.98200 0.98200 0.98598 0.98715

 Alpha virt. eigenvalues -- 0.98715 0.99712 0.99712 0.99790 1.00335

 Alpha virt. eigenvalues -- 1.01401 1.02164 1.02344 1.02685 1.02685

 Alpha virt. eigenvalues -- 1.03582 1.03960 1.03960 1.05403 1.05563

 Alpha virt. eigenvalues -- 1.06382 1.06382 1.07102 1.07102 1.07318

 Alpha virt. eigenvalues -- 1.09000 1.09995 1.10031 1.10031 1.10335

 Alpha virt. eigenvalues -- 1.10617 1.11232 1.11232 1.11369 1.11503

 Alpha virt. eigenvalues -- 1.11610 1.11610 1.12371 1.12606 1.12611

 Alpha virt. eigenvalues -- 1.12640 1.12640 1.13727 1.14152 1.14195

 Alpha virt. eigenvalues -- 1.14722 1.14722 1.16652 1.16652 1.16686

 Alpha virt. eigenvalues -- 1.17184 1.17184 1.17366 1.17858 1.18387

 Alpha virt. eigenvalues -- 1.19032 1.19032 1.19653 1.20824 1.21810

 Alpha virt. eigenvalues -- 1.21810 1.21821 1.21825 1.21945 1.22533

 Alpha virt. eigenvalues -- 1.22630 1.22630 1.23306 1.24723 1.24723

 Alpha virt. eigenvalues -- 1.25633 1.25633 1.25880 1.26660 1.26682

 Alpha virt. eigenvalues -- 1.27425 1.27425 1.27813 1.27876 1.28567

 Alpha virt. eigenvalues -- 1.29235 1.29728 1.30400 1.30515 1.30515

 Alpha virt. eigenvalues -- 1.33426 1.33427 1.34481 1.34875 1.35389

 Alpha virt. eigenvalues -- 1.35389 1.36231 1.37787 1.38626 1.38997

 Alpha virt. eigenvalues -- 1.39330 1.39330 1.40125 1.40126 1.40466

 Alpha virt. eigenvalues -- 1.42627 1.42733 1.42733 1.44672 1.44744

 Alpha virt. eigenvalues -- 1.44821 1.44821 1.44959 1.45833 1.45833

 Alpha virt. eigenvalues -- 1.46315 1.47276 1.48626 1.48626 1.48987

 Alpha virt. eigenvalues -- 1.51615 1.51616 1.51654 1.51837 1.51837

 Alpha virt. eigenvalues -- 1.51931 1.51991 1.52101 1.52219 1.52372

 Alpha virt. eigenvalues -- 1.52372 1.52740 1.53125 1.53125 1.53136

 Alpha virt. eigenvalues -- 1.53299 1.54342 1.54395 1.54395 1.55157

 Alpha virt. eigenvalues -- 1.56293 1.56743 1.56743 1.57850 1.58259

 Alpha virt. eigenvalues -- 1.60975 1.60975 1.64285 1.64576 1.64920

 Alpha virt. eigenvalues -- 1.65089 1.65089 1.65328 1.67001 1.68320

 Alpha virt. eigenvalues -- 1.68320 1.69567 1.69581 1.69581 1.70892

 Alpha virt. eigenvalues -- 1.71230 1.71230 1.71962 1.72232 1.72589

 Alpha virt. eigenvalues -- 1.73560 1.74238 1.74238 1.75526 1.75634

 Alpha virt. eigenvalues -- 1.77028 1.77028 1.77612 1.78085 1.78086

 Alpha virt. eigenvalues -- 1.78087 1.79315 1.80151 1.80151 1.81282

 Alpha virt. eigenvalues -- 1.82017 1.82146 1.82210 1.82210 1.82760

 Alpha virt. eigenvalues -- 1.83096 1.83097 1.83686 1.84782 1.84782

 Alpha virt. eigenvalues -- 1.86212 1.86674 1.86688 1.86688 1.87254

 Alpha virt. eigenvalues -- 1.87330 1.88146 1.88750 1.88750 1.88955

 Alpha virt. eigenvalues -- 1.89322 1.89645 1.89645 1.90115 1.90547

 Alpha virt. eigenvalues -- 1.91631 1.91660 1.91660 1.92152 1.92461

 Alpha virt. eigenvalues -- 1.92461 1.92526 1.92655 1.92655 1.92675

 Alpha virt. eigenvalues -- 1.92794 1.94304 1.94742 1.94924 1.95112

 Alpha virt. eigenvalues -- 1.95112 1.95284 1.95284 1.95752 1.96607

 Alpha virt. eigenvalues -- 1.96607 1.96622 1.97099 1.97361 1.97693

 Alpha virt. eigenvalues -- 1.97693 1.98114 1.99514 1.99853 1.99853

 Alpha virt. eigenvalues -- 2.02267 2.02695 2.04092 2.04788 2.04788

 Alpha virt. eigenvalues -- 2.05118 2.07386 2.08441 2.08441 2.09649

 Alpha virt. eigenvalues -- 2.12307 2.13202 2.13202 2.15224 2.15224

 Alpha virt. eigenvalues -- 2.15545 2.15843 2.18731 2.18731 2.18958

 Alpha virt. eigenvalues -- 2.19812 2.21385 2.21385 2.21869 2.21938

 Alpha virt. eigenvalues -- 2.22310 2.22310 2.22352 2.22540 2.22856

 Alpha virt. eigenvalues -- 2.24463 2.24835 2.24835 2.24986 2.26298

 Alpha virt. eigenvalues -- 2.26442 2.26442 2.27605 2.27870 2.28342

 Alpha virt. eigenvalues -- 2.28342 2.30072 2.31424 2.31616 2.31776

 Alpha virt. eigenvalues -- 2.31776 2.31890 2.32430 2.33920 2.33920

 Alpha virt. eigenvalues -- 2.35025 2.35025 2.35054 2.35350 2.36246

 Alpha virt. eigenvalues -- 2.36503 2.36503 2.38606 2.39832 2.39833

 Alpha virt. eigenvalues -- 2.40660 2.42884 2.43548 2.44129 2.44692

 Alpha virt. eigenvalues -- 2.44692 2.45583 2.45583 2.45649 2.46500

 Alpha virt. eigenvalues -- 2.47715 2.49965 2.49965 2.51306 2.51898

 Alpha virt. eigenvalues -- 2.51898 2.52492 2.53088 2.53166 2.53493

 Alpha virt. eigenvalues -- 2.53493 2.54048 2.55194 2.55194 2.55447

 Alpha virt. eigenvalues -- 2.56041 2.56041 2.56099 2.56194 2.57098

 Alpha virt. eigenvalues -- 2.57574 2.57574 2.57867 2.59006 2.61029

 Alpha virt. eigenvalues -- 2.63201 2.65008 2.65008 2.65208 2.65208

 Alpha virt. eigenvalues -- 2.65697 2.68119 2.68831 2.69586 2.69726

 Alpha virt. eigenvalues -- 2.69726 2.70965 2.70965 2.71226 2.71438

 Alpha virt. eigenvalues -- 2.72151 2.72151 2.72647 2.73624 2.73678

 Alpha virt. eigenvalues -- 2.73980 2.74016 2.74058 2.74058 2.74595

 Alpha virt. eigenvalues -- 2.74664 2.75448 2.75449 2.75861 2.75861

 Alpha virt. eigenvalues -- 2.78157 2.80250 2.80740 2.80740 2.80930

 Alpha virt. eigenvalues -- 2.81689 2.82380 2.82380 2.82784 2.82956

 Alpha virt. eigenvalues -- 2.82957 2.83735 2.84999 2.86527 2.86831

 Alpha virt. eigenvalues -- 2.86831 2.86941 2.87640 2.87640 2.87842

 Alpha virt. eigenvalues -- 2.88042 2.88820 2.89590 2.89590 2.89642

 Alpha virt. eigenvalues -- 2.91138 2.93056 2.93056 2.93823 2.93937

 Alpha virt. eigenvalues -- 2.96939 2.96939 2.98990 3.02520 3.03218

 Alpha virt. eigenvalues -- 3.03218 3.03997 3.04182 3.05040 3.05576

 Alpha virt. eigenvalues -- 3.05576 3.07640 3.09302 3.09302 3.15071

 Alpha virt. eigenvalues -- 3.15628 3.15628 3.15914 3.16857 3.17823

 Alpha virt. eigenvalues -- 3.17823 3.18973 3.19378 3.20410 3.20453

 Alpha virt. eigenvalues -- 3.20453 3.20543 3.21429 3.21490 3.21490

 Alpha virt. eigenvalues -- 3.22520 3.23171 3.23642 3.24560 3.24560

 Alpha virt. eigenvalues -- 3.26333 3.26919 3.27350 3.27350 3.28367

 Alpha virt. eigenvalues -- 3.28564 3.28564 3.28652 3.29131 3.29268

 Alpha virt. eigenvalues -- 3.29268 3.29318 3.31630 3.31945 3.31945

 Alpha virt. eigenvalues -- 3.32475 3.32492 3.33917 3.33917 3.34024

 Alpha virt. eigenvalues -- 3.34786 3.35114 3.35114 3.37586 3.39907

 Alpha virt. eigenvalues -- 3.41283 3.41283 3.42165 3.42249 3.42918

 Alpha virt. eigenvalues -- 3.42918 3.43685 3.46785 3.47140 3.47140

 Alpha virt. eigenvalues -- 3.47758 3.51636 3.52115 3.52115 3.53003

 Alpha virt. eigenvalues -- 3.53195 3.53195 3.53299 3.53378 3.55311

 Alpha virt. eigenvalues -- 3.60086 3.60086 3.62491 3.62754 3.63168

 Alpha virt. eigenvalues -- 3.63168 3.70490 3.71011 3.71011 3.71799

 Alpha virt. eigenvalues -- 3.75101 3.75726 3.75727 3.76843 3.82954

 Alpha virt. eigenvalues -- 3.83514 3.83700 3.83700 3.87439 3.88297

 Alpha virt. eigenvalues -- 3.88670 3.89369 3.89369 3.89717 3.90055

 Alpha virt. eigenvalues -- 3.90055 3.91022 4.00805 4.01153 4.01153

 Alpha virt. eigenvalues -- 4.02326 4.03151 4.03584 4.03584 4.06130

 Alpha virt. eigenvalues -- 4.11841 4.13033 4.13033 4.20896 4.24176

 Alpha virt. eigenvalues -- 4.28844 4.28844 4.38992 4.40996 4.42965

 Alpha virt. eigenvalues -- 4.44978 4.44978 4.47195 4.53231 4.53231

 Alpha virt. eigenvalues -- 4.54457 4.75875 4.75875 4.75880 4.75900

 Alpha virt. eigenvalues -- 4.79029 4.79094 4.79094 4.79233 5.12469

 Alpha virt. eigenvalues -- 5.12469 5.13467 5.16221 5.23133 5.37058

 Alpha virt. eigenvalues -- 5.37058 5.52396 7.82539 7.87339 7.87339

 Alpha virt. eigenvalues -- 7.88520 8.10137 11.10218 23.20698 23.22355

 Alpha virt. eigenvalues -- 23.22355 23.23287 23.56491 23.58438 23.58438

 Alpha virt. eigenvalues -- 23.59415 23.72291 23.72492 23.72492 23.72670

 Alpha virt. eigenvalues -- 23.81416 23.81477 23.81790 23.81790 23.82217

 Alpha virt. eigenvalues -- 23.82982 23.82982 23.84834 23.88936 23.89861

 Alpha virt. eigenvalues -- 23.89861 23.90535 23.92355 23.92506 23.92524

 Alpha virt. eigenvalues -- 23.92524 23.98130 23.98241 23.98241 23.98437

 Alpha virt. eigenvalues -- 24.06942 24.06949 24.06949 24.06961 24.10069

 Alpha virt. eigenvalues -- 24.10069 24.10115 24.10118 24.14086 24.14171

 Alpha virt. eigenvalues -- 24.14171 24.14257 24.14478 24.14646 24.14646

 Alpha virt. eigenvalues -- 24.15189 35.56578 35.60124 35.60124 35.61462

 Alpha virt. eigenvalues -- 35.69267 35.70143 35.70143 35.70242

 Condensed to atoms (all electrons):

 Mulliken charges:

 1

 1 C 0.386683

 2 N -0.645418

 3 C 0.386683

 4 C -0.072858

 5 C -0.072858

 6 N -0.403973

 7 C 0.386682

 8 N -0.645417

 9 C 0.386682

 10 C -0.072857

 11 C -0.072857

 12 N -0.403973

 13 C -0.072857

 14 C -0.072857

 15 C 0.386682

 16 N -0.645417

 17 C 0.386682

 18 N -0.403973

 19 N -0.645418

 20 C 0.386683

 21 C -0.072858

 22 C -0.072858

 23 C 0.386683

 24 N -0.403973

 25 Zn 1.404122

 26 C -0.210552

 27 C 0.009122

 28 C 0.009122

 29 C -0.210552

 30 C -0.210552

 31 C 0.009122

 32 C 0.009122

 33 C -0.210552

 34 C -0.210552

 35 C 0.009122

 36 C 0.009122

 37 C -0.210552

 38 C -0.210552

 39 C 0.009122

 40 C 0.009122

 41 C -0.210552

 42 C -0.229471

 43 C -0.222402

 44 C -0.222402

 45 C -0.229471

 46 C -0.229471

 47 C -0.222402

 48 C -0.222402

 49 C -0.229471

 50 C -0.229471

 51 C -0.222402

 52 C -0.222402

 53 C -0.229471

 54 C -0.229471

 55 C -0.222402

 56 C -0.222402

 57 C -0.229471

 58 H 0.230376

 59 H 0.230376

 60 H 0.230376

 61 H 0.230376

 62 H 0.230376

 63 H 0.230376

 64 H 0.230376

 65 H 0.230376

 66 H 0.229879

 67 H 0.228402

 68 H 0.228402

 69 H 0.229879

 70 H 0.229879

 71 H 0.228402

 72 H 0.228402

 73 H 0.229879

 74 H 0.229879

 75 H 0.228402

 76 H 0.228402

 77 H 0.229879

 78 H 0.229879

 79 H 0.228402

 80 H 0.228402

 81 H 0.229879

 Sum of Mulliken charges = -0.00000

 Mulliken charges with hydrogens summed into heavy atoms:

 1

 1 C 0.386683

 2 N -0.645418

 3 C 0.386683

 4 C -0.072858

 5 C -0.072858

 6 N -0.403973

 7 C 0.386682

 8 N -0.645417

 9 C 0.386682

 10 C -0.072857

 11 C -0.072857

 12 N -0.403973

 13 C -0.072857

 14 C -0.072857

 15 C 0.386682

 16 N -0.645417

 17 C 0.386682

 18 N -0.403973

 19 N -0.645418

 20 C 0.386683

 21 C -0.072858

 22 C -0.072858

 23 C 0.386683

 24 N -0.403973

 25 Zn 1.404122

 26 C 0.019824

 27 C 0.009122

 28 C 0.009122

 29 C 0.019824

 30 C 0.019824

 31 C 0.009122

 32 C 0.009122

 33 C 0.019824

 34 C 0.019824

 35 C 0.009122

 36 C 0.009122

 37 C 0.019824

 38 C 0.019824

 39 C 0.009122

 40 C 0.009122

 41 C 0.019824

 42 C 0.000408

 43 C 0.006000

 44 C 0.006000

 45 C 0.000408

 46 C 0.000409

 47 C 0.006000

 48 C 0.006000

 49 C 0.000409

 50 C 0.000408

 51 C 0.006000

 52 C 0.006000

 53 C 0.000408

 54 C 0.000409

 55 C 0.006000

 56 C 0.006000

 57 C 0.000409

 Electronic spatial extent (au): <R\*\*2>= 50409.6148

 Charge= 0.0000 electrons

 Dipole moment (field-independent basis, Debye):

 X= 0.0000 Y= -0.0000 Z= 2.6053 Tot= 2.6053

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

 XX= -268.3099 YY= -268.3103 ZZ= -337.6642

 XY= -0.0000 XZ= -0.0000 YZ= 0.0000

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

 XX= 23.1183 YY= 23.1179 ZZ= -46.2361

 XY= -0.0000 XZ= -0.0000 YZ= 0.0000

 Octapole moment (field-independent basis, Debye-Ang\*\*2):

 XXX= -0.0000 YYY= 0.0000 ZZZ= 60.4769 XYY= 0.0000

 XXY= -0.0000 XXZ= -40.2036 XZZ= 0.0000 YZZ= 0.0000

 YYZ= -40.2213 XYZ= 0.0000

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

 XXXX= -28224.7506 YYYY= -28224.7172 ZZZZ= -486.6928 XXXY= 0.0000

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

 ZZZY= 0.0000 XXYY= -10322.7273 XXZZ= -6609.7966 YYZZ= -6609.7506

 XXYZ= 0.0000 YYXZ= -0.0000 ZZXY= -0.0000

 N-N= 6.888572816868D+03 E-N=-1.931954521448D+04 KE= 2.388757903125D+03

 Symmetry A1 KE= 6.742197496188D+02

 Symmetry A2 KE= 5.331437604629D+02

 Symmetry B1 KE= 5.906971971451D+02

 Symmetry B2 KE= 5.906971958986D+02

 Leave Link 601 at Thu Sep 19 01:06:36 2019, MaxMem= 1342177280 cpu: 46.3

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

 Test job not archived.

 1\1\ WCSS.PL-BEM-DHCP-129-94-98-136\SP\RB3LYP TD-FC\GenECP\C48H24N8Zn1

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

 nt=dmso,smd) empiricaldispersion=gd3bj IOp(9/40=3)\\ZnNPC0td\\0,1\C,0,

 1.122077,2.793021,0.172784\N,0,0.,2.020361,0.259821\C,0,-1.122077,2.79

 3021,0.172784\C,0,-0.714524,4.194635,0.051468\C,0,0.714524,4.194635,0.

 051468\N,0,-2.389506,2.389505,0.154613\C,0,-2.793023,1.122077,0.172801

 \N,0,-2.020362,0.,0.259826\C,0,-2.793023,-1.122077,0.172801\C,0,-4.194

 641,-0.714524,0.051526\C,0,-4.194641,0.714524,0.051526\N,0,2.389506,2.

 389505,0.154613\C,0,4.194641,0.714524,0.051526\C,0,4.194641,-0.714524,

 0.051526\C,0,2.793023,-1.122077,0.172801\N,0,2.020362,0.,0.259826\C,0,

 2.793023,1.122077,0.172801\N,0,2.389506,-2.389505,0.154613\N,0,0.,-2.0

 20361,0.259821\C,0,1.122077,-2.793021,0.172784\C,0,0.714524,-4.194635,

 0.051468\C,0,-0.714524,-4.194635,0.051468\C,0,-1.122077,-2.793021,0.17

 2784\N,0,-2.389506,-2.389505,0.154613\Zn,0,0.,0.,0.777528\C,0,5.363492

 ,1.427454,-0.054616\C,0,6.58861,0.72073,-0.156377\C,0,6.58861,-0.72073

 ,-0.156377\C,0,5.363492,-1.427454,-0.054616\C,0,-1.427454,-5.363483,-0

 .054708\C,0,-0.72073,-6.588598,-0.156501\C,0,0.72073,-6.588598,-0.1565

 01\C,0,1.427454,-5.363483,-0.054708\C,0,-5.363492,1.427454,-0.054616\C

 ,0,-6.58861,0.72073,-0.156377\C,0,-6.58861,-0.72073,-0.156377\C,0,-5.3

 63492,-1.427454,-0.054616\C,0,1.427454,5.363483,-0.054708\C,0,0.72073,

 6.588598,-0.156501\C,0,-0.72073,6.588598,-0.156501\C,0,-1.427454,5.363

 483,-0.054708\C,0,1.402412,-7.830417,-0.258961\C,0,0.708074,-9.011507,

 -0.356784\C,0,-0.708074,-9.011507,-0.356784\C,0,-1.402412,-7.830417,-0

 .258961\C,0,7.830431,-1.402412,-0.258803\C,0,9.011524,-0.708074,-0.356

 593\C,0,9.011524,0.708074,-0.356593\C,0,7.830431,1.402412,-0.258803\C,

 0,-1.402412,7.830417,-0.258961\C,0,-0.708074,9.011507,-0.356784\C,0,0.

 708074,9.011507,-0.356784\C,0,1.402412,7.830417,-0.258961\C,0,-7.83043

 1,-1.402412,-0.258803\C,0,-9.011524,-0.708074,-0.356593\C,0,-9.011524,

 0.708074,-0.356593\C,0,-7.830431,1.402412,-0.258803\H,0,5.364985,2.512

 421,-0.058211\H,0,5.364985,-2.512421,-0.058211\H,0,-2.512421,-5.364975

 ,-0.058303\H,0,2.512421,-5.364975,-0.058303\H,0,-5.364985,2.512421,-0.

 058211\H,0,-5.364985,-2.512421,-0.058211\H,0,2.512421,5.364975,-0.0583

 03\H,0,-2.512421,5.364975,-0.058303\H,0,2.487843,-7.828541,-0.258814\H

 ,0,1.243262,-9.951788,-0.435088\H,0,-1.243262,-9.951788,-0.435088\H,0,

 -2.487843,-7.828541,-0.258814\H,0,7.828556,-2.487843,-0.258655\H,0,9.9

 51808,-1.243262,-0.43487\H,0,9.951808,1.243262,-0.43487\H,0,7.828556,2

 .487843,-0.258655\H,0,-2.487843,7.828541,-0.258814\H,0,-1.243262,9.951

 788,-0.435088\H,0,1.243262,9.951788,-0.435088\H,0,2.487843,7.828541,-0

 .258814\H,0,-7.828556,-2.487843,-0.258655\H,0,-9.951808,-1.243262,-0.4

 3487\H,0,-9.951808,1.243262,-0.43487\H,0,-7.828556,2.487843,-0.258655\

 \Version=ES64L-G09RevE.01\State=1-A1\HF=-2348.1645354\RMSD=5.058e-09\P

 G=C02V [C2(Zn1),SGV(N2),SGV'(N2),X(C48H24N4)]\\@

 THE SECRET OF SUCCESS IN LIFE IS TO EAT WHAT YOU LIKE, AND LET THE FOOD

 FIGHT IT OUT INSIDE YOU. -- FROM A FORTUNE COOKIE

 Job cpu time: 0 days 4 hours 36 minutes 47.4 seconds.

 File lengths (MBytes): RWF= 4517 Int= 0 D2E= 0 Chk= 459 Scr= 1

 Normal termination of Gaussian 09 at Thu Sep 19 01:07:17 2019.