Entering Gaussian System, Link 0=g09

 Input=ZnOMPC0td.com

 Output=ZnOMPC0td.log

 Initial command:

 /home/blab/g09/l1.exe "/home/blab/g09/scratch/Gau-47507.inp" -scrdir="/home/blab/g09/scratch/"

 Entering Link 1 = /home/blab/g09/l1.exe PID= 47514.

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 Cite this work as:

 Gaussian 09, Revision E.01,

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

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

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

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

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

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

 19-Sep-2019

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

 %nprocshared=9

 Will use up to 9 processors via shared memory.

 %mem=10GB

 %chk=ZnOMPC0td.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 00:35:41 2019, MaxMem= 1342177280 cpu: 0.4

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

 ---------

 ZnOMPC0td

 ---------

 Symbolic Z-matrix:

 Charge = 0 Multiplicity = 1

 C -1.12695 2.81013 0.01354

 N 0. 2.04085 -0.0007

 C 1.12695 2.81013 0.01354

 C 0.70839 4.21655 0.04302

 C -0.70839 4.21655 0.04302

 N 2.39223 2.39223 0.

 C 2.81013 1.12695 -0.01354

 N 2.04085 0. 0.0007

 C 2.81013 -1.12695 -0.01354

 C 4.21655 -0.70839 -0.04302

 C 4.21655 0.70839 -0.04302

 N -2.39223 2.39223 0.

 C -4.21655 0.70839 -0.04302

 C -4.21655 -0.70839 -0.04302

 C -2.81013 -1.12695 -0.01354

 N -2.04085 0. 0.0007

 C -2.81013 1.12695 -0.01354

 N -2.39223 -2.39223 0.

 N 0. -2.04085 -0.0007

 C -1.12695 -2.81013 0.01354

 C -0.70839 -4.21655 0.04302

 C 0.70839 -4.21655 0.04302

 C 1.12695 -2.81013 0.01354

 N 2.39223 -2.39223 0.

 Zn 0. 0. 0.

 C -5.42079 1.43282 -0.07184

 C -6.61032 0.6998 -0.09831

 C -6.61032 -0.6998 -0.09831

 C -5.42079 -1.43282 -0.07184

 C 1.43282 -5.42079 0.07184

 C 0.6998 -6.61032 0.09831

 C -0.6998 -6.61032 0.09831

 C -1.43282 -5.42079 0.07184

 C 5.42079 1.43282 -0.07184

 C 6.61032 0.6998 -0.09831

 C 6.61032 -0.6998 -0.09831

 C 5.42079 -1.43282 -0.07184

 C -1.43282 5.42079 0.07184

 C -0.6998 6.61032 0.09831

 C 0.6998 6.61032 0.09831

 C 1.43282 5.42079 0.07184

 H 7.56515 1.20789 -0.12097

 H 7.56515 -1.20789 -0.12097

 H 1.20789 7.56515 0.12097

 H -1.20789 7.56515 0.12097

 H -7.56515 1.20789 -0.12097

 H -7.56515 -1.20789 -0.12097

 H -1.20789 -7.56515 0.12097

 H 1.20789 -7.56515 0.12097

 O 2.78394 5.3576 0.07395

 O -2.78394 5.3576 0.07395

 O 5.3576 2.78394 -0.07395

 O 5.3576 -2.78394 -0.07395

 O 2.78394 -5.3576 0.07395

 O -2.78394 -5.3576 0.07395

 O -5.3576 -2.78394 -0.07395

 O -5.3576 2.78394 -0.07395

 C 3.51435 6.58061 0.1027

 H 3.30356 7.19436 -0.77851

 H 4.56446 6.29392 0.09971

 C 6.58061 3.51435 -0.1027

 H 7.19436 3.30356 0.77851

 H 6.29392 4.56446 -0.09971

 C 6.58061 -3.51435 -0.1027

 H 7.19436 -3.30356 0.77851

 H 6.29392 -4.56446 -0.09971

 C -3.51435 6.58061 0.1027

 H -3.30356 7.19436 -0.77851

 H -4.56446 6.29392 0.09971

 C -6.58061 3.51435 -0.1027

 H -7.19436 3.30356 0.77851

 H -6.29392 4.56446 -0.09971

 C -6.58061 -3.51435 -0.1027

 H -7.19436 -3.30356 0.77851

 H -6.29392 -4.56446 -0.09971

 C -3.51435 -6.58061 0.1027

 H -3.30356 -7.19436 -0.77851

 H -4.56446 -6.29392 0.09971

 C 3.51435 -6.58061 0.1027

 H 3.30356 -7.19436 -0.77851

 H 4.56446 -6.29392 0.09971

 H 3.29834 -7.15574 1.00833

 H -3.29834 -7.15574 1.00833

 H -7.15574 -3.29834 -1.00833

 H -7.15574 3.29834 -1.00833

 H 3.29834 7.15574 1.00833

 H -3.29834 7.15574 1.00833

 H 7.15574 -3.29834 -1.00833

 H 7.15574 3.29834 -1.00833

 NAtoms= 89 NQM= 89 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 1 1 1 1 1 1 1 1 16

 AtmWgt= 12.0000000 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 15.9949146

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

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

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

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

 AtZNuc= 6.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 8.0000000

 Atom 51 52 53 54 55 56 57 58 59 60

 IAtWgt= 16 16 16 16 16 16 16 12 1 1

 AtmWgt= 15.9949146 15.9949146 15.9949146 15.9949146 15.9949146 15.9949146 15.9949146 12.0000000 1.0078250 1.0078250

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

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

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

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

 AtZNuc= 8.0000000 8.0000000 8.0000000 8.0000000 8.0000000 8.0000000 8.0000000 6.0000000 1.0000000 1.0000000

 Atom 61 62 63 64 65 66 67 68 69 70

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

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

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

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

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

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

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

 Atom 71 72 73 74 75 76 77 78 79 80

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

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

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

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

 Atom 81 82 83 84 85 86 87 88 89

 IAtWgt= 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

 NucSpn= 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

 NQMom= 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

 AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

 Leave Link 101 at Thu Sep 19 00:35:41 2019, MaxMem= 1342177280 cpu: 0.8

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

 Stoichiometry C40H32N8O8Zn

 Framework group D2D[O(Zn),2SGD(N2),X(C40H32N4O8)]

 Deg. of freedom 32

 Full point group D2D NOp 8

 Largest Abelian subgroup C2V NOp 4

 Largest concise Abelian subgroup C2V NOp 4

 Standard orientation:

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

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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

 1 6 0 -1.126947 2.810131 0.013541

 2 7 0 0.000000 2.040854 -0.000700

 3 6 0 1.126947 2.810131 0.013541

 4 6 0 0.708388 4.216552 0.043016

 5 6 0 -0.708388 4.216552 0.043016

 6 7 0 2.392227 2.392227 -0.000000

 7 6 0 2.810131 1.126947 -0.013541

 8 7 0 2.040854 -0.000000 0.000700

 9 6 0 2.810131 -1.126947 -0.013541

 10 6 0 4.216552 -0.708388 -0.043016

 11 6 0 4.216552 0.708388 -0.043016

 12 7 0 -2.392227 2.392227 -0.000000

 13 6 0 -4.216552 0.708388 -0.043016

 14 6 0 -4.216552 -0.708388 -0.043016

 15 6 0 -2.810131 -1.126947 -0.013541

 16 7 0 -2.040854 0.000000 0.000700

 17 6 0 -2.810131 1.126947 -0.013541

 18 7 0 -2.392227 -2.392227 -0.000000

 19 7 0 -0.000000 -2.040854 -0.000700

 20 6 0 -1.126947 -2.810131 0.013541

 21 6 0 -0.708388 -4.216552 0.043016

 22 6 0 0.708388 -4.216552 0.043016

 23 6 0 1.126947 -2.810131 0.013541

 24 7 0 2.392227 -2.392227 -0.000000

 25 30 0 0.000000 0.000000 0.000000

 26 6 0 -5.420785 1.432821 -0.071840

 27 6 0 -6.610317 0.699802 -0.098313

 28 6 0 -6.610317 -0.699802 -0.098313

 29 6 0 -5.420785 -1.432821 -0.071840

 30 6 0 1.432821 -5.420785 0.071840

 31 6 0 0.699802 -6.610317 0.098313

 32 6 0 -0.699802 -6.610317 0.098313

 33 6 0 -1.432821 -5.420785 0.071840

 34 6 0 5.420785 1.432821 -0.071840

 35 6 0 6.610317 0.699802 -0.098313

 36 6 0 6.610317 -0.699802 -0.098313

 37 6 0 5.420785 -1.432821 -0.071840

 38 6 0 -1.432821 5.420785 0.071840

 39 6 0 -0.699802 6.610317 0.098313

 40 6 0 0.699802 6.610317 0.098313

 41 6 0 1.432821 5.420785 0.071840

 42 1 0 7.565152 1.207886 -0.120969

 43 1 0 7.565152 -1.207886 -0.120969

 44 1 0 1.207886 7.565152 0.120969

 45 1 0 -1.207886 7.565152 0.120969

 46 1 0 -7.565152 1.207886 -0.120969

 47 1 0 -7.565152 -1.207886 -0.120969

 48 1 0 -1.207886 -7.565152 0.120969

 49 1 0 1.207886 -7.565152 0.120969

 50 8 0 2.783942 5.357598 0.073945

 51 8 0 -2.783942 5.357598 0.073945

 52 8 0 5.357598 2.783942 -0.073945

 53 8 0 5.357598 -2.783942 -0.073945

 54 8 0 2.783942 -5.357598 0.073945

 55 8 0 -2.783942 -5.357598 0.073945

 56 8 0 -5.357598 -2.783942 -0.073945

 57 8 0 -5.357598 2.783942 -0.073945

 58 6 0 3.514352 6.580615 0.102700

 59 1 0 3.303559 7.194357 -0.778514

 60 1 0 4.564460 6.293917 0.099713

 61 6 0 6.580615 3.514352 -0.102700

 62 1 0 7.194357 3.303559 0.778514

 63 1 0 6.293917 4.564460 -0.099713

 64 6 0 6.580615 -3.514352 -0.102700

 65 1 0 7.194357 -3.303559 0.778514

 66 1 0 6.293917 -4.564460 -0.099713

 67 6 0 -3.514352 6.580615 0.102700

 68 1 0 -3.303559 7.194357 -0.778514

 69 1 0 -4.564460 6.293917 0.099713

 70 6 0 -6.580615 3.514352 -0.102700

 71 1 0 -7.194357 3.303559 0.778514

 72 1 0 -6.293917 4.564460 -0.099713

 73 6 0 -6.580615 -3.514352 -0.102700

 74 1 0 -7.194357 -3.303559 0.778514

 75 1 0 -6.293917 -4.564460 -0.099713

 76 6 0 -3.514352 -6.580615 0.102700

 77 1 0 -3.303559 -7.194357 -0.778514

 78 1 0 -4.564460 -6.293917 0.099713

 79 6 0 3.514352 -6.580615 0.102700

 80 1 0 3.303559 -7.194357 -0.778514

 81 1 0 4.564460 -6.293917 0.099713

 82 1 0 3.298342 -7.155737 1.008335

 83 1 0 -3.298342 -7.155737 1.008335

 84 1 0 -7.155737 -3.298342 -1.008335

 85 1 0 -7.155737 3.298342 -1.008335

 86 1 0 3.298342 7.155737 1.008335

 87 1 0 -3.298342 7.155737 1.008335

 88 1 0 7.155737 -3.298342 -1.008335

 89 1 0 7.155737 3.298342 -1.008335

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

 Rotational constants (GHZ): 0.0443773 0.0443773 0.0222211

 Leave Link 202 at Thu Sep 19 00:35:41 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: 42 43 44 45 46 47 48 49 59 60

 Centers: 62 63 65 66 68 69 71 72 74 75

 Centers: 77 78 80 81 82 83 84 85 86 87

 Centers: 88 89 1 3 4 5 7 9 10 11

 Centers: 13 14 15 17 20 21 22 23 26 27

 Centers: 28 29 30 31 32 33 34 35 36 37

 Centers: 38 39 40 41 58 61 64 67 70 73

 Centers: 76 79 2 6 8 12 16 18 19 24

 Centers: 50 51 52 53 54 55 56 57

 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

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 28 6

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 58 6

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 59 1

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 88 1

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 89 1

 No pseudopotential on this center.

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

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

 There are 313 symmetry adapted cartesian basis functions of A1 symmetry.

 There are 284 symmetry adapted cartesian basis functions of A2 symmetry.

 There are 295 symmetry adapted cartesian basis functions of B1 symmetry.

 There are 295 symmetry adapted cartesian basis functions of B2 symmetry.

 There are 295 symmetry adapted basis functions of A1 symmetry.

 There are 271 symmetry adapted basis functions of A2 symmetry.

 There are 281 symmetry adapted basis functions of B1 symmetry.

 There are 281 symmetry adapted basis functions of B2 symmetry.

 1128 basis functions, 1991 primitive gaussians, 1187 cartesian basis functions

 202 alpha electrons 202 beta electrons

 nuclear repulsion energy 8035.3666833908 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= 89 NActive= 89 NUniq= 13 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T Big=F

 Integral buffers will be 131072 words long.

 Regular integral format.

 Two-electron integral symmetry is turned on.

 R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2282224176 Hartrees.

 Nuclear repulsion after empirical dispersion term = 8035.1384609732 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= 89.

 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 = 89

 GePol: Total number of spheres = 89

 GePol: Number of exposed spheres = 89 (100.00%)

 GePol: Number of points = 6354

 GePol: Average weight of points = 0.11

 GePol: Minimum weight of points = 0.46D-09

 GePol: Maximum weight of points = 0.18390

 GePol: Number of points with low weight = 400

 GePol: Fraction of low-weight points (<1% of avg) = 6.30%

 GePol: Cavity surface area = 706.313 Ang\*\*2

 GePol: Cavity volume = 803.517 Ang\*\*3

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

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

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

 PCM non-electrostatic energy = -0.0073357608 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 8035.1311252125 Hartrees.

 Leave Link 301 at Thu Sep 19 00:35:42 2019, MaxMem= 1342177280 cpu: 1.6

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

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

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

 One-electron integrals computed using PRISM.

 One-electron integral symmetry used in STVInt

 8 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 73920 NPrTT= 356010 LenC2= 44165 LenP2D= 111006.

 LDataN: DoStor=T MaxTD1= 5 Len= 102

 NBasis= 1128 RedAO= T EigKep= 2.70D-05 NBF= 295 271 281 281

 NBsUse= 1128 1.00D-06 EigRej= -1.00D+00 NBFU= 295 271 281 281

 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= 1124 1124 1140 1148 1148 MxSgAt= 89 MxSgA2= 89.

 Leave Link 302 at Thu Sep 19 00:35:44 2019, MaxMem= 1342177280 cpu: 17.5

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

 Leave Link 308 at Thu Sep 19 00:35:44 2019, MaxMem= 1342177280 cpu: 2.9

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

 DipDrv: MaxL=1.

 Leave Link 303 at Thu Sep 19 00:35:44 2019, MaxMem= 1342177280 cpu: 2.0

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

 ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 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= -2650.06149826476

 JPrj=0 DoOrth=F DoCkMO=F.

 Initial guess orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

 Leave Link 401 at Thu Sep 19 00:35:48 2019, MaxMem= 1342177280 cpu: 30.2

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

 Closed shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 4271036 IEndB= 4271036 NGot= 1342177280 MDV= 1339333041

 LenX= 1339333041 LenY= 1337922885

 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= 450000000 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 1.01D-14 for 6349.

 Iteration 1 A\*A^-1 deviation from orthogonality is 4.50D-15 for 4766 1350.

 Iteration 1 A^-1\*A deviation from unit magnitude is 1.05D-14 for 6349.

 Iteration 1 A^-1\*A deviation from orthogonality is 1.43D-12 for 5704 5477.

 E= -2648.75788848665

 DIIS: error= 9.56D-02 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -2648.75788848665 IErMin= 1 ErrMin= 9.56D-02

 ErrMax= 9.56D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.49D+00 BMatP= 1.49D+00

 IDIUse=3 WtCom= 4.44D-02 WtEn= 9.56D-01

 Coeff-Com: 0.100D+01

 Coeff-En: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.082 Goal= None Shift= 0.000

 GapD= 0.082 DampG=0.500 DampE=0.250 DampFc=0.1250 IDamp=-1.

 Damping current iteration by 1.25D-01

 RMSDP=2.57D-03 MaxDP=1.55D-01 OVMax= 1.91D-01

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 3.22D-04 CP: 1.00D+00

 E= -2648.98139279677 Delta-E= -0.223504310123 Rises=F Damp=T

 DIIS: error= 6.80D-02 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -2648.98139279677 IErMin= 2 ErrMin= 6.80D-02

 ErrMax= 6.80D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.63D-01 BMatP= 1.49D+00

 IDIUse=3 WtCom= 3.20D-01 WtEn= 6.80D-01

 Coeff-Com: -0.292D+01 0.392D+01

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

 Coeff: -0.936D+00 0.194D+01

 Gap= 0.073 Goal= None Shift= 0.000

 RMSDP=1.60D-03 MaxDP=9.07D-02 DE=-2.24D-01 OVMax= 6.88D-02

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 9.75D-04 CP: 9.96D-01 3.00D+00

 E= -2649.59095133369 Delta-E= -0.609558536920 Rises=F Damp=F

 DIIS: error= 5.07D-02 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 3 EnMin= -2649.59095133369 IErMin= 3 ErrMin= 5.07D-02

 ErrMax= 5.07D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.11D-01 BMatP= 8.63D-01

 IDIUse=3 WtCom= 4.93D-01 WtEn= 5.07D-01

 EnCoef did 100 forward-backward iterations

 Coeff-Com: 0.259D+01-0.276D+01 0.117D+01

 Coeff-En: 0.108D+00 0.234D-02 0.889D+00

 Coeff: 0.133D+01-0.136D+01 0.103D+01

 Gap= 0.071 Goal= None Shift= 0.000

 RMSDP=7.83D-04 MaxDP=5.28D-02 DE=-6.10D-01 OVMax= 6.98D-02

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 3.72D-04 CP: 9.95D-01 3.00D+00 2.93D-01

 E= -2649.78394714515 Delta-E= -0.192995811463 Rises=F Damp=F

 DIIS: error= 1.96D-02 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -2649.78394714515 IErMin= 4 ErrMin= 1.96D-02

 ErrMax= 1.96D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.81D-02 BMatP= 3.11D-01

 IDIUse=3 WtCom= 8.04D-01 WtEn= 1.96D-01

 Coeff-Com: -0.430D+00 0.537D+00 0.217D+00 0.675D+00

 Coeff-En: 0.000D+00 0.000D+00 0.120D+00 0.880D+00

 Coeff: -0.345D+00 0.432D+00 0.198D+00 0.715D+00

 Gap= 0.071 Goal= None Shift= 0.000

 RMSDP=2.10D-04 MaxDP=1.09D-02 DE=-1.93D-01 OVMax= 3.69D-02

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 7.00D-05 CP: 9.94D-01 3.00D+00 4.58D-01 6.93D-01

 E= -2649.82609640052 Delta-E= -0.042149255371 Rises=F Damp=F

 DIIS: error= 1.41D-03 at cycle 5 NSaved= 5.

 NSaved= 5 IEnMin= 5 EnMin= -2649.82609640052 IErMin= 5 ErrMin= 1.41D-03

 ErrMax= 1.41D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.65D-03 BMatP= 5.81D-02

 IDIUse=3 WtCom= 9.86D-01 WtEn= 1.41D-02

 Coeff-Com: -0.263D+00 0.308D+00 0.685D-01 0.405D+00 0.481D+00

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

 Coeff: -0.259D+00 0.304D+00 0.675D-01 0.399D+00 0.489D+00

 Gap= 0.070 Goal= None Shift= 0.000

 RMSDP=3.46D-05 MaxDP=2.58D-03 DE=-4.21D-02 OVMax= 9.42D-03

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 1.69D-05 CP: 9.94D-01 3.00D+00 4.48D-01 7.35D-01 6.60D-01

 E= -2649.82835453875 Delta-E= -0.002258138229 Rises=F Damp=F

 DIIS: error= 2.26D-04 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -2649.82835453875 IErMin= 6 ErrMin= 2.26D-04

 ErrMax= 2.26D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.31D-05 BMatP= 2.65D-03

 IDIUse=3 WtCom= 9.98D-01 WtEn= 2.26D-03

 Coeff-Com: -0.140D+00 0.161D+00 0.110D-01 0.156D+00 0.214D+00 0.598D+00

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

 Coeff: -0.140D+00 0.161D+00 0.110D-01 0.156D+00 0.213D+00 0.598D+00

 Gap= 0.070 Goal= None Shift= 0.000

 RMSDP=8.29D-06 MaxDP=4.22D-04 DE=-2.26D-03 OVMax= 1.32D-03

 Cycle 7 Pass 1 IDiag 1:

 RMSU= 5.85D-06 CP: 9.94D-01 3.00D+00 4.49D-01 7.34D-01 6.70D-01

 CP: 6.63D-01

 E= -2649.82838509610 Delta-E= -0.000030557345 Rises=F Damp=F

 DIIS: error= 1.07D-04 at cycle 7 NSaved= 7.

 NSaved= 7 IEnMin= 7 EnMin= -2649.82838509610 IErMin= 7 ErrMin= 1.07D-04

 ErrMax= 1.07D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.08D-05 BMatP= 4.31D-05

 IDIUse=3 WtCom= 9.99D-01 WtEn= 1.07D-03

 Coeff-Com: -0.593D-01 0.678D-01 0.122D-02 0.571D-01 0.756D-01 0.376D+00

 Coeff-Com: 0.481D+00

 Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.181D+00

 Coeff-En: 0.819D+00

 Coeff: -0.592D-01 0.678D-01 0.122D-02 0.570D-01 0.755D-01 0.376D+00

 Coeff: 0.482D+00

 Gap= 0.070 Goal= None Shift= 0.000

 RMSDP=3.29D-06 MaxDP=1.73D-04 DE=-3.06D-05 OVMax= 4.01D-04

 Cycle 8 Pass 1 IDiag 1:

 RMSU= 2.03D-06 CP: 9.94D-01 3.00D+00 4.49D-01 7.36D-01 6.66D-01

 CP: 7.42D-01 6.39D-01

 E= -2649.82839357634 Delta-E= -0.000008480240 Rises=F Damp=F

 DIIS: error= 3.38D-05 at cycle 8 NSaved= 8.

 NSaved= 8 IEnMin= 8 EnMin= -2649.82839357634 IErMin= 8 ErrMin= 3.38D-05

 ErrMax= 3.38D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.67D-07 BMatP= 1.08D-05

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

 Coeff-Com: -0.669D-02 0.753D-02-0.264D-04 0.581D-02 0.292D-02 0.987D-01

 Coeff-Com: 0.165D+00 0.727D+00

 Coeff: -0.669D-02 0.753D-02-0.264D-04 0.581D-02 0.292D-02 0.987D-01

 Coeff: 0.165D+00 0.727D+00

 Gap= 0.070 Goal= None Shift= 0.000

 RMSDP=7.27D-07 MaxDP=4.16D-05 DE=-8.48D-06 OVMax= 8.77D-05

 Cycle 9 Pass 1 IDiag 1:

 RMSU= 5.87D-07 CP: 9.94D-01 3.00D+00 4.49D-01 7.36D-01 6.68D-01

 CP: 7.60D-01 6.37D-01 8.86D-01

 E= -2649.82839378545 Delta-E= -0.000000209109 Rises=F Damp=F

 DIIS: error= 2.10D-05 at cycle 9 NSaved= 9.

 NSaved= 9 IEnMin= 9 EnMin= -2649.82839378545 IErMin= 9 ErrMin= 2.10D-05

 ErrMax= 2.10D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.17D-07 BMatP= 3.67D-07

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

 Coeff-Com: 0.109D-02-0.133D-02-0.889D-04-0.123D-02-0.486D-02 0.235D-01

 Coeff-Com: 0.426D-01 0.438D+00 0.502D+00

 Coeff: 0.109D-02-0.133D-02-0.889D-04-0.123D-02-0.486D-02 0.235D-01

 Coeff: 0.426D-01 0.438D+00 0.502D+00

 Gap= 0.070 Goal= None Shift= 0.000

 RMSDP=2.98D-07 MaxDP=2.36D-05 DE=-2.09D-07 OVMax= 6.82D-05

 Cycle 10 Pass 1 IDiag 1:

 RMSU= 1.98D-07 CP: 9.94D-01 3.00D+00 4.49D-01 7.36D-01 6.67D-01

 CP: 7.62D-01 6.46D-01 8.98D-01 6.78D-01

 E= -2649.82839388226 Delta-E= -0.000000096819 Rises=F Damp=F

 DIIS: error= 2.79D-06 at cycle 10 NSaved= 10.

 NSaved=10 IEnMin=10 EnMin= -2649.82839388226 IErMin=10 ErrMin= 2.79D-06

 ErrMax= 2.79D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.46D-09 BMatP= 1.17D-07

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

 Coeff-Com: 0.117D-02-0.138D-02-0.171D-04-0.106D-02-0.269D-02 0.504D-02

 Coeff-Com: 0.891D-02 0.171D+00 0.247D+00 0.572D+00

 Coeff: 0.117D-02-0.138D-02-0.171D-04-0.106D-02-0.269D-02 0.504D-02

 Coeff: 0.891D-02 0.171D+00 0.247D+00 0.572D+00

 Gap= 0.070 Goal= None Shift= 0.000

 RMSDP=1.08D-07 MaxDP=4.76D-06 DE=-9.68D-08 OVMax= 1.25D-05

 Cycle 11 Pass 1 IDiag 1:

 RMSU= 8.55D-08 CP: 9.94D-01 3.00D+00 4.49D-01 7.36D-01 6.67D-01

 CP: 7.62D-01 6.41D-01 8.91D-01 7.16D-01 8.60D-01

 E= -2649.82839388592 Delta-E= -0.000000003658 Rises=F Damp=F

 DIIS: error= 9.34D-07 at cycle 11 NSaved= 11.

 NSaved=11 IEnMin=11 EnMin= -2649.82839388592 IErMin=11 ErrMin= 9.34D-07

 ErrMax= 9.34D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.08D-09 BMatP= 5.46D-09

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

 Coeff-Com: 0.306D-03-0.354D-03-0.105D-04-0.285D-03-0.546D-03-0.129D-03

 Coeff-Com: -0.118D-02 0.224D-01 0.485D-01 0.326D+00 0.605D+00

 Coeff: 0.306D-03-0.354D-03-0.105D-04-0.285D-03-0.546D-03-0.129D-03

 Coeff: -0.118D-02 0.224D-01 0.485D-01 0.326D+00 0.605D+00

 Gap= 0.070 Goal= None Shift= 0.000

 RMSDP=3.48D-08 MaxDP=2.00D-06 DE=-3.66D-09 OVMax= 4.73D-06

 Cycle 12 Pass 1 IDiag 1:

 RMSU= 1.95D-08 CP: 9.94D-01 3.00D+00 4.49D-01 7.36D-01 6.67D-01

 CP: 7.63D-01 6.41D-01 8.94D-01 7.17D-01 8.99D-01

 CP: 8.99D-01

 E= -2649.82839388654 Delta-E= -0.000000000622 Rises=F Damp=F

 DIIS: error= 2.90D-07 at cycle 12 NSaved= 12.

 NSaved=12 IEnMin=12 EnMin= -2649.82839388654 IErMin=12 ErrMin= 2.90D-07

 ErrMax= 2.90D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.55D-11 BMatP= 1.08D-09

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

 Coeff-Com: -0.528D-04 0.620D-04-0.137D-04 0.651D-05 0.177D-04-0.248D-03

 Coeff-Com: -0.100D-02-0.474D-02-0.649D-03 0.927D-01 0.271D+00 0.643D+00

 Coeff: -0.528D-04 0.620D-04-0.137D-04 0.651D-05 0.177D-04-0.248D-03

 Coeff: -0.100D-02-0.474D-02-0.649D-03 0.927D-01 0.271D+00 0.643D+00

 Gap= 0.070 Goal= None Shift= 0.000

 RMSDP=1.02D-08 MaxDP=5.27D-07 DE=-6.22D-10 OVMax= 1.63D-06

 Cycle 13 Pass 1 IDiag 1:

 RMSU= 6.98D-09 CP: 9.94D-01 3.00D+00 4.49D-01 7.36D-01 6.67D-01

 CP: 7.63D-01 6.41D-01 8.94D-01 7.17D-01 9.15D-01

 CP: 9.05D-01 7.28D-01

 E= -2649.82839388658 Delta-E= -0.000000000035 Rises=F Damp=F

 DIIS: error= 3.94D-07 at cycle 13 NSaved= 13.

 NSaved=13 IEnMin=13 EnMin= -2649.82839388658 IErMin=12 ErrMin= 2.90D-07

 ErrMax= 3.94D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.64D-11 BMatP= 7.55D-11

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

 Coeff-Com: -0.214D-04 0.255D-04-0.761D-05-0.780D-05-0.699D-05-0.223D-03

 Coeff-Com: -0.518D-03-0.403D-02-0.325D-02 0.186D-01 0.876D-01 0.369D+00

 Coeff-Com: 0.533D+00

 Coeff: -0.214D-04 0.255D-04-0.761D-05-0.780D-05-0.699D-05-0.223D-03

 Coeff: -0.518D-03-0.403D-02-0.325D-02 0.186D-01 0.876D-01 0.369D+00

 Coeff: 0.533D+00

 Gap= 0.070 Goal= None Shift= 0.000

 RMSDP=4.40D-09 MaxDP=1.73D-07 DE=-3.46D-11 OVMax= 8.20D-07

 Error on total polarization charges = 0.07340

 SCF Done: E(RB3LYP) = -2649.82839389 A.U. after 13 cycles

 NFock= 13 Conv=0.44D-08 -V/T= 1.9850

 KE= 2.690097641994D+03 PE=-2.234733588692D+04 EE= 8.972278725823D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.60

 (included in total energy above)

 Leave Link 502 at Thu Sep 19 00:39:51 2019, MaxMem= 1342177280 cpu: 2155.5

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

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

 ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 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 5.14D-05

 Largest core mixing into a valence orbital is 2.46D-05

 Range of M.O.s used for correlation: 57 1128

 NBasis= 1128 NAE= 202 NBE= 202 NFC= 56 NFV= 0

 NROrb= 1072 NOA= 146 NOB= 146 NVA= 926 NVB= 926

 \*\*\*\* Warning!!: The largest alpha MO coefficient is 0.13233268D+02

 \*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.70030460D-01

 Leave Link 801 at Thu Sep 19 00:39:56 2019, MaxMem= 1342177280 cpu: 4.5

 (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 252071400000 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 9.66D-15 for 6352.

 Iteration 1 A\*A^-1 deviation from orthogonality is 2.66D-15 for 6352 747.

 Iteration 1 A^-1\*A deviation from unit magnitude is 9.55D-15 for 6352.

 Iteration 1 A^-1\*A deviation from orthogonality is 1.80D-15 for 2677 2027.

 Making orbital integer symmetry assigments:

 Orbital symmetries:

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

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

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

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

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

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

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

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

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

 (A2)

 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: 270392

 Iteration 1 Dimension 40 NMult 0 NNew 40

 CISAX will form 40 AO SS matrices at one time.

 NMat= 40 NSing= 40 JSym2X=-1.

 FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

 IRaf= 0 NMat= 80 IRICut= 100 DoRegI=T DoRafI=T ISym2E=-1.

 New state 1 was old state 2

 New state 2 was old state 1

 New state 3 was old state 7

 New state 4 was old state 6

 New state 5 was old state 3

 New state 6 was old state 4

 New state 7 was old state 5

 New state 9 was old state 12

 New state 10 was old state 13

 Excitation Energies [eV] at current iteration:

 Root 1 : 1.900181167959592

 Root 2 : 1.900181167962491

 Root 3 : 2.484361198846707

 Root 4 : 2.583202314384637

 Root 5 : 2.600007276620242

 Root 6 : 2.600007276626787

 Root 7 : 2.692646640914146

 Root 8 : 2.903190826581534

 Root 9 : 3.133039755525036

 Root 10 : 3.133039755525115

 Root 11 : 3.272023548535302

 Root 12 : 3.321641925066158

 Root 13 : 3.321641925068831

 Root 14 : 3.575335076057715

 Root 15 : 3.575335076060520

 Root 16 : 3.591708845242723

 Root 17 : 3.591708845256204

 Root 18 : 3.597090404400112

 Root 19 : 3.611498540993447

 Root 20 : 3.631857304973446

 Root 21 : 3.641497150757556

 Root 22 : 3.661601738624640

 Root 23 : 3.679427398487915

 Root 24 : 3.784492961789394

 Root 25 : 3.823158333978653

 Root 26 : 3.900212539688958

 Root 27 : 3.900212539690033

 Root 28 : 4.022220642153778

 Root 29 : 4.022220642162383

 Root 30 : 4.184368936600251

 Root 31 : 4.205568621858740

 Root 32 : 4.319135554485383

 Root 33 : 4.319135554486715

 Root 34 : 4.376219730551119

 Root 35 : 4.376219730552508

 Root 36 : 4.409177647231946

 Root 37 : 4.799635976650545

 Root 38 : 4.799635976650699

 Root 39 : 5.020884230945949

 Root 40 : 5.198377823645767

 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 0.057231313645281

 Root 2 not converged, maximum delta is 0.057231313644880

 Root 3 not converged, maximum delta is 0.020269679046072

 New state 4 was old state 5

 Root 4 not converged, maximum delta is 0.049093039924765

 New state 5 was old state 6

 Root 5 not converged, maximum delta is 0.049093039922728

 New state 6 was old state 4

 Root 6 not converged, maximum delta is 0.050219065977987

 Root 7 not converged, maximum delta is 0.065641748071347

 Root 8 not converged, maximum delta is 0.102613532499864

 Root 9 not converged, maximum delta is 0.392421749244570

 Root 10 not converged, maximum delta is 0.392421749242944

 Excitation Energies [eV] at current iteration:

 Root 1 : 1.719166794607738 Change is -0.181014373351854

 Root 2 : 1.719166794610989 Change is -0.181014373351501

 Root 3 : 2.466419677395415 Change is -0.017941521451292

 Root 4 : 2.496998476169038 Change is -0.103008800451204

 Root 5 : 2.496998476177334 Change is -0.103008800449453

 Root 6 : 2.507286167569716 Change is -0.075916146814921

 Root 7 : 2.543048643823086 Change is -0.149597997091060

 Root 8 : 2.665916903084227 Change is -0.237273923497308

 Root 9 : 3.077962826907945 Change is -0.055076928617091

 Root 10 : 3.077962826909841 Change is -0.055076928615274

 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 0.017947308209105

 Root 2 not converged, maximum delta is 0.017947308208187

 Root 3 not converged, maximum delta is 0.002494424463759

 Root 4 not converged, maximum delta is 0.006621684521004

 Root 5 not converged, maximum delta is 0.006621684521185

 Root 6 not converged, maximum delta is 0.006420946865318

 Root 7 not converged, maximum delta is 0.051879899740317

 Root 8 not converged, maximum delta is 0.011785879574896

 Root 9 not converged, maximum delta is 0.010714193160829

 Root 10 not converged, maximum delta is 0.010714193167414

 Excitation Energies [eV] at current iteration:

 Root 1 : 1.705030418556449 Change is -0.014136376051289

 Root 2 : 1.705030418560499 Change is -0.014136376050490

 Root 3 : 2.465642197857280 Change is -0.000777479538134

 Root 4 : 2.492954181575997 Change is -0.004044294593040

 Root 5 : 2.492954181584406 Change is -0.004044294592928

 Root 6 : 2.504442458077695 Change is -0.002843709492021

 Root 7 : 2.530021227200907 Change is -0.013027416622179

 Root 8 : 2.654477217193296 Change is -0.011439685890931

 Root 9 : 3.075977584626894 Change is -0.001985242281050

 Root 10 : 3.075977584628204 Change is -0.001985242281637

 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 0.011301101627306

 Root 2 not converged, maximum delta is 0.011301101627295

 Root 3 has converged.

 Root 4 not converged, maximum delta is 0.002083397827316

 Root 5 not converged, maximum delta is 0.002083397827773

 Root 6 not converged, maximum delta is 0.003994277321353

 Root 7 not converged, maximum delta is 0.003100540038221

 Root 8 not converged, maximum delta is 0.003203379810082

 Root 9 not converged, maximum delta is 0.005316419307843

 Root 10 not converged, maximum delta is 0.005316419305105

 Excitation Energies [eV] at current iteration:

 Root 1 : 1.703735422937954 Change is -0.001294995618495

 Root 2 : 1.703735422941958 Change is -0.001294995618541

 Root 3 : 2.465516339827831 Change is -0.000125858029449

 Root 4 : 2.492343270709044 Change is -0.000610910866952

 Root 5 : 2.492343270717192 Change is -0.000610910867215

 Root 6 : 2.503920463157269 Change is -0.000521994920426

 Root 7 : 2.528718080662327 Change is -0.001303146538580

 Root 8 : 2.653191803404130 Change is -0.001285413789165

 Root 9 : 3.075704930226319 Change is -0.000272654400576

 Root 10 : 3.075704930227816 Change is -0.000272654400388

 Iteration 5 Dimension 118 NMult 100 NNew 18

 CISAX will form 18 AO SS matrices at one time.

 NMat= 18 NSing= 18 JSym2X=-1.

 Root 1 not converged, maximum delta is 0.011300784358852

 Root 2 not converged, maximum delta is 0.011300784358842

 Root 3 has converged.

 Root 4 has converged.

 Root 5 has converged.

 Root 6 has converged.

 Root 7 has converged.

 Root 8 has converged.

 Root 9 not converged, maximum delta is 0.002742753269541

 Root 10 not converged, maximum delta is 0.002742753265360

 Excitation Energies [eV] at current iteration:

 Root 1 : 1.703592254557351 Change is -0.000143168380603

 Root 2 : 1.703592254561549 Change is -0.000143168380409

 Root 3 : 2.465516339827864 Change is 0.000000000000033

 Root 4 : 2.492302379000745 Change is -0.000040891708300

 Root 5 : 2.492302379008794 Change is -0.000040891708398

 Root 6 : 2.503860227245328 Change is -0.000060235911941

 Root 7 : 2.528600019293039 Change is -0.000118061369288

 Root 8 : 2.652996303208161 Change is -0.000195500195969

 Root 9 : 3.075669241324304 Change is -0.000035688902015

 Root 10 : 3.075669241325881 Change is -0.000035688901934

 Iteration 6 Dimension 126 NMult 118 NNew 8

 CISAX will form 8 AO SS matrices at one time.

 NMat= 8 NSing= 8 JSym2X=-1.

 Root 1 has converged.

 Root 2 has converged.

 Root 3 has converged.

 Root 4 has converged.

 Root 5 has converged.

 Root 6 has converged.

 Root 7 has converged.

 Root 8 has converged.

 Root 9 has converged.

 Root 10 has converged.

 Excitation Energies [eV] at current iteration:

 Root 1 : 1.703582990164302 Change is -0.000009264393049

 Root 2 : 1.703582990168645 Change is -0.000009264392904

 Root 3 : 2.465516339827864 Change is 0.000000000000000

 Root 4 : 2.492301355074880 Change is -0.000001023925865

 Root 5 : 2.492301355083126 Change is -0.000001023925667

 Root 6 : 2.503860227245328 Change is 0.000000000000000

 Root 7 : 2.528600019293039 Change is 0.000000000000000

 Root 8 : 2.652996303208161 Change is 0.000000000000000

 Root 9 : 3.075665165743650 Change is -0.000004075580654

 Root 10 : 3.075665165745120 Change is -0.000004075580761

 Convergence achieved on expansion vectors.

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

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

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

 1PDM for each excited state written to RWF 633

 Ground to excited state transition densities written to RWF 633

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

 state X Y Z Dip. S. Osc.

 1 -0.0000 4.0038 0.0000 16.0308 0.6691

 2 -4.0038 -0.0000 -0.0000 16.0308 0.6691

 3 -0.0000 0.0000 0.0000 0.0000 0.0000

 4 -1.9979 0.0000 0.0000 3.9916 0.2437

 5 -0.0000 -1.9979 -0.0000 3.9916 0.2437

 6 -0.0000 -0.0000 -0.0000 0.0000 0.0000

 7 -0.0000 -0.0000 0.0590 0.0035 0.0002

 8 0.0000 -0.0000 -0.0000 0.0000 0.0000

 9 -0.1377 -0.0000 -0.0000 0.0189 0.0014

 10 -0.0000 0.1377 0.0000 0.0189 0.0014

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

 state X Y Z Dip. S. Osc.

 1 0.0000 -0.2509 -0.0000 0.0630 0.6704

 2 0.2509 0.0000 0.0000 0.0630 0.6704

 3 0.0000 -0.0000 -0.0000 0.0000 0.0000

 4 0.1806 -0.0000 -0.0000 0.0326 0.2373

 5 0.0000 0.1806 0.0000 0.0326 0.2373

 6 0.0000 0.0000 0.0000 0.0000 0.0000

 7 0.0000 0.0000 -0.0056 0.0000 0.0002

 8 -0.0000 0.0000 -0.0000 0.0000 0.0000

 9 0.0162 0.0000 0.0000 0.0003 0.0015

 10 -0.0000 -0.0162 -0.0000 0.0003 0.0015

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

 state X Y Z

 1 -0.0126 0.0000 0.0000

 2 0.0000 0.0126 0.0000

 3 -0.0000 0.0000 1.2582

 4 0.0000 0.0111 0.0000

 5 0.0111 0.0000 0.0000

 6 0.0000 0.0000 -0.0000

 7 0.0000 -0.0000 -0.0000

 8 0.0000 0.0000 -0.0000

 9 0.0000 0.4245 0.0000

 10 -0.4245 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 -0.0369

 2 0.0000 0.0000 0.0000 -0.0000 -0.0369 0.0000

 3 0.0000 -0.0000 0.0000 0.0000 -0.0000 -0.0000

 4 0.0000 0.0000 0.0000 0.0000 -0.0435 -0.0000

 5 -0.0000 0.0000 -0.0000 0.0000 -0.0000 0.0435

 6 -0.0000 -0.0000 -0.0000 -0.3812 -0.0000 0.0000

 7 2.0536 -2.0536 -0.0000 0.0000 0.0000 0.0000

 8 1.5007 1.5007 0.0100 -0.0000 -0.0000 0.0000

 9 -0.0000 0.0000 -0.0000 0.0000 -0.1071 0.0000

 10 0.0000 -0.0000 0.0000 0.0000 0.0000 -0.1071

 <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 -1.0046 -0.0000 1.0046 0.6697

 2 -1.0046 -0.0000 -0.0000 1.0046 0.6697

 3 -0.0000 -0.0000 -0.0000 0.0000 0.0000

 4 -0.3607 -0.0000 -0.0000 0.3607 0.2405

 5 -0.0000 -0.3607 -0.0000 0.3607 0.2405

 6 -0.0000 -0.0000 -0.0000 0.0000 0.0000

 7 -0.0000 -0.0000 -0.0003 0.0003 0.0002

 8 -0.0000 -0.0000 0.0000 -0.0000 -0.0000

 9 -0.0022 -0.0000 -0.0000 0.0022 0.0015

 10 0.0000 -0.0022 -0.0000 0.0022 0.0015

 Excitation energies and oscillator strengths:

 Excited State 1: Singlet-E 1.7036 eV 727.78 nm f=0.6691 <S\*\*2>=0.000

 71 -> 289 -0.00104

 72 -> 282 -0.00106

 90 -> 272 0.00115

 97 -> 256 0.00109

 101 -> 282 0.00107

 102 -> 272 0.00107

 105 -> 291 -0.00184

 105 -> 334 -0.00128

 110 -> 222 -0.00136

 110 -> 227 0.00129

 110 -> 246 0.00119

 110 -> 272 -0.00103

 111 -> 266 -0.00107

 112 -> 291 0.00120

 114 -> 225 0.00159

 114 -> 229 -0.00100

 115 -> 258 -0.00237

 115 -> 265 0.00105

 115 -> 272 0.00163

 115 -> 287 -0.00212

 116 -> 266 0.00212

 116 -> 280 0.00115

 116 -> 285 -0.00183

 116 -> 288 -0.00103

 116 -> 314 -0.00149

 116 -> 389 0.00169

 116 -> 402 0.00118

 116 -> 435 0.00103

 117 -> 232 0.00202

 118 -> 230 0.00199

 118 -> 235 0.00147

 118 -> 236 0.00256

 120 -> 228 -0.00116

 120 -> 232 0.00198

 120 -> 278 -0.00107

 122 -> 216 -0.00102

 122 -> 222 -0.00104

 123 -> 230 0.00128

 123 -> 266 0.00102

 125 -> 220 -0.00155

 125 -> 232 0.00132

 125 -> 256 0.00114

 125 -> 263 0.00116

 125 -> 269 -0.00314

 125 -> 278 0.00280

 125 -> 301 -0.00128

 125 -> 322 0.00105

 125 -> 372 -0.00134

 125 -> 443 -0.00115

 126 -> 256 -0.00105

 126 -> 274 -0.00117

 127 -> 227 -0.00220

 127 -> 234 -0.00148

 127 -> 258 0.00135

 127 -> 267 -0.00187

 127 -> 275 0.00123

 127 -> 293 0.00117

 128 -> 230 0.00110

 128 -> 254 0.00110

 128 -> 257 -0.00108

 129 -> 203 0.00131

 129 -> 237 -0.00110

 129 -> 247 0.00133

 129 -> 318 -0.00124

 130 -> 213 -0.00114

 131 -> 205 0.00171

 132 -> 203 -0.00150

 133 -> 225 -0.00164

 133 -> 229 0.00112

 137 -> 204 -0.00109

 138 -> 207 0.00178

 138 -> 237 -0.00230

 138 -> 239 -0.00114

 138 -> 247 0.00102

 138 -> 318 -0.00137

 139 -> 228 -0.00151

 139 -> 244 -0.00110

 139 -> 256 0.00160

 139 -> 263 0.00224

 139 -> 269 0.00150

 139 -> 274 -0.00173

 139 -> 281 -0.00259

 140 -> 218 0.00182

 140 -> 222 -0.00174

 140 -> 227 0.00122

 140 -> 231 -0.00145

 140 -> 234 -0.00180

 140 -> 242 0.00144

 140 -> 258 0.00257

 140 -> 272 0.00101

 141 -> 289 -0.00189

 142 -> 224 -0.00128

 142 -> 232 0.00100

 142 -> 256 0.00127

 142 -> 263 -0.00123

 143 -> 206 -0.00303

 143 -> 209 -0.00262

 143 -> 213 -0.00289

 143 -> 221 0.00232

 143 -> 241 -0.00168

 143 -> 253 -0.00144

 143 -> 348 0.00114

 144 -> 205 0.00232

 144 -> 223 -0.00272

 144 -> 260 -0.00125

 145 -> 225 -0.00181

 145 -> 229 0.00132

 145 -> 243 -0.00191

 145 -> 282 -0.00172

 145 -> 284 0.00102

 146 -> 217 -0.00250

 146 -> 226 -0.00179

 146 -> 235 0.00104

 146 -> 254 0.00156

 146 -> 257 -0.00150

 146 -> 266 -0.00105

 146 -> 270 0.00155

 148 -> 214 0.00200

 148 -> 224 -0.00169

 148 -> 244 0.00105

 148 -> 256 0.00154

 148 -> 269 0.00103

 149 -> 203 -0.00585

 149 -> 207 0.00114

 149 -> 212 -0.00160

 149 -> 318 -0.00175

 150 -> 215 -0.00154

 150 -> 225 -0.00171

 150 -> 243 -0.00234

 150 -> 273 -0.00135

 151 -> 216 -0.00297

 151 -> 222 -0.00236

 151 -> 231 -0.00114

 151 -> 242 0.00274

 151 -> 246 -0.00154

 151 -> 265 0.00104

 152 -> 217 0.00135

 153 -> 215 0.00296

 153 -> 219 -0.00126

 153 -> 233 -0.00146

 153 -> 243 0.00170

 154 -> 239 0.00144

 154 -> 243 -0.00205

 155 -> 216 -0.00178

 155 -> 234 0.00212

 155 -> 246 0.00178

 155 -> 258 0.00138

 156 -> 235 0.00182

 156 -> 257 0.00129

 156 -> 266 0.00111

 156 -> 285 -0.00116

 156 -> 289 0.00194

 157 -> 228 -0.00144

 157 -> 244 -0.00102

 157 -> 256 0.00168

 157 -> 283 -0.00118

 158 -> 226 0.00104

 158 -> 230 -0.00109

 158 -> 235 0.00155

 158 -> 236 0.00117

 158 -> 257 0.00117

 158 -> 276 0.00148

 158 -> 280 -0.00105

 158 -> 289 -0.00189

 158 -> 303 0.00124

 158 -> 315 0.00118

 158 -> 326 -0.00103

 159 -> 218 0.00131

 159 -> 246 0.00165

 159 -> 258 0.00269

 159 -> 267 -0.00116

 159 -> 275 0.00151

 159 -> 286 0.00121

 160 -> 219 -0.00139

 160 -> 239 0.00135

 160 -> 268 -0.00130

 160 -> 282 0.00252

 160 -> 284 -0.00149

 160 -> 302 -0.00113

 160 -> 333 0.00120

 161 -> 416 -0.00103

 162 -> 204 0.00550

 162 -> 208 -0.00168

 162 -> 211 0.00194

 162 -> 262 -0.00145

 162 -> 319 -0.00131

 162 -> 336 -0.00124

 163 -> 204 0.00140

 163 -> 240 0.00222

 163 -> 263 0.00171

 163 -> 274 -0.00266

 163 -> 281 -0.00135

 164 -> 203 0.00328

 164 -> 207 -0.00137

 164 -> 237 0.00121

 164 -> 335 0.00181

 165 -> 206 -0.00353

 165 -> 209 -0.00221

 165 -> 213 -0.00130

 165 -> 221 0.00149

 165 -> 241 -0.00123

 165 -> 325 -0.00146

 165 -> 327 -0.00150

 165 -> 346 -0.00104

 165 -> 348 0.00116

 166 -> 223 -0.00152

 167 -> 203 -0.00619

 167 -> 207 0.00360

 167 -> 212 -0.00230

 167 -> 335 -0.00188

 168 -> 209 0.00139

 168 -> 221 -0.00101

 169 -> 223 0.00196

 169 -> 259 -0.00133

 169 -> 339 0.00122

 169 -> 357 -0.00156

 170 -> 238 -0.00108

 170 -> 354 -0.00119

 171 -> 204 -0.00552

 171 -> 208 0.00209

 171 -> 211 -0.00296

 172 -> 239 -0.00113

 172 -> 243 -0.00122

 172 -> 264 -0.00122

 173 -> 254 -0.00116

 173 -> 288 -0.00114

 174 -> 218 -0.00161

 174 -> 222 -0.00102

 174 -> 231 0.00116

 174 -> 234 -0.00146

 174 -> 242 -0.00145

 174 -> 265 -0.00196

 174 -> 267 -0.00142

 175 -> 225 0.00100

 175 -> 239 -0.00156

 175 -> 243 -0.00102

 175 -> 264 -0.00127

 176 -> 230 0.00102

 176 -> 257 0.00140

 176 -> 266 0.00234

 176 -> 276 -0.00115

 176 -> 285 -0.00297

 176 -> 314 -0.00121

 176 -> 343 0.00121

 177 -> 216 -0.00215

 177 -> 218 0.00651

 177 -> 258 0.00353

 177 -> 265 -0.00100

 177 -> 267 0.00233

 177 -> 272 -0.00106

 177 -> 287 -0.00263

 178 -> 256 -0.00257

 178 -> 278 0.00192

 179 -> 218 0.00461

 179 -> 258 0.00110

 179 -> 267 0.00115

 179 -> 275 -0.00233

 179 -> 287 -0.00220

 180 -> 235 0.00118

 180 -> 254 0.00276

 180 -> 257 -0.00195

 180 -> 266 0.00211

 180 -> 276 0.00102

 180 -> 288 0.00164

 180 -> 314 -0.00211

 181 -> 256 0.00264

 181 -> 281 0.00212

 181 -> 283 0.00136

 181 -> 291 0.00134

 182 -> 206 -0.00336

 182 -> 209 0.00467

 182 -> 213 0.00108

 182 -> 221 0.00338

 182 -> 271 0.00129

 183 -> 205 0.00539

 183 -> 210 -0.00544

 183 -> 223 -0.00210

 183 -> 259 0.00122

 183 -> 339 -0.00163

 183 -> 368 -0.00113

 184 -> 203 -0.00463

 184 -> 207 -0.00456

 184 -> 212 -0.00252

 184 -> 237 -0.00245

 184 -> 239 -0.00123

 184 -> 247 -0.00116

 185 -> 203 -0.00116

 185 -> 207 -0.00447

 185 -> 212 -0.00406

 185 -> 237 -0.00146

 185 -> 247 -0.00199

 185 -> 335 -0.00123

 186 -> 206 0.00659

 186 -> 209 0.00358

 186 -> 213 -0.00273

 186 -> 221 0.00220

 186 -> 241 -0.00293

 186 -> 245 -0.00232

 186 -> 346 -0.00146

 186 -> 348 0.00106

 187 -> 205 0.00312

 187 -> 210 -0.00282

 187 -> 223 -0.00236

 188 -> 233 0.00139

 188 -> 268 -0.00159

 188 -> 279 0.00207

 188 -> 284 -0.00134

 188 -> 292 0.00163

 189 -> 216 -0.00115

 189 -> 218 0.00389

 189 -> 234 -0.00102

 189 -> 265 0.00365

 189 -> 271 -0.00162

 189 -> 272 0.00602

 189 -> 287 -0.00219

 189 -> 293 0.00185

 189 -> 310 -0.00171

 190 -> 205 -0.00114

 190 -> 230 0.00152

 190 -> 266 0.00250

 190 -> 285 -0.00236

 190 -> 300 0.00115

 190 -> 314 -0.00153

 190 -> 324 -0.00107

 190 -> 337 -0.00172

 191 -> 203 0.00271

 191 -> 215 0.00164

 191 -> 219 0.00262

 191 -> 233 -0.00144

 191 -> 255 -0.00118

 191 -> 264 -0.00183

 191 -> 268 0.00441

 191 -> 279 -0.00402

 191 -> 282 0.00151

 191 -> 284 -0.00255

 191 -> 302 -0.00152

 191 -> 309 -0.00192

 191 -> 312 0.00259

 191 -> 321 -0.00115

 191 -> 353 -0.00125

 191 -> 400 0.00101

 191 -> 416 0.00141

 192 -> 203 0.02474

 192 -> 207 -0.00215

 192 -> 212 -0.00175

 192 -> 247 -0.00177

 192 -> 261 -0.00220

 192 -> 335 -0.00106

 192 -> 355 0.00139

 192 -> 363 -0.00144

 193 -> 206 -0.00616

 193 -> 209 -0.00860

 193 -> 213 -0.00457

 193 -> 221 0.00242

 193 -> 241 -0.00224

 193 -> 245 0.00115

 193 -> 253 -0.00338

 193 -> 271 -0.00151

 193 -> 346 0.00166

 193 -> 348 -0.00151

 193 -> 375 -0.00122

 194 -> 205 -0.00663

 194 -> 210 -0.00549

 194 -> 223 -0.00332

 194 -> 259 0.00232

 194 -> 260 -0.00294

 195 -> 203 -0.00661

 195 -> 207 0.00924

 195 -> 212 -0.00479

 195 -> 237 -0.00166

 195 -> 247 0.00210

 195 -> 261 -0.00227

 195 -> 355 -0.00113

 195 -> 363 0.00176

 196 -> 203 -0.10434

 196 -> 207 0.00643

 196 -> 212 -0.01187

 196 -> 261 -0.00198

 197 -> 204 -0.00682

 197 -> 220 0.00153

 197 -> 263 -0.00231

 197 -> 274 0.00240

 197 -> 278 -0.00260

 197 -> 283 0.00239

 197 -> 291 -0.00374

 197 -> 299 -0.00104

 197 -> 301 -0.00129

 197 -> 322 0.00108

 198 -> 204 -0.03894

 198 -> 208 -0.00637

 198 -> 211 -0.00250

 198 -> 238 0.00105

 198 -> 248 -0.00129

 198 -> 250 0.00204

 198 -> 262 -0.00110

 198 -> 354 0.00197

 199 -> 205 -0.02850

 199 -> 210 0.00998

 199 -> 223 0.00346

 199 -> 249 -0.00339

 199 -> 252 -0.00310

 199 -> 259 -0.00276

 199 -> 357 0.00167

 199 -> 368 0.00137

 200 -> 206 -0.01057

 200 -> 209 -0.00386

 200 -> 213 0.00333

 200 -> 221 0.01216

 200 -> 241 0.00204

 200 -> 245 0.00124

 200 -> 253 0.00204

 201 -> 204 0.03625

 201 -> 208 -0.00378

 201 -> 211 0.01051

 201 -> 238 -0.00359

 201 -> 240 -0.00174

 201 -> 248 0.00238

 201 -> 250 0.00391

 201 -> 262 -0.00144

 201 -> 354 0.00120

 201 -> 364 0.00101

 202 -> 204 0.70059

 202 -> 208 -0.00145

 202 -> 211 0.00160

 202 -> 238 -0.00154

 202 -> 250 -0.00300

 202 -> 262 0.00181

 202 -> 364 -0.00111

 202 -> 381 -0.00209

 202 -> 425 0.00114

 90 <- 272 0.00107

 105 <- 291 -0.00159

 105 <- 334 -0.00113

 110 <- 222 -0.00108

 110 <- 227 0.00102

 112 <- 291 0.00103

 114 <- 225 0.00126

 115 <- 258 -0.00202

 115 <- 272 0.00145

 115 <- 287 -0.00188

 116 <- 266 0.00177

 116 <- 280 0.00102

 116 <- 285 -0.00155

 116 <- 314 -0.00130

 116 <- 389 0.00150

 116 <- 402 0.00104

 117 <- 232 0.00161

 118 <- 230 0.00157

 118 <- 235 0.00117

 118 <- 236 0.00203

 120 <- 232 0.00156

 123 <- 230 0.00101

 125 <- 220 -0.00124

 125 <- 232 0.00107

 125 <- 269 -0.00265

 125 <- 278 0.00241

 125 <- 301 -0.00111

 125 <- 372 -0.00118

 125 <- 443 -0.00103

 127 <- 227 -0.00171

 127 <- 234 -0.00117

 127 <- 258 0.00111

 127 <- 267 -0.00153

 127 <- 275 0.00102

 129 <- 203 0.00107

 129 <- 247 0.00109

 129 <- 318 -0.00108

 133 <- 225 -0.00125

 138 <- 207 0.00127

 138 <- 237 -0.00190

 138 <- 318 -0.00123

 139 <- 228 -0.00117

 139 <- 256 0.00128

 139 <- 263 0.00186

 139 <- 269 0.00123

 139 <- 274 -0.00145

 139 <- 281 -0.00219

 140 <- 218 0.00134

 140 <- 222 -0.00131

 140 <- 231 -0.00112

 140 <- 234 -0.00141

 140 <- 242 0.00113

 140 <- 258 0.00208

 141 <- 289 -0.00160

 142 <- 256 0.00101

 143 <- 206 -0.00219

 143 <- 209 -0.00191

 143 <- 213 -0.00217

 143 <- 221 0.00189

 143 <- 241 -0.00153

 143 <- 253 -0.00138

 144 <- 205 0.00146

 144 <- 223 -0.00192

 145 <- 225 -0.00135

 145 <- 243 -0.00149

 145 <- 282 -0.00142

 146 <- 217 -0.00187

 146 <- 226 -0.00135

 146 <- 254 0.00123

 146 <- 257 -0.00118

 146 <- 270 0.00124

 148 <- 214 0.00149

 148 <- 224 -0.00127

 148 <- 256 0.00122

 149 <- 203 -0.00305

 149 <- 212 -0.00124

 149 <- 318 -0.00143

 150 <- 215 -0.00113

 150 <- 225 -0.00127

 150 <- 243 -0.00179

 150 <- 273 -0.00109

 151 <- 216 -0.00218

 151 <- 222 -0.00174

 151 <- 242 0.00210

 151 <- 246 -0.00118

 152 <- 217 0.00100

 153 <- 215 0.00217

 153 <- 233 -0.00111

 153 <- 243 0.00130

 154 <- 239 0.00107

 154 <- 243 -0.00156

 155 <- 216 -0.00129

 155 <- 234 0.00157

 155 <- 246 0.00134

 155 <- 258 0.00113

 156 <- 235 0.00137

 156 <- 289 0.00158

 157 <- 228 -0.00107

 157 <- 256 0.00129

 158 <- 235 0.00115

 158 <- 276 0.00118

 158 <- 289 -0.00160

 158 <- 303 0.00103

 159 <- 246 0.00124

 159 <- 258 0.00214

 159 <- 275 0.00123

 160 <- 219 -0.00103

 160 <- 268 -0.00107

 160 <- 282 0.00206

 160 <- 284 -0.00122

 160 <- 333 0.00101

 162 <- 204 0.00423

 162 <- 211 0.00130

 162 <- 238 0.00103

 162 <- 262 -0.00112

 162 <- 319 -0.00104

 162 <- 336 -0.00104

 163 <- 204 0.00107

 163 <- 240 0.00174

 163 <- 263 0.00137

 163 <- 274 -0.00214

 163 <- 281 -0.00112

 164 <- 203 0.00269

 164 <- 207 -0.00105

 164 <- 237 0.00103

 164 <- 335 0.00155

 165 <- 206 -0.00258

 165 <- 209 -0.00164

 165 <- 221 0.00110

 165 <- 241 -0.00109

 165 <- 325 -0.00116

 165 <- 327 -0.00125

 165 <- 348 0.00103

 166 <- 223 -0.00125

 167 <- 203 -0.00268

 167 <- 207 0.00284

 167 <- 212 -0.00188

 167 <- 335 -0.00151

 168 <- 209 0.00119

 169 <- 259 -0.00113

 169 <- 357 -0.00132

 170 <- 354 -0.00100

 171 <- 204 -0.00438

 171 <- 211 -0.00165

 174 <- 218 -0.00112

 174 <- 234 -0.00107

 174 <- 242 -0.00106

 174 <- 265 -0.00152

 174 <- 267 -0.00110

 175 <- 239 -0.00113

 176 <- 257 0.00104

 176 <- 266 0.00182

 176 <- 285 -0.00236

 176 <- 343 0.00100

 177 <- 216 -0.00148

 177 <- 218 0.00449

 177 <- 258 0.00265

 177 <- 267 0.00181

 177 <- 287 -0.00209

 178 <- 256 -0.00192

 178 <- 278 0.00151

 179 <- 218 0.00315

 179 <- 275 -0.00186

 179 <- 287 -0.00177

 180 <- 254 0.00205

 180 <- 257 -0.00145

 180 <- 266 0.00161

 180 <- 288 0.00129

 180 <- 314 -0.00174

 181 <- 256 0.00196

 181 <- 281 0.00168

 181 <- 283 0.00107

 181 <- 291 0.00110

 182 <- 206 -0.00160

 182 <- 209 0.00279

 182 <- 213 0.00103

 182 <- 221 0.00117

 182 <- 271 0.00124

 183 <- 210 -0.00404

 183 <- 339 -0.00120

 184 <- 203 -0.00259

 184 <- 207 -0.00247

 184 <- 212 -0.00160

 184 <- 237 -0.00178

 185 <- 207 -0.00194

 185 <- 212 -0.00265

 185 <- 237 -0.00140

 185 <- 247 -0.00109

 185 <- 335 -0.00104

 186 <- 206 0.00311

 186 <- 209 0.00177

 186 <- 213 -0.00183

 186 <- 221 0.00212

 186 <- 241 -0.00217

 186 <- 245 -0.00150

 186 <- 346 -0.00122

 187 <- 210 -0.00205

 188 <- 268 -0.00118

 188 <- 279 0.00157

 188 <- 284 -0.00105

 188 <- 292 0.00129

 189 <- 218 0.00248

 189 <- 265 0.00273

 189 <- 271 -0.00117

 189 <- 272 0.00454

 189 <- 287 -0.00173

 189 <- 293 0.00148

 189 <- 310 -0.00139

 190 <- 230 0.00104

 190 <- 266 0.00187

 190 <- 285 -0.00181

 190 <- 314 -0.00122

 190 <- 337 -0.00141

 191 <- 203 0.00143

 191 <- 215 0.00104

 191 <- 219 0.00167

 191 <- 264 -0.00131

 191 <- 268 0.00328

 191 <- 279 -0.00306

 191 <- 282 0.00111

 191 <- 284 -0.00196

 191 <- 302 -0.00120

 191 <- 309 -0.00156

 191 <- 312 0.00203

 191 <- 353 -0.00100

 191 <- 416 0.00120

 192 <- 203 0.01295

 192 <- 207 -0.00235

 192 <- 212 -0.00142

 192 <- 247 -0.00119

 192 <- 261 -0.00184

 192 <- 355 0.00120

 192 <- 363 -0.00121

 193 <- 206 -0.00495

 193 <- 209 -0.00592

 193 <- 213 -0.00264

 193 <- 221 0.00173

 193 <- 241 -0.00163

 193 <- 253 -0.00233

 193 <- 271 -0.00103

 193 <- 346 0.00131

 193 <- 348 -0.00122

 193 <- 375 -0.00110

 194 <- 205 -0.00449

 194 <- 210 -0.00461

 194 <- 223 -0.00211

 194 <- 259 0.00216

 194 <- 260 -0.00235

 195 <- 203 -0.00268

 195 <- 207 0.00671

 195 <- 212 -0.00317

 195 <- 237 -0.00136

 195 <- 247 0.00153

 195 <- 261 -0.00191

 195 <- 363 0.00155

 196 <- 203 -0.04613

 196 <- 207 0.00554

 196 <- 212 -0.00940

 196 <- 261 -0.00205

 197 <- 204 -0.00226

 197 <- 263 -0.00169

 197 <- 274 0.00179

 197 <- 278 -0.00199

 197 <- 283 0.00184

 197 <- 291 -0.00293

 197 <- 301 -0.00100

 198 <- 204 -0.01838

 198 <- 208 -0.00290

 198 <- 211 -0.00353

 198 <- 248 -0.00117

 198 <- 250 0.00152

 198 <- 354 0.00167

 199 <- 205 -0.00222

 199 <- 210 0.00430

 199 <- 223 0.00172

 199 <- 249 -0.00245

 199 <- 252 -0.00234

 199 <- 259 -0.00162

 199 <- 357 0.00123

 199 <- 368 0.00120

 200 <- 206 -0.00199

 200 <- 209 -0.00279

 200 <- 213 0.00218

 200 <- 221 0.00619

 200 <- 241 0.00125

 200 <- 253 0.00144

 201 <- 204 0.01270

 201 <- 208 0.00158

 201 <- 211 0.00424

 201 <- 238 -0.00166

 201 <- 248 0.00115

 201 <- 250 0.00273

 202 <- 204 -0.07028

 202 <- 211 -0.00180

 202 <- 250 -0.00210

 202 <- 381 -0.00179

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

 Total Energy, E(TD-HF/TD-KS) = -2649.76578836

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

 Excited State 2: Singlet-E 1.7036 eV 727.78 nm f=0.6691 <S\*\*2>=0.000

 70 -> 289 0.00104

 72 -> 281 0.00106

 91 -> 272 -0.00115

 97 -> 255 -0.00109

 101 -> 281 0.00107

 103 -> 272 -0.00107

 105 -> 292 0.00184

 105 -> 333 -0.00128

 110 -> 266 0.00107

 111 -> 222 -0.00136

 111 -> 227 -0.00129

 111 -> 246 0.00119

 111 -> 272 -0.00103

 112 -> 292 -0.00120

 114 -> 224 0.00159

 114 -> 228 -0.00100

 115 -> 266 -0.00212

 115 -> 280 -0.00115

 115 -> 285 0.00183

 115 -> 288 -0.00103

 115 -> 314 0.00149

 115 -> 389 0.00169

 115 -> 402 0.00118

 115 -> 435 0.00103

 116 -> 258 0.00237

 116 -> 265 0.00105

 116 -> 272 0.00163

 116 -> 287 0.00212

 117 -> 233 -0.00202

 119 -> 230 -0.00199

 119 -> 235 -0.00147

 119 -> 236 0.00256

 120 -> 229 -0.00116

 120 -> 233 0.00198

 120 -> 279 -0.00107

 122 -> 230 -0.00128

 122 -> 266 -0.00102

 123 -> 216 0.00102

 123 -> 222 -0.00104

 125 -> 219 -0.00155

 125 -> 233 0.00132

 125 -> 255 0.00114

 125 -> 264 0.00116

 125 -> 268 -0.00314

 125 -> 279 0.00280

 125 -> 302 0.00128

 125 -> 321 0.00105

 125 -> 371 -0.00134

 125 -> 444 -0.00115

 126 -> 255 0.00105

 126 -> 273 0.00117

 127 -> 230 -0.00110

 127 -> 254 -0.00110

 127 -> 257 -0.00108

 128 -> 227 0.00220

 128 -> 234 0.00148

 128 -> 258 -0.00135

 128 -> 267 0.00187

 128 -> 275 -0.00123

 128 -> 293 0.00117

 129 -> 204 -0.00131

 129 -> 238 -0.00110

 129 -> 248 0.00133

 129 -> 319 0.00124

 130 -> 205 -0.00171

 131 -> 213 0.00114

 132 -> 204 -0.00150

 133 -> 224 0.00164

 133 -> 228 -0.00112

 137 -> 203 -0.00109

 138 -> 208 -0.00178

 138 -> 238 -0.00230

 138 -> 240 -0.00114

 138 -> 248 0.00102

 138 -> 319 0.00137

 139 -> 229 -0.00151

 139 -> 243 -0.00110

 139 -> 255 0.00160

 139 -> 264 0.00224

 139 -> 268 0.00150

 139 -> 273 -0.00173

 139 -> 282 -0.00259

 140 -> 289 0.00189

 141 -> 218 -0.00182

 141 -> 222 -0.00174

 141 -> 227 -0.00122

 141 -> 231 -0.00145

 141 -> 234 0.00180

 141 -> 242 -0.00144

 141 -> 258 -0.00257

 141 -> 272 0.00101

 142 -> 225 0.00128

 142 -> 233 -0.00100

 142 -> 255 -0.00127

 142 -> 264 0.00123

 143 -> 205 -0.00232

 143 -> 223 0.00272

 143 -> 260 0.00125

 144 -> 206 -0.00303

 144 -> 209 0.00262

 144 -> 213 0.00289

 144 -> 221 0.00232

 144 -> 241 0.00168

 144 -> 253 0.00144

 144 -> 348 -0.00114

 145 -> 224 -0.00181

 145 -> 228 0.00132

 145 -> 244 -0.00191

 145 -> 281 -0.00172

 145 -> 283 0.00102

 147 -> 217 0.00250

 147 -> 226 -0.00179

 147 -> 235 -0.00104

 147 -> 254 -0.00156

 147 -> 257 -0.00150

 147 -> 266 0.00105

 147 -> 270 0.00155

 148 -> 215 0.00200

 148 -> 225 -0.00169

 148 -> 243 0.00105

 148 -> 255 0.00154

 148 -> 268 0.00103

 149 -> 204 -0.00585

 149 -> 208 0.00114

 149 -> 211 -0.00160

 149 -> 319 -0.00175

 150 -> 214 0.00154

 150 -> 224 0.00171

 150 -> 244 0.00234

 150 -> 274 0.00135

 151 -> 217 -0.00135

 152 -> 216 0.00297

 152 -> 222 -0.00236

 152 -> 231 -0.00114

 152 -> 242 -0.00274

 152 -> 246 -0.00154

 152 -> 265 0.00104

 153 -> 214 0.00296

 153 -> 220 -0.00126

 153 -> 232 -0.00146

 153 -> 244 0.00170

 154 -> 240 -0.00144

 154 -> 244 0.00205

 155 -> 235 0.00182

 155 -> 257 -0.00129

 155 -> 266 0.00111

 155 -> 285 -0.00116

 155 -> 289 0.00194

 156 -> 216 -0.00178

 156 -> 234 0.00212

 156 -> 246 -0.00178

 156 -> 258 0.00138

 157 -> 229 0.00144

 157 -> 243 0.00102

 157 -> 255 -0.00168

 157 -> 284 0.00118

 158 -> 218 -0.00131

 158 -> 246 0.00165

 158 -> 258 -0.00269

 158 -> 267 0.00116

 158 -> 275 -0.00151

 158 -> 286 0.00121

 159 -> 226 0.00104

 159 -> 230 0.00109

 159 -> 235 -0.00155

 159 -> 236 0.00117

 159 -> 257 0.00117

 159 -> 276 0.00148

 159 -> 280 0.00105

 159 -> 289 0.00189

 159 -> 303 -0.00124

 159 -> 315 0.00118

 159 -> 326 0.00103

 160 -> 220 -0.00139

 160 -> 240 0.00135

 160 -> 269 -0.00130

 160 -> 281 0.00252

 160 -> 283 -0.00149

 160 -> 301 0.00113

 160 -> 334 -0.00120

 161 -> 417 0.00103

 162 -> 203 -0.00550

 162 -> 207 0.00168

 162 -> 212 -0.00194

 162 -> 261 -0.00145

 162 -> 318 0.00131

 162 -> 335 0.00124

 163 -> 203 -0.00140

 163 -> 239 0.00222

 163 -> 264 0.00171

 163 -> 273 -0.00266

 163 -> 282 -0.00135

 164 -> 204 -0.00328

 164 -> 208 0.00137

 164 -> 238 0.00121

 164 -> 336 -0.00181

 165 -> 223 0.00152

 166 -> 206 -0.00353

 166 -> 209 0.00221

 166 -> 213 0.00130

 166 -> 221 0.00149

 166 -> 241 0.00123

 166 -> 325 -0.00146

 166 -> 327 0.00150

 166 -> 346 -0.00104

 166 -> 348 -0.00116

 167 -> 204 -0.00619

 167 -> 208 0.00360

 167 -> 211 -0.00230

 167 -> 336 -0.00188

 168 -> 223 -0.00196

 168 -> 259 -0.00133

 168 -> 339 -0.00122

 168 -> 357 -0.00156

 169 -> 209 -0.00139

 169 -> 221 -0.00101

 170 -> 237 0.00108

 170 -> 355 -0.00119

 171 -> 203 0.00552

 171 -> 207 -0.00209

 171 -> 212 0.00296

 172 -> 240 0.00113

 172 -> 244 0.00122

 172 -> 263 0.00122

 173 -> 218 0.00161

 173 -> 222 -0.00102

 173 -> 231 0.00116

 173 -> 234 0.00146

 173 -> 242 0.00145

 173 -> 265 -0.00196

 173 -> 267 0.00142

 174 -> 254 0.00116

 174 -> 288 -0.00114

 175 -> 224 0.00100

 175 -> 240 -0.00156

 175 -> 244 -0.00102

 175 -> 263 -0.00127

 176 -> 216 0.00215

 176 -> 218 -0.00651

 176 -> 258 -0.00353

 176 -> 265 -0.00100

 176 -> 267 -0.00233

 176 -> 272 -0.00106

 176 -> 287 0.00263

 177 -> 230 -0.00102

 177 -> 257 0.00140

 177 -> 266 -0.00234

 177 -> 276 -0.00115

 177 -> 285 0.00297

 177 -> 314 0.00121

 177 -> 343 -0.00121

 178 -> 255 0.00257

 178 -> 279 -0.00192

 179 -> 235 -0.00118

 179 -> 254 -0.00276

 179 -> 257 -0.00195

 179 -> 266 -0.00211

 179 -> 276 0.00102

 179 -> 288 0.00164

 179 -> 314 0.00211

 180 -> 218 -0.00461

 180 -> 258 -0.00110

 180 -> 267 -0.00115

 180 -> 275 0.00233

 180 -> 287 0.00220

 181 -> 255 0.00264

 181 -> 282 0.00212

 181 -> 284 0.00136

 181 -> 292 0.00134

 182 -> 205 0.00539

 182 -> 210 0.00544

 182 -> 223 -0.00210

 182 -> 259 -0.00122

 182 -> 339 -0.00163

 182 -> 368 -0.00113

 183 -> 206 0.00336

 183 -> 209 0.00467

 183 -> 213 0.00108

 183 -> 221 -0.00338

 183 -> 271 0.00129

 184 -> 204 0.00463

 184 -> 208 0.00456

 184 -> 211 0.00252

 184 -> 238 -0.00245

 184 -> 240 -0.00123

 184 -> 248 -0.00116

 185 -> 204 -0.00116

 185 -> 208 -0.00447

 185 -> 211 -0.00406

 185 -> 238 0.00146

 185 -> 248 0.00199

 185 -> 336 -0.00123

 186 -> 205 -0.00312

 186 -> 210 -0.00282

 186 -> 223 0.00236

 187 -> 206 0.00659

 187 -> 209 -0.00358

 187 -> 213 0.00273

 187 -> 221 0.00220

 187 -> 241 0.00293

 187 -> 245 -0.00232

 187 -> 346 -0.00146

 187 -> 348 -0.00106

 188 -> 232 -0.00139

 188 -> 269 0.00159

 188 -> 278 -0.00207

 188 -> 283 0.00134

 188 -> 291 -0.00163

 189 -> 205 -0.00114

 189 -> 230 -0.00152

 189 -> 266 -0.00250

 189 -> 285 0.00236

 189 -> 300 0.00115

 189 -> 314 0.00153

 189 -> 324 -0.00107

 189 -> 337 -0.00172

 190 -> 216 0.00115

 190 -> 218 -0.00389

 190 -> 234 0.00102

 190 -> 265 0.00365

 190 -> 271 -0.00162

 190 -> 272 0.00602

 190 -> 287 0.00219

 190 -> 293 0.00185

 190 -> 310 -0.00171

 191 -> 204 -0.00271

 191 -> 214 0.00164

 191 -> 220 0.00262

 191 -> 232 -0.00144

 191 -> 256 -0.00118

 191 -> 263 -0.00183

 191 -> 269 0.00441

 191 -> 278 -0.00402

 191 -> 281 0.00151

 191 -> 283 -0.00255

 191 -> 301 0.00152

 191 -> 308 -0.00192

 191 -> 313 0.00259

 191 -> 322 -0.00115

 191 -> 352 -0.00125

 191 -> 401 0.00101

 191 -> 417 0.00141

 192 -> 204 -0.02474

 192 -> 208 0.00215

 192 -> 211 0.00175

 192 -> 248 -0.00177

 192 -> 262 -0.00220

 192 -> 336 0.00106

 192 -> 354 -0.00139

 192 -> 364 0.00144

 193 -> 205 0.00663

 193 -> 210 -0.00549

 193 -> 223 0.00332

 193 -> 259 0.00232

 193 -> 260 0.00294

 194 -> 206 -0.00616

 194 -> 209 0.00860

 194 -> 213 0.00457

 194 -> 221 0.00242

 194 -> 241 0.00224

 194 -> 245 0.00115

 194 -> 253 0.00338

 194 -> 271 0.00151

 194 -> 346 0.00166

 194 -> 348 0.00151

 194 -> 375 0.00122

 195 -> 204 -0.00661

 195 -> 208 0.00924

 195 -> 211 -0.00479

 195 -> 238 0.00166

 195 -> 248 -0.00210

 195 -> 262 0.00227

 195 -> 354 -0.00113

 195 -> 364 0.00176

 196 -> 204 0.10434

 196 -> 208 -0.00643

 196 -> 211 0.01187

 196 -> 262 -0.00198

 197 -> 203 -0.00682

 197 -> 219 -0.00153

 197 -> 264 0.00231

 197 -> 273 -0.00240

 197 -> 279 0.00260

 197 -> 284 -0.00239

 197 -> 292 0.00374

 197 -> 298 0.00104

 197 -> 302 -0.00129

 197 -> 321 -0.00108

 198 -> 203 -0.03894

 198 -> 207 -0.00637

 198 -> 212 -0.00250

 198 -> 237 -0.00105

 198 -> 247 0.00129

 198 -> 251 0.00204

 198 -> 261 0.00110

 198 -> 355 0.00197

 199 -> 206 -0.01057

 199 -> 209 0.00386

 199 -> 213 -0.00333

 199 -> 221 0.01216

 199 -> 241 -0.00204

 199 -> 245 0.00124

 199 -> 253 -0.00204

 200 -> 205 0.02850

 200 -> 210 0.00998

 200 -> 223 -0.00346

 200 -> 249 0.00339

 200 -> 252 -0.00310

 200 -> 259 -0.00276

 200 -> 357 0.00167

 200 -> 368 -0.00137

 201 -> 203 -0.03625

 201 -> 207 0.00378

 201 -> 212 -0.01051

 201 -> 237 -0.00359

 201 -> 239 -0.00174

 201 -> 247 0.00238

 201 -> 251 -0.00391

 201 -> 261 -0.00144

 201 -> 355 -0.00120

 201 -> 363 -0.00101

 202 -> 203 0.70059

 202 -> 207 -0.00145

 202 -> 212 0.00160

 202 -> 237 0.00154

 202 -> 251 -0.00300

 202 -> 261 -0.00181

 202 -> 363 -0.00111

 202 -> 380 -0.00209

 202 -> 424 0.00114

 91 <- 272 -0.00107

 105 <- 292 0.00159

 105 <- 333 -0.00113

 111 <- 222 -0.00108

 111 <- 227 -0.00102

 112 <- 292 -0.00103

 114 <- 224 0.00126

 115 <- 266 -0.00177

 115 <- 280 -0.00102

 115 <- 285 0.00155

 115 <- 314 0.00130

 115 <- 389 0.00150

 115 <- 402 0.00104

 116 <- 258 0.00202

 116 <- 272 0.00145

 116 <- 287 0.00188

 117 <- 233 -0.00161

 119 <- 230 -0.00157

 119 <- 235 -0.00117

 119 <- 236 0.00203

 120 <- 233 0.00156

 122 <- 230 -0.00101

 125 <- 219 -0.00124

 125 <- 233 0.00107

 125 <- 268 -0.00265

 125 <- 279 0.00241

 125 <- 302 0.00111

 125 <- 371 -0.00118

 125 <- 444 -0.00103

 128 <- 227 0.00171

 128 <- 234 0.00117

 128 <- 258 -0.00111

 128 <- 267 0.00153

 128 <- 275 -0.00102

 129 <- 204 -0.00107

 129 <- 248 0.00109

 129 <- 319 0.00108

 133 <- 224 0.00125

 138 <- 208 -0.00127

 138 <- 238 -0.00190

 138 <- 319 0.00123

 139 <- 229 -0.00117

 139 <- 255 0.00128

 139 <- 264 0.00186

 139 <- 268 0.00123

 139 <- 273 -0.00145

 139 <- 282 -0.00219

 140 <- 289 0.00160

 141 <- 218 -0.00134

 141 <- 222 -0.00131

 141 <- 231 -0.00112

 141 <- 234 0.00141

 141 <- 242 -0.00113

 141 <- 258 -0.00208

 142 <- 255 -0.00101

 143 <- 205 -0.00146

 143 <- 223 0.00192

 144 <- 206 -0.00219

 144 <- 209 0.00191

 144 <- 213 0.00217

 144 <- 221 0.00189

 144 <- 241 0.00153

 144 <- 253 0.00138

 145 <- 224 -0.00135

 145 <- 244 -0.00149

 145 <- 281 -0.00142

 147 <- 217 0.00187

 147 <- 226 -0.00135

 147 <- 254 -0.00123

 147 <- 257 -0.00118

 147 <- 270 0.00124

 148 <- 215 0.00149

 148 <- 225 -0.00127

 148 <- 255 0.00122

 149 <- 204 -0.00305

 149 <- 211 -0.00124

 149 <- 319 -0.00143

 150 <- 214 0.00113

 150 <- 224 0.00127

 150 <- 244 0.00179

 150 <- 274 0.00109

 151 <- 217 -0.00100

 152 <- 216 0.00218

 152 <- 222 -0.00174

 152 <- 242 -0.00210

 152 <- 246 -0.00118

 153 <- 214 0.00217

 153 <- 232 -0.00111

 153 <- 244 0.00130

 154 <- 240 -0.00107

 154 <- 244 0.00156

 155 <- 235 0.00137

 155 <- 289 0.00158

 156 <- 216 -0.00129

 156 <- 234 0.00157

 156 <- 246 -0.00134

 156 <- 258 0.00113

 157 <- 229 0.00107

 157 <- 255 -0.00129

 158 <- 246 0.00124

 158 <- 258 -0.00214

 158 <- 275 -0.00123

 159 <- 235 -0.00115

 159 <- 276 0.00118

 159 <- 289 0.00160

 159 <- 303 -0.00103

 160 <- 220 -0.00103

 160 <- 269 -0.00107

 160 <- 281 0.00206

 160 <- 283 -0.00122

 160 <- 334 -0.00101

 162 <- 203 -0.00423

 162 <- 212 -0.00130

 162 <- 237 0.00103

 162 <- 261 -0.00112

 162 <- 318 0.00104

 162 <- 335 0.00104

 163 <- 203 -0.00107

 163 <- 239 0.00174

 163 <- 264 0.00137

 163 <- 273 -0.00214

 163 <- 282 -0.00112

 164 <- 204 -0.00269

 164 <- 208 0.00105

 164 <- 238 0.00103

 164 <- 336 -0.00155

 165 <- 223 0.00125

 166 <- 206 -0.00258

 166 <- 209 0.00164

 166 <- 221 0.00110

 166 <- 241 0.00109

 166 <- 325 -0.00116

 166 <- 327 0.00125

 166 <- 348 -0.00103

 167 <- 204 -0.00268

 167 <- 208 0.00284

 167 <- 211 -0.00188

 167 <- 336 -0.00151

 168 <- 259 -0.00113

 168 <- 357 -0.00132

 169 <- 209 -0.00119

 170 <- 355 -0.00100

 171 <- 203 0.00438

 171 <- 212 0.00165

 173 <- 218 0.00112

 173 <- 234 0.00107

 173 <- 242 0.00106

 173 <- 265 -0.00152

 173 <- 267 0.00110

 175 <- 240 -0.00113

 176 <- 216 0.00148

 176 <- 218 -0.00449

 176 <- 258 -0.00265

 176 <- 267 -0.00181

 176 <- 287 0.00209

 177 <- 257 0.00104

 177 <- 266 -0.00182

 177 <- 285 0.00236

 177 <- 343 -0.00100

 178 <- 255 0.00192

 178 <- 279 -0.00151

 179 <- 254 -0.00205

 179 <- 257 -0.00145

 179 <- 266 -0.00161

 179 <- 288 0.00129

 179 <- 314 0.00174

 180 <- 218 -0.00315

 180 <- 275 0.00186

 180 <- 287 0.00177

 181 <- 255 0.00196

 181 <- 282 0.00168

 181 <- 284 0.00107

 181 <- 292 0.00110

 182 <- 210 0.00404

 182 <- 339 -0.00120

 183 <- 206 0.00160

 183 <- 209 0.00279

 183 <- 213 0.00103

 183 <- 221 -0.00117

 183 <- 271 0.00124

 184 <- 204 0.00259

 184 <- 208 0.00247

 184 <- 211 0.00160

 184 <- 238 -0.00178

 185 <- 208 -0.00194

 185 <- 211 -0.00265

 185 <- 238 0.00140

 185 <- 248 0.00109

 185 <- 336 -0.00104

 186 <- 210 -0.00205

 187 <- 206 0.00311

 187 <- 209 -0.00177

 187 <- 213 0.00183

 187 <- 221 0.00212

 187 <- 241 0.00217

 187 <- 245 -0.00150

 187 <- 346 -0.00122

 188 <- 269 0.00118

 188 <- 278 -0.00157

 188 <- 283 0.00105

 188 <- 291 -0.00129

 189 <- 230 -0.00104

 189 <- 266 -0.00187

 189 <- 285 0.00181

 189 <- 314 0.00122

 189 <- 337 -0.00141

 190 <- 218 -0.00248

 190 <- 265 0.00273

 190 <- 271 -0.00117

 190 <- 272 0.00454

 190 <- 287 0.00173

 190 <- 293 0.00148

 190 <- 310 -0.00139

 191 <- 204 -0.00143

 191 <- 214 0.00104

 191 <- 220 0.00167

 191 <- 263 -0.00131

 191 <- 269 0.00328

 191 <- 278 -0.00306

 191 <- 281 0.00111

 191 <- 283 -0.00196

 191 <- 301 0.00120

 191 <- 308 -0.00156

 191 <- 313 0.00203

 191 <- 352 -0.00100

 191 <- 417 0.00120

 192 <- 204 -0.01295

 192 <- 208 0.00235

 192 <- 211 0.00142

 192 <- 248 -0.00119

 192 <- 262 -0.00184

 192 <- 354 -0.00120

 192 <- 364 0.00121

 193 <- 205 0.00449

 193 <- 210 -0.00461

 193 <- 223 0.00211

 193 <- 259 0.00216

 193 <- 260 0.00235

 194 <- 206 -0.00495

 194 <- 209 0.00592

 194 <- 213 0.00264

 194 <- 221 0.00173

 194 <- 241 0.00163

 194 <- 253 0.00233

 194 <- 271 0.00103

 194 <- 346 0.00131

 194 <- 348 0.00122

 194 <- 375 0.00110

 195 <- 204 -0.00268

 195 <- 208 0.00671

 195 <- 211 -0.00317

 195 <- 238 0.00136

 195 <- 248 -0.00153

 195 <- 262 0.00191

 195 <- 364 0.00155

 196 <- 204 0.04613

 196 <- 208 -0.00554

 196 <- 211 0.00940

 196 <- 262 -0.00205

 197 <- 203 -0.00226

 197 <- 264 0.00169

 197 <- 273 -0.00179

 197 <- 279 0.00199

 197 <- 284 -0.00184

 197 <- 292 0.00293

 197 <- 302 -0.00100

 198 <- 203 -0.01838

 198 <- 207 -0.00290

 198 <- 212 -0.00353

 198 <- 247 0.00117

 198 <- 251 0.00152

 198 <- 355 0.00167

 199 <- 206 -0.00199

 199 <- 209 0.00279

 199 <- 213 -0.00218

 199 <- 221 0.00619

 199 <- 241 -0.00125

 199 <- 253 -0.00144

 200 <- 205 0.00222

 200 <- 210 0.00430

 200 <- 223 -0.00172

 200 <- 249 0.00245

 200 <- 252 -0.00234

 200 <- 259 -0.00162

 200 <- 357 0.00123

 200 <- 368 -0.00120

 201 <- 203 -0.01270

 201 <- 207 -0.00158

 201 <- 212 -0.00424

 201 <- 237 -0.00166

 201 <- 247 0.00115

 201 <- 251 -0.00273

 202 <- 203 -0.07028

 202 <- 212 -0.00180

 202 <- 251 -0.00210

 202 <- 380 -0.00179

 Excited State 3: Singlet-E 2.4655 eV 502.87 nm f=0.0000 <S\*\*2>=0.000

 132 -> 205 -0.00125

 143 -> 204 -0.00123

 144 -> 203 0.00123

 149 -> 205 -0.00155

 162 -> 206 -0.00123

 164 -> 210 0.00105

 167 -> 205 -0.00168

 167 -> 223 0.00168

 171 -> 221 -0.00214

 182 -> 204 0.01016

 182 -> 211 0.00123

 183 -> 203 0.01016

 183 -> 212 0.00123

 185 -> 205 -0.00639

 185 -> 223 0.00229

 186 -> 204 -0.00467

 187 -> 203 0.00467

 192 -> 210 0.00249

 192 -> 259 -0.00169

 193 -> 204 -0.00827

 193 -> 208 0.00143

 193 -> 211 -0.00294

 193 -> 262 0.00177

 194 -> 203 0.00827

 194 -> 207 -0.00143

 194 -> 212 0.00294

 194 -> 261 0.00177

 195 -> 205 -0.00211

 195 -> 223 0.00317

 195 -> 260 0.00190

 196 -> 210 0.00183

 198 -> 209 0.00216

 199 -> 203 -0.49935

 199 -> 207 0.00318

 199 -> 212 -0.00987

 199 -> 237 -0.00204

 199 -> 247 0.00201

 200 -> 204 0.49935

 200 -> 208 -0.00318

 200 -> 211 0.00987

 200 -> 238 -0.00204

 200 -> 248 0.00201

 201 -> 206 -0.01911

 201 -> 221 0.01272

 201 -> 245 0.00163

 202 -> 209 -0.00808

 202 -> 213 0.00112

 149 <- 205 -0.00134

 182 <- 204 0.00118

 183 <- 203 0.00118

 193 <- 204 0.00235

 194 <- 203 -0.00235

 195 <- 205 0.00233

 196 <- 210 0.00145

 198 <- 209 0.00179

 198 <- 213 -0.00112

 199 <- 203 0.00268

 199 <- 207 -0.00235

 199 <- 212 -0.00129

 200 <- 204 -0.00268

 200 <- 208 0.00235

 200 <- 211 0.00129

 201 <- 206 0.00328

 201 <- 221 0.00109

 202 <- 209 -0.00226

 Excited State 4: Singlet-E 2.4923 eV 497.47 nm f=0.2437 <S\*\*2>=0.000

 104 -> 255 0.00132

 111 -> 222 -0.00114

 111 -> 227 -0.00131

 114 -> 224 0.00119

 119 -> 230 -0.00114

 119 -> 236 0.00116

 120 -> 233 0.00116

 123 -> 310 0.00112

 123 -> 311 -0.00128

 124 -> 308 0.00112

 126 -> 255 0.00126

 127 -> 230 -0.00119

 127 -> 254 -0.00109

 127 -> 257 -0.00127

 129 -> 208 0.00130

 131 -> 206 0.00116

 133 -> 244 0.00124

 134 -> 203 0.00177

 136 -> 205 0.00111

 138 -> 204 -0.00153

 139 -> 255 0.00129

 141 -> 234 0.00116

 141 -> 246 -0.00132

 144 -> 206 0.00171

 145 -> 244 -0.00114

 145 -> 330 -0.00100

 147 -> 217 0.00196

 147 -> 226 -0.00110

 147 -> 254 -0.00109

 147 -> 257 -0.00101

 147 -> 270 0.00114

 148 -> 215 0.00153

 148 -> 225 -0.00116

 149 -> 204 0.00196

 149 -> 208 -0.00187

 149 -> 211 -0.00139

 150 -> 214 0.00141

 150 -> 224 0.00111

 150 -> 244 0.00111

 152 -> 216 0.00231

 152 -> 222 -0.00177

 152 -> 242 -0.00166

 152 -> 265 0.00101

 153 -> 214 0.00207

 153 -> 220 -0.00109

 153 -> 240 0.00104

 153 -> 244 0.00119

 154 -> 281 -0.00105

 154 -> 372 -0.00103

 155 -> 235 0.00115

 156 -> 216 -0.00109

 156 -> 227 -0.00103

 156 -> 258 0.00150

 156 -> 293 0.00148

 156 -> 310 0.00118

 156 -> 311 -0.00107

 157 -> 233 0.00105

 157 -> 268 -0.00145

 157 -> 341 0.00121

 158 -> 293 -0.00117

 159 -> 235 -0.00153

 159 -> 266 -0.00185

 159 -> 276 0.00124

 159 -> 300 0.00102

 159 -> 343 0.00145

 160 -> 263 -0.00144

 160 -> 308 -0.00114

 161 -> 283 -0.00105

 162 -> 203 -0.00202

 163 -> 233 0.00104

 163 -> 239 0.00113

 163 -> 268 -0.00128

 164 -> 204 0.00161

 164 -> 208 0.00165

 165 -> 205 -0.00115

 166 -> 209 0.00182

 166 -> 221 -0.00178

 166 -> 327 0.00106

 167 -> 204 0.00223

 167 -> 211 0.00119

 168 -> 205 0.00128

 168 -> 210 0.00101

 168 -> 259 -0.00159

 168 -> 260 0.00149

 169 -> 221 0.00168

 170 -> 203 -0.00365

 170 -> 207 -0.00117

 170 -> 261 0.00162

 171 -> 203 0.00112

 171 -> 207 0.00116

 171 -> 212 -0.00237

 171 -> 261 -0.00121

 173 -> 234 0.00115

 175 -> 240 -0.00116

 176 -> 218 -0.00123

 178 -> 255 0.00118

 178 -> 292 0.00165

 179 -> 285 -0.00118

 181 -> 255 0.00117

 181 -> 292 0.00181

 182 -> 205 -0.00568

 182 -> 210 -0.00232

 183 -> 206 0.00270

 183 -> 209 -0.00173

 183 -> 241 -0.00107

 184 -> 204 -0.00292

 184 -> 208 0.00315

 184 -> 248 -0.00221

 185 -> 204 0.00249

 185 -> 208 -0.00315

 185 -> 248 0.00167

 186 -> 205 0.00578

 186 -> 210 0.00124

 186 -> 223 -0.00141

 187 -> 206 0.00664

 187 -> 209 -0.00397

 187 -> 241 0.00104

 187 -> 245 -0.00205

 187 -> 253 -0.00170

 187 -> 346 -0.00105

 189 -> 324 -0.00101

 190 -> 323 -0.00118

 192 -> 204 -0.00606

 192 -> 208 0.01465

 192 -> 211 0.00541

 192 -> 238 -0.00100

 192 -> 262 0.00116

 192 -> 336 0.00179

 193 -> 205 0.00137

 193 -> 210 0.00196

 193 -> 259 -0.00114

 193 -> 260 -0.00124

 194 -> 206 -0.01430

 194 -> 209 0.01563

 194 -> 213 -0.00281

 194 -> 221 -0.00613

 194 -> 241 -0.00110

 194 -> 253 -0.00122

 194 -> 325 0.00143

 194 -> 327 -0.00168

 194 -> 346 0.00134

 194 -> 348 0.00109

 195 -> 204 -0.01708

 195 -> 208 0.01391

 195 -> 211 0.00720

 195 -> 238 -0.00133

 195 -> 248 0.00102

 195 -> 336 0.00157

 196 -> 204 -0.01367

 196 -> 208 -0.00264

 196 -> 211 -0.00220

 196 -> 238 -0.00161

 197 -> 203 -0.00125

 197 -> 353 0.00119

 198 -> 203 0.01198

 198 -> 207 -0.00645

 198 -> 212 0.00520

 198 -> 237 0.00166

 198 -> 247 -0.00133

 198 -> 251 0.00148

 198 -> 261 -0.00101

 199 -> 206 0.01367

 199 -> 221 -0.00796

 199 -> 245 -0.00119

 199 -> 271 -0.00101

 200 -> 205 0.02397

 200 -> 210 0.00195

 200 -> 223 -0.00341

 200 -> 249 0.00234

 200 -> 252 -0.00222

 200 -> 260 -0.00175

 201 -> 203 0.70435

 201 -> 207 -0.00372

 201 -> 212 0.00832

 201 -> 237 0.00118

 201 -> 247 -0.00162

 201 -> 251 -0.00204

 201 -> 261 0.00128

 202 -> 203 0.03959

 202 -> 207 -0.01254

 202 -> 212 0.00798

 202 -> 251 -0.00298

 202 -> 261 0.00103

 104 <- 255 0.00101

 123 <- 311 -0.00104

 144 <- 206 0.00136

 147 <- 217 0.00128

 149 <- 204 0.00138

 149 <- 208 -0.00152

 149 <- 211 -0.00116

 152 <- 216 0.00147

 152 <- 222 -0.00113

 152 <- 242 -0.00112

 153 <- 214 0.00131

 156 <- 258 0.00109

 156 <- 293 0.00112

 157 <- 268 -0.00105

 159 <- 266 -0.00132

 159 <- 343 0.00115

 160 <- 263 -0.00106

 162 <- 203 -0.00132

 164 <- 208 0.00120

 166 <- 209 0.00136

 167 <- 204 0.00155

 168 <- 205 0.00186

 168 <- 210 0.00113

 168 <- 259 -0.00128

 168 <- 260 0.00118

 170 <- 203 -0.00230

 170 <- 207 -0.00146

 170 <- 261 0.00127

 171 <- 203 0.00358

 171 <- 212 -0.00120

 171 <- 261 -0.00103

 178 <- 292 0.00121

 181 <- 292 0.00132

 182 <- 205 -0.00330

 182 <- 210 -0.00140

 183 <- 206 0.00225

 183 <- 209 -0.00215

 185 <- 204 0.00118

 185 <- 208 -0.00126

 187 <- 206 0.00174

 187 <- 209 -0.00167

 187 <- 245 -0.00108

 192 <- 204 -0.00133

 192 <- 208 0.00796

 192 <- 211 0.00321

 192 <- 336 0.00122

 193 <- 205 -0.00146

 194 <- 206 -0.00744

 194 <- 209 0.00787

 194 <- 213 -0.00155

 194 <- 221 -0.00316

 194 <- 327 -0.00113

 195 <- 204 -0.00366

 195 <- 208 0.00671

 195 <- 211 0.00398

 195 <- 336 0.00105

 196 <- 208 -0.00203

 196 <- 211 -0.00166

 196 <- 238 -0.00104

 198 <- 203 0.00455

 198 <- 212 0.00128

 198 <- 251 0.00115

 198 <- 261 -0.00104

 199 <- 206 -0.00218

 200 <- 205 -0.00842

 200 <- 210 -0.00354

 200 <- 249 0.00169

 200 <- 252 -0.00161

 200 <- 259 0.00204

 200 <- 260 -0.00145

 201 <- 203 -0.01431

 201 <- 207 -0.00129

 201 <- 212 0.00299

 201 <- 247 -0.00101

 201 <- 251 -0.00153

 201 <- 261 0.00174

 202 <- 203 -0.01787

 202 <- 207 -0.00724

 202 <- 212 0.00672

 202 <- 237 0.00102

 202 <- 251 -0.00128

 202 <- 261 0.00146

 Excited State 5: Singlet-E 2.4923 eV 497.47 nm f=0.2437 <S\*\*2>=0.000

 104 -> 256 -0.00132

 110 -> 222 0.00114

 110 -> 227 -0.00131

 114 -> 225 -0.00119

 118 -> 230 -0.00114

 118 -> 236 -0.00116

 120 -> 232 -0.00116

 122 -> 310 -0.00112

 122 -> 311 -0.00128

 124 -> 309 -0.00112

 126 -> 256 0.00126

 128 -> 230 -0.00119

 128 -> 254 -0.00109

 128 -> 257 0.00127

 129 -> 207 0.00130

 130 -> 206 -0.00116

 133 -> 243 0.00124

 134 -> 204 0.00177

 135 -> 205 0.00111

 138 -> 203 -0.00153

 139 -> 256 -0.00129

 140 -> 234 0.00116

 140 -> 246 0.00132

 143 -> 206 -0.00171

 145 -> 243 0.00114

 145 -> 331 0.00100

 146 -> 217 0.00196

 146 -> 226 0.00110

 146 -> 254 -0.00109

 146 -> 257 0.00101

 146 -> 270 -0.00114

 148 -> 214 -0.00153

 148 -> 224 0.00116

 149 -> 203 -0.00196

 149 -> 207 0.00187

 149 -> 212 0.00139

 150 -> 215 0.00141

 150 -> 225 0.00111

 150 -> 243 0.00111

 151 -> 216 0.00231

 151 -> 222 0.00177

 151 -> 242 -0.00166

 151 -> 265 -0.00101

 153 -> 215 -0.00207

 153 -> 219 0.00109

 153 -> 239 -0.00104

 153 -> 243 -0.00119

 154 -> 282 -0.00105

 154 -> 371 -0.00103

 155 -> 216 0.00109

 155 -> 227 0.00103

 155 -> 258 -0.00150

 155 -> 293 0.00148

 155 -> 310 0.00118

 155 -> 311 0.00107

 156 -> 235 -0.00115

 157 -> 232 0.00105

 157 -> 269 -0.00145

 157 -> 340 0.00121

 158 -> 235 -0.00153

 158 -> 266 -0.00185

 158 -> 276 -0.00124

 158 -> 300 -0.00102

 158 -> 343 0.00145

 159 -> 293 0.00117

 160 -> 264 0.00144

 160 -> 309 0.00114

 161 -> 284 -0.00105

 162 -> 204 -0.00202

 163 -> 232 -0.00104

 163 -> 240 -0.00113

 163 -> 269 0.00128

 164 -> 203 0.00161

 164 -> 207 0.00165

 165 -> 209 0.00182

 165 -> 221 0.00178

 165 -> 327 0.00106

 166 -> 205 -0.00115

 167 -> 203 -0.00223

 167 -> 212 -0.00119

 168 -> 221 -0.00168

 169 -> 205 0.00128

 169 -> 210 -0.00101

 169 -> 259 0.00159

 169 -> 260 0.00149

 170 -> 204 0.00365

 170 -> 208 0.00117

 170 -> 262 0.00162

 171 -> 204 0.00112

 171 -> 208 0.00116

 171 -> 211 -0.00237

 171 -> 262 0.00121

 174 -> 234 0.00115

 175 -> 239 0.00116

 177 -> 218 -0.00123

 178 -> 256 0.00118

 178 -> 291 0.00165

 180 -> 285 -0.00118

 181 -> 256 -0.00117

 181 -> 291 -0.00181

 182 -> 206 0.00270

 182 -> 209 0.00173

 182 -> 241 0.00107

 183 -> 205 0.00568

 183 -> 210 -0.00232

 184 -> 203 -0.00292

 184 -> 207 0.00315

 184 -> 247 0.00221

 185 -> 203 -0.00249

 185 -> 207 0.00315

 185 -> 247 0.00167

 186 -> 206 -0.00664

 186 -> 209 -0.00397

 186 -> 241 0.00104

 186 -> 245 0.00205

 186 -> 253 -0.00170

 186 -> 346 0.00105

 187 -> 205 0.00578

 187 -> 210 -0.00124

 187 -> 223 -0.00141

 189 -> 323 -0.00118

 190 -> 324 0.00101

 192 -> 203 -0.00606

 192 -> 207 0.01465

 192 -> 212 0.00541

 192 -> 237 0.00100

 192 -> 261 -0.00116

 192 -> 335 0.00179

 193 -> 206 0.01430

 193 -> 209 0.01563

 193 -> 213 -0.00281

 193 -> 221 0.00613

 193 -> 241 -0.00110

 193 -> 253 -0.00122

 193 -> 325 -0.00143

 193 -> 327 -0.00168

 193 -> 346 -0.00134

 193 -> 348 0.00109

 194 -> 205 0.00137

 194 -> 210 -0.00196

 194 -> 259 0.00114

 194 -> 260 -0.00124

 195 -> 203 0.01708

 195 -> 207 -0.01391

 195 -> 212 -0.00720

 195 -> 237 -0.00133

 195 -> 247 0.00102

 195 -> 335 -0.00157

 196 -> 203 -0.01367

 196 -> 207 -0.00264

 196 -> 212 -0.00220

 196 -> 237 0.00161

 197 -> 204 0.00125

 197 -> 352 0.00119

 198 -> 204 -0.01198

 198 -> 208 0.00645

 198 -> 211 -0.00520

 198 -> 238 0.00166

 198 -> 248 -0.00133

 198 -> 250 -0.00148

 198 -> 262 -0.00101

 199 -> 205 0.02397

 199 -> 210 -0.00195

 199 -> 223 -0.00341

 199 -> 249 0.00234

 199 -> 252 0.00222

 199 -> 260 -0.00175

 200 -> 206 -0.01367

 200 -> 221 0.00796

 200 -> 245 0.00119

 200 -> 271 -0.00101

 201 -> 204 0.70435

 201 -> 208 -0.00372

 201 -> 211 0.00832

 201 -> 238 -0.00118

 201 -> 248 0.00162

 201 -> 250 -0.00204

 201 -> 262 -0.00128

 202 -> 204 -0.03959

 202 -> 208 0.01254

 202 -> 211 -0.00798

 202 -> 250 0.00298

 202 -> 262 0.00103

 104 <- 256 -0.00101

 122 <- 311 -0.00104

 143 <- 206 -0.00136

 146 <- 217 0.00128

 149 <- 203 -0.00138

 149 <- 207 0.00152

 149 <- 212 0.00116

 151 <- 216 0.00147

 151 <- 222 0.00113

 151 <- 242 -0.00112

 153 <- 215 -0.00131

 155 <- 258 -0.00109

 155 <- 293 0.00112

 157 <- 269 -0.00105

 158 <- 266 -0.00132

 158 <- 343 0.00115

 160 <- 264 0.00106

 162 <- 204 -0.00132

 164 <- 207 0.00120

 165 <- 209 0.00136

 167 <- 203 -0.00155

 169 <- 205 0.00186

 169 <- 210 -0.00113

 169 <- 259 0.00128

 169 <- 260 0.00118

 170 <- 204 0.00230

 170 <- 208 0.00146

 170 <- 262 0.00127

 171 <- 204 0.00358

 171 <- 211 -0.00120

 171 <- 262 0.00103

 178 <- 291 0.00121

 181 <- 291 -0.00132

 182 <- 206 0.00225

 182 <- 209 0.00215

 183 <- 205 0.00330

 183 <- 210 -0.00140

 185 <- 203 -0.00118

 185 <- 207 0.00126

 186 <- 206 -0.00174

 186 <- 209 -0.00167

 186 <- 245 0.00108

 192 <- 203 -0.00133

 192 <- 207 0.00796

 192 <- 212 0.00321

 192 <- 335 0.00122

 193 <- 206 0.00744

 193 <- 209 0.00787

 193 <- 213 -0.00155

 193 <- 221 0.00316

 193 <- 327 -0.00113

 194 <- 205 -0.00146

 195 <- 203 0.00366

 195 <- 207 -0.00671

 195 <- 212 -0.00398

 195 <- 335 -0.00105

 196 <- 207 -0.00203

 196 <- 212 -0.00166

 196 <- 237 0.00104

 198 <- 204 -0.00455

 198 <- 211 -0.00128

 198 <- 250 -0.00115

 198 <- 262 -0.00104

 199 <- 205 -0.00842

 199 <- 210 0.00354

 199 <- 249 0.00169

 199 <- 252 0.00161

 199 <- 259 -0.00204

 199 <- 260 -0.00145

 200 <- 206 0.00218

 201 <- 204 -0.01431

 201 <- 208 -0.00129

 201 <- 211 0.00299

 201 <- 248 0.00101

 201 <- 250 -0.00153

 201 <- 262 -0.00174

 202 <- 204 0.01787

 202 <- 208 0.00724

 202 <- 211 -0.00672

 202 <- 238 0.00102

 202 <- 250 0.00128

 202 <- 262 0.00146

 Excited State 6: Singlet-E 2.5039 eV 495.17 nm f=0.0000 <S\*\*2>=0.000

 69 -> 258 0.00111

 125 -> 272 -0.00194

 129 -> 223 0.00104

 138 -> 205 -0.00241

 138 -> 223 0.00180

 143 -> 204 -0.00262

 143 -> 238 -0.00107

 144 -> 203 -0.00262

 144 -> 237 0.00107

 154 -> 289 -0.00101

 162 -> 209 0.00183

 162 -> 241 0.00132

 162 -> 253 0.00143

 164 -> 205 0.00183

 165 -> 204 -0.00435

 166 -> 203 -0.00435

 168 -> 204 -0.00421

 168 -> 211 -0.00161

 169 -> 203 -0.00421

 169 -> 212 -0.00161

 170 -> 221 0.00238

 171 -> 241 -0.00159

 182 -> 204 -0.01025

 182 -> 211 -0.00164

 182 -> 238 -0.00121

 183 -> 203 0.01025

 183 -> 212 0.00164

 183 -> 237 -0.00121

 184 -> 205 0.00384

 184 -> 223 -0.00128

 185 -> 210 0.00107

 186 -> 204 0.00388

 186 -> 211 0.00117

 187 -> 203 0.00388

 187 -> 212 0.00117

 188 -> 230 0.00171

 188 -> 266 0.00101

 188 -> 407 -0.00120

 189 -> 204 0.00150

 189 -> 274 0.00104

 189 -> 278 -0.00165

 189 -> 281 0.00105

 189 -> 291 -0.00149

 189 -> 299 -0.00147

 189 -> 352 0.00112

 190 -> 203 -0.00150

 190 -> 273 0.00104

 190 -> 279 -0.00165

 190 -> 282 0.00105

 190 -> 292 -0.00149

 190 -> 298 -0.00147

 190 -> 353 0.00112

 192 -> 205 0.00819

 192 -> 260 0.00143

 193 -> 204 -0.01680

 193 -> 208 -0.00169

 193 -> 211 0.00208

 193 -> 262 -0.00180

 194 -> 203 -0.01680

 194 -> 207 -0.00169

 194 -> 212 0.00208

 194 -> 261 0.00180

 195 -> 210 0.00340

 195 -> 259 -0.00184

 196 -> 205 -0.00580

 196 -> 223 0.00514

 196 -> 260 0.00195

 196 -> 339 0.00112

 197 -> 206 0.00138

 197 -> 221 -0.00101

 197 -> 267 -0.00155

 197 -> 287 -0.00233

 197 -> 290 0.00196

 197 -> 323 -0.00197

 197 -> 347 -0.00133

 197 -> 367 -0.00176

 197 -> 386 0.00107

 198 -> 206 0.01700

 198 -> 221 -0.01262

 198 -> 245 -0.00159

 199 -> 203 0.49916

 199 -> 207 -0.00246

 199 -> 212 0.00897

 199 -> 237 0.00388

 199 -> 239 0.00189

 199 -> 247 -0.00309

 200 -> 204 0.49916

 200 -> 208 -0.00246

 200 -> 211 0.00897

 200 -> 238 -0.00388

 200 -> 240 -0.00189

 200 -> 248 0.00309

 201 -> 209 -0.00532

 201 -> 213 0.00101

 201 -> 241 0.00166

 201 -> 253 0.00205

 201 -> 271 -0.00155

 202 -> 206 0.00410

 202 -> 221 0.00271

 125 <- 272 -0.00150

 138 <- 205 -0.00119

 138 <- 223 0.00129

 143 <- 204 -0.00134

 144 <- 203 -0.00134

 162 <- 209 0.00186

 162 <- 241 0.00112

 162 <- 253 0.00112

 164 <- 205 0.00109

 165 <- 204 -0.00185

 166 <- 203 -0.00185

 168 <- 204 -0.00126

 169 <- 203 -0.00126

 182 <- 204 -0.00599

 182 <- 211 -0.00184

 183 <- 203 0.00599

 183 <- 212 0.00184

 186 <- 204 0.00226

 186 <- 211 0.00113

 187 <- 203 0.00226

 187 <- 212 0.00113

 189 <- 278 -0.00113

 189 <- 291 -0.00103

 189 <- 299 -0.00104

 190 <- 279 -0.00113

 190 <- 292 -0.00103

 190 <- 298 -0.00104

 192 <- 205 0.00310

 193 <- 204 -0.00153

 193 <- 211 0.00167

 193 <- 262 -0.00119

 194 <- 203 -0.00153

 194 <- 212 0.00167

 194 <- 261 0.00119

 195 <- 210 0.00199

 195 <- 259 -0.00107

 196 <- 205 -0.00398

 196 <- 223 0.00469

 196 <- 260 0.00175

 197 <- 287 -0.00160

 197 <- 290 0.00134

 197 <- 323 -0.00143

 197 <- 367 -0.00134

 198 <- 221 -0.00394

 199 <- 203 -0.00201

 199 <- 207 0.00246

 199 <- 237 0.00136

 199 <- 247 -0.00119

 200 <- 204 -0.00201

 200 <- 208 0.00246

 200 <- 238 -0.00136

 200 <- 248 0.00119

 201 <- 209 -0.00309

 201 <- 213 0.00102

 201 <- 253 0.00126

 202 <- 206 0.00603

 202 <- 221 -0.00306

 Excited State 7: Singlet-E 2.5286 eV 490.33 nm f=0.0002 <S\*\*2>=0.000

 96 -> 227 -0.00101

 97 -> 300 0.00122

 98 -> 222 0.00100

 98 -> 231 0.00103

 98 -> 286 -0.00114

 98 -> 293 0.00126

 99 -> 292 -0.00102

 100 -> 291 -0.00102

 101 -> 242 -0.00102

 101 -> 290 -0.00111

 102 -> 243 -0.00107

 102 -> 255 0.00129

 102 -> 312 0.00111

 103 -> 244 -0.00107

 103 -> 256 0.00129

 103 -> 313 0.00111

 104 -> 254 0.00177

 104 -> 266 0.00146

 104 -> 280 -0.00110

 104 -> 343 -0.00125

 110 -> 225 0.00127

 111 -> 224 -0.00127

 113 -> 222 -0.00141

 113 -> 246 0.00111

 114 -> 227 0.00191

 117 -> 236 0.00143

 117 -> 257 0.00103

 118 -> 232 0.00145

 119 -> 233 -0.00145

 120 -> 230 0.00169

 121 -> 246 -0.00104

 121 -> 277 -0.00104

 121 -> 286 0.00108

 121 -> 293 -0.00114

 121 -> 310 -0.00141

 122 -> 284 0.00117

 122 -> 309 0.00120

 123 -> 283 -0.00117

 123 -> 308 -0.00120

 124 -> 267 -0.00115

 124 -> 290 -0.00132

 124 -> 311 0.00172

 126 -> 257 0.00152

 126 -> 270 0.00104

 127 -> 229 0.00121

 127 -> 255 -0.00137

 128 -> 228 -0.00121

 128 -> 256 0.00137

 129 -> 206 0.00229

 130 -> 207 -0.00135

 131 -> 208 0.00135

 132 -> 209 0.00112

 133 -> 246 0.00158

 133 -> 286 0.00109

 133 -> 338 0.00108

 134 -> 210 0.00101

 135 -> 204 -0.00180

 136 -> 203 0.00180

 137 -> 205 -0.00156

 138 -> 206 0.00273

 139 -> 230 0.00125

 139 -> 254 0.00150

 140 -> 243 0.00142

 140 -> 284 0.00108

 141 -> 244 -0.00142

 141 -> 283 -0.00108

 142 -> 226 -0.00141

 142 -> 257 -0.00115

 142 -> 270 0.00138

 143 -> 203 0.00198

 143 -> 207 -0.00257

 144 -> 204 -0.00198

 144 -> 208 0.00257

 145 -> 234 0.00183

 145 -> 329 0.00151

 146 -> 214 0.00129

 146 -> 224 -0.00168

 146 -> 256 0.00128

 147 -> 215 -0.00129

 147 -> 225 0.00168

 147 -> 255 -0.00128

 148 -> 217 -0.00286

 148 -> 254 0.00127

 148 -> 266 -0.00128

 149 -> 209 0.00294

 149 -> 213 -0.00181

 150 -> 222 0.00225

 150 -> 231 0.00118

 150 -> 246 0.00101

 150 -> 265 -0.00131

 151 -> 215 0.00240

 151 -> 219 -0.00124

 151 -> 243 0.00143

 152 -> 214 -0.00240

 152 -> 220 0.00124

 152 -> 244 -0.00143

 153 -> 216 -0.00328

 153 -> 218 -0.00100

 153 -> 234 0.00101

 153 -> 242 0.00219

 153 -> 332 -0.00115

 154 -> 277 0.00111

 154 -> 293 -0.00190

 154 -> 310 -0.00160

 154 -> 365 -0.00133

 155 -> 215 0.00115

 155 -> 229 0.00102

 155 -> 268 -0.00129

 155 -> 309 -0.00158

 155 -> 331 -0.00104

 155 -> 371 0.00105

 156 -> 214 0.00115

 156 -> 228 0.00102

 156 -> 269 -0.00129

 156 -> 308 -0.00158

 156 -> 330 -0.00104

 156 -> 372 0.00105

 157 -> 236 -0.00135

 157 -> 270 0.00117

 157 -> 276 -0.00197

 157 -> 300 -0.00121

 157 -> 337 0.00125

 158 -> 240 0.00115

 158 -> 263 0.00131

 158 -> 269 -0.00125

 158 -> 274 -0.00106

 158 -> 283 0.00104

 158 -> 340 0.00129

 159 -> 239 -0.00115

 159 -> 264 -0.00131

 159 -> 268 0.00125

 159 -> 273 0.00106

 159 -> 284 -0.00104

 159 -> 341 -0.00129

 160 -> 216 -0.00105

 160 -> 227 -0.00137

 160 -> 258 0.00180

 160 -> 267 -0.00122

 160 -> 290 0.00107

 160 -> 311 -0.00152

 160 -> 332 0.00122

 160 -> 386 0.00138

 163 -> 235 0.00231

 163 -> 266 0.00212

 163 -> 343 -0.00203

 164 -> 221 0.00361

 164 -> 325 0.00105

 165 -> 203 0.00193

 165 -> 212 0.00184

 165 -> 237 0.00160

 165 -> 247 -0.00141

 166 -> 204 -0.00193

 166 -> 211 -0.00184

 166 -> 238 0.00160

 166 -> 248 -0.00141

 167 -> 253 0.00111

 167 -> 271 -0.00135

 167 -> 327 -0.00134

 168 -> 207 0.00143

 168 -> 212 -0.00150

 168 -> 261 -0.00194

 169 -> 208 -0.00143

 169 -> 211 0.00150

 169 -> 262 -0.00194

 170 -> 205 -0.00198

 170 -> 223 -0.00141

 170 -> 260 -0.00221

 171 -> 210 0.00314

 171 -> 259 -0.00195

 171 -> 357 -0.00128

 172 -> 222 -0.00120

 172 -> 265 -0.00139

 172 -> 310 -0.00118

 173 -> 240 0.00109

 173 -> 263 0.00126

 174 -> 239 -0.00109

 174 -> 264 -0.00126

 175 -> 234 -0.00160

 175 -> 242 -0.00123

 175 -> 275 -0.00119

 175 -> 323 0.00111

 176 -> 269 -0.00105

 176 -> 281 -0.00112

 176 -> 291 -0.00120

 177 -> 268 0.00105

 177 -> 282 0.00112

 177 -> 292 0.00120

 178 -> 236 0.00105

 178 -> 257 0.00140

 178 -> 270 -0.00138

 178 -> 288 -0.00159

 178 -> 300 0.00132

 179 -> 229 -0.00111

 179 -> 255 -0.00125

 179 -> 292 -0.00163

 180 -> 228 0.00111

 180 -> 256 0.00125

 180 -> 291 0.00163

 181 -> 230 -0.00142

 181 -> 254 0.00153

 181 -> 266 -0.00118

 181 -> 285 0.00176

 181 -> 303 0.00103

 182 -> 203 -0.00210

 182 -> 212 0.00365

 182 -> 247 -0.00108

 183 -> 204 -0.00210

 183 -> 211 0.00365

 183 -> 248 0.00108

 184 -> 206 0.00641

 184 -> 221 -0.00158

 184 -> 245 -0.00266

 185 -> 209 0.00455

 185 -> 213 -0.00118

 185 -> 241 -0.00124

 185 -> 253 0.00230

 185 -> 348 0.00112

 186 -> 203 0.00433

 186 -> 207 -0.00466

 186 -> 212 -0.00231

 186 -> 247 -0.00244

 187 -> 204 -0.00433

 187 -> 208 0.00466

 187 -> 211 0.00231

 187 -> 248 -0.00244

 188 -> 265 0.00120

 188 -> 272 0.00211

 189 -> 279 0.00122

 190 -> 278 -0.00122

 191 -> 216 -0.00204

 191 -> 218 0.00557

 191 -> 258 0.00221

 191 -> 267 0.00136

 191 -> 287 -0.00131

 191 -> 420 -0.00106

 191 -> 428 0.00109

 192 -> 206 0.01569

 192 -> 221 0.00936

 192 -> 325 -0.00213

 192 -> 346 -0.00172

 193 -> 203 -0.01284

 193 -> 207 0.01616

 193 -> 212 0.00713

 193 -> 237 0.00304

 193 -> 239 0.00151

 193 -> 247 -0.00201

 193 -> 318 -0.00146

 193 -> 335 0.00184

 194 -> 204 0.01284

 194 -> 208 -0.01616

 194 -> 211 -0.00713

 194 -> 238 0.00304

 194 -> 240 0.00151

 194 -> 248 -0.00201

 194 -> 319 0.00146

 194 -> 336 -0.00184

 195 -> 209 -0.01880

 195 -> 213 0.00302

 195 -> 241 0.00263

 195 -> 253 0.00282

 195 -> 271 -0.00145

 195 -> 327 0.00229

 195 -> 348 -0.00123

 196 -> 206 0.00100

 196 -> 221 -0.00319

 197 -> 205 -0.00371

 197 -> 288 0.00114

 197 -> 324 -0.00195

 198 -> 205 -0.03688

 198 -> 223 0.00497

 198 -> 249 -0.00165

 198 -> 260 0.00242

 199 -> 204 -0.49780

 199 -> 211 -0.00656

 199 -> 250 0.00289

 199 -> 262 0.00249

 200 -> 203 0.49780

 200 -> 212 0.00656

 200 -> 251 -0.00289

 200 -> 261 0.00249

 201 -> 252 -0.00293

 201 -> 259 0.00149

 202 -> 205 -0.04246

 202 -> 223 -0.00661

 202 -> 249 0.00365

 202 -> 368 -0.00105

 97 <- 300 0.00102

 98 <- 293 0.00103

 104 <- 254 0.00135

 104 <- 266 0.00115

 104 <- 343 -0.00110

 114 <- 227 0.00136

 117 <- 236 0.00101

 118 <- 232 0.00102

 119 <- 233 -0.00102

 120 <- 230 0.00118

 121 <- 310 -0.00114

 124 <- 290 -0.00102

 124 <- 311 0.00139

 126 <- 257 0.00112

 127 <- 255 -0.00101

 128 <- 256 0.00101

 129 <- 206 0.00135

 133 <- 246 0.00112

 137 <- 205 -0.00109

 138 <- 206 0.00209

 139 <- 254 0.00108

 143 <- 203 0.00125

 143 <- 207 -0.00207

 144 <- 204 -0.00125

 144 <- 208 0.00207

 145 <- 234 0.00126

 145 <- 329 0.00117

 146 <- 224 -0.00111

 147 <- 225 0.00111

 148 <- 217 -0.00186

 149 <- 209 0.00263

 149 <- 213 -0.00134

 150 <- 222 0.00144

 151 <- 215 0.00152

 152 <- 214 -0.00152

 153 <- 216 -0.00207

 153 <- 242 0.00146

 154 <- 293 -0.00145

 154 <- 310 -0.00125

 154 <- 365 -0.00103

 155 <- 309 -0.00122

 156 <- 308 -0.00122

 157 <- 276 -0.00142

 158 <- 340 0.00102

 159 <- 341 -0.00102

 160 <- 258 0.00131

 160 <- 311 -0.00118

 160 <- 386 0.00109

 163 <- 235 0.00149

 163 <- 266 0.00151

 163 <- 343 -0.00160

 164 <- 221 0.00201

 165 <- 203 0.00104

 165 <- 212 0.00104

 166 <- 204 -0.00104

 166 <- 211 -0.00104

 168 <- 203 0.00193

 168 <- 207 0.00166

 168 <- 212 -0.00116

 168 <- 261 -0.00156

 169 <- 204 -0.00193

 169 <- 208 -0.00166

 169 <- 211 0.00116

 169 <- 262 -0.00156

 170 <- 205 -0.00293

 170 <- 260 -0.00173

 171 <- 210 0.00231

 171 <- 259 -0.00160

 178 <- 288 -0.00115

 179 <- 292 -0.00120

 180 <- 291 0.00120

 181 <- 285 0.00124

 182 <- 203 -0.00297

 182 <- 207 0.00147

 182 <- 212 0.00188

 183 <- 204 -0.00297

 183 <- 208 0.00147

 183 <- 211 0.00188

 184 <- 245 -0.00140

 185 <- 209 0.00137

 186 <- 203 0.00218

 186 <- 207 -0.00174

 186 <- 247 -0.00117

 187 <- 204 -0.00218

 187 <- 208 0.00174

 187 <- 248 -0.00117

 188 <- 272 0.00140

 191 <- 216 -0.00101

 191 <- 218 0.00274

 191 <- 258 0.00130

 192 <- 206 0.00857

 192 <- 221 0.00531

 192 <- 325 -0.00143

 192 <- 346 -0.00121

 193 <- 203 -0.00183

 193 <- 207 0.00775

 193 <- 212 0.00446

 193 <- 237 0.00173

 193 <- 247 -0.00134

 193 <- 335 0.00127

 194 <- 204 0.00183

 194 <- 208 -0.00775

 194 <- 211 -0.00446

 194 <- 238 0.00173

 194 <- 248 -0.00134

 194 <- 336 -0.00127

 195 <- 209 -0.00944

 195 <- 213 0.00177

 195 <- 241 0.00134

 195 <- 253 0.00167

 195 <- 327 0.00154

 196 <- 206 -0.00348

 197 <- 324 -0.00139

 198 <- 205 0.00151

 198 <- 249 -0.00148

 198 <- 260 0.00190

 199 <- 204 0.01364

 199 <- 208 0.00264

 199 <- 211 -0.00349

 199 <- 250 0.00197

 199 <- 262 0.00259

 200 <- 203 -0.01364

 200 <- 207 -0.00264

 200 <- 212 0.00349

 200 <- 251 -0.00197

 200 <- 261 0.00259

 201 <- 210 -0.00552

 201 <- 252 -0.00213

 201 <- 259 0.00295

 202 <- 205 -0.02169

 202 <- 223 -0.00218

 202 <- 249 0.00160

 202 <- 260 -0.00124

 Excited State 8: Singlet-E 2.6530 eV 467.34 nm f=0.0000 <S\*\*2>=0.000

 69 -> 280 0.00111

 72 -> 258 0.00111

 96 -> 286 0.00110

 96 -> 293 -0.00113

 97 -> 266 -0.00106

 98 -> 275 -0.00101

 98 -> 290 0.00148

 98 -> 311 -0.00116

 99 -> 284 0.00155

 100 -> 283 -0.00155

 102 -> 255 0.00100

 102 -> 292 -0.00107

 103 -> 256 -0.00100

 103 -> 291 0.00107

 104 -> 257 0.00136

 104 -> 270 0.00144

 104 -> 300 -0.00167

 113 -> 227 -0.00118

 114 -> 222 0.00109

 117 -> 254 0.00103

 117 -> 266 0.00107

 117 -> 314 0.00107

 118 -> 301 0.00106

 119 -> 302 -0.00106

 121 -> 218 -0.00132

 121 -> 258 -0.00136

 121 -> 267 -0.00104

 121 -> 290 -0.00164

 121 -> 311 0.00179

 122 -> 282 0.00131

 122 -> 284 -0.00194

 122 -> 309 -0.00137

 122 -> 331 -0.00102

 123 -> 281 0.00131

 123 -> 283 -0.00194

 123 -> 308 -0.00137

 123 -> 330 -0.00102

 124 -> 277 -0.00128

 124 -> 286 0.00184

 124 -> 293 -0.00169

 124 -> 310 -0.00172

 126 -> 230 0.00182

 126 -> 254 0.00165

 126 -> 266 0.00177

 126 -> 289 -0.00168

 126 -> 326 0.00135

 126 -> 343 -0.00139

 127 -> 229 0.00116

 127 -> 255 -0.00153

 127 -> 264 -0.00173

 127 -> 279 0.00135

 127 -> 312 -0.00124

 128 -> 228 0.00116

 128 -> 256 -0.00153

 128 -> 263 -0.00173

 128 -> 278 0.00135

 128 -> 313 -0.00124

 129 -> 209 -0.00131

 130 -> 207 0.00108

 131 -> 208 0.00108

 132 -> 206 -0.00129

 133 -> 218 -0.00125

 133 -> 234 -0.00212

 133 -> 258 0.00111

 133 -> 267 -0.00203

 133 -> 275 0.00135

 134 -> 205 0.00187

 135 -> 204 0.00197

 135 -> 211 -0.00101

 136 -> 203 0.00197

 136 -> 212 -0.00101

 137 -> 210 -0.00134

 138 -> 209 -0.00127

 138 -> 213 -0.00155

 138 -> 348 0.00102

 139 -> 257 0.00141

 139 -> 270 0.00104

 139 -> 300 -0.00111

 140 -> 239 0.00118

 140 -> 268 0.00103

 140 -> 273 -0.00113

 140 -> 284 -0.00127

 140 -> 317 -0.00106

 140 -> 331 -0.00105

 141 -> 240 0.00118

 141 -> 269 0.00103

 141 -> 274 -0.00113

 141 -> 283 -0.00127

 141 -> 316 0.00106

 141 -> 330 -0.00105

 143 -> 203 -0.00372

 143 -> 207 0.00121

 143 -> 318 -0.00161

 144 -> 204 -0.00372

 144 -> 208 0.00121

 144 -> 319 -0.00161

 145 -> 231 0.00105

 145 -> 246 -0.00115

 145 -> 265 -0.00118

 145 -> 277 0.00154

 145 -> 286 -0.00204

 145 -> 310 0.00136

 145 -> 338 -0.00158

 148 -> 270 -0.00109

 149 -> 206 -0.00375

 150 -> 216 -0.00144

 151 -> 264 -0.00110

 152 -> 263 -0.00110

 153 -> 222 0.00137

 154 -> 227 0.00157

 154 -> 234 0.00282

 154 -> 242 -0.00151

 154 -> 258 -0.00297

 154 -> 267 0.00187

 154 -> 275 -0.00112

 154 -> 290 -0.00209

 154 -> 311 0.00178

 154 -> 332 -0.00162

 154 -> 386 -0.00129

 155 -> 239 0.00159

 155 -> 243 -0.00197

 155 -> 264 0.00269

 155 -> 273 -0.00168

 155 -> 282 -0.00190

 155 -> 284 0.00147

 155 -> 309 0.00125

 155 -> 312 0.00162

 155 -> 331 0.00128

 155 -> 341 0.00113

 155 -> 371 -0.00113

 156 -> 240 -0.00159

 156 -> 244 0.00197

 156 -> 263 -0.00269

 156 -> 274 0.00168

 156 -> 281 0.00190

 156 -> 283 -0.00147

 156 -> 308 -0.00125

 156 -> 313 -0.00162

 156 -> 330 -0.00128

 156 -> 340 -0.00113

 156 -> 372 0.00113

 157 -> 230 0.00162

 157 -> 235 0.00126

 157 -> 254 0.00119

 157 -> 266 0.00338

 157 -> 280 -0.00112

 157 -> 289 -0.00176

 157 -> 343 -0.00241

 158 -> 232 -0.00168

 158 -> 244 -0.00133

 158 -> 256 -0.00112

 158 -> 269 0.00301

 158 -> 278 0.00105

 158 -> 281 -0.00118

 158 -> 291 0.00172

 158 -> 301 0.00194

 158 -> 308 0.00169

 158 -> 316 0.00120

 159 -> 233 -0.00168

 159 -> 243 -0.00133

 159 -> 255 -0.00112

 159 -> 268 0.00301

 159 -> 279 0.00105

 159 -> 282 -0.00118

 159 -> 292 0.00172

 159 -> 302 -0.00194

 159 -> 309 0.00169

 159 -> 317 -0.00120

 160 -> 231 -0.00151

 160 -> 246 0.00296

 160 -> 265 0.00217

 160 -> 277 -0.00164

 160 -> 293 0.00434

 160 -> 310 0.00192

 160 -> 320 -0.00102

 160 -> 328 0.00141

 160 -> 365 0.00127

 161 -> 227 0.00218

 161 -> 234 0.00113

 161 -> 267 0.00166

 161 -> 275 -0.00175

 161 -> 290 0.00275

 161 -> 311 -0.00204

 161 -> 329 0.00100

 162 -> 205 -0.00482

 162 -> 339 0.00198

 163 -> 205 -0.00120

 163 -> 236 -0.00158

 163 -> 257 0.00130

 163 -> 270 0.00254

 163 -> 276 -0.00196

 163 -> 300 -0.00244

 163 -> 315 0.00147

 163 -> 337 0.00181

 164 -> 209 -0.00283

 164 -> 213 0.00222

 165 -> 203 -0.00202

 165 -> 207 -0.00308

 165 -> 212 -0.00146

 165 -> 318 -0.00107

 166 -> 204 -0.00202

 166 -> 208 -0.00308

 166 -> 211 -0.00146

 166 -> 319 -0.00107

 167 -> 221 0.00213

 167 -> 325 0.00133

 168 -> 203 0.00470

 168 -> 207 0.00126

 168 -> 212 -0.00227

 168 -> 261 -0.00172

 169 -> 204 0.00470

 169 -> 208 0.00126

 169 -> 211 -0.00227

 169 -> 262 0.00172

 170 -> 210 -0.00343

 170 -> 259 0.00173

 171 -> 205 0.00944

 171 -> 223 0.00183

 171 -> 260 0.00195

 171 -> 339 -0.00161

 176 -> 220 0.00155

 176 -> 224 -0.00134

 176 -> 228 0.00165

 176 -> 274 0.00135

 176 -> 278 0.00125

 176 -> 283 0.00175

 176 -> 291 0.00149

 176 -> 308 0.00115

 177 -> 219 0.00155

 177 -> 225 -0.00134

 177 -> 229 0.00165

 177 -> 273 0.00135

 177 -> 279 0.00125

 177 -> 284 0.00175

 177 -> 292 0.00149

 177 -> 309 0.00115

 178 -> 230 -0.00113

 178 -> 266 -0.00179

 178 -> 280 0.00141

 178 -> 289 0.00104

 178 -> 343 0.00123

 179 -> 219 0.00110

 179 -> 225 -0.00133

 179 -> 268 -0.00167

 179 -> 273 0.00123

 179 -> 284 0.00197

 179 -> 292 -0.00152

 179 -> 317 0.00107

 179 -> 353 -0.00113

 180 -> 220 0.00110

 180 -> 224 -0.00133

 180 -> 269 -0.00167

 180 -> 274 0.00123

 180 -> 283 0.00197

 180 -> 291 -0.00152

 180 -> 316 -0.00107

 180 -> 352 -0.00113

 181 -> 270 -0.00192

 181 -> 300 0.00230

 181 -> 337 -0.00179

 182 -> 203 -0.00335

 182 -> 207 -0.00891

 182 -> 212 0.00362

 182 -> 237 0.00161

 182 -> 335 -0.00116

 182 -> 355 -0.00151

 183 -> 204 0.00335

 183 -> 208 0.00891

 183 -> 211 -0.00362

 183 -> 238 0.00161

 183 -> 336 0.00116

 183 -> 354 0.00151

 184 -> 209 0.00165

 184 -> 253 -0.00115

 185 -> 206 -0.00410

 185 -> 221 0.00167

 185 -> 245 0.00149

 186 -> 203 -0.00139

 186 -> 207 0.00407

 186 -> 212 -0.00141

 186 -> 247 0.00170

 187 -> 204 -0.00139

 187 -> 208 0.00407

 187 -> 211 -0.00141

 187 -> 248 -0.00170

 188 -> 216 0.00148

 188 -> 242 -0.00161

 188 -> 258 0.00199

 188 -> 267 -0.00129

 188 -> 275 0.00149

 188 -> 287 0.00149

 188 -> 323 -0.00237

 188 -> 329 -0.00101

 188 -> 347 -0.00153

 188 -> 351 -0.00195

 188 -> 367 -0.00126

 188 -> 411 -0.00120

 188 -> 440 -0.00210

 189 -> 215 -0.00214

 189 -> 233 0.00170

 189 -> 255 -0.00102

 189 -> 264 -0.00188

 189 -> 273 0.00124

 189 -> 282 0.00136

 189 -> 292 0.00140

 189 -> 298 -0.00169

 189 -> 317 0.00137

 189 -> 331 0.00108

 189 -> 333 -0.00118

 189 -> 353 0.00157

 189 -> 362 0.00154

 189 -> 382 0.00100

 189 -> 390 0.00103

 189 -> 403 0.00110

 189 -> 427 0.00103

 189 -> 437 -0.00101

 189 -> 447 0.00128

 190 -> 214 -0.00214

 190 -> 232 0.00170

 190 -> 256 -0.00102

 190 -> 263 -0.00188

 190 -> 274 0.00124

 190 -> 281 0.00136

 190 -> 291 0.00140

 190 -> 299 -0.00169

 190 -> 316 -0.00137

 190 -> 330 0.00108

 190 -> 334 0.00118

 190 -> 352 0.00157

 190 -> 361 0.00154

 190 -> 383 0.00100

 190 -> 391 0.00103

 190 -> 404 -0.00110

 190 -> 426 -0.00103

 190 -> 436 -0.00101

 190 -> 448 0.00128

 191 -> 222 0.00279

 191 -> 231 0.00279

 191 -> 246 -0.00126

 191 -> 277 0.00241

 191 -> 286 -0.00298

 191 -> 310 0.00128

 191 -> 338 -0.00140

 192 -> 209 -0.03196

 192 -> 213 0.00759

 192 -> 241 -0.00103

 192 -> 271 0.00176

 192 -> 327 0.00245

 192 -> 348 -0.00120

 193 -> 203 0.03635

 193 -> 207 -0.02994

 193 -> 212 -0.01248

 193 -> 247 0.00118

 193 -> 318 0.00133

 193 -> 335 -0.00227

 194 -> 204 0.03635

 194 -> 208 -0.02994

 194 -> 211 -0.01248

 194 -> 248 -0.00118

 194 -> 319 0.00133

 194 -> 336 -0.00227

 195 -> 206 0.03807

 195 -> 221 0.00742

 195 -> 245 0.00146

 195 -> 325 -0.00216

 195 -> 346 -0.00153

 195 -> 415 0.00125

 195 -> 514 -0.00111

 196 -> 209 0.00550

 196 -> 213 0.00193

 196 -> 241 0.00217

 196 -> 253 0.00181

 196 -> 348 0.00108

 196 -> 450 -0.00196

 197 -> 210 -0.00161

 197 -> 217 0.00138

 197 -> 230 0.00289

 197 -> 235 0.00125

 197 -> 254 -0.00119

 197 -> 280 0.00350

 197 -> 285 0.00110

 197 -> 303 0.00116

 197 -> 314 0.00101

 197 -> 349 0.00188

 197 -> 366 0.00153

 197 -> 378 -0.00108

 197 -> 394 0.00123

 197 -> 412 -0.00198

 197 -> 433 -0.00155

 197 -> 442 -0.00131

 198 -> 210 -0.01371

 198 -> 357 0.00112

 199 -> 204 0.49616

 199 -> 208 -0.00559

 199 -> 211 0.00511

 199 -> 262 -0.00337

 200 -> 203 0.49616

 200 -> 207 -0.00559

 200 -> 212 0.00511

 200 -> 261 0.00337

 201 -> 205 0.01060

 201 -> 223 -0.00427

 201 -> 249 0.00126

 201 -> 260 -0.00435

 202 -> 210 -0.04253

 202 -> 252 -0.00249

 202 -> 259 0.00517

 202 -> 357 0.00157

 98 <- 290 0.00118

 99 <- 284 0.00122

 100 <- 283 -0.00122

 104 <- 257 0.00102

 104 <- 270 0.00111

 104 <- 300 -0.00137

 121 <- 258 -0.00101

 121 <- 290 -0.00125

 121 <- 311 0.00143

 122 <- 284 -0.00149

 122 <- 309 -0.00109

 123 <- 283 -0.00149

 123 <- 308 -0.00109

 124 <- 286 0.00141

 124 <- 293 -0.00129

 124 <- 310 -0.00136

 126 <- 230 0.00125

 126 <- 254 0.00119

 126 <- 266 0.00132

 126 <- 289 -0.00135

 126 <- 326 0.00109

 126 <- 343 -0.00112

 127 <- 255 -0.00110

 127 <- 264 -0.00128

 127 <- 279 0.00104

 128 <- 256 -0.00110

 128 <- 263 -0.00128

 128 <- 278 0.00104

 133 <- 234 -0.00146

 133 <- 267 -0.00147

 134 <- 205 0.00117

 137 <- 210 -0.00109

 138 <- 209 -0.00101

 139 <- 257 0.00100

 143 <- 203 -0.00208

 143 <- 318 -0.00119

 144 <- 204 -0.00208

 144 <- 319 -0.00119

 145 <- 277 0.00113

 145 <- 286 -0.00152

 145 <- 310 0.00105

 145 <- 338 -0.00123

 149 <- 206 -0.00276

 154 <- 227 0.00100

 154 <- 234 0.00189

 154 <- 242 -0.00101

 154 <- 258 -0.00209

 154 <- 267 0.00133

 154 <- 290 -0.00153

 154 <- 311 0.00137

 154 <- 332 -0.00124

 154 <- 386 -0.00101

 155 <- 239 0.00106

 155 <- 243 -0.00132

 155 <- 264 0.00190

 155 <- 273 -0.00119

 155 <- 282 -0.00137

 155 <- 284 0.00107

 155 <- 312 0.00122

 156 <- 240 -0.00106

 156 <- 244 0.00132

 156 <- 263 -0.00190

 156 <- 274 0.00119

 156 <- 281 0.00137

 156 <- 283 -0.00107

 156 <- 313 -0.00122

 157 <- 230 0.00103

 157 <- 266 0.00236

 157 <- 289 -0.00134

 157 <- 343 -0.00188

 158 <- 232 -0.00106

 158 <- 269 0.00210

 158 <- 291 0.00127

 158 <- 301 0.00146

 158 <- 308 0.00129

 159 <- 233 -0.00106

 159 <- 268 0.00210

 159 <- 292 0.00127

 159 <- 302 -0.00146

 159 <- 309 0.00129

 160 <- 246 0.00196

 160 <- 265 0.00152

 160 <- 277 -0.00118

 160 <- 293 0.00318

 160 <- 310 0.00145

 160 <- 328 0.00107

 161 <- 227 0.00136

 161 <- 267 0.00115

 161 <- 275 -0.00125

 161 <- 290 0.00201

 161 <- 311 -0.00154

 162 <- 205 -0.00251

 162 <- 339 0.00151

 163 <- 270 0.00178

 163 <- 276 -0.00138

 163 <- 300 -0.00183

 163 <- 315 0.00115

 163 <- 337 0.00141

 164 <- 209 -0.00183

 164 <- 213 0.00130

 165 <- 207 -0.00193

 166 <- 208 -0.00193

 168 <- 203 0.00397

 168 <- 212 -0.00160

 168 <- 261 -0.00136

 169 <- 204 0.00397

 169 <- 211 -0.00160

 169 <- 262 0.00136

 170 <- 210 -0.00243

 170 <- 259 0.00147

 171 <- 205 0.00621

 171 <- 260 0.00150

 171 <- 339 -0.00113

 176 <- 283 0.00122

 176 <- 291 0.00108

 177 <- 284 0.00122

 177 <- 292 0.00108

 178 <- 266 -0.00120

 179 <- 268 -0.00113

 179 <- 284 0.00137

 179 <- 292 -0.00108

 180 <- 269 -0.00113

 180 <- 283 0.00137

 180 <- 291 -0.00108

 181 <- 270 -0.00129

 181 <- 300 0.00166

 181 <- 337 -0.00135

 182 <- 203 -0.00174

 182 <- 207 -0.00529

 182 <- 212 0.00131

 182 <- 355 -0.00105

 183 <- 204 0.00174

 183 <- 208 0.00529

 183 <- 211 -0.00131

 183 <- 354 0.00105

 184 <- 209 0.00192

 188 <- 258 0.00121

 188 <- 287 0.00102

 188 <- 323 -0.00170

 188 <- 347 -0.00113

 188 <- 351 -0.00146

 188 <- 440 -0.00169

 189 <- 215 -0.00102

 189 <- 264 -0.00119

 189 <- 298 -0.00116

 189 <- 353 0.00115

 189 <- 362 0.00117

 189 <- 447 0.00101

 190 <- 214 -0.00102

 190 <- 263 -0.00119

 190 <- 299 -0.00116

 190 <- 352 0.00115

 190 <- 361 0.00117

 190 <- 448 0.00101

 191 <- 222 0.00141

 191 <- 231 0.00155

 191 <- 277 0.00158

 191 <- 286 -0.00201

 191 <- 338 -0.00102

 192 <- 209 -0.01453

 192 <- 213 0.00380

 192 <- 271 0.00119

 192 <- 327 0.00163

 193 <- 203 0.00567

 193 <- 207 -0.01311

 193 <- 212 -0.00570

 193 <- 335 -0.00150

 194 <- 204 0.00567

 194 <- 208 -0.01311

 194 <- 211 -0.00570

 194 <- 336 -0.00150

 195 <- 206 0.01563

 195 <- 221 0.00353

 195 <- 325 -0.00146

 195 <- 346 -0.00102

 196 <- 209 0.00350

 196 <- 241 0.00105

 196 <- 450 -0.00164

 197 <- 230 0.00150

 197 <- 280 0.00224

 197 <- 349 0.00137

 197 <- 366 0.00115

 197 <- 412 -0.00156

 197 <- 433 -0.00122

 197 <- 442 -0.00103

 198 <- 210 -0.00332

 198 <- 259 -0.00105

 199 <- 204 -0.02454

 199 <- 208 -0.00492

 199 <- 211 0.00261

 199 <- 238 -0.00166

 199 <- 248 0.00108

 199 <- 262 -0.00303

 200 <- 203 -0.02454

 200 <- 207 -0.00492

 200 <- 212 0.00261

 200 <- 237 0.00166

 200 <- 247 -0.00108

 200 <- 261 0.00303

 201 <- 205 -0.01847

 201 <- 249 0.00110

 201 <- 260 -0.00327

 202 <- 210 -0.01959

 202 <- 252 -0.00118

 202 <- 259 0.00476

 Excited State 9: Singlet-E 3.0757 eV 403.11 nm f=0.0014 <S\*\*2>=0.000

 65 -> 204 -0.00125

 66 -> 223 0.00104

 69 -> 203 -0.00180

 70 -> 205 -0.00117

 70 -> 223 0.00116

 72 -> 204 -0.00111

 97 -> 203 0.00233

 105 -> 203 0.00330

 105 -> 212 0.00131

 112 -> 203 -0.00200

 115 -> 205 0.00159

 115 -> 223 -0.00154

 116 -> 206 0.00143

 116 -> 221 -0.00155

 125 -> 207 -0.00172

 125 -> 237 0.00225

 125 -> 239 0.00106

 125 -> 247 -0.00134

 142 -> 203 -0.00171

 143 -> 205 0.00110

 143 -> 223 -0.00120

 144 -> 206 0.00157

 144 -> 209 -0.00125

 149 -> 204 0.00216

 149 -> 208 -0.00108

 154 -> 208 0.00128

 154 -> 238 0.00109

 155 -> 205 0.00122

 155 -> 223 -0.00117

 156 -> 206 -0.00112

 157 -> 212 0.00120

 159 -> 205 0.00138

 161 -> 204 0.00140

 161 -> 208 0.00119

 161 -> 238 0.00127

 162 -> 203 0.00312

 163 -> 207 -0.00151

 166 -> 206 0.00101

 166 -> 221 -0.00143

 167 -> 204 0.00323

 170 -> 212 0.00104

 171 -> 207 0.00110

 171 -> 212 -0.00125

 172 -> 208 -0.00204

 172 -> 238 -0.00211

 172 -> 248 0.00114

 173 -> 206 -0.00175

 173 -> 221 0.00199

 174 -> 205 -0.00248

 174 -> 210 0.00106

 174 -> 223 0.00185

 176 -> 206 -0.00433

 176 -> 209 0.00179

 176 -> 221 0.00325

 176 -> 241 0.00110

 177 -> 205 -0.00738

 177 -> 210 0.00149

 177 -> 223 0.00438

 178 -> 203 -0.01602

 178 -> 207 0.00118

 178 -> 212 -0.00393

 179 -> 205 -0.00469

 179 -> 210 -0.00177

 180 -> 206 -0.00156

 181 -> 203 0.00319

 181 -> 207 0.00215

 181 -> 212 -0.00108

 182 -> 205 -0.00460

 182 -> 210 -0.00232

 183 -> 206 -0.00140

 183 -> 209 -0.00128

 183 -> 221 0.00177

 183 -> 258 -0.00107

 184 -> 204 -0.00238

 185 -> 204 0.00155

 185 -> 208 -0.00103

 188 -> 208 0.01287

 188 -> 211 -0.00214

 188 -> 238 0.00780

 188 -> 240 0.00364

 188 -> 248 -0.00461

 188 -> 250 -0.00106

 188 -> 262 -0.00152

 188 -> 477 -0.00129

 189 -> 205 0.05437

 189 -> 210 -0.00511

 189 -> 223 -0.01581

 189 -> 260 -0.00203

 189 -> 472 0.00160

 190 -> 206 0.02928

 190 -> 209 -0.00648

 190 -> 213 -0.00132

 190 -> 218 0.00153

 190 -> 221 -0.01655

 190 -> 241 -0.00333

 190 -> 245 -0.00139

 190 -> 253 -0.00323

 190 -> 271 0.00148

 190 -> 450 0.00200

 191 -> 204 -0.00114

 192 -> 204 -0.00357

 192 -> 208 0.00426

 192 -> 211 0.00223

 192 -> 238 -0.00106

 193 -> 205 0.00282

 193 -> 223 -0.00101

 194 -> 206 -0.00452

 194 -> 209 0.00432

 194 -> 213 -0.00175

 194 -> 221 -0.00276

 194 -> 241 -0.00102

 194 -> 253 -0.00131

 195 -> 204 0.01015

 195 -> 208 0.00361

 195 -> 211 0.00342

 195 -> 238 -0.00107

 196 -> 204 -0.09075

 196 -> 208 0.00159

 196 -> 211 -0.00422

 196 -> 281 0.00112

 197 -> 203 0.63703

 197 -> 207 -0.00831

 197 -> 212 0.02255

 197 -> 237 -0.00186

 197 -> 239 -0.00103

 197 -> 261 0.00193

 197 -> 438 -0.00181

 197 -> 476 0.00145

 198 -> 203 -0.28249

 198 -> 207 0.00199

 198 -> 212 -0.00477

 199 -> 206 -0.00205

 199 -> 209 0.00165

 199 -> 221 0.00107

 200 -> 205 0.00332

 200 -> 210 -0.00199

 200 -> 223 -0.00132

 200 -> 259 0.00101

 200 -> 260 -0.00115

 201 -> 203 0.00372

 201 -> 207 -0.00156

 201 -> 261 0.00118

 202 -> 203 0.00408

 202 -> 207 -0.00157

 202 -> 212 0.00447

 162 <- 203 0.00144

 172 <- 204 0.00109

 183 <- 258 -0.00101

 183 <- 287 -0.00164

 183 <- 367 -0.00103

 188 <- 204 -0.00416

 188 <- 208 -0.00131

 188 <- 211 -0.00109

 188 <- 238 -0.00216

 188 <- 240 -0.00113

 188 <- 248 0.00124

 188 <- 262 0.00114

 189 <- 205 -0.00437

 189 <- 223 0.00349

 189 <- 260 0.00120

 190 <- 209 0.00179

 190 <- 241 0.00185

 190 <- 253 0.00176

 190 <- 271 -0.00115

 192 <- 208 0.00166

 192 <- 211 0.00119

 194 <- 206 -0.00124

 194 <- 209 0.00168

 194 <- 221 -0.00154

 195 <- 208 0.00137

 195 <- 211 0.00131

 196 <- 204 -0.00435

 196 <- 211 -0.00115

 196 <- 269 -0.00141

 196 <- 278 0.00197

 196 <- 283 -0.00107

 196 <- 299 0.00108

 197 <- 203 -0.00547

 197 <- 207 -0.00103

 197 <- 212 -0.00141

 197 <- 237 0.00215

 197 <- 247 -0.00120

 197 <- 261 -0.00122

 198 <- 203 0.00325

 198 <- 292 -0.00108

 200 <- 205 -0.00278

 200 <- 210 -0.00163

 201 <- 203 -0.00186

 201 <- 207 -0.00150

 202 <- 207 -0.00106

 202 <- 212 0.00197

 202 <- 279 -0.00163

 202 <- 284 0.00111

 202 <- 292 -0.00177

 Excited State 10: Singlet-E 3.0757 eV 403.11 nm f=0.0014 <S\*\*2>=0.000

 65 -> 203 -0.00125

 67 -> 223 0.00104

 69 -> 204 -0.00180

 71 -> 205 -0.00117

 71 -> 223 0.00116

 72 -> 203 -0.00111

 97 -> 204 0.00233

 105 -> 204 0.00330

 105 -> 211 0.00131

 112 -> 204 -0.00200

 115 -> 206 -0.00143

 115 -> 221 0.00155

 116 -> 205 0.00159

 116 -> 223 -0.00154

 125 -> 208 0.00172

 125 -> 238 0.00225

 125 -> 240 0.00106

 125 -> 248 -0.00134

 142 -> 204 -0.00171

 143 -> 206 0.00157

 143 -> 209 0.00125

 144 -> 205 -0.00110

 144 -> 223 0.00120

 149 -> 203 0.00216

 149 -> 207 -0.00108

 154 -> 207 0.00128

 154 -> 237 -0.00109

 155 -> 206 -0.00112

 156 -> 205 -0.00122

 156 -> 223 0.00117

 157 -> 211 0.00120

 158 -> 205 0.00138

 161 -> 203 0.00140

 161 -> 207 0.00119

 161 -> 237 -0.00127

 162 -> 204 -0.00312

 163 -> 208 0.00151

 165 -> 206 0.00101

 165 -> 221 -0.00143

 167 -> 203 0.00323

 170 -> 211 0.00104

 171 -> 208 -0.00110

 171 -> 211 0.00125

 172 -> 207 -0.00204

 172 -> 237 0.00211

 172 -> 247 -0.00114

 173 -> 205 -0.00248

 173 -> 210 -0.00106

 173 -> 223 0.00185

 174 -> 206 0.00175

 174 -> 221 -0.00199

 176 -> 205 -0.00738

 176 -> 210 -0.00149

 176 -> 223 0.00438

 177 -> 206 0.00433

 177 -> 209 0.00179

 177 -> 221 -0.00325

 177 -> 241 0.00110

 178 -> 204 -0.01602

 178 -> 208 0.00118

 178 -> 211 -0.00393

 179 -> 206 0.00156

 180 -> 205 -0.00469

 180 -> 210 0.00177

 181 -> 204 -0.00319

 181 -> 208 -0.00215

 181 -> 211 0.00108

 182 -> 206 0.00140

 182 -> 209 -0.00128

 182 -> 221 -0.00177

 182 -> 258 0.00107

 183 -> 205 -0.00460

 183 -> 210 0.00232

 184 -> 203 0.00238

 185 -> 203 0.00155

 185 -> 207 -0.00103

 188 -> 207 0.01287

 188 -> 212 -0.00214

 188 -> 237 -0.00780

 188 -> 239 -0.00364

 188 -> 247 0.00461

 188 -> 251 -0.00106

 188 -> 261 0.00152

 188 -> 476 0.00129

 189 -> 206 -0.02928

 189 -> 209 -0.00648

 189 -> 213 -0.00132

 189 -> 218 -0.00153

 189 -> 221 0.01655

 189 -> 241 -0.00333

 189 -> 245 0.00139

 189 -> 253 -0.00323

 189 -> 271 0.00148

 189 -> 450 0.00200

 190 -> 205 0.05437

 190 -> 210 0.00511

 190 -> 223 -0.01581

 190 -> 260 -0.00203

 190 -> 472 0.00160

 191 -> 203 0.00114

 192 -> 203 0.00357

 192 -> 207 -0.00426

 192 -> 212 -0.00223

 192 -> 237 -0.00106

 193 -> 206 -0.00452

 193 -> 209 -0.00432

 193 -> 213 0.00175

 193 -> 221 -0.00276

 193 -> 241 0.00102

 193 -> 253 0.00131

 194 -> 205 -0.00282

 194 -> 223 0.00101

 195 -> 203 0.01015

 195 -> 207 0.00361

 195 -> 212 0.00342

 195 -> 237 0.00107

 196 -> 203 0.09075

 196 -> 207 -0.00159

 196 -> 212 0.00422

 196 -> 282 0.00112

 197 -> 204 0.63703

 197 -> 208 -0.00831

 197 -> 211 0.02255

 197 -> 238 0.00186

 197 -> 240 0.00103

 197 -> 262 -0.00193

 197 -> 439 -0.00181

 197 -> 477 -0.00145

 198 -> 204 -0.28249

 198 -> 208 0.00199

 198 -> 211 -0.00477

 199 -> 205 -0.00332

 199 -> 210 -0.00199

 199 -> 223 0.00132

 199 -> 259 0.00101

 199 -> 260 0.00115

 200 -> 206 -0.00205

 200 -> 209 -0.00165

 200 -> 221 0.00107

 201 -> 204 -0.00372

 201 -> 208 0.00156

 201 -> 262 0.00118

 202 -> 204 0.00408

 202 -> 208 -0.00157

 202 -> 211 0.00447

 162 <- 204 -0.00144

 172 <- 203 0.00109

 182 <- 258 0.00101

 182 <- 287 0.00164

 182 <- 367 0.00103

 188 <- 203 -0.00416

 188 <- 207 -0.00131

 188 <- 212 -0.00109

 188 <- 237 0.00216

 188 <- 239 0.00113

 188 <- 247 -0.00124

 188 <- 261 -0.00114

 189 <- 209 0.00179

 189 <- 241 0.00185

 189 <- 253 0.00176

 189 <- 271 -0.00115

 190 <- 205 -0.00437

 190 <- 223 0.00349

 190 <- 260 0.00120

 192 <- 207 -0.00166

 192 <- 212 -0.00119

 193 <- 206 -0.00124

 193 <- 209 -0.00168

 193 <- 221 -0.00154

 195 <- 207 0.00137

 195 <- 212 0.00131

 196 <- 203 0.00435

 196 <- 212 0.00115

 196 <- 268 -0.00141

 196 <- 279 0.00197

 196 <- 284 -0.00107

 196 <- 298 0.00108

 197 <- 204 -0.00547

 197 <- 208 -0.00103

 197 <- 211 -0.00141

 197 <- 238 -0.00215

 197 <- 248 0.00120

 197 <- 262 0.00122

 198 <- 204 0.00325

 198 <- 291 0.00108

 199 <- 205 0.00278

 199 <- 210 -0.00163

 201 <- 204 0.00186

 201 <- 208 0.00150

 202 <- 208 -0.00106

 202 <- 211 0.00197

 202 <- 278 0.00163

 202 <- 283 -0.00111

 202 <- 291 0.00177

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

 Leave Link 914 at Thu Sep 19 01:07:36 2019, MaxMem= 1342177280 cpu: 14856.9

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

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

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

 Population analysis using the SCF density.

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

 Orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

 (A2)

 The electronic state is 1-A1.

 Alpha occ. eigenvalues -- -19.14404 -19.14404 -19.14404 -19.14404 -19.14404

 Alpha occ. eigenvalues -- -19.14404 -19.14404 -19.14404 -14.30822 -14.30822

 Alpha occ. eigenvalues -- -14.30822 -14.30821 -14.30414 -14.30414 -14.30414

 Alpha occ. eigenvalues -- -14.30413 -10.24427 -10.24427 -10.24427 -10.24427

 Alpha occ. eigenvalues -- -10.24425 -10.24425 -10.24425 -10.24425 -10.23497

 Alpha occ. eigenvalues -- -10.23497 -10.23497 -10.23497 -10.23496 -10.23496

 Alpha occ. eigenvalues -- -10.23496 -10.23495 -10.20789 -10.20789 -10.20789

 Alpha occ. eigenvalues -- -10.20789 -10.20789 -10.20789 -10.20789 -10.20789

 Alpha occ. eigenvalues -- -10.18012 -10.18012 -10.18012 -10.18012 -10.17966

 Alpha occ. eigenvalues -- -10.17966 -10.17966 -10.17966 -10.17357 -10.17357

 Alpha occ. eigenvalues -- -10.17357 -10.17357 -10.17307 -10.17307 -10.17307

 Alpha occ. eigenvalues -- -10.17307 -1.06559 -1.06543 -1.06543 -1.06521

 Alpha occ. eigenvalues -- -1.06457 -1.06438 -1.06438 -1.06424 -0.99814

 Alpha occ. eigenvalues -- -0.98449 -0.98449 -0.95886 -0.93392 -0.89465

 Alpha occ. eigenvalues -- -0.89465 -0.86464 -0.84946 -0.84936 -0.84936

 Alpha occ. eigenvalues -- -0.84766 -0.77405 -0.76418 -0.76418 -0.76254

 Alpha occ. eigenvalues -- -0.76141 -0.75991 -0.75991 -0.75865 -0.72588

 Alpha occ. eigenvalues -- -0.71284 -0.71121 -0.71121 -0.71041 -0.69469

 Alpha occ. eigenvalues -- -0.69469 -0.67875 -0.67758 -0.67758 -0.67758

 Alpha occ. eigenvalues -- -0.63624 -0.63149 -0.61717 -0.61356 -0.61356

 Alpha occ. eigenvalues -- -0.60090 -0.59601 -0.59601 -0.59557 -0.59355

 Alpha occ. eigenvalues -- -0.57263 -0.56364 -0.55873 -0.55873 -0.55077

 Alpha occ. eigenvalues -- -0.55077 -0.54958 -0.54887 -0.53796 -0.53322

 Alpha occ. eigenvalues -- -0.53322 -0.51758 -0.51505 -0.51505 -0.51309

 Alpha occ. eigenvalues -- -0.50701 -0.50406 -0.50406 -0.50154 -0.49760

 Alpha occ. eigenvalues -- -0.48878 -0.47731 -0.47731 -0.47091 -0.46808

 Alpha occ. eigenvalues -- -0.46808 -0.46656 -0.46412 -0.46123 -0.46084

 Alpha occ. eigenvalues -- -0.46084 -0.46051 -0.44957 -0.44948 -0.44659

 Alpha occ. eigenvalues -- -0.44659 -0.43697 -0.43603 -0.43603 -0.43572

 Alpha occ. eigenvalues -- -0.43280 -0.43280 -0.42902 -0.41380 -0.41025

 Alpha occ. eigenvalues -- -0.40715 -0.40715 -0.40386 -0.40383 -0.39343

 Alpha occ. eigenvalues -- -0.39343 -0.39090 -0.38228 -0.38228 -0.38148

 Alpha occ. eigenvalues -- -0.38146 -0.37943 -0.37789 -0.37760 -0.37693

 Alpha occ. eigenvalues -- -0.37693 -0.36182 -0.35057 -0.35057 -0.34934

 Alpha occ. eigenvalues -- -0.34310 -0.34144 -0.33761 -0.33761 -0.33111

 Alpha occ. eigenvalues -- -0.33094 -0.33094 -0.32978 -0.31946 -0.31946

 Alpha occ. eigenvalues -- -0.31848 -0.31178 -0.31178 -0.29275 -0.29072

 Alpha occ. eigenvalues -- -0.29003 -0.29003 -0.28554 -0.26009 -0.26009

 Alpha occ. eigenvalues -- -0.25980 -0.25605 -0.24940 -0.24940 -0.24729

 Alpha occ. eigenvalues -- -0.24379 -0.24176 -0.23285 -0.20812 -0.20812

 Alpha occ. eigenvalues -- -0.20666 -0.16896

 Alpha virt. eigenvalues -- -0.09893 -0.09893 -0.04395 -0.01131 -0.00085

 Alpha virt. eigenvalues -- -0.00085 0.00073 0.02154 0.02998 0.02998

 Alpha virt. eigenvalues -- 0.04107 0.05049 0.05049 0.05129 0.05446

 Alpha virt. eigenvalues -- 0.05861 0.06071 0.06071 0.06305 0.06444

 Alpha virt. eigenvalues -- 0.06491 0.06937 0.06937 0.07960 0.08108

 Alpha virt. eigenvalues -- 0.09322 0.09322 0.09923 0.11112 0.11325

 Alpha virt. eigenvalues -- 0.11325 0.11539 0.11570 0.11734 0.11767

 Alpha virt. eigenvalues -- 0.11767 0.11785 0.11785 0.12142 0.12702

 Alpha virt. eigenvalues -- 0.12861 0.12861 0.12969 0.13144 0.13200

 Alpha virt. eigenvalues -- 0.13200 0.13254 0.13326 0.13326 0.13372

 Alpha virt. eigenvalues -- 0.13477 0.16949 0.16984 0.16984 0.17011

 Alpha virt. eigenvalues -- 0.17593 0.18565 0.18888 0.18997 0.18997

 Alpha virt. eigenvalues -- 0.20418 0.20418 0.20484 0.20715 0.20989

 Alpha virt. eigenvalues -- 0.21449 0.21449 0.22002 0.22304 0.22821

 Alpha virt. eigenvalues -- 0.23609 0.23609 0.24252 0.24662 0.24691

 Alpha virt. eigenvalues -- 0.24981 0.24981 0.25130 0.25837 0.25837

 Alpha virt. eigenvalues -- 0.26312 0.26312 0.26647 0.27787 0.28613

 Alpha virt. eigenvalues -- 0.28824 0.29310 0.29813 0.30191 0.30191

 Alpha virt. eigenvalues -- 0.30345 0.31079 0.31082 0.31082 0.31274

 Alpha virt. eigenvalues -- 0.31489 0.31489 0.32404 0.32622 0.32622

 Alpha virt. eigenvalues -- 0.33322 0.33672 0.33730 0.33730 0.33800

 Alpha virt. eigenvalues -- 0.34790 0.34790 0.34803 0.35138 0.35343

 Alpha virt. eigenvalues -- 0.35343 0.36017 0.36104 0.36925 0.36925

 Alpha virt. eigenvalues -- 0.37337 0.37337 0.37910 0.38168 0.38168

 Alpha virt. eigenvalues -- 0.38271 0.38406 0.38575 0.38771 0.39263

 Alpha virt. eigenvalues -- 0.39366 0.39532 0.39828 0.39828 0.39959

 Alpha virt. eigenvalues -- 0.40011 0.40011 0.40848 0.40848 0.41201

 Alpha virt. eigenvalues -- 0.41318 0.41674 0.41922 0.41922 0.42196

 Alpha virt. eigenvalues -- 0.43000 0.43458 0.43458 0.43649 0.43824

 Alpha virt. eigenvalues -- 0.43998 0.44420 0.44459 0.44496 0.44543

 Alpha virt. eigenvalues -- 0.44543 0.45350 0.45350 0.46313 0.46384

 Alpha virt. eigenvalues -- 0.46428 0.46428 0.46995 0.48304 0.48304

 Alpha virt. eigenvalues -- 0.48588 0.48588 0.49121 0.49168 0.49241

 Alpha virt. eigenvalues -- 0.49503 0.49601 0.49601 0.50292 0.50292

 Alpha virt. eigenvalues -- 0.50327 0.50330 0.50343 0.50585 0.50585

 Alpha virt. eigenvalues -- 0.51294 0.51884 0.52565 0.52565 0.52705

 Alpha virt. eigenvalues -- 0.52705 0.52870 0.53319 0.53372 0.53614

 Alpha virt. eigenvalues -- 0.54420 0.54700 0.55225 0.55225 0.55700

 Alpha virt. eigenvalues -- 0.55700 0.56153 0.56914 0.57268 0.57268

 Alpha virt. eigenvalues -- 0.57680 0.57700 0.58104 0.58104 0.58531

 Alpha virt. eigenvalues -- 0.58723 0.58723 0.59219 0.59307 0.59483

 Alpha virt. eigenvalues -- 0.59967 0.59967 0.60333 0.61306 0.61393

 Alpha virt. eigenvalues -- 0.61784 0.61784 0.62015 0.62663 0.62663

 Alpha virt. eigenvalues -- 0.63131 0.63202 0.63311 0.63588 0.63674

 Alpha virt. eigenvalues -- 0.63674 0.63912 0.63912 0.64278 0.64278

 Alpha virt. eigenvalues -- 0.64454 0.64941 0.65013 0.65013 0.65124

 Alpha virt. eigenvalues -- 0.65216 0.65716 0.65789 0.65889 0.65889

 Alpha virt. eigenvalues -- 0.67509 0.67509 0.67700 0.67702 0.69277

 Alpha virt. eigenvalues -- 0.69798 0.69798 0.70430 0.70720 0.70995

 Alpha virt. eigenvalues -- 0.70995 0.72276 0.72393 0.72693 0.72755

 Alpha virt. eigenvalues -- 0.72755 0.73031 0.73031 0.73638 0.75361

 Alpha virt. eigenvalues -- 0.75361 0.75988 0.76354 0.76747 0.77548

 Alpha virt. eigenvalues -- 0.77548 0.78373 0.78591 0.78785 0.78804

 Alpha virt. eigenvalues -- 0.78882 0.78882 0.79099 0.79995 0.80846

 Alpha virt. eigenvalues -- 0.81383 0.81396 0.81396 0.81559 0.81559

 Alpha virt. eigenvalues -- 0.82502 0.83140 0.83175 0.83175 0.83696

 Alpha virt. eigenvalues -- 0.83696 0.84371 0.85132 0.85450 0.85570

 Alpha virt. eigenvalues -- 0.85570 0.85834 0.86367 0.86670 0.87651

 Alpha virt. eigenvalues -- 0.87651 0.87687 0.88526 0.88526 0.88678

 Alpha virt. eigenvalues -- 0.90499 0.91621 0.91621 0.91900 0.92217

 Alpha virt. eigenvalues -- 0.92217 0.93391 0.93717 0.93803 0.94049

 Alpha virt. eigenvalues -- 0.94049 0.95081 0.95081 0.95549 0.95558

 Alpha virt. eigenvalues -- 0.96314 0.96814 0.97125 0.98312 0.98312

 Alpha virt. eigenvalues -- 0.98654 0.98654 0.98858 0.99274 0.99295

 Alpha virt. eigenvalues -- 0.99295 0.99851 1.00230 1.02368 1.02368

 Alpha virt. eigenvalues -- 1.03127 1.03341 1.04372 1.04996 1.04996

 Alpha virt. eigenvalues -- 1.07550 1.07550 1.08028 1.08028 1.08042

 Alpha virt. eigenvalues -- 1.08081 1.08332 1.08355 1.09459 1.11503

 Alpha virt. eigenvalues -- 1.11546 1.11546 1.11611 1.11761 1.11843

 Alpha virt. eigenvalues -- 1.12200 1.12200 1.13088 1.14098 1.14098

 Alpha virt. eigenvalues -- 1.14189 1.14330 1.14330 1.15433 1.15984

 Alpha virt. eigenvalues -- 1.17756 1.18191 1.18191 1.18461 1.18946

 Alpha virt. eigenvalues -- 1.19375 1.19375 1.19565 1.19682 1.19682

 Alpha virt. eigenvalues -- 1.19967 1.22238 1.22402 1.23612 1.23673

 Alpha virt. eigenvalues -- 1.23770 1.23790 1.23790 1.24103 1.24103

 Alpha virt. eigenvalues -- 1.25528 1.25528 1.26277 1.27204 1.27204

 Alpha virt. eigenvalues -- 1.27498 1.27996 1.28039 1.28498 1.30165

 Alpha virt. eigenvalues -- 1.30662 1.31695 1.31894 1.31894 1.33481

 Alpha virt. eigenvalues -- 1.33591 1.33591 1.33730 1.34526 1.34909

 Alpha virt. eigenvalues -- 1.34909 1.35394 1.35720 1.36267 1.36267

 Alpha virt. eigenvalues -- 1.37733 1.38282 1.38282 1.38405 1.39400

 Alpha virt. eigenvalues -- 1.41037 1.41928 1.43943 1.43943 1.44782

 Alpha virt. eigenvalues -- 1.44782 1.46388 1.47683 1.47683 1.48266

 Alpha virt. eigenvalues -- 1.48322 1.48660 1.48660 1.50384 1.50384

 Alpha virt. eigenvalues -- 1.50397 1.50583 1.51255 1.51550 1.51550

 Alpha virt. eigenvalues -- 1.51646 1.51797 1.52001 1.52497 1.52595

 Alpha virt. eigenvalues -- 1.52785 1.52859 1.52859 1.52978 1.52978

 Alpha virt. eigenvalues -- 1.53092 1.53259 1.54266 1.54266 1.54655

 Alpha virt. eigenvalues -- 1.55597 1.55965 1.56286 1.56286 1.56529

 Alpha virt. eigenvalues -- 1.56718 1.56718 1.57920 1.57920 1.58591

 Alpha virt. eigenvalues -- 1.59033 1.59640 1.59640 1.59643 1.59792

 Alpha virt. eigenvalues -- 1.61043 1.61311 1.61830 1.61830 1.62446

 Alpha virt. eigenvalues -- 1.64410 1.64410 1.64617 1.64617 1.64754

 Alpha virt. eigenvalues -- 1.66535 1.66535 1.67016 1.68655 1.69049

 Alpha virt. eigenvalues -- 1.69094 1.69643 1.69643 1.70359 1.71146

 Alpha virt. eigenvalues -- 1.71215 1.71964 1.71964 1.72456 1.74038

 Alpha virt. eigenvalues -- 1.74038 1.74600 1.75150 1.75407 1.75407

 Alpha virt. eigenvalues -- 1.75502 1.77555 1.77555 1.77713 1.78867

 Alpha virt. eigenvalues -- 1.79136 1.79568 1.80026 1.80026 1.80147

 Alpha virt. eigenvalues -- 1.80147 1.80539 1.80966 1.81177 1.82014

 Alpha virt. eigenvalues -- 1.82014 1.82252 1.84198 1.84198 1.84328

 Alpha virt. eigenvalues -- 1.85543 1.87405 1.88031 1.88158 1.88158

 Alpha virt. eigenvalues -- 1.89180 1.89286 1.89286 1.89384 1.90494

 Alpha virt. eigenvalues -- 1.90673 1.90673 1.90794 1.90871 1.91191

 Alpha virt. eigenvalues -- 1.91953 1.91953 1.95203 1.96362 1.96362

 Alpha virt. eigenvalues -- 1.96493 1.97083 1.98383 1.98452 1.98452

 Alpha virt. eigenvalues -- 1.99209 1.99299 1.99299 2.00030 2.01487

 Alpha virt. eigenvalues -- 2.01730 2.01730 2.02692 2.03485 2.07975

 Alpha virt. eigenvalues -- 2.08945 2.08999 2.09135 2.09258 2.09258

 Alpha virt. eigenvalues -- 2.10109 2.11316 2.11316 2.13550 2.13550

 Alpha virt. eigenvalues -- 2.14628 2.15639 2.16339 2.16339 2.18559

 Alpha virt. eigenvalues -- 2.19721 2.20806 2.20806 2.21423 2.22291

 Alpha virt. eigenvalues -- 2.24182 2.24254 2.25636 2.25636 2.25730

 Alpha virt. eigenvalues -- 2.25730 2.26658 2.27461 2.27952 2.28358

 Alpha virt. eigenvalues -- 2.28358 2.28541 2.30059 2.30059 2.31218

 Alpha virt. eigenvalues -- 2.31978 2.32005 2.33555 2.33555 2.34094

 Alpha virt. eigenvalues -- 2.34200 2.34200 2.34304 2.34344 2.34519

 Alpha virt. eigenvalues -- 2.34657 2.34657 2.34736 2.35190 2.35284

 Alpha virt. eigenvalues -- 2.36760 2.36760 2.37968 2.39356 2.39800

 Alpha virt. eigenvalues -- 2.39800 2.40336 2.40336 2.40339 2.41410

 Alpha virt. eigenvalues -- 2.43240 2.43597 2.43597 2.44116 2.44353

 Alpha virt. eigenvalues -- 2.44353 2.45063 2.47556 2.48798 2.48798

 Alpha virt. eigenvalues -- 2.49592 2.50111 2.50564 2.51257 2.51257

 Alpha virt. eigenvalues -- 2.51662 2.51662 2.51728 2.51824 2.54097

 Alpha virt. eigenvalues -- 2.54789 2.56978 2.56978 2.58167 2.59071

 Alpha virt. eigenvalues -- 2.59071 2.61379 2.62439 2.63062 2.64476

 Alpha virt. eigenvalues -- 2.64476 2.64699 2.65142 2.67022 2.67022

 Alpha virt. eigenvalues -- 2.67402 2.67402 2.67721 2.68057 2.68467

 Alpha virt. eigenvalues -- 2.72792 2.73171 2.74096 2.74281 2.74281

 Alpha virt. eigenvalues -- 2.74285 2.74622 2.74622 2.78111 2.78111

 Alpha virt. eigenvalues -- 2.79141 2.79256 2.79733 2.80146 2.80146

 Alpha virt. eigenvalues -- 2.81796 2.81942 2.81942 2.82068 2.83220

 Alpha virt. eigenvalues -- 2.83429 2.83429 2.83841 2.84993 2.85619

 Alpha virt. eigenvalues -- 2.86727 2.86938 2.86938 2.87132 2.87132

 Alpha virt. eigenvalues -- 2.87545 2.87808 2.87808 2.89028 2.89227

 Alpha virt. eigenvalues -- 2.90319 2.91151 2.94018 2.94018 2.94750

 Alpha virt. eigenvalues -- 2.94871 2.95132 2.95132 2.96084 2.96268

 Alpha virt. eigenvalues -- 2.98764 2.98764 2.99422 3.00515 3.00515

 Alpha virt. eigenvalues -- 3.00831 3.00996 3.01748 3.02942 3.02942

 Alpha virt. eigenvalues -- 3.03803 3.05070 3.06208 3.06208 3.06414

 Alpha virt. eigenvalues -- 3.07922 3.07922 3.08917 3.11748 3.13121

 Alpha virt. eigenvalues -- 3.13387 3.13387 3.13979 3.14115 3.14848

 Alpha virt. eigenvalues -- 3.14848 3.15511 3.15884 3.16284 3.16427

 Alpha virt. eigenvalues -- 3.16427 3.17612 3.17795 3.17795 3.18339

 Alpha virt. eigenvalues -- 3.19344 3.19393 3.20304 3.20388 3.20388

 Alpha virt. eigenvalues -- 3.20454 3.21215 3.21261 3.21261 3.21303

 Alpha virt. eigenvalues -- 3.21563 3.21563 3.22011 3.22359 3.22359

 Alpha virt. eigenvalues -- 3.23327 3.24933 3.26407 3.26407 3.27005

 Alpha virt. eigenvalues -- 3.28785 3.28842 3.28842 3.29147 3.29227

 Alpha virt. eigenvalues -- 3.30447 3.30447 3.31320 3.31422 3.32987

 Alpha virt. eigenvalues -- 3.32987 3.35669 3.37154 3.37576 3.38167

 Alpha virt. eigenvalues -- 3.38167 3.41075 3.41075 3.41216 3.41316

 Alpha virt. eigenvalues -- 3.41509 3.42051 3.42051 3.43262 3.45569

 Alpha virt. eigenvalues -- 3.47203 3.47203 3.49013 3.55631 3.60857

 Alpha virt. eigenvalues -- 3.60857 3.61368 3.61970 3.62685 3.62685

 Alpha virt. eigenvalues -- 3.67814 3.68015 3.68015 3.68769 3.76619

 Alpha virt. eigenvalues -- 3.76926 3.77999 3.77999 3.78833 3.80124

 Alpha virt. eigenvalues -- 3.80124 3.81311 3.82890 3.82890 3.83043

 Alpha virt. eigenvalues -- 3.84845 3.87215 3.89364 3.89535 3.89535

 Alpha virt. eigenvalues -- 3.92111 3.95742 3.96880 3.96880 3.97741

 Alpha virt. eigenvalues -- 3.98613 3.98613 3.98917 3.99600 4.01922

 Alpha virt. eigenvalues -- 4.01922 4.02579 4.02641 4.11584 4.15126

 Alpha virt. eigenvalues -- 4.15126 4.17185 4.18203 4.18203 4.19775

 Alpha virt. eigenvalues -- 4.21838 4.23261 4.24626 4.24626 4.27271

 Alpha virt. eigenvalues -- 4.35398 4.41755 4.41755 4.42486 4.46963

 Alpha virt. eigenvalues -- 4.52114 4.61512 4.61512 4.82427 4.82429

 Alpha virt. eigenvalues -- 4.82429 4.82576 4.87818 4.88250 4.88250

 Alpha virt. eigenvalues -- 4.89138 4.89179 4.89852 4.89852 4.90121

 Alpha virt. eigenvalues -- 5.13633 5.13642 5.13642 5.17251 5.21812

 Alpha virt. eigenvalues -- 5.25966 5.26628 5.26628 5.27311 5.29964

 Alpha virt. eigenvalues -- 5.30289 5.30289 5.31285 5.38394 5.38394

 Alpha virt. eigenvalues -- 5.56086 5.67529 5.69050 5.69050 5.69387

 Alpha virt. eigenvalues -- 5.75818 5.76216 5.76216 5.77002 7.77599

 Alpha virt. eigenvalues -- 7.77599 7.88709 7.95021 8.20751 11.17031

 Alpha virt. eigenvalues -- 23.34464 23.37771 23.37771 23.39775 23.44693

 Alpha virt. eigenvalues -- 23.45091 23.45091 23.45571 23.46199 23.46424

 Alpha virt. eigenvalues -- 23.46424 23.46555 23.77721 23.79473 23.79473

 Alpha virt. eigenvalues -- 23.80893 23.82802 23.83201 23.83201 23.83532

 Alpha virt. eigenvalues -- 23.88876 23.88876 23.89012 23.89254 23.89453

 Alpha virt. eigenvalues -- 23.90784 23.90784 23.91003 24.02322 24.02329

 Alpha virt. eigenvalues -- 24.02329 24.02440 24.03595 24.03885 24.03885

 Alpha virt. eigenvalues -- 24.04443 24.11459 24.11489 24.11489 24.11630

 Alpha virt. eigenvalues -- 35.58110 35.61417 35.61417 35.62327 35.70076

 Alpha virt. eigenvalues -- 35.71260 35.71260 35.71424 49.92018 49.92454

 Alpha virt. eigenvalues -- 49.92454 49.92730 49.92893 49.93264 49.93264

 Alpha virt. eigenvalues -- 49.93495

 Condensed to atoms (all electrons):

 Mulliken charges:

 1

 1 C 0.385494

 2 N -0.687379

 3 C 0.385494

 4 C -0.092977

 5 C -0.092977

 6 N -0.342451

 7 C 0.385494

 8 N -0.687379

 9 C 0.385494

 10 C -0.092977

 11 C -0.092977

 12 N -0.342451

 13 C -0.092977

 14 C -0.092977

 15 C 0.385494

 16 N -0.687379

 17 C 0.385494

 18 N -0.342451

 19 N -0.687379

 20 C 0.385494

 21 C -0.092977

 22 C -0.092977

 23 C 0.385494

 24 N -0.342451

 25 Zn 1.449984

 26 C 0.202394

 27 C -0.307078

 28 C -0.307078

 29 C 0.202394

 30 C 0.202394

 31 C -0.307078

 32 C -0.307078

 33 C 0.202394

 34 C 0.202394

 35 C -0.307078

 36 C -0.307078

 37 C 0.202394

 38 C 0.202394

 39 C -0.307078

 40 C -0.307078

 41 C 0.202394

 42 H 0.255919

 43 H 0.255919

 44 H 0.255919

 45 H 0.255919

 46 H 0.255919

 47 H 0.255919

 48 H 0.255919

 49 H 0.255919

 50 O -0.315694

 51 O -0.315694

 52 O -0.315694

 53 O -0.315694

 54 O -0.315694

 55 O -0.315694

 56 O -0.315694

 57 O -0.315694

 58 C -0.505457

 59 H 0.227146

 60 H 0.256628

 61 C -0.505457

 62 H 0.227146

 63 H 0.256628

 64 C -0.505457

 65 H 0.227146

 66 H 0.256628

 67 C -0.505457

 68 H 0.227146

 69 H 0.256628

 70 C -0.505457

 71 H 0.227146

 72 H 0.256628

 73 C -0.505457

 74 H 0.227146

 75 H 0.256628

 76 C -0.505457

 77 H 0.227146

 78 H 0.256628

 79 C -0.505457

 80 H 0.227146

 81 H 0.256628

 82 H 0.227293

 83 H 0.227293

 84 H 0.227293

 85 H 0.227293

 86 H 0.227293

 87 H 0.227293

 88 H 0.227293

 89 H 0.227293

 Sum of Mulliken charges = -0.00000

 Mulliken charges with hydrogens summed into heavy atoms:

 1

 1 C 0.385494

 2 N -0.687379

 3 C 0.385494

 4 C -0.092977

 5 C -0.092977

 6 N -0.342451

 7 C 0.385494

 8 N -0.687379

 9 C 0.385494

 10 C -0.092977

 11 C -0.092977

 12 N -0.342451

 13 C -0.092977

 14 C -0.092977

 15 C 0.385494

 16 N -0.687379

 17 C 0.385494

 18 N -0.342451

 19 N -0.687379

 20 C 0.385494

 21 C -0.092977

 22 C -0.092977

 23 C 0.385494

 24 N -0.342451

 25 Zn 1.449984

 26 C 0.202394

 27 C -0.051160

 28 C -0.051160

 29 C 0.202394

 30 C 0.202394

 31 C -0.051160

 32 C -0.051160

 33 C 0.202394

 34 C 0.202394

 35 C -0.051160

 36 C -0.051160

 37 C 0.202394

 38 C 0.202394

 39 C -0.051160

 40 C -0.051160

 41 C 0.202394

 50 O -0.315694

 51 O -0.315694

 52 O -0.315694

 53 O -0.315694

 54 O -0.315694

 55 O -0.315694

 56 O -0.315694

 57 O -0.315694

 58 C 0.205610

 61 C 0.205610

 64 C 0.205610

 67 C 0.205610

 70 C 0.205610

 73 C 0.205610

 76 C 0.205610

 79 C 0.205610

 Electronic spatial extent (au): <R\*\*2>= 44666.7531

 Charge= -0.0000 electrons

 Dipole moment (field-independent basis, Debye):

 X= 0.0000 Y= 0.0000 Z= 0.0000 Tot= 0.0000

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

 XX= -199.1244 YY= -199.1244 ZZ= -336.1852

 XY= 0.0000 XZ= -0.0000 YZ= 0.0000

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

 XX= 45.6869 YY= 45.6869 ZZ= -91.3738

 XY= 0.0000 XZ= -0.0000 YZ= 0.0000

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

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

 XXY= 0.0000 XXZ= -16.6252 XZZ= -0.0000 YZZ= -0.0000

 YYZ= 16.6252 XYZ= -0.0000

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

 XXXX= -20661.0950 YYYY= -20661.0950 ZZZZ= -414.7972 XXXY= 0.0000

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

 ZZZY= -0.0000 XXYY= -6637.0002 XXZZ= -5203.0866 YYZZ= -5203.0866

 XXYZ= 0.0000 YYXZ= -0.0000 ZZXY= 0.0000

 N-N= 8.035131125212D+03 E-N=-2.234733592132D+04 KE= 2.690097641994D+03

 Symmetry A1 KE= 7.472512070613D+02

 Symmetry A2 KE= 6.108286470496D+02

 Symmetry B1 KE= 6.660088939415D+02

 Symmetry B2 KE= 6.660088939415D+02

 Leave Link 601 at Thu Sep 19 01:08:08 2019, MaxMem= 1342177280 cpu: 45.9

 (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\C40H32N8O8Z

 n1\BLAB\19-Sep-2019\0\\#p td(root=1,nstates=10) b3lyp/genecp scrf=(sol

 vent=dmso,smd) empiricaldispersion=gd3bj IOp(9/40=3)\\ZnOMPC0td\\0,1\C

 ,0,-1.126947,2.810131,0.013541\N,0,0.,2.040854,-0.0007\C,0,1.126947,2.

 810131,0.013541\C,0,0.708388,4.216552,0.043016\C,0,-0.708388,4.216552,

 0.043016\N,0,2.392227,2.392227,0.\C,0,2.810131,1.126947,-0.013541\N,0,

 2.040854,0.,0.0007\C,0,2.810131,-1.126947,-0.013541\C,0,4.216552,-0.70

 8388,-0.043016\C,0,4.216552,0.708388,-0.043016\N,0,-2.392227,2.392227,

 0.\C,0,-4.216552,0.708388,-0.043016\C,0,-4.216552,-0.708388,-0.043016\

 C,0,-2.810131,-1.126947,-0.013541\N,0,-2.040854,0.,0.0007\C,0,-2.81013

 1,1.126947,-0.013541\N,0,-2.392227,-2.392227,0.\N,0,0.,-2.040854,-0.00

 07\C,0,-1.126947,-2.810131,0.013541\C,0,-0.708388,-4.216552,0.043016\C

 ,0,0.708388,-4.216552,0.043016\C,0,1.126947,-2.810131,0.013541\N,0,2.3

 92227,-2.392227,0.\Zn,0,0.,0.,0.\C,0,-5.420785,1.432821,-0.07184\C,0,-

 6.610317,0.699802,-0.098313\C,0,-6.610317,-0.699802,-0.098313\C,0,-5.4

 20785,-1.432821,-0.07184\C,0,1.432821,-5.420785,0.07184\C,0,0.699802,-

 6.610317,0.098313\C,0,-0.699802,-6.610317,0.098313\C,0,-1.432821,-5.42

 0785,0.07184\C,0,5.420785,1.432821,-0.07184\C,0,6.610317,0.699802,-0.0

 98313\C,0,6.610317,-0.699802,-0.098313\C,0,5.420785,-1.432821,-0.07184

 \C,0,-1.432821,5.420785,0.07184\C,0,-0.699802,6.610317,0.098313\C,0,0.

 699802,6.610317,0.098313\C,0,1.432821,5.420785,0.07184\H,0,7.565152,1.

 207886,-0.120969\H,0,7.565152,-1.207886,-0.120969\H,0,1.207886,7.56515

 2,0.120969\H,0,-1.207886,7.565152,0.120969\H,0,-7.565152,1.207886,-0.1

 20969\H,0,-7.565152,-1.207886,-0.120969\H,0,-1.207886,-7.565152,0.1209

 69\H,0,1.207886,-7.565152,0.120969\O,0,2.783942,5.357598,0.073945\O,0,

 -2.783942,5.357598,0.073945\O,0,5.357598,2.783942,-0.073945\O,0,5.3575

 98,-2.783942,-0.073945\O,0,2.783942,-5.357598,0.073945\O,0,-2.783942,-

 5.357598,0.073945\O,0,-5.357598,-2.783942,-0.073945\O,0,-5.357598,2.78

 3942,-0.073945\C,0,3.514352,6.580615,0.1027\H,0,3.303559,7.194357,-0.7

 78514\H,0,4.56446,6.293917,0.099713\C,0,6.580615,3.514352,-0.1027\H,0,

 7.194357,3.303559,0.778514\H,0,6.293917,4.56446,-0.099713\C,0,6.580615

 ,-3.514352,-0.1027\H,0,7.194357,-3.303559,0.778514\H,0,6.293917,-4.564

 46,-0.099713\C,0,-3.514352,6.580615,0.1027\H,0,-3.303559,7.194357,-0.7

 78514\H,0,-4.56446,6.293917,0.099713\C,0,-6.580615,3.514352,-0.1027\H,

 0,-7.194357,3.303559,0.778514\H,0,-6.293917,4.56446,-0.099713\C,0,-6.5

 80615,-3.514352,-0.1027\H,0,-7.194357,-3.303559,0.778514\H,0,-6.293917

 ,-4.56446,-0.099713\C,0,-3.514352,-6.580615,0.1027\H,0,-3.303559,-7.19

 4357,-0.778514\H,0,-4.56446,-6.293917,0.099713\C,0,3.514352,-6.580615,

 0.1027\H,0,3.303559,-7.194357,-0.778514\H,0,4.56446,-6.293917,0.099713

 \H,0,3.298342,-7.155737,1.008335\H,0,-3.298342,-7.155737,1.008335\H,0,

 -7.155737,-3.298342,-1.008335\H,0,-7.155737,3.298342,-1.008335\H,0,3.2

 98342,7.155737,1.008335\H,0,-3.298342,7.155737,1.008335\H,0,7.155737,-

 3.298342,-1.008335\H,0,7.155737,3.298342,-1.008335\\Version=ES64L-G09R

 evE.01\State=1-A1\HF=-2649.8283939\RMSD=4.396e-09\PG=D02D [O(Zn1),2SGD

 (N2),X(C40H32N4O8)]\\@

 A people that values its privileges above its principles soon loses both.

 -- Dwight D. Eisenhower

 Job cpu time: 0 days 4 hours 45 minutes 24.8 seconds.

 File lengths (MBytes): RWF= 4848 Int= 0 D2E= 0 Chk= 488 Scr= 1

 Normal termination of Gaussian 09 at Thu Sep 19 01:09:03 2019.