Entering Gaussian System, Link 0=g09

 Input=ZnPC0td.com

 Output=ZnPC0td.log

 Initial command:

 /home/blab/g09/l1.exe "/home/blab/g09/scratch/Gau-46803.inp" -scrdir="/home/blab/g09/scratch/"

 Entering Link 1 = /home/blab/g09/l1.exe PID= 46810.

 Copyright (c) 1988,1990,1992,1993,1995,1998,2003,2009,2015,

 Gaussian, Inc. All Rights Reserved.

 This is part of the Gaussian(R) 09 program. It is based on

 the Gaussian(R) 03 system (copyright 2003, Gaussian, Inc.),

 the Gaussian(R) 98 system (copyright 1998, Gaussian, Inc.),

 the Gaussian(R) 94 system (copyright 1995, Gaussian, Inc.),

 the Gaussian 92(TM) system (copyright 1992, Gaussian, Inc.),

 the Gaussian 90(TM) system (copyright 1990, Gaussian, Inc.),

 the Gaussian 88(TM) system (copyright 1988, Gaussian, Inc.),

 the Gaussian 86(TM) system (copyright 1986, Carnegie Mellon

 University), and the Gaussian 82(TM) system (copyright 1983,

 Carnegie Mellon University). Gaussian is a federally registered

 trademark of Gaussian, Inc.

 This software contains proprietary and confidential information,

 including trade secrets, belonging to Gaussian, Inc.

 This software is provided under written license and may be

 used, copied, transmitted, or stored only in accord with that

 written license.

 The following legend is applicable only to US Government

 contracts under FAR:

 RESTRICTED RIGHTS LEGEND

 Use, reproduction and disclosure by the US Government is

 subject to restrictions as set forth in subparagraphs (a)

 and (c) of the Commercial Computer Software - Restricted

 Rights clause in FAR 52.227-19.

 Gaussian, Inc.

 340 Quinnipiac St., Bldg. 40, Wallingford CT 06492

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

 Warning -- This program may not be used in any manner that

 competes with the business of Gaussian, Inc. or will provide

 assistance to any competitor of Gaussian, Inc. The licensee

 of this program is prohibited from giving any competitor of

 Gaussian, Inc. access to this program. By using this program,

 the user acknowledges that Gaussian, Inc. is engaged in the

 business of creating and licensing software in the field of

 computational chemistry and represents and warrants to the

 licensee that it is not a competitor of Gaussian, Inc. and that

 it will not use this program in any manner prohibited above.

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

 Cite this work as:

 Gaussian 09, Revision E.01,

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

 M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,

 G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,

 A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,

 M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,

 Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,

 J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,

 K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand,

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

 M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,

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

 O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,

 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=ZnPC0td.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 00:35:27 2019, MaxMem= 1342177280 cpu: 0.6

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

 -------

 ZnPC0td

 -------

 Symbolic Z-matrix:

 Charge = 0 Multiplicity = 1

 C 2.76651 1.18235 0.01953

 N 1.4247 1.4247 0.06819

 C 1.18235 2.76651 0.01953

 C 2.46772 3.46649 -0.04739

 C 3.46649 2.46772 -0.04739

 N 0. 3.37815 0.00933

 C -1.18235 2.76651 0.01953

 N -1.4247 1.4247 0.06819

 C -2.76651 1.18235 0.01953

 C -3.46649 2.46772 -0.04739

 C -2.46772 3.46649 -0.04739

 N 3.37815 0. 0.00933

 C 3.46649 -2.46772 -0.04739

 C 2.46772 -3.46649 -0.04739

 C 1.18235 -2.76651 0.01953

 N 1.4247 -1.4247 0.06819

 C 2.76651 -1.18235 0.01953

 N 0. -3.37815 0.00933

 N -1.4247 -1.4247 0.06819

 C -1.18235 -2.76651 0.01953

 C -2.46772 -3.46649 -0.04739

 C -3.46649 -2.46772 -0.04739

 C -2.76651 -1.18235 0.01953

 N -3.37815 0. 0.00933

 Zn 0. 0. 0.51047

 C 4.81585 -2.80418 -0.11201

 C 5.14916 -4.1562 -0.16919

 C 4.1562 -5.14916 -0.16919

 C 2.80418 -4.81585 -0.11201

 C -4.81585 -2.80418 -0.11201

 C -5.14916 -4.1562 -0.16919

 C -4.1562 -5.14916 -0.16919

 C -2.80418 -4.81585 -0.11201

 C -2.80418 4.81585 -0.11201

 C -4.1562 5.14916 -0.16919

 C -5.14916 4.1562 -0.16919

 C -4.81585 2.80418 -0.11201

 C 4.81585 2.80418 -0.11201

 C 5.14916 4.1562 -0.16919

 C 4.1562 5.14916 -0.16919

 C 2.80418 4.81585 -0.11201

 H 5.58269 -2.03739 -0.11563

 H 2.03739 -5.58269 -0.11563

 H -5.58269 -2.03739 -0.11563

 H -2.03739 -5.58269 -0.11563

 H -2.03739 5.58269 -0.11563

 H -5.58269 2.03739 -0.11563

 H 5.58269 2.03739 -0.11563

 H 2.03739 5.58269 -0.11563

 H -4.44927 6.19242 -0.21565

 H -6.19242 4.44927 -0.21565

 H 4.44927 6.19242 -0.21565

 H 6.19242 4.44927 -0.21565

 H 6.19242 -4.44927 -0.21565

 H 4.44927 -6.19242 -0.21565

 H -4.44927 -6.19242 -0.21565

 H -6.19242 -4.44927 -0.21565

 NAtoms= 57 NQM= 57 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 1

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

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

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

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

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

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

 Atom 51 52 53 54 55 56 57

 IAtWgt= 1 1 1 1 1 1 1

 AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

 NucSpn= 1 1 1 1 1 1 1

 AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

 NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

 NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

 AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

 Leave Link 101 at Thu Sep 19 00:35:27 2019, MaxMem= 1342177280 cpu: 0.8

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

 Stoichiometry C32H16N8Zn

 Framework group C4V[C4(Zn),2SGV(N2),2SGD(N2),X(C32H16)]

 Deg. of freedom 22

 Full point group C4V 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 2.766507 1.182350 0.019533

 2 7 0 1.424701 1.424701 0.068191

 3 6 0 1.182350 2.766507 0.019533

 4 6 0 2.467721 3.466489 -0.047388

 5 6 0 3.466489 2.467721 -0.047388

 6 7 0 0.000000 3.378152 0.009330

 7 6 0 -1.182350 2.766507 0.019533

 8 7 0 -1.424701 1.424701 0.068191

 9 6 0 -2.766507 1.182350 0.019533

 10 6 0 -3.466489 2.467721 -0.047388

 11 6 0 -2.467721 3.466489 -0.047388

 12 7 0 3.378152 -0.000000 0.009330

 13 6 0 3.466489 -2.467721 -0.047388

 14 6 0 2.467721 -3.466489 -0.047388

 15 6 0 1.182350 -2.766507 0.019533

 16 7 0 1.424701 -1.424701 0.068191

 17 6 0 2.766507 -1.182350 0.019533

 18 7 0 -0.000000 -3.378152 0.009330

 19 7 0 -1.424701 -1.424701 0.068191

 20 6 0 -1.182350 -2.766507 0.019533

 21 6 0 -2.467721 -3.466489 -0.047388

 22 6 0 -3.466489 -2.467721 -0.047388

 23 6 0 -2.766507 -1.182350 0.019533

 24 7 0 -3.378152 0.000000 0.009330

 25 30 0 0.000000 0.000000 0.510466

 26 6 0 4.815847 -2.804179 -0.112010

 27 6 0 5.149164 -4.156200 -0.169185

 28 6 0 4.156200 -5.149164 -0.169185

 29 6 0 2.804179 -4.815847 -0.112010

 30 6 0 -4.815847 -2.804179 -0.112010

 31 6 0 -5.149164 -4.156200 -0.169185

 32 6 0 -4.156200 -5.149164 -0.169185

 33 6 0 -2.804179 -4.815847 -0.112010

 34 6 0 -2.804179 4.815847 -0.112010

 35 6 0 -4.156200 5.149164 -0.169185

 36 6 0 -5.149164 4.156200 -0.169185

 37 6 0 -4.815847 2.804179 -0.112010

 38 6 0 4.815847 2.804179 -0.112010

 39 6 0 5.149164 4.156200 -0.169185

 40 6 0 4.156200 5.149164 -0.169185

 41 6 0 2.804179 4.815847 -0.112010

 42 1 0 5.582686 -2.037386 -0.115625

 43 1 0 2.037386 -5.582686 -0.115625

 44 1 0 -5.582686 -2.037386 -0.115625

 45 1 0 -2.037386 -5.582686 -0.115625

 46 1 0 -2.037386 5.582686 -0.115625

 47 1 0 -5.582686 2.037386 -0.115625

 48 1 0 5.582686 2.037386 -0.115625

 49 1 0 2.037386 5.582686 -0.115625

 50 1 0 -4.449274 6.192416 -0.215654

 51 1 0 -6.192416 4.449274 -0.215654

 52 1 0 4.449274 6.192416 -0.215654

 53 1 0 6.192416 4.449274 -0.215654

 54 1 0 6.192416 -4.449274 -0.215654

 55 1 0 4.449274 -6.192416 -0.215654

 56 1 0 -4.449274 -6.192416 -0.215654

 57 1 0 -6.192416 -4.449274 -0.215654

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

 Rotational constants (GHZ): 0.0882342 0.0882342 0.0442839

 Leave Link 202 at Thu Sep 19 00:35:27 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 50 51

 Centers: 52 53 54 55 56 57 1 3 4 5

 Centers: 7 9 10 11 13 14 15 17 20 21

 Centers: 22 23 26 27 28 29 30 31 32 33

 Centers: 34 35 36 37 38 39 40 41 2 6

 Centers: 8 12 16 18 19 24

 6-311G\*

 \*\*\*\*

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

 Pseudopotential Parameters

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

 Center Atomic Valence Angular Power

 Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

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

 1 6

 No pseudopotential on this center.

 2 7

 No pseudopotential on this center.

 3 6

 No pseudopotential on this center.

 4 6

 No pseudopotential on this center.

 5 6

 No pseudopotential on this center.

 6 7

 No pseudopotential on this center.

 7 6

 No pseudopotential on this center.

 8 7

 No pseudopotential on this center.

 9 6

 No pseudopotential on this center.

 10 6

 No pseudopotential on this center.

 11 6

 No pseudopotential on this center.

 12 7

 No pseudopotential on this center.

 13 6

 No pseudopotential on this center.

 14 6

 No pseudopotential on this center.

 15 6

 No pseudopotential on this center.

 16 7

 No pseudopotential on this center.

 17 6

 No pseudopotential on this center.

 18 7

 No pseudopotential on this center.

 19 7

 No pseudopotential on this center.

 20 6

 No pseudopotential on this center.

 21 6

 No pseudopotential on this center.

 22 6

 No pseudopotential on this center.

 23 6

 No pseudopotential on this center.

 24 7

 No pseudopotential on this center.

 25 30 12

 F and up

 1 386.7379660 -18.00000000 0.00000000

 2 72.8587359 -124.35274030 0.00000000

 2 15.9066170 -30.66018220 0.00000000

 2 4.3502340 -10.63589890 0.00000000

 2 1.2842199 -0.76836230 0.00000000

 S - F

 0 19.0867858 3.00000000 0.00000000

 1 5.0231080 22.52342250 0.00000000

 2 1.2701744 48.44659420 0.00000000

 2 1.0671287 -44.55601190 0.00000000

 2 0.9264190 12.99839580 0.00000000

 P - F

 0 43.4927750 5.00000000 0.00000000

 1 20.8692669 20.74355890 0.00000000

 2 21.7118378 90.30271580 0.00000000

 2 6.3616915 74.66103160 0.00000000

 2 1.2291195 9.88944240 0.00000000

 D - F

 2 13.5851800 -4.84903590 0.00000000

 2 9.8373050 3.69133790 0.00000000

 2 0.8373113 -0.50373190 0.00000000

 26 6

 No pseudopotential on this center.

 27 6

 No pseudopotential on this center.

 28 6

 No pseudopotential on this center.

 29 6

 No pseudopotential on this center.

 30 6

 No pseudopotential on this center.

 31 6

 No pseudopotential on this center.

 32 6

 No pseudopotential on this center.

 33 6

 No pseudopotential on this center.

 34 6

 No pseudopotential on this center.

 35 6

 No pseudopotential on this center.

 36 6

 No pseudopotential on this center.

 37 6

 No pseudopotential on this center.

 38 6

 No pseudopotential on this center.

 39 6

 No pseudopotential on this center.

 40 6

 No pseudopotential on this center.

 41 6

 No pseudopotential on this center.

 42 1

 No pseudopotential on this center.

 43 1

 No pseudopotential on this center.

 44 1

 No pseudopotential on this center.

 45 1

 No pseudopotential on this center.

 46 1

 No pseudopotential on this center.

 47 1

 No pseudopotential on this center.

 48 1

 No pseudopotential on this center.

 49 1

 No pseudopotential on this center.

 50 1

 No pseudopotential on this center.

 51 1

 No pseudopotential on this center.

 52 1

 No pseudopotential on this center.

 53 1

 No pseudopotential on this center.

 54 1

 No pseudopotential on this center.

 55 1

 No pseudopotential on this center.

 56 1

 No pseudopotential on this center.

 57 1

 No pseudopotential on this center.

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

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

 There are 225 symmetry adapted cartesian basis functions of A1 symmetry.

 There are 196 symmetry adapted cartesian basis functions of A2 symmetry.

 There are 207 symmetry adapted cartesian basis functions of B1 symmetry.

 There are 207 symmetry adapted cartesian basis functions of B2 symmetry.

 There are 211 symmetry adapted basis functions of A1 symmetry.

 There are 187 symmetry adapted basis functions of A2 symmetry.

 There are 197 symmetry adapted basis functions of B1 symmetry.

 There are 197 symmetry adapted basis functions of B2 symmetry.

 792 basis functions, 1399 primitive gaussians, 835 cartesian basis functions

 138 alpha electrons 138 beta electrons

 nuclear repulsion energy 4381.1283324348 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= 57 NActive= 57 NUniq= 9 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F 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= -0.1642256700 Hartrees.

 Nuclear repulsion after empirical dispersion term = 4380.9641067648 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= 57.

 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 = 57

 GePol: Total number of spheres = 57

 GePol: Number of exposed spheres = 57 (100.00%)

 GePol: Number of points = 4638

 GePol: Average weight of points = 0.10

 GePol: Minimum weight of points = 0.18D-07

 GePol: Maximum weight of points = 0.18390

 GePol: Number of points with low weight = 288

 GePol: Fraction of low-weight points (<1% of avg) = 6.21%

 GePol: Cavity surface area = 486.300 Ang\*\*2

 GePol: Cavity volume = 504.060 Ang\*\*3

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

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

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

 PCM non-electrostatic energy = -0.0144004639 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 4380.9497063008 Hartrees.

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

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

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

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

 One-electron integrals computed using PRISM.

 One-electron integral symmetry used in STVInt

 8 Symmetry operations used in ECPInt.

 ECPInt: NShTT= 32896 NPrTT= 163506 LenC2= 22909 LenP2D= 61418.

 LDataN: DoStor=T MaxTD1= 5 Len= 102

 NBasis= 792 RedAO= T EigKep= 3.47D-05 NBF= 211 187 197 197

 NBsUse= 792 1.00D-06 EigRej= -1.00D+00 NBFU= 211 187 197 197

 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= 802 802 802 802 802 MxSgAt= 57 MxSgA2= 57.

 Leave Link 302 at Thu Sep 19 00:35:29 2019, MaxMem= 1342177280 cpu: 10.3

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

 Leave Link 308 at Thu Sep 19 00:35:29 2019, MaxMem= 1342177280 cpu: 1.8

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

 DipDrv: MaxL=1.

 Leave Link 303 at Thu Sep 19 00:35:29 2019, MaxMem= 1342177280 cpu: 1.0

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

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

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

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

 ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

 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= -1733.63499390998

 JPrj=0 DoOrth=F DoCkMO=F.

 Initial guess orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

 Leave Link 401 at Thu Sep 19 00:35:31 2019, MaxMem= 1342177280 cpu: 17.1

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

 Closed shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 2128092 IEndB= 2128092 NGot= 1342177280 MDV= 1340763889

 LenX= 1340763889 LenY= 1340065829

 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= 560000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

 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= 64533132.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 6.88D-15 for 4618.

 Iteration 1 A\*A^-1 deviation from orthogonality is 3.55D-15 for 3711 1219.

 Iteration 1 A^-1\*A deviation from unit magnitude is 6.88D-15 for 4618.

 Iteration 1 A^-1\*A deviation from orthogonality is 1.65D-13 for 4103 4062.

 E= -1732.57712527219

 DIIS: error= 9.59D-02 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -1732.57712527219 IErMin= 1 ErrMin= 9.59D-02

 ErrMax= 9.59D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.09D+00 BMatP= 1.09D+00

 IDIUse=3 WtCom= 4.08D-02 WtEn= 9.59D-01

 Coeff-Com: 0.100D+01

 Coeff-En: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.102 Goal= None Shift= 0.000

 GapD= 0.102 DampG=1.000 DampE=0.250 DampFc=0.2500 IDamp=-1.

 Damping current iteration by 2.50D-01

 RMSDP=2.49D-03 MaxDP=8.89D-02 OVMax= 2.02D-01

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 6.21D-04 CP: 9.96D-01

 E= -1732.86602177788 Delta-E= -0.288896505691 Rises=F Damp=T

 DIIS: error= 4.02D-02 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -1732.86602177788 IErMin= 2 ErrMin= 4.02D-02

 ErrMax= 4.02D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.04D-01 BMatP= 1.09D+00

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

 Coeff-Com: -0.933D+00 0.193D+01

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

 Coeff: -0.558D+00 0.156D+01

 Gap= 0.093 Goal= None Shift= 0.000

 RMSDP=9.43D-04 MaxDP=3.52D-02 DE=-2.89D-01 OVMax= 1.13D-01

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 5.43D-04 CP: 9.84D-01 2.23D+00

 E= -1733.36536603604 Delta-E= -0.499344258163 Rises=F Damp=F

 DIIS: error= 6.81D-03 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 3 EnMin= -1733.36536603604 IErMin= 3 ErrMin= 6.81D-03

 ErrMax= 6.81D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.45D-02 BMatP= 3.04D-01

 IDIUse=3 WtCom= 9.32D-01 WtEn= 6.81D-02

 Coeff-Com: -0.692D-01 0.317D+00 0.753D+00

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

 Coeff: -0.645D-01 0.295D+00 0.769D+00

 Gap= 0.080 Goal= None Shift= 0.000

 RMSDP=3.36D-04 MaxDP=1.39D-02 DE=-4.99D-01 OVMax= 2.53D-02

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 2.17D-04 CP: 9.85D-01 1.85D+00 8.28D-01

 E= -1733.38537578344 Delta-E= -0.020009747391 Rises=F Damp=F

 DIIS: error= 2.71D-03 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -1733.38537578344 IErMin= 4 ErrMin= 2.71D-03

 ErrMax= 2.71D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.05D-03 BMatP= 2.45D-02

 IDIUse=3 WtCom= 9.73D-01 WtEn= 2.71D-02

 Coeff-Com: 0.448D-01-0.173D-01 0.367D+00 0.606D+00

 Coeff-En: 0.000D+00 0.000D+00 0.100D-01 0.990D+00

 Coeff: 0.436D-01-0.168D-01 0.357D+00 0.616D+00

 Gap= 0.080 Goal= None Shift= 0.000

 RMSDP=1.00D-04 MaxDP=4.79D-03 DE=-2.00D-02 OVMax= 1.37D-02

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 5.74D-05 CP: 9.85D-01 1.89D+00 8.69D-01 6.53D-01

 E= -1733.38897217707 Delta-E= -0.003596393634 Rises=F Damp=F

 DIIS: error= 1.33D-03 at cycle 5 NSaved= 5.

 NSaved= 5 IEnMin= 5 EnMin= -1733.38897217707 IErMin= 5 ErrMin= 1.33D-03

 ErrMax= 1.33D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.04D-04 BMatP= 4.05D-03

 IDIUse=3 WtCom= 9.87D-01 WtEn= 1.33D-02

 Coeff-Com: 0.293D-01-0.333D-01 0.146D+00 0.362D+00 0.496D+00

 Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.847D-01 0.915D+00

 Coeff: 0.289D-01-0.329D-01 0.144D+00 0.358D+00 0.502D+00

 Gap= 0.080 Goal= None Shift= 0.000

 RMSDP=3.51D-05 MaxDP=1.36D-03 DE=-3.60D-03 OVMax= 4.09D-03

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 1.66D-05 CP: 9.85D-01 1.90D+00 8.87D-01 6.65D-01 5.36D-01

 E= -1733.38962565896 Delta-E= -0.000653481887 Rises=F Damp=F

 DIIS: error= 3.71D-04 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -1733.38962565896 IErMin= 6 ErrMin= 3.71D-04

 ErrMax= 3.71D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.73D-05 BMatP= 7.04D-04

 IDIUse=3 WtCom= 9.96D-01 WtEn= 3.71D-03

 Coeff-Com: 0.113D-01-0.150D-01 0.460D-01 0.134D+00 0.243D+00 0.581D+00

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

 Coeff: 0.112D-01-0.149D-01 0.459D-01 0.133D+00 0.242D+00 0.582D+00

 Gap= 0.080 Goal= None Shift= 0.000

 RMSDP=8.01D-06 MaxDP=3.92D-04 DE=-6.53D-04 OVMax= 1.01D-03

 Cycle 7 Pass 1 IDiag 1:

 RMSU= 3.80D-06 CP: 9.85D-01 1.90D+00 8.85D-01 6.79D-01 5.78D-01

 CP: 6.95D-01

 E= -1733.38964419353 Delta-E= -0.000018534576 Rises=F Damp=F

 DIIS: error= 1.26D-04 at cycle 7 NSaved= 7.

 NSaved= 7 IEnMin= 7 EnMin= -1733.38964419353 IErMin= 7 ErrMin= 1.26D-04

 ErrMax= 1.26D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.87D-06 BMatP= 2.73D-05

 IDIUse=3 WtCom= 9.99D-01 WtEn= 1.26D-03

 Coeff-Com: 0.484D-02-0.675D-02 0.180D-01 0.569D-01 0.112D+00 0.345D+00

 Coeff-Com: 0.469D+00

 Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.448D-01

 Coeff-En: 0.955D+00

 Coeff: 0.484D-02-0.674D-02 0.180D-01 0.569D-01 0.112D+00 0.345D+00

 Coeff: 0.470D+00

 Gap= 0.080 Goal= None Shift= 0.000

 RMSDP=2.39D-06 MaxDP=1.18D-04 DE=-1.85D-05 OVMax= 3.50D-04

 Cycle 8 Pass 1 IDiag 1:

 RMSU= 1.39D-06 CP: 9.85D-01 1.90D+00 8.86D-01 6.78D-01 5.78D-01

 CP: 7.38D-01 5.59D-01

 E= -1733.38964721732 Delta-E= -0.000003023791 Rises=F Damp=F

 DIIS: error= 2.35D-05 at cycle 8 NSaved= 8.

 NSaved= 8 IEnMin= 8 EnMin= -1733.38964721732 IErMin= 8 ErrMin= 2.35D-05

 ErrMax= 2.35D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.13D-07 BMatP= 3.87D-06

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

 Coeff-Com: 0.914D-03-0.133D-02 0.280D-02 0.102D-01 0.215D-01 0.855D-01

 Coeff-Com: 0.227D+00 0.654D+00

 Coeff: 0.914D-03-0.133D-02 0.280D-02 0.102D-01 0.215D-01 0.855D-01

 Coeff: 0.227D+00 0.654D+00

 Gap= 0.080 Goal= None Shift= 0.000

 RMSDP=6.48D-07 MaxDP=3.41D-05 DE=-3.02D-06 OVMax= 9.87D-05

 Cycle 9 Pass 1 IDiag 1:

 RMSU= 4.03D-07 CP: 9.85D-01 1.90D+00 8.86D-01 6.79D-01 5.79D-01

 CP: 7.39D-01 6.21D-01 7.49D-01

 E= -1733.38964737174 Delta-E= -0.000000154413 Rises=F Damp=F

 DIIS: error= 2.28D-05 at cycle 9 NSaved= 9.

 NSaved= 9 IEnMin= 9 EnMin= -1733.38964737174 IErMin= 9 ErrMin= 2.28D-05

 ErrMax= 2.28D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.30D-08 BMatP= 2.13D-07

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

 Coeff-Com: 0.892D-04-0.162D-03-0.139D-03 0.195D-03 0.946D-03 0.134D-01

 Coeff-Com: 0.861D-01 0.387D+00 0.512D+00

 Coeff: 0.892D-04-0.162D-03-0.139D-03 0.195D-03 0.946D-03 0.134D-01

 Coeff: 0.861D-01 0.387D+00 0.512D+00

 Gap= 0.080 Goal= None Shift= 0.000

 RMSDP=1.93D-07 MaxDP=1.04D-05 DE=-1.54D-07 OVMax= 2.36D-05

 Cycle 10 Pass 1 IDiag 1:

 RMSU= 1.13D-07 CP: 9.85D-01 1.90D+00 8.86D-01 6.79D-01 5.79D-01

 CP: 7.40D-01 6.26D-01 8.02D-01 6.84D-01

 E= -1733.38964740089 Delta-E= -0.000000029156 Rises=F Damp=F

 DIIS: error= 1.03D-06 at cycle 10 NSaved= 10.

 NSaved=10 IEnMin=10 EnMin= -1733.38964740089 IErMin=10 ErrMin= 1.03D-06

 ErrMax= 1.03D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.79D-10 BMatP= 4.30D-08

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

 Coeff-Com: -0.294D-04 0.352D-04-0.200D-03-0.628D-03-0.113D-02-0.190D-02

 Coeff-Com: 0.103D-01 0.673D-01 0.127D+00 0.799D+00

 Coeff: -0.294D-04 0.352D-04-0.200D-03-0.628D-03-0.113D-02-0.190D-02

 Coeff: 0.103D-01 0.673D-01 0.127D+00 0.799D+00

 Gap= 0.080 Goal= None Shift= 0.000

 RMSDP=3.70D-08 MaxDP=1.15D-06 DE=-2.92D-08 OVMax= 7.82D-06

 Cycle 11 Pass 1 IDiag 1:

 RMSU= 2.47D-08 CP: 9.85D-01 1.90D+00 8.86D-01 6.79D-01 5.79D-01

 CP: 7.41D-01 6.28D-01 8.13D-01 6.99D-01 9.32D-01

 E= -1733.38964740118 Delta-E= -0.000000000286 Rises=F Damp=F

 DIIS: error= 5.92D-07 at cycle 11 NSaved= 11.

 NSaved=11 IEnMin=11 EnMin= -1733.38964740118 IErMin=11 ErrMin= 5.92D-07

 ErrMax= 5.92D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.15D-10 BMatP= 3.79D-10

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

 Coeff-Com: -0.187D-04 0.244D-04-0.104D-03-0.359D-03-0.654D-03-0.150D-02

 Coeff-Com: 0.258D-02 0.218D-01 0.443D-01 0.434D+00 0.500D+00

 Coeff: -0.187D-04 0.244D-04-0.104D-03-0.359D-03-0.654D-03-0.150D-02

 Coeff: 0.258D-02 0.218D-01 0.443D-01 0.434D+00 0.500D+00

 Gap= 0.080 Goal= None Shift= 0.000

 RMSDP=1.75D-08 MaxDP=6.91D-07 DE=-2.86D-10 OVMax= 2.52D-06

 Cycle 12 Pass 1 IDiag 1:

 RMSU= 1.08D-08 CP: 9.85D-01 1.90D+00 8.86D-01 6.79D-01 5.79D-01

 CP: 7.41D-01 6.28D-01 8.13D-01 7.05D-01 9.85D-01

 CP: 7.11D-01

 E= -1733.38964740134 Delta-E= -0.000000000164 Rises=F Damp=F

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

 NSaved=12 IEnMin=12 EnMin= -1733.38964740134 IErMin=12 ErrMin= 1.51D-07

 ErrMax= 1.51D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.25D-12 BMatP= 1.15D-10

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

 Coeff-Com: -0.207D-05 0.299D-05-0.858D-05-0.521D-04-0.908D-04-0.354D-03

 Coeff-Com: -0.691D-03-0.276D-02-0.600D-02 0.580D-01 0.202D+00 0.750D+00

 Coeff: -0.207D-05 0.299D-05-0.858D-05-0.521D-04-0.908D-04-0.354D-03

 Coeff: -0.691D-03-0.276D-02-0.600D-02 0.580D-01 0.202D+00 0.750D+00

 Gap= 0.080 Goal= None Shift= 0.000

 RMSDP=5.00D-09 MaxDP=1.47D-07 DE=-1.64D-10 OVMax= 1.22D-06

 Error on total polarization charges = 0.07181

 SCF Done: E(RB3LYP) = -1733.38964740 A.U. after 12 cycles

 NFock= 12 Conv=0.50D-08 -V/T= 1.9757

 KE= 1.776541638178D+03 PE=-1.287661464976D+04 EE= 4.985733657885D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -9.04

 (included in total energy above)

 Leave Link 502 at Thu Sep 19 00:37:18 2019, MaxMem= 1342177280 cpu: 944.4

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

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

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

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

 ICtDFT= 12500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

 Largest core mixing into a valence orbital is 2.25D-05

 Range of M.O.s used for correlation: 41 792

 NBasis= 792 NAE= 138 NBE= 138 NFC= 40 NFV= 0

 NROrb= 752 NOA= 98 NOB= 98 NVA= 654 NVB= 654

 \*\*\*\* Warning!!: The largest alpha MO coefficient is 0.12959119D+02

 \*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.80140569D-01

 Leave Link 801 at Thu Sep 19 00:37:19 2019, MaxMem= 1342177280 cpu: 2.8

 (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 60292500000 words for in-memory AO integral storage.

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

 Inv3: Mode=1 IEnd= 64533132.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 8.22D-15 for 4627.

 Iteration 1 A\*A^-1 deviation from orthogonality is 2.99D-15 for 4630 3760.

 Iteration 1 A^-1\*A deviation from unit magnitude is 8.22D-15 for 4627.

 Iteration 1 A^-1\*A deviation from orthogonality is 1.78D-15 for 4633 4609.

 Making orbital integer symmetry assigments:

 Orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

 (A2)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

 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: 128184

 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 5

 New state 5 was old state 7

 New state 6 was old state 9

 New state 7 was old state 26

 New state 8 was old state 27

 New state 9 was old state 25

 New state 10 was old state 24

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.260807998217566

 Root 2 : 2.260807998224620

 Root 3 : 3.457428761343296

 Root 4 : 3.457428761346411

 Root 5 : 3.468717621705896

 Root 6 : 3.489833386634942

 Root 7 : 3.579469781343652

 Root 8 : 3.579469781358811

 Root 9 : 3.590696141983564

 Root 10 : 3.590696141989334

 Root 11 : 3.618743841667010

 Root 12 : 3.676359187609923

 Root 13 : 3.704616573459891

 Root 14 : 3.729453254352031

 Root 15 : 3.735579215217723

 Root 16 : 3.755248424184478

 Root 17 : 3.755248424190279

 Root 18 : 3.848660248869227

 Root 19 : 3.848660248878092

 Root 20 : 3.945378968962145

 Root 21 : 4.008267469238258

 Root 22 : 4.008267469245128

 Root 23 : 4.023658395473614

 Root 24 : 4.034464615116606

 Root 25 : 4.038310244438326

 Root 26 : 4.062343964567411

 Root 27 : 4.066978394101302

 Root 28 : 4.083618928872398

 Root 29 : 4.111250622589590

 Root 30 : 4.168743718125652

 Root 31 : 4.168743718125692

 Root 32 : 4.830614947804804

 Root 33 : 4.830614947808276

 Root 34 : 4.862426119805578

 Root 35 : 4.862426119813643

 Root 36 : 5.272471588444855

 Root 37 : 5.315989537378972

 Root 38 : 5.315989537382929

 Root 39 : 5.531889283617966

 Root 40 : 5.725020830369886

 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 0.051794436019275

 Root 2 not converged, maximum delta is 0.051794436019433

 Root 3 not converged, maximum delta is 0.046754364880017

 Root 4 not converged, maximum delta is 0.046754364880358

 Root 5 not converged, maximum delta is 0.106984290190375

 Root 6 not converged, maximum delta is 0.036229801857750

 New state 7 was old state 9

 Root 7 not converged, maximum delta is 0.438241206409545

 New state 8 was old state 10

 Root 8 not converged, maximum delta is 0.438241205662629

 New state 9 was old state 7

 Root 9 not converged, maximum delta is 0.429824601382394

 New state 10 was old state 8

 Root 10 not converged, maximum delta is 0.429824600655773

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.012194999998586 Change is -0.248612998218980

 Root 2 : 2.012195000006430 Change is -0.248612998218190

 Root 3 : 3.335838681312229 Change is -0.121590080031067

 Root 4 : 3.335838681313757 Change is -0.121590080032654

 Root 5 : 3.341778660155455 Change is -0.126938961550441

 Root 6 : 3.346703459191904 Change is -0.143129927443038

 Root 7 : 3.536556122233153 Change is -0.054140019750411

 Root 8 : 3.536556122246961 Change is -0.054140019742373

 Root 9 : 3.547240293331287 Change is -0.032229488012365

 Root 10 : 3.547240293337429 Change is -0.032229488021381

 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 0.025594509613801

 Root 2 not converged, maximum delta is 0.025594509615225

 Root 3 not converged, maximum delta is 0.029011773416201

 Root 4 not converged, maximum delta is 0.029011773415995

 Root 5 not converged, maximum delta is 0.008125897073670

 Root 6 not converged, maximum delta is 0.004421255593668

 Root 7 not converged, maximum delta is 0.005007772400976

 Root 8 not converged, maximum delta is 0.005007772403527

 Root 9 not converged, maximum delta is 0.003860706353288

 Root 10 not converged, maximum delta is 0.003860706358977

 Excitation Energies [eV] at current iteration:

 Root 1 : 1.991459156606346 Change is -0.020735843392240

 Root 2 : 1.991459156612579 Change is -0.020735843393851

 Root 3 : 3.328534804325345 Change is -0.007303876986884

 Root 4 : 3.328534804326258 Change is -0.007303876987499

 Root 5 : 3.335654475723512 Change is -0.006124184431943

 Root 6 : 3.340330632719558 Change is -0.006372826472346

 Root 7 : 3.535068983313655 Change is -0.001487138919498

 Root 8 : 3.535068983327003 Change is -0.001487138919958

 Root 9 : 3.546052810293530 Change is -0.001187483037757

 Root 10 : 3.546052810299882 Change is -0.001187483037547

 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 0.002671964295458

 Root 2 not converged, maximum delta is 0.002671964295560

 Root 3 not converged, maximum delta is 0.002789337360566

 Root 4 not converged, maximum delta is 0.002789337360924

 Root 5 not converged, maximum delta is 0.003142960503575

 Root 6 not converged, maximum delta is 0.004415172495125

 Root 7 not converged, maximum delta is 0.003394898050984

 Root 8 not converged, maximum delta is 0.003394898059712

 Root 9 not converged, maximum delta is 0.003136249529189

 Root 10 not converged, maximum delta is 0.003136249537544

 Excitation Energies [eV] at current iteration:

 Root 1 : 1.989283700182521 Change is -0.002175456423825

 Root 2 : 1.989283700188844 Change is -0.002175456423735

 Root 3 : 3.327597607736869 Change is -0.000937196588476

 Root 4 : 3.327597607737758 Change is -0.000937196588501

 Root 5 : 3.334669440577445 Change is -0.000985035146067

 Root 6 : 3.339212294070485 Change is -0.001118338649073

 Root 7 : 3.534902582323987 Change is -0.000166400989667

 Root 8 : 3.534902582337150 Change is -0.000166400989852

 Root 9 : 3.545810180691952 Change is -0.000242629601579

 Root 10 : 3.545810180698420 Change is -0.000242629601463

 Iteration 5 Dimension 120 NMult 100 NNew 20

 CISAX will form 20 AO SS matrices at one time.

 NMat= 20 NSing= 20 JSym2X=-1.

 Root 1 has converged.

 Root 2 has converged.

 Root 3 not converged, maximum delta is 0.001703385137473

 Root 4 not converged, maximum delta is 0.001703385139258

 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 : 1.989116946614429 Change is -0.000166753568092

 Root 2 : 1.989116946620918 Change is -0.000166753567926

 Root 3 : 3.327515090394606 Change is -0.000082517342262

 Root 4 : 3.327515090395348 Change is -0.000082517342410

 Root 5 : 3.334587553711279 Change is -0.000081886866166

 Root 6 : 3.339056369279984 Change is -0.000155924790501

 Root 7 : 3.534878973849753 Change is -0.000023608474234

 Root 8 : 3.534878973863056 Change is -0.000023608474095

 Root 9 : 3.545792620846008 Change is -0.000017559845944

 Root 10 : 3.545792620852522 Change is -0.000017559845897

 Iteration 6 Dimension 124 NMult 120 NNew 4

 CISAX will form 4 AO SS matrices at one time.

 NMat= 4 NSing= 4 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 not converged, maximum delta is 0.004609101758526

 Root 8 not converged, maximum delta is 0.004609101757096

 Root 9 has converged.

 Root 10 has converged.

 Excitation Energies [eV] at current iteration:

 Root 1 : 1.989116913943556 Change is -0.000000032670873

 Root 2 : 1.989116913949756 Change is -0.000000032671162

 Root 3 : 3.327509834292781 Change is -0.000005256101826

 Root 4 : 3.327509834293497 Change is -0.000005256101851

 Root 5 : 3.334587553711304 Change is 0.000000000000025

 Root 6 : 3.339056369279910 Change is -0.000000000000074

 Root 7 : 3.534878966542337 Change is -0.000000007307417

 Root 8 : 3.534878966555523 Change is -0.000000007307533

 Root 9 : 3.545792610120685 Change is -0.000000010725323

 Root 10 : 3.545792610127269 Change is -0.000000010725253

 Convergence on energies, max DE= 5.26D-06.

 Convergence on expansion vectors.

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

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

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

 1PDM for each excited state written to RWF 633

 Ground to excited state transition densities written to RWF 633

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

 state X Y Z Dip. S. Osc.

 1 0.0000 3.6174 -0.0000 13.0858 0.6377

 2 -3.6174 0.0000 0.0000 13.0858 0.6377

 3 0.0000 -0.6734 -0.0000 0.4535 0.0370

 4 -0.6734 -0.0000 0.0000 0.4535 0.0370

 5 0.0000 0.0000 0.0000 0.0000 0.0000

 6 -0.0000 -0.0000 -0.0000 0.0000 0.0000

 7 0.1364 0.0009 -0.0000 0.0186 0.0016

 8 0.0009 -0.1364 -0.0000 0.0186 0.0016

 9 -0.0533 -0.0000 -0.0000 0.0028 0.0002

 10 0.0000 -0.0533 -0.0000 0.0028 0.0002

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

 state X Y Z Dip. S. Osc.

 1 -0.0000 -0.2631 -0.0000 0.0692 0.6314

 2 0.2631 -0.0000 0.0000 0.0692 0.6314

 3 -0.0000 0.0761 0.0000 0.0058 0.0316

 4 0.0761 0.0000 -0.0000 0.0058 0.0316

 5 -0.0000 -0.0000 -0.0000 0.0000 0.0000

 6 0.0000 0.0000 0.0000 0.0000 0.0000

 7 -0.0177 -0.0001 -0.0000 0.0003 0.0016

 8 -0.0001 0.0177 -0.0000 0.0003 0.0016

 9 0.0098 0.0000 0.0000 0.0001 0.0005

 10 -0.0000 0.0098 0.0000 0.0001 0.0005

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

 state X Y Z

 1 0.0256 -0.0000 0.0000

 2 0.0000 0.0256 -0.0000

 3 -0.1166 -0.0000 0.0000

 4 -0.0000 0.1166 -0.0000

 5 0.0000 -0.0000 1.8419

 6 -0.0000 0.0000 0.0000

 7 -0.0029 0.4202 0.0000

 8 0.4202 0.0029 -0.0000

 9 -0.0000 0.4162 0.0000

 10 -0.4162 -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 0.0457

 2 0.0000 -0.0000 -0.0000 0.0000 -0.0457 0.0000

 3 0.0000 -0.0000 -0.0000 -0.0000 0.0000 -0.0131

 4 -0.0000 0.0000 -0.0000 0.0000 -0.0131 -0.0000

 5 0.0000 -0.0000 0.0000 -0.0000 0.0000 0.0000

 6 -0.4336 0.4336 0.0000 -0.0000 -0.0000 0.0000

 7 0.0000 -0.0000 -0.0000 0.0000 -0.1166 -0.0008

 8 -0.0000 -0.0000 -0.0000 -0.0000 -0.0008 0.1166

 9 -0.0000 0.0000 -0.0000 0.0000 0.0125 0.0000

 10 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 0.0125

 <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 -0.1776 0.1776 0.0000 -0.0000 90.00

 8 0.1776 -0.1776 -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 0.2781 -0.2781 0.0000 0.0000

 8 -0.2781 0.2781 -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 -0.9518 0.0000 0.9518 0.6345

 2 -0.9518 -0.0000 0.0000 0.9518 0.6345

 3 -0.0000 -0.0512 -0.0000 0.0512 0.0342

 4 -0.0512 -0.0000 -0.0000 0.0512 0.0342

 5 -0.0000 -0.0000 -0.0000 0.0000 0.0000

 6 -0.0000 -0.0000 -0.0000 0.0000 0.0000

 7 -0.0024 -0.0000 0.0000 0.0024 0.0016

 8 -0.0000 -0.0024 0.0000 0.0024 0.0016

 9 -0.0005 -0.0000 -0.0000 0.0005 0.0003

 10 -0.0000 -0.0005 -0.0000 0.0005 0.0003

 Excitation energies and oscillator strengths:

 Excited State 1: Singlet-E 1.9891 eV 623.31 nm f=0.6377 <S\*\*2>=0.000

 41 ->186 0.00106

 42 ->207 0.00107

 44 ->181 0.00107

 45 ->186 0.00143

 46 ->178 -0.00103

 46 ->182 0.00105

 46 ->207 0.00152

 47 ->214 0.00111

 48 ->186 0.00114

 48 ->195 0.00104

 48 ->212 -0.00119

 53 ->181 -0.00114

 61 ->181 -0.00174

 62 ->179 -0.00136

 63 ->183 -0.00195

 63 ->187 -0.00144

 63 ->218 0.00107

 63 ->232 -0.00130

 63 ->239 -0.00104

 64 ->181 0.00114

 64 ->185 0.00170

 64 ->327 -0.00102

 68 ->196 0.00122

 69 ->185 0.00146

 69 ->197 0.00103

 70 ->189 0.00137

 70 ->195 0.00120

 70 ->196 -0.00170

 70 ->203 0.00133

 70 ->212 -0.00109

 70 ->216 -0.00110

 70 ->234 0.00116

 70 ->249 0.00114

 71 ->163 -0.00106

 71 ->183 0.00173

 71 ->214 0.00111

 72 ->169 -0.00104

 72 ->182 -0.00172

 72 ->210 -0.00123

 72 ->211 -0.00111

 73 ->166 -0.00125

 73 ->181 0.00163

 73 ->185 -0.00121

 73 ->194 0.00117

 73 ->197 0.00140

 77 ->149 0.00106

 78 ->180 -0.00111

 78 ->189 -0.00143

 78 ->196 0.00104

 78 ->203 -0.00131

 78 ->234 -0.00103

 79 ->157 0.00125

 79 ->183 0.00239

 79 ->187 0.00160

 79 ->257 -0.00146

 79 ->260 -0.00199

 79 ->297 -0.00168

 80 ->178 -0.00109

 80 ->179 0.00314

 80 ->193 0.00187

 80 ->205 -0.00159

 80 ->211 -0.00190

 80 ->259 -0.00105

 81 ->152 0.00143

 81 ->156 -0.00110

 81 ->186 -0.00137

 82 ->154 0.00236

 82 ->162 -0.00140

 82 ->169 0.00115

 82 ->178 -0.00249

 82 ->179 0.00246

 82 ->184 0.00101

 82 ->193 0.00111

 82 ->205 -0.00133

 82 ->207 -0.00176

 82 ->211 -0.00205

 82 ->266 0.00120

 83 ->157 -0.00157

 83 ->257 -0.00126

 83 ->260 -0.00106

 83 ->282 0.00109

 83 ->297 -0.00189

 83 ->320 0.00125

 84 ->151 -0.00208

 84 ->155 0.00198

 84 ->185 -0.00109

 84 ->190 -0.00149

 84 ->194 0.00102

 85 ->151 -0.00216

 85 ->166 -0.00137

 85 ->172 0.00108

 85 ->181 -0.00534

 85 ->197 -0.00114

 85 ->199 -0.00170

 85 ->204 -0.00114

 85 ->209 0.00184

 85 ->213 0.00152

 85 ->241 0.00105

 85 ->250 0.00170

 85 ->252 0.00135

 85 ->280 -0.00100

 85 ->290 0.00160

 85 ->302 -0.00125

 85 ->327 -0.00108

 86 ->167 -0.00109

 86 ->186 0.00251

 86 ->203 0.00102

 86 ->261 0.00110

 86 ->272 -0.00104

 87 ->154 0.00205

 87 ->158 -0.00107

 87 ->169 -0.00159

 87 ->178 -0.00212

 87 ->182 0.00398

 87 ->207 -0.00123

 87 ->258 -0.00137

 87 ->271 -0.00149

 88 ->173 0.00189

 88 ->183 0.00127

 88 ->192 0.00133

 88 ->214 0.00140

 89 ->156 0.00185

 89 ->180 0.00112

 89 ->195 0.00141

 89 ->203 0.00110

 90 ->149 0.00129

 90 ->154 0.00207

 90 ->162 0.00140

 90 ->179 0.00216

 90 ->193 0.00189

 91 ->157 -0.00220

 91 ->187 -0.00118

 91 ->192 0.00101

 91 ->206 -0.00114

 92 ->139 -0.00119

 92 ->145 0.00344

 92 ->164 -0.00454

 92 ->177 -0.00178

 92 ->212 0.00102

 92 ->216 -0.00198

 93 ->160 -0.00168

 93 ->172 0.00273

 93 ->185 0.00332

 93 ->194 -0.00204

 93 ->197 -0.00106

 93 ->209 -0.00117

 94 ->151 -0.00107

 94 ->155 0.00145

 94 ->181 -0.00144

 94 ->197 0.00154

 95 ->142 0.00438

 95 ->150 -0.00355

 95 ->219 -0.00139

 96 ->141 0.00408

 96 ->143 -0.00423

 96 ->149 -0.00355

 96 ->153 -0.00401

 96 ->158 0.00169

 96 ->168 0.00325

 96 ->175 -0.00195

 96 ->220 0.00135

 96 ->230 -0.00101

 96 ->243 0.00158

 97 ->152 -0.00106

 97 ->156 0.00277

 97 ->161 -0.00150

 97 ->186 -0.00184

 98 ->154 0.00226

 98 ->159 0.00386

 98 ->182 0.00134

 99 ->157 -0.00103

 99 ->163 -0.00216

 99 ->173 0.00254

 100 ->161 -0.00307

 100 ->171 0.00245

 100 ->227 -0.00117

 101 ->151 0.00218

 101 ->155 -0.00164

 101 ->160 0.00288

 101 ->185 0.00344

 101 ->194 -0.00180

 101 ->197 -0.00100

 102 ->157 0.00340

 102 ->163 -0.00206

 102 ->183 -0.00128

 102 ->192 -0.00147

 102 ->206 -0.00155

 102 ->226 0.00141

 103 ->149 -0.00117

 103 ->158 -0.00126

 103 ->159 0.00172

 103 ->162 -0.00261

 103 ->178 -0.00296

 103 ->182 0.00104

 103 ->188 0.00198

 103 ->207 -0.00260

 103 ->210 0.00159

 104 ->140 0.00546

 104 ->144 -0.00138

 104 ->148 -0.00124

 104 ->155 -0.00252

 104 ->160 -0.00109

 104 ->166 -0.00130

 104 ->190 -0.00163

 104 ->213 0.00171

 104 ->217 -0.00160

 105 ->140 0.00796

 105 ->144 -0.00221

 105 ->148 -0.00180

 105 ->155 0.00133

 105 ->166 0.00102

 105 ->190 0.00158

 105 ->194 -0.00105

 105 ->204 0.00148

 105 ->217 -0.00132

 106 ->156 -0.00159

 106 ->186 0.00121

 106 ->234 0.00103

 106 ->281 0.00103

 107 ->139 -0.01027

 107 ->145 -0.00152

 107 ->147 -0.00425

 107 ->177 -0.00190

 107 ->216 -0.00151

 107 ->234 0.00108

 108 ->161 0.00162

 108 ->167 -0.00269

 108 ->171 0.00157

 108 ->186 -0.00249

 108 ->195 0.00163

 108 ->235 0.00103

 109 ->141 -0.00219

 109 ->149 -0.00264

 109 ->153 -0.00213

 109 ->168 0.00265

 109 ->220 -0.00186

 109 ->230 -0.00126

 109 ->243 0.00119

 110 ->142 0.00237

 110 ->150 -0.00475

 110 ->219 0.00205

 111 ->159 0.00115

 111 ->162 0.00106

 111 ->169 -0.00314

 111 ->178 0.00141

 111 ->182 -0.00338

 111 ->188 0.00111

 111 ->207 0.00117

 111 ->237 -0.00106

 112 ->163 -0.00288

 112 ->173 -0.00136

 112 ->191 0.00243

 112 ->192 0.00186

 113 ->139 -0.00627

 113 ->145 0.00111

 113 ->164 0.00315

 113 ->224 0.00202

 114 ->160 -0.00165

 114 ->166 0.00263

 114 ->185 0.00402

 114 ->190 -0.00246

 114 ->194 -0.00221

 115 ->161 0.00119

 115 ->167 0.00231

 115 ->171 0.00344

 115 ->186 -0.00180

 115 ->189 -0.00135

 116 ->140 0.00964

 116 ->144 -0.00144

 116 ->148 -0.00550

 116 ->165 -0.00168

 116 ->176 0.00103

 116 ->223 -0.00205

 116 ->244 0.00115

 117 ->149 0.00255

 117 ->154 0.00185

 117 ->158 0.00238

 117 ->159 0.00128

 117 ->162 -0.00308

 117 ->178 0.00385

 117 ->184 -0.00121

 117 ->207 0.00254

 117 ->211 -0.00111

 118 ->170 -0.00385

 118 ->173 -0.00112

 118 ->192 0.00250

 119 ->151 0.00134

 119 ->160 0.00253

 119 ->166 0.00242

 119 ->172 0.00144

 119 ->190 -0.00207

 119 ->194 0.00273

 119 ->222 0.00182

 119 ->233 -0.00103

 119 ->241 0.00116

 120 ->142 0.00237

 120 ->146 -0.00231

 120 ->150 -0.00139

 120 ->157 0.00155

 120 ->170 0.00180

 120 ->183 -0.00264

 120 ->192 -0.00140

 120 ->214 -0.00106

 120 ->260 0.00115

 120 ->282 -0.00104

 121 ->141 -0.00220

 121 ->143 0.00283

 121 ->149 0.00632

 121 ->153 0.00155

 121 ->158 0.00597

 121 ->162 0.00104

 121 ->175 0.00101

 121 ->178 0.00360

 121 ->179 0.00404

 121 ->182 0.00202

 121 ->193 0.00195

 121 ->201 0.00206

 121 ->205 -0.00315

 121 ->207 -0.00221

 121 ->211 -0.00296

 121 ->229 0.00155

 121 ->298 0.00113

 122 ->142 0.00392

 122 ->146 -0.00577

 122 ->150 -0.00146

 122 ->174 0.00171

 122 ->183 0.00115

 122 ->240 0.00153

 122 ->246 0.00154

 123 ->141 -0.00543

 123 ->143 0.00559

 123 ->153 0.00394

 123 ->158 -0.00332

 123 ->168 -0.00152

 123 ->175 0.00125

 123 ->178 -0.00121

 123 ->179 -0.00161

 123 ->184 0.00238

 123 ->205 0.00121

 123 ->211 0.00100

 123 ->230 -0.00230

 124 ->152 -0.00132

 124 ->171 -0.00106

 124 ->180 -0.00359

 124 ->186 -0.00109

 124 ->189 0.00171

 124 ->196 -0.00221

 124 ->203 0.00111

 124 ->216 -0.00137

 124 ->251 0.00100

 125 ->170 -0.00220

 125 ->173 -0.00129

 125 ->183 0.00796

 125 ->187 -0.00172

 125 ->191 -0.00119

 125 ->192 0.00120

 125 ->215 0.00218

 125 ->218 -0.00147

 125 ->226 0.00217

 125 ->257 -0.00100

 126 ->149 0.00393

 126 ->158 0.00449

 126 ->169 0.00123

 126 ->178 0.00170

 126 ->179 0.00466

 126 ->182 -0.00159

 126 ->193 0.00129

 126 ->201 0.00119

 126 ->205 -0.00179

 126 ->207 -0.00125

 126 ->211 -0.00310

 126 ->229 0.00128

 126 ->278 0.00115

 127 ->140 0.01459

 127 ->144 0.00761

 127 ->148 0.00165

 127 ->165 -0.00112

 127 ->176 -0.00173

 127 ->241 -0.00104

 127 ->244 0.00260

 128 ->140 -0.00308

 128 ->151 0.00281

 128 ->155 0.00267

 128 ->160 -0.00158

 128 ->172 -0.00128

 128 ->181 0.00665

 128 ->185 0.00127

 128 ->190 -0.00315

 128 ->194 0.00281

 128 ->199 0.00268

 128 ->204 -0.00135

 128 ->209 -0.00254

 128 ->213 -0.00190

 128 ->217 -0.00139

 128 ->222 -0.00205

 128 ->223 -0.00107

 128 ->233 0.00181

 128 ->273 -0.00121

 128 ->276 -0.00103

 128 ->290 -0.00144

 128 ->295 0.00138

 128 ->302 0.00125

 129 ->147 -0.00160

 129 ->156 0.00219

 129 ->171 0.00288

 129 ->180 0.00331

 129 ->186 -0.00181

 129 ->189 -0.00310

 129 ->195 -0.00153

 129 ->196 0.00369

 129 ->203 -0.00164

 129 ->208 0.00120

 129 ->212 0.00124

 129 ->216 0.00201

 129 ->281 -0.00137

 130 ->139 -0.00635

 130 ->145 -0.00117

 130 ->147 -0.01102

 130 ->164 0.00393

 130 ->177 -0.00229

 130 ->245 0.00225

 131 ->142 0.00526

 131 ->146 -0.01001

 131 ->150 -0.01159

 131 ->174 0.00304

 131 ->246 -0.00246

 132 ->141 0.02370

 132 ->143 0.00175

 132 ->175 0.00209

 132 ->230 -0.00103

 132 ->253 -0.00215

 133 ->139 -0.01412

 133 ->145 0.00437

 133 ->147 0.00177

 133 ->164 0.00213

 133 ->177 0.00284

 133 ->245 0.00104

 133 ->249 -0.00119

 133 ->255 -0.00132

 134 ->139 0.15135

 134 ->147 0.01571

 134 ->164 -0.00186

 134 ->177 0.00224

 134 ->434 0.00120

 135 ->142 -0.00171

 135 ->146 0.00869

 135 ->150 -0.00164

 135 ->174 -0.00375

 135 ->240 0.00158

 135 ->279 0.00149

 136 ->143 -0.00313

 136 ->149 -0.00718

 136 ->153 -0.00383

 136 ->154 0.00111

 136 ->158 0.00239

 136 ->168 0.00536

 136 ->175 -0.00295

 136 ->184 -0.00219

 136 ->243 -0.00136

 136 ->263 0.00142

 137 ->140 0.00789

 137 ->144 -0.00297

 137 ->148 -0.00888

 137 ->165 -0.00419

 137 ->176 0.00267

 137 ->250 -0.00164

 137 ->256 0.00151

 138 ->140 0.69448

 138 ->144 -0.00891

 138 ->148 0.00537

 138 ->165 -0.00138

 138 ->176 -0.00199

 138 ->209 0.00118

 138 ->223 -0.00106

 138 ->250 -0.00127

 138 ->256 0.00158

 138 ->262 0.00192

 138 ->267 -0.00206

 138 ->288 -0.00197

 138 ->305 -0.00117

 138 ->314 -0.00102

 45 <-186 0.00125

 46 <-207 0.00133

 47 <-214 0.00112

 48 <-186 0.00100

 48 <-212 -0.00111

 61 <-181 -0.00148

 62 <-179 -0.00111

 63 <-183 -0.00173

 63 <-187 -0.00116

 63 <-232 -0.00117

 64 <-185 0.00149

 68 <-196 0.00109

 69 <-185 0.00128

 70 <-189 0.00112

 70 <-195 0.00103

 70 <-196 -0.00149

 70 <-203 0.00115

 70 <-234 0.00103

 71 <-183 0.00144

 72 <-182 -0.00144

 72 <-210 -0.00104

 73 <-181 0.00134

 73 <-185 -0.00102

 73 <-194 0.00101

 73 <-197 0.00117

 78 <-189 -0.00116

 78 <-203 -0.00111

 79 <-183 0.00206

 79 <-187 0.00129

 79 <-257 -0.00126

 79 <-260 -0.00173

 79 <-297 -0.00147

 80 <-179 0.00253

 80 <-193 0.00159

 80 <-205 -0.00137

 80 <-211 -0.00159

 81 <-152 0.00109

 81 <-186 -0.00110

 82 <-154 0.00182

 82 <-162 -0.00111

 82 <-178 -0.00206

 82 <-179 0.00200

 82 <-205 -0.00116

 82 <-207 -0.00153

 82 <-211 -0.00172

 82 <-266 0.00108

 83 <-157 -0.00118

 83 <-257 -0.00107

 83 <-297 -0.00164

 83 <-320 0.00109

 84 <-151 -0.00158

 84 <-155 0.00148

 84 <-190 -0.00122

 85 <-151 -0.00167

 85 <-166 -0.00107

 85 <-181 -0.00434

 85 <-199 -0.00144

 85 <-204 -0.00102

 85 <-209 0.00154

 85 <-213 0.00128

 85 <-250 0.00145

 85 <-252 0.00112

 85 <-290 0.00141

 85 <-302 -0.00112

 86 <-186 0.00199

 87 <-154 0.00152

 87 <-169 -0.00120

 87 <-178 -0.00170

 87 <-182 0.00317

 87 <-207 -0.00108

 87 <-258 -0.00113

 87 <-271 -0.00127

 88 <-173 0.00145

 88 <-192 0.00108

 88 <-214 0.00119

 89 <-156 0.00135

 89 <-195 0.00111

 90 <-154 0.00150

 90 <-162 0.00102

 90 <-179 0.00170

 90 <-193 0.00150

 91 <-157 -0.00160

 92 <-145 0.00242

 92 <-164 -0.00364

 92 <-177 -0.00161

 92 <-216 -0.00171

 93 <-160 -0.00124

 93 <-172 0.00209

 93 <-185 0.00272

 93 <-194 -0.00166

 94 <-155 0.00105

 94 <-181 -0.00111

 94 <-197 0.00123

 95 <-142 0.00304

 95 <-150 -0.00276

 95 <-219 -0.00123

 96 <-141 0.00235

 96 <-143 -0.00306

 96 <-149 -0.00253

 96 <-153 -0.00272

 96 <-158 0.00121

 96 <-168 0.00298

 96 <-175 -0.00145

 96 <-220 0.00112

 96 <-243 0.00131

 97 <-156 0.00200

 97 <-161 -0.00109

 97 <-186 -0.00144

 98 <-154 0.00161

 98 <-159 0.00278

 98 <-182 0.00104

 99 <-163 -0.00158

 99 <-173 0.00192

 100 <-161 -0.00223

 100 <-171 0.00183

 101 <-151 0.00156

 101 <-155 -0.00118

 101 <-160 0.00208

 101 <-185 0.00275

 101 <-194 -0.00144

 102 <-157 0.00242

 102 <-163 -0.00150

 102 <-183 -0.00100

 102 <-192 -0.00115

 102 <-206 -0.00123

 102 <-226 0.00116

 103 <-159 0.00124

 103 <-162 -0.00192

 103 <-178 -0.00233

 103 <-188 0.00160

 103 <-207 -0.00214

 103 <-210 0.00129

 104 <-140 0.00266

 104 <-144 -0.00111

 104 <-155 -0.00178

 104 <-166 -0.00100

 104 <-190 -0.00131

 104 <-213 0.00138

 104 <-217 -0.00128

 105 <-140 0.00384

 105 <-144 -0.00174

 105 <-148 -0.00138

 105 <-165 -0.00132

 105 <-190 0.00121

 105 <-204 0.00114

 105 <-217 -0.00103

 106 <-156 -0.00109

 107 <-139 -0.00721

 107 <-147 -0.00258

 107 <-164 -0.00167

 107 <-177 -0.00147

 107 <-216 -0.00116

 108 <-161 0.00112

 108 <-167 -0.00191

 108 <-171 0.00112

 108 <-186 -0.00190

 108 <-195 0.00127

 109 <-149 -0.00162

 109 <-153 -0.00195

 109 <-168 0.00219

 109 <-220 -0.00150

 109 <-230 -0.00101

 109 <-243 0.00103

 110 <-142 0.00142

 110 <-150 -0.00301

 110 <-219 0.00158

 111 <-169 -0.00222

 111 <-178 0.00107

 111 <-182 -0.00256

 112 <-163 -0.00201

 112 <-191 0.00184

 112 <-192 0.00145

 113 <-139 -0.00447

 113 <-164 0.00246

 113 <-224 0.00164

 114 <-160 -0.00114

 114 <-166 0.00184

 114 <-185 0.00311

 114 <-190 -0.00185

 114 <-194 -0.00169

 115 <-167 0.00161

 115 <-171 0.00248

 115 <-186 -0.00135

 115 <-189 -0.00103

 116 <-140 0.00365

 116 <-144 -0.00162

 116 <-148 -0.00409

 116 <-165 -0.00209

 116 <-223 -0.00158

 116 <-244 0.00102

 117 <-149 0.00162

 117 <-154 0.00121

 117 <-158 0.00157

 117 <-162 -0.00211

 117 <-178 0.00287

 117 <-207 0.00202

 118 <-170 -0.00273

 118 <-192 0.00191

 119 <-160 0.00173

 119 <-166 0.00169

 119 <-172 0.00101

 119 <-190 -0.00156

 119 <-194 0.00211

 119 <-222 0.00146

 120 <-146 -0.00174

 120 <-157 0.00102

 120 <-170 0.00127

 120 <-183 -0.00194

 120 <-192 -0.00105

 121 <-143 0.00158

 121 <-149 0.00400

 121 <-158 0.00386

 121 <-178 0.00258

 121 <-179 0.00300

 121 <-182 0.00155

 121 <-193 0.00154

 121 <-201 0.00158

 121 <-205 -0.00243

 121 <-207 -0.00178

 121 <-211 -0.00233

 121 <-229 0.00122

 122 <-146 -0.00444

 122 <-174 0.00130

 122 <-240 0.00119

 122 <-246 0.00136

 123 <-141 0.00128

 123 <-143 0.00314

 123 <-158 -0.00227

 123 <-168 -0.00125

 123 <-179 -0.00113

 123 <-184 0.00192

 123 <-230 -0.00167

 124 <-180 -0.00259

 124 <-189 0.00128

 124 <-196 -0.00164

 124 <-216 -0.00110

 125 <-170 -0.00152

 125 <-183 0.00575

 125 <-187 -0.00123

 125 <-215 0.00175

 125 <-218 -0.00115

 125 <-226 0.00171

 126 <-149 0.00225

 126 <-158 0.00279

 126 <-178 0.00114

 126 <-179 0.00333

 126 <-182 -0.00111

 126 <-193 0.00101

 126 <-205 -0.00137

 126 <-211 -0.00239

 126 <-229 0.00102

 127 <-140 0.01115

 127 <-144 0.00372

 127 <-148 -0.00100

 127 <-165 -0.00104

 127 <-244 0.00214

 128 <-151 0.00166

 128 <-155 0.00160

 128 <-181 0.00468

 128 <-190 -0.00227

 128 <-194 0.00204

 128 <-199 0.00199

 128 <-209 -0.00196

 128 <-213 -0.00143

 128 <-217 -0.00106

 128 <-222 -0.00162

 128 <-233 0.00141

 128 <-290 -0.00121

 128 <-295 0.00115

 128 <-302 0.00106

 129 <-156 0.00134

 129 <-171 0.00196

 129 <-180 0.00237

 129 <-186 -0.00129

 129 <-189 -0.00230

 129 <-195 -0.00113

 129 <-196 0.00273

 129 <-203 -0.00125

 129 <-216 0.00158

 129 <-281 -0.00114

 130 <-139 -0.00598

 130 <-145 0.00133

 130 <-147 -0.00502

 130 <-164 0.00196

 130 <-177 -0.00136

 130 <-245 0.00169

 131 <-142 0.00111

 131 <-146 -0.00494

 131 <-150 -0.00616

 131 <-174 0.00180

 131 <-246 -0.00192

 132 <-141 0.00502

 132 <-143 0.00194

 132 <-175 0.00133

 132 <-253 -0.00176

 133 <-139 -0.00641

 133 <-145 0.00129

 133 <-147 0.00132

 133 <-164 0.00154

 133 <-177 0.00231

 133 <-255 -0.00107

 134 <-139 0.05392

 134 <-147 0.01116

 134 <-164 -0.00149

 134 <-177 0.00209

 134 <-434 0.00129

 135 <-146 0.00596

 135 <-150 -0.00152

 135 <-174 -0.00309

 135 <-240 0.00127

 135 <-279 0.00121

 136 <-141 -0.00249

 136 <-143 -0.00199

 136 <-149 -0.00386

 136 <-153 -0.00229

 136 <-158 0.00147

 136 <-168 0.00345

 136 <-175 -0.00237

 136 <-184 -0.00154

 136 <-243 -0.00104

 136 <-263 0.00120

 137 <-140 0.00293

 137 <-144 -0.00243

 137 <-148 -0.00548

 137 <-165 -0.00281

 137 <-176 0.00218

 137 <-250 -0.00129

 137 <-256 0.00122

 138 <-140 -0.07206

 138 <-144 -0.00240

 138 <-148 0.00640

 138 <-176 -0.00111

 138 <-256 0.00118

 138 <-262 0.00153

 138 <-267 -0.00167

 138 <-288 -0.00166

 138 <-305 -0.00101

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

 Total Energy, E(TD-HF/TD-KS) = -1733.31654870

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

 Excited State 2: Singlet-E 1.9891 eV 623.31 nm f=0.6377 <S\*\*2>=0.000

 41 ->185 -0.00106

 43 ->207 0.00107

 44 ->180 -0.00107

 45 ->185 0.00143

 46 ->214 0.00111

 47 ->178 0.00103

 47 ->182 -0.00105

 47 ->207 0.00152

 48 ->185 -0.00114

 48 ->194 0.00104

 48 ->213 0.00119

 53 ->180 -0.00114

 61 ->180 -0.00174

 62 ->183 0.00195

 62 ->187 -0.00144

 62 ->218 -0.00107

 62 ->232 0.00130

 62 ->239 -0.00104

 63 ->179 -0.00136

 64 ->180 -0.00114

 64 ->186 -0.00170

 64 ->328 0.00102

 68 ->197 0.00122

 69 ->186 -0.00146

 69 ->196 -0.00103

 70 ->190 -0.00137

 70 ->194 -0.00120

 70 ->197 -0.00170

 70 ->204 -0.00133

 70 ->213 -0.00109

 70 ->217 -0.00110

 70 ->233 0.00116

 70 ->250 -0.00114

 71 ->169 -0.00104

 71 ->182 0.00172

 71 ->210 0.00123

 71 ->211 -0.00111

 72 ->163 -0.00106

 72 ->183 -0.00173

 72 ->214 0.00111

 73 ->167 0.00125

 73 ->180 0.00163

 73 ->186 -0.00121

 73 ->195 -0.00117

 73 ->196 0.00140

 76 ->149 -0.00106

 78 ->181 -0.00111

 78 ->190 0.00143

 78 ->197 0.00104

 78 ->204 0.00131

 78 ->233 -0.00103

 79 ->178 0.00109

 79 ->179 0.00314

 79 ->193 -0.00187

 79 ->205 0.00159

 79 ->211 -0.00190

 79 ->259 0.00105

 80 ->157 -0.00125

 80 ->183 -0.00239

 80 ->187 0.00160

 80 ->257 -0.00146

 80 ->260 -0.00199

 80 ->297 -0.00168

 81 ->151 -0.00143

 81 ->155 0.00110

 81 ->185 0.00137

 82 ->157 0.00157

 82 ->257 -0.00126

 82 ->260 -0.00106

 82 ->282 -0.00109

 82 ->297 -0.00189

 82 ->320 -0.00125

 83 ->154 -0.00236

 83 ->162 0.00140

 83 ->169 0.00115

 83 ->178 0.00249

 83 ->179 0.00246

 83 ->184 -0.00101

 83 ->193 -0.00111

 83 ->205 0.00133

 83 ->207 -0.00176

 83 ->211 -0.00205

 83 ->266 -0.00120

 84 ->152 0.00208

 84 ->156 -0.00198

 84 ->186 0.00109

 84 ->189 -0.00149

 84 ->195 0.00102

 85 ->152 -0.00216

 85 ->167 0.00137

 85 ->171 -0.00108

 85 ->180 -0.00534

 85 ->196 -0.00114

 85 ->200 -0.00170

 85 ->203 0.00114

 85 ->208 0.00184

 85 ->212 0.00152

 85 ->242 -0.00105

 85 ->249 -0.00170

 85 ->251 0.00135

 85 ->281 -0.00100

 85 ->291 0.00160

 85 ->301 -0.00125

 85 ->328 -0.00108

 86 ->166 0.00109

 86 ->185 0.00251

 86 ->204 -0.00102

 86 ->262 0.00110

 86 ->273 -0.00104

 87 ->173 -0.00189

 87 ->183 0.00127

 87 ->192 0.00133

 87 ->214 -0.00140

 88 ->154 0.00205

 88 ->158 -0.00107

 88 ->169 0.00159

 88 ->178 -0.00212

 88 ->182 0.00398

 88 ->207 0.00123

 88 ->258 0.00137

 88 ->271 0.00149

 89 ->155 -0.00185

 89 ->181 -0.00112

 89 ->194 0.00141

 89 ->204 0.00110

 90 ->157 0.00220

 90 ->187 -0.00118

 90 ->192 -0.00101

 90 ->206 0.00114

 91 ->149 -0.00129

 91 ->154 -0.00207

 91 ->162 -0.00140

 91 ->179 0.00216

 91 ->193 -0.00189

 92 ->140 0.00119

 92 ->144 0.00344

 92 ->165 0.00454

 92 ->176 0.00178

 92 ->213 -0.00102

 92 ->217 0.00198

 93 ->161 0.00168

 93 ->171 -0.00273

 93 ->186 0.00332

 93 ->195 0.00204

 93 ->196 -0.00106

 93 ->208 -0.00117

 94 ->152 0.00107

 94 ->156 -0.00145

 94 ->180 0.00144

 94 ->196 -0.00154

 95 ->141 0.00408

 95 ->143 0.00423

 95 ->149 0.00355

 95 ->153 -0.00401

 95 ->158 -0.00169

 95 ->168 -0.00325

 95 ->175 -0.00195

 95 ->220 -0.00135

 95 ->230 -0.00101

 95 ->243 -0.00158

 96 ->142 -0.00438

 96 ->150 0.00355

 96 ->219 0.00139

 97 ->151 0.00106

 97 ->155 -0.00277

 97 ->160 -0.00150

 97 ->185 0.00184

 98 ->157 0.00103

 98 ->163 -0.00216

 98 ->173 0.00254

 99 ->154 -0.00226

 99 ->159 0.00386

 99 ->182 -0.00134

 100 ->160 0.00307

 100 ->172 -0.00245

 100 ->228 0.00117

 101 ->152 0.00218

 101 ->156 -0.00164

 101 ->161 -0.00288

 101 ->186 0.00344

 101 ->195 0.00180

 101 ->196 -0.00100

 102 ->149 0.00117

 102 ->158 0.00126

 102 ->159 0.00172

 102 ->162 0.00261

 102 ->178 0.00296

 102 ->182 -0.00104

 102 ->188 0.00198

 102 ->207 -0.00260

 102 ->210 -0.00159

 103 ->157 -0.00340

 103 ->163 -0.00206

 103 ->183 0.00128

 103 ->192 0.00147

 103 ->206 0.00155

 103 ->226 0.00141

 104 ->139 -0.00546

 104 ->145 -0.00138

 104 ->147 -0.00124

 104 ->156 0.00252

 104 ->161 -0.00109

 104 ->167 -0.00130

 104 ->189 -0.00163

 104 ->212 -0.00171

 104 ->216 0.00160

 105 ->139 -0.00796

 105 ->145 -0.00221

 105 ->147 -0.00180

 105 ->156 -0.00133

 105 ->167 0.00102

 105 ->189 0.00158

 105 ->195 -0.00105

 105 ->203 0.00148

 105 ->216 0.00132

 106 ->155 0.00159

 106 ->185 -0.00121

 106 ->233 -0.00103

 106 ->280 -0.00103

 107 ->140 -0.01027

 107 ->144 0.00152

 107 ->148 0.00425

 107 ->176 -0.00190

 107 ->217 -0.00151

 107 ->233 0.00108

 108 ->160 -0.00162

 108 ->166 0.00269

 108 ->172 -0.00157

 108 ->185 -0.00249

 108 ->194 -0.00163

 108 ->236 -0.00103

 109 ->142 -0.00237

 109 ->150 0.00475

 109 ->219 -0.00205

 110 ->141 -0.00219

 110 ->149 0.00264

 110 ->153 -0.00213

 110 ->168 -0.00265

 110 ->220 0.00186

 110 ->230 -0.00126

 110 ->243 -0.00119

 111 ->163 -0.00288

 111 ->173 -0.00136

 111 ->191 0.00243

 111 ->192 -0.00186

 112 ->159 0.00115

 112 ->162 -0.00106

 112 ->169 -0.00314

 112 ->178 -0.00141

 112 ->182 0.00338

 112 ->188 0.00111

 112 ->207 0.00117

 112 ->237 -0.00106

 113 ->140 0.00627

 113 ->144 0.00111

 113 ->165 -0.00315

 113 ->223 -0.00202

 114 ->161 0.00165

 114 ->167 -0.00263

 114 ->186 0.00402

 114 ->189 0.00246

 114 ->195 0.00221

 115 ->160 0.00119

 115 ->166 0.00231

 115 ->172 0.00344

 115 ->185 0.00180

 115 ->190 -0.00135

 116 ->139 -0.00964

 116 ->145 -0.00144

 116 ->147 -0.00550

 116 ->164 0.00168

 116 ->177 -0.00103

 116 ->224 0.00205

 116 ->245 -0.00115

 117 ->170 0.00385

 117 ->173 -0.00112

 117 ->192 -0.00250

 118 ->149 -0.00255

 118 ->154 -0.00185

 118 ->158 -0.00238

 118 ->159 0.00128

 118 ->162 0.00308

 118 ->178 -0.00385

 118 ->184 0.00121

 118 ->207 0.00254

 118 ->211 -0.00111

 119 ->152 -0.00134

 119 ->161 0.00253

 119 ->167 0.00242

 119 ->171 0.00144

 119 ->189 -0.00207

 119 ->195 0.00273

 119 ->221 -0.00182

 119 ->234 0.00103

 119 ->242 0.00116

 120 ->141 -0.00220

 120 ->143 -0.00283

 120 ->149 -0.00632

 120 ->153 0.00155

 120 ->158 -0.00597

 120 ->162 -0.00104

 120 ->175 0.00101

 120 ->178 -0.00360

 120 ->179 0.00404

 120 ->182 -0.00202

 120 ->193 -0.00195

 120 ->201 -0.00206

 120 ->205 0.00315

 120 ->207 -0.00221

 120 ->211 -0.00296

 120 ->229 0.00155

 120 ->298 -0.00113

 121 ->142 -0.00237

 121 ->146 -0.00231

 121 ->150 0.00139

 121 ->157 -0.00155

 121 ->170 -0.00180

 121 ->183 0.00264

 121 ->192 0.00140

 121 ->214 -0.00106

 121 ->260 0.00115

 121 ->282 0.00104

 122 ->141 -0.00543

 122 ->143 -0.00559

 122 ->153 0.00394

 122 ->158 0.00332

 122 ->168 0.00152

 122 ->175 0.00125

 122 ->178 0.00121

 122 ->179 -0.00161

 122 ->184 -0.00238

 122 ->205 -0.00121

 122 ->211 0.00100

 122 ->230 -0.00230

 123 ->142 -0.00392

 123 ->146 -0.00577

 123 ->150 0.00146

 123 ->174 0.00171

 123 ->183 -0.00115

 123 ->240 -0.00153

 123 ->246 0.00154

 124 ->151 0.00132

 124 ->172 -0.00106

 124 ->181 0.00359

 124 ->185 0.00109

 124 ->190 0.00171

 124 ->197 0.00221

 124 ->204 0.00111

 124 ->217 0.00137

 124 ->252 -0.00100

 125 ->149 -0.00393

 125 ->158 -0.00449

 125 ->169 0.00123

 125 ->178 -0.00170

 125 ->179 0.00466

 125 ->182 0.00159

 125 ->193 -0.00129

 125 ->201 -0.00119

 125 ->205 0.00179

 125 ->207 -0.00125

 125 ->211 -0.00310

 125 ->229 0.00128

 125 ->278 0.00115

 126 ->170 0.00220

 126 ->173 -0.00129

 126 ->183 -0.00796

 126 ->187 -0.00172

 126 ->191 -0.00119

 126 ->192 -0.00120

 126 ->215 -0.00218

 126 ->218 0.00147

 126 ->226 0.00217

 126 ->257 -0.00100

 127 ->139 0.01459

 127 ->145 -0.00761

 127 ->147 -0.00165

 127 ->164 -0.00112

 127 ->177 -0.00173

 127 ->242 0.00104

 127 ->245 0.00260

 128 ->139 0.00308

 128 ->152 -0.00281

 128 ->156 -0.00267

 128 ->161 -0.00158

 128 ->171 -0.00128

 128 ->180 -0.00665

 128 ->186 -0.00127

 128 ->189 -0.00315

 128 ->195 0.00281

 128 ->200 -0.00268

 128 ->203 -0.00135

 128 ->208 0.00254

 128 ->212 0.00190

 128 ->216 0.00139

 128 ->221 0.00205

 128 ->224 0.00107

 128 ->234 -0.00181

 128 ->272 0.00121

 128 ->277 0.00103

 128 ->291 0.00144

 128 ->294 -0.00138

 128 ->301 -0.00125

 129 ->148 0.00160

 129 ->155 0.00219

 129 ->172 -0.00288

 129 ->181 0.00331

 129 ->185 -0.00181

 129 ->190 0.00310

 129 ->194 0.00153

 129 ->197 0.00369

 129 ->204 0.00164

 129 ->209 0.00120

 129 ->213 0.00124

 129 ->217 0.00201

 129 ->280 -0.00137

 130 ->140 -0.00635

 130 ->144 0.00117

 130 ->148 0.01102

 130 ->165 0.00393

 130 ->176 -0.00229

 130 ->244 0.00225

 131 ->141 -0.02370

 131 ->143 0.00175

 131 ->175 -0.00209

 131 ->230 0.00103

 131 ->253 0.00215

 132 ->142 0.00526

 132 ->146 0.01001

 132 ->150 -0.01159

 132 ->174 -0.00304

 132 ->246 0.00246

 133 ->140 0.01412

 133 ->144 0.00437

 133 ->148 0.00177

 133 ->165 -0.00213

 133 ->176 -0.00284

 133 ->244 -0.00104

 133 ->250 -0.00119

 133 ->256 0.00132

 134 ->140 -0.15135

 134 ->148 0.01571

 134 ->165 0.00186

 134 ->176 -0.00224

 134 ->433 -0.00120

 135 ->143 0.00313

 135 ->149 0.00718

 135 ->153 -0.00383

 135 ->154 -0.00111

 135 ->158 -0.00239

 135 ->168 -0.00536

 135 ->175 -0.00295

 135 ->184 0.00219

 135 ->243 0.00136

 135 ->263 -0.00142

 136 ->142 0.00171

 136 ->146 0.00869

 136 ->150 0.00164

 136 ->174 -0.00375

 136 ->240 -0.00158

 136 ->279 -0.00149

 137 ->139 -0.00789

 137 ->145 -0.00297

 137 ->147 -0.00888

 137 ->164 0.00419

 137 ->177 -0.00267

 137 ->249 -0.00164

 137 ->255 -0.00151

 138 ->139 0.69448

 138 ->145 0.00891

 138 ->147 -0.00537

 138 ->164 -0.00138

 138 ->177 -0.00199

 138 ->208 0.00118

 138 ->224 -0.00106

 138 ->249 0.00127

 138 ->255 0.00158

 138 ->261 0.00192

 138 ->268 -0.00206

 138 ->287 -0.00197

 138 ->304 0.00117

 138 ->313 -0.00102

 45 <-185 0.00125

 46 <-214 0.00112

 47 <-207 0.00133

 48 <-185 -0.00100

 48 <-213 0.00111

 61 <-180 -0.00148

 62 <-183 0.00173

 62 <-187 -0.00116

 62 <-232 0.00117

 63 <-179 -0.00111

 64 <-186 -0.00149

 68 <-197 0.00109

 69 <-186 -0.00128

 70 <-190 -0.00112

 70 <-194 -0.00103

 70 <-197 -0.00149

 70 <-204 -0.00115

 70 <-233 0.00103

 71 <-182 0.00144

 71 <-210 0.00104

 72 <-183 -0.00144

 73 <-180 0.00134

 73 <-186 -0.00102

 73 <-195 -0.00101

 73 <-196 0.00117

 78 <-190 0.00116

 78 <-204 0.00111

 79 <-179 0.00253

 79 <-193 -0.00159

 79 <-205 0.00137

 79 <-211 -0.00159

 80 <-183 -0.00206

 80 <-187 0.00129

 80 <-257 -0.00126

 80 <-260 -0.00173

 80 <-297 -0.00147

 81 <-151 -0.00109

 81 <-185 0.00110

 82 <-157 0.00118

 82 <-257 -0.00107

 82 <-297 -0.00164

 82 <-320 -0.00109

 83 <-154 -0.00182

 83 <-162 0.00111

 83 <-178 0.00206

 83 <-179 0.00200

 83 <-205 0.00116

 83 <-207 -0.00153

 83 <-211 -0.00172

 83 <-266 -0.00108

 84 <-152 0.00158

 84 <-156 -0.00148

 84 <-189 -0.00122

 85 <-152 -0.00167

 85 <-167 0.00107

 85 <-180 -0.00434

 85 <-200 -0.00144

 85 <-203 0.00102

 85 <-208 0.00154

 85 <-212 0.00128

 85 <-249 -0.00145

 85 <-251 0.00112

 85 <-291 0.00141

 85 <-301 -0.00112

 86 <-185 0.00199

 87 <-173 -0.00145

 87 <-192 0.00108

 87 <-214 -0.00119

 88 <-154 0.00152

 88 <-169 0.00120

 88 <-178 -0.00170

 88 <-182 0.00317

 88 <-207 0.00108

 88 <-258 0.00113

 88 <-271 0.00127

 89 <-155 -0.00135

 89 <-194 0.00111

 90 <-157 0.00160

 91 <-154 -0.00150

 91 <-162 -0.00102

 91 <-179 0.00170

 91 <-193 -0.00150

 92 <-144 0.00242

 92 <-165 0.00364

 92 <-176 0.00161

 92 <-217 0.00171

 93 <-161 0.00124

 93 <-171 -0.00209

 93 <-186 0.00272

 93 <-195 0.00166

 94 <-156 -0.00105

 94 <-180 0.00111

 94 <-196 -0.00123

 95 <-141 0.00235

 95 <-143 0.00306

 95 <-149 0.00253

 95 <-153 -0.00272

 95 <-158 -0.00121

 95 <-168 -0.00298

 95 <-175 -0.00145

 95 <-220 -0.00112

 95 <-243 -0.00131

 96 <-142 -0.00304

 96 <-150 0.00276

 96 <-219 0.00123

 97 <-155 -0.00200

 97 <-160 -0.00109

 97 <-185 0.00144

 98 <-163 -0.00158

 98 <-173 0.00192

 99 <-154 -0.00161

 99 <-159 0.00278

 99 <-182 -0.00104

 100 <-160 0.00223

 100 <-172 -0.00183

 101 <-152 0.00156

 101 <-156 -0.00118

 101 <-161 -0.00208

 101 <-186 0.00275

 101 <-195 0.00144

 102 <-159 0.00124

 102 <-162 0.00192

 102 <-178 0.00233

 102 <-188 0.00160

 102 <-207 -0.00214

 102 <-210 -0.00129

 103 <-157 -0.00242

 103 <-163 -0.00150

 103 <-183 0.00100

 103 <-192 0.00115

 103 <-206 0.00123

 103 <-226 0.00116

 104 <-139 -0.00266

 104 <-145 -0.00111

 104 <-156 0.00178

 104 <-167 -0.00100

 104 <-189 -0.00131

 104 <-212 -0.00138

 104 <-216 0.00128

 105 <-139 -0.00384

 105 <-145 -0.00174

 105 <-147 -0.00138

 105 <-164 0.00132

 105 <-189 0.00121

 105 <-203 0.00114

 105 <-216 0.00103

 106 <-155 0.00109

 107 <-140 -0.00721

 107 <-148 0.00258

 107 <-165 -0.00167

 107 <-176 -0.00147

 107 <-217 -0.00116

 108 <-160 -0.00112

 108 <-166 0.00191

 108 <-172 -0.00112

 108 <-185 -0.00190

 108 <-194 -0.00127

 109 <-142 -0.00142

 109 <-150 0.00301

 109 <-219 -0.00158

 110 <-149 0.00162

 110 <-153 -0.00195

 110 <-168 -0.00219

 110 <-220 0.00150

 110 <-230 -0.00101

 110 <-243 -0.00103

 111 <-163 -0.00201

 111 <-191 0.00184

 111 <-192 -0.00145

 112 <-169 -0.00222

 112 <-178 -0.00107

 112 <-182 0.00256

 113 <-140 0.00447

 113 <-165 -0.00246

 113 <-223 -0.00164

 114 <-161 0.00114

 114 <-167 -0.00184

 114 <-186 0.00311

 114 <-189 0.00185

 114 <-195 0.00169

 115 <-166 0.00161

 115 <-172 0.00248

 115 <-185 0.00135

 115 <-190 -0.00103

 116 <-139 -0.00365

 116 <-145 -0.00162

 116 <-147 -0.00409

 116 <-164 0.00209

 116 <-224 0.00158

 116 <-245 -0.00102

 117 <-170 0.00273

 117 <-192 -0.00191

 118 <-149 -0.00162

 118 <-154 -0.00121

 118 <-158 -0.00157

 118 <-162 0.00211

 118 <-178 -0.00287

 118 <-207 0.00202

 119 <-161 0.00173

 119 <-167 0.00169

 119 <-171 0.00101

 119 <-189 -0.00156

 119 <-195 0.00211

 119 <-221 -0.00146

 120 <-143 -0.00158

 120 <-149 -0.00400

 120 <-158 -0.00386

 120 <-178 -0.00258

 120 <-179 0.00300

 120 <-182 -0.00155

 120 <-193 -0.00154

 120 <-201 -0.00158

 120 <-205 0.00243

 120 <-207 -0.00178

 120 <-211 -0.00233

 120 <-229 0.00122

 121 <-146 -0.00174

 121 <-157 -0.00102

 121 <-170 -0.00127

 121 <-183 0.00194

 121 <-192 0.00105

 122 <-141 0.00128

 122 <-143 -0.00314

 122 <-158 0.00227

 122 <-168 0.00125

 122 <-179 -0.00113

 122 <-184 -0.00192

 122 <-230 -0.00167

 123 <-146 -0.00444

 123 <-174 0.00130

 123 <-240 -0.00119

 123 <-246 0.00136

 124 <-181 0.00259

 124 <-190 0.00128

 124 <-197 0.00164

 124 <-217 0.00110

 125 <-149 -0.00225

 125 <-158 -0.00279

 125 <-178 -0.00114

 125 <-179 0.00333

 125 <-182 0.00111

 125 <-193 -0.00101

 125 <-205 0.00137

 125 <-211 -0.00239

 125 <-229 0.00102

 126 <-170 0.00152

 126 <-183 -0.00575

 126 <-187 -0.00123

 126 <-215 -0.00175

 126 <-218 0.00115

 126 <-226 0.00171

 127 <-139 0.01115

 127 <-145 -0.00372

 127 <-147 0.00100

 127 <-164 -0.00104

 127 <-245 0.00214

 128 <-152 -0.00166

 128 <-156 -0.00160

 128 <-180 -0.00468

 128 <-189 -0.00227

 128 <-195 0.00204

 128 <-200 -0.00199

 128 <-208 0.00196

 128 <-212 0.00143

 128 <-216 0.00106

 128 <-221 0.00162

 128 <-234 -0.00141

 128 <-291 0.00121

 128 <-294 -0.00115

 128 <-301 -0.00106

 129 <-155 0.00134

 129 <-172 -0.00196

 129 <-181 0.00237

 129 <-185 -0.00129

 129 <-190 0.00230

 129 <-194 0.00113

 129 <-197 0.00273

 129 <-204 0.00125

 129 <-217 0.00158

 129 <-280 -0.00114

 130 <-140 -0.00598

 130 <-144 -0.00133

 130 <-148 0.00502

 130 <-165 0.00196

 130 <-176 -0.00136

 130 <-244 0.00169

 131 <-141 -0.00502

 131 <-143 0.00194

 131 <-175 -0.00133

 131 <-253 0.00176

 132 <-142 0.00111

 132 <-146 0.00494

 132 <-150 -0.00616

 132 <-174 -0.00180

 132 <-246 0.00192

 133 <-140 0.00641

 133 <-144 0.00129

 133 <-148 0.00132

 133 <-165 -0.00154

 133 <-176 -0.00231

 133 <-256 0.00107

 134 <-140 -0.05392

 134 <-148 0.01116

 134 <-165 0.00149

 134 <-176 -0.00209

 134 <-433 -0.00129

 135 <-141 -0.00249

 135 <-143 0.00199

 135 <-149 0.00386

 135 <-153 -0.00229

 135 <-158 -0.00147

 135 <-168 -0.00345

 135 <-175 -0.00237

 135 <-184 0.00154

 135 <-243 0.00104

 135 <-263 -0.00120

 136 <-146 0.00596

 136 <-150 0.00152

 136 <-174 -0.00309

 136 <-240 -0.00127

 136 <-279 -0.00121

 137 <-139 -0.00293

 137 <-145 -0.00243

 137 <-147 -0.00548

 137 <-164 0.00281

 137 <-177 -0.00218

 137 <-249 -0.00129

 137 <-255 -0.00122

 138 <-139 -0.07206

 138 <-145 0.00240

 138 <-147 -0.00640

 138 <-177 -0.00111

 138 <-255 0.00118

 138 <-261 0.00153

 138 <-268 -0.00167

 138 <-287 -0.00166

 138 <-304 0.00101

 Excited State 3: Singlet-E 3.3275 eV 372.60 nm f=0.0370 <S\*\*2>=0.000

 56 ->189 -0.00113

 57 ->188 0.00122

 58 ->191 0.00104

 66 ->207 -0.00145

 67 ->231 -0.00104

 69 ->222 0.00101

 72 ->225 -0.00103

 73 ->197 -0.00113

 80 ->179 -0.00131

 80 ->188 0.00127

 81 ->180 -0.00118

 83 ->187 -0.00103

 84 ->185 0.00117

 85 ->181 0.00159

 85 ->213 -0.00127

 86 ->161 -0.00115

 86 ->186 -0.00134

 87 ->154 -0.00101

 87 ->162 -0.00131

 87 ->182 -0.00170

 88 ->187 -0.00108

 88 ->192 -0.00142

 88 ->215 -0.00108

 92 ->139 -0.00632

 92 ->177 0.00124

 93 ->160 0.00119

 93 ->166 0.00108

 93 ->185 -0.00180

 95 ->142 -0.00228

 95 ->146 -0.00135

 95 ->174 0.00164

 96 ->141 0.00319

 96 ->175 0.00104

 97 ->180 -0.00152

 97 ->196 0.00142

 97 ->265 -0.00136

 98 ->159 -0.00121

 99 ->187 0.00132

 101 ->185 -0.00130

 102 ->157 -0.00117

 102 ->187 -0.00139

 102 ->191 -0.00102

 102 ->226 -0.00117

 102 ->257 0.00145

 102 ->297 -0.00129

 103 ->179 0.00183

 103 ->182 -0.00117

 103 ->198 -0.00150

 103 ->207 0.00115

 103 ->271 -0.00123

 103 ->278 -0.00142

 104 ->144 0.00141

 104 ->181 -0.00140

 104 ->204 0.00121

 104 ->264 -0.00125

 105 ->144 0.00218

 105 ->148 0.00114

 105 ->165 0.00115

 105 ->176 -0.00151

 106 ->208 0.00129

 106 ->234 -0.00112

 107 ->139 -0.00387

 107 ->145 0.00110

 107 ->147 -0.00146

 108 ->156 0.00106

 108 ->161 -0.00105

 108 ->171 -0.00107

 109 ->141 0.00669

 109 ->153 -0.00327

 109 ->175 -0.00292

 110 ->174 -0.00193

 111 ->162 -0.00131

 111 ->182 0.00153

 112 ->157 -0.00105

 112 ->187 -0.00107

 112 ->206 -0.00106

 113 ->139 0.01639

 113 ->145 -0.00103

 113 ->147 0.00195

 113 ->177 0.00235

 114 ->166 -0.00108

 114 ->181 0.00128

 114 ->185 -0.00166

 115 ->180 -0.00142

 115 ->189 -0.00123

 115 ->195 -0.00181

 115 ->227 0.00135

 116 ->140 0.02953

 116 ->144 0.00287

 116 ->148 -0.00183

 116 ->165 0.00177

 116 ->176 0.00233

 117 ->179 -0.00229

 117 ->188 0.00165

 117 ->237 0.00108

 118 ->163 0.00107

 118 ->170 0.00111

 118 ->187 0.00147

 118 ->191 -0.00193

 118 ->192 -0.00104

 118 ->231 -0.00131

 119 ->166 -0.00155

 119 ->181 -0.00209

 119 ->190 0.00180

 119 ->228 -0.00110

 119 ->264 -0.00113

 120 ->142 0.00252

 120 ->150 -0.00236

 120 ->260 -0.00150

 121 ->143 -0.00122

 121 ->182 -0.00117

 121 ->184 0.00111

 121 ->207 0.00111

 121 ->211 0.00159

 121 ->225 0.00106

 121 ->229 -0.00102

 122 ->142 0.00432

 122 ->150 -0.00358

 123 ->141 -0.00761

 123 ->143 -0.00358

 123 ->168 0.00139

 124 ->152 0.00114

 124 ->161 -0.00129

 124 ->180 -0.00101

 124 ->189 -0.00130

 124 ->265 -0.00131

 125 ->183 -0.00158

 125 ->187 -0.00135

 125 ->191 0.00106

 125 ->192 -0.00120

 125 ->218 0.00119

 125 ->226 -0.00100

 126 ->141 0.00189

 126 ->154 0.00111

 126 ->159 -0.00140

 126 ->188 -0.00102

 126 ->207 0.00105

 126 ->210 0.00158

 126 ->271 -0.00143

 127 ->140 -0.01533

 127 ->144 0.00282

 127 ->165 0.00161

 127 ->176 0.00155

 128 ->140 0.04742

 128 ->148 -0.00222

 128 ->185 -0.00180

 128 ->222 0.00135

 129 ->145 0.00108

 129 ->152 0.00129

 129 ->189 0.00140

 129 ->196 -0.00219

 130 ->139 0.02207

 130 ->145 0.00745

 130 ->164 -0.00257

 131 ->142 -0.00568

 131 ->146 0.00227

 131 ->219 -0.00129

 132 ->141 -0.00668

 132 ->143 0.00991

 132 ->153 0.00510

 132 ->168 -0.00231

 132 ->220 0.00143

 133 ->139 0.20586

 133 ->145 -0.00338

 133 ->147 0.01284

 133 ->164 0.00355

 134 ->139 0.13849

 134 ->145 0.00679

 134 ->147 0.00249

 134 ->164 -0.00452

 134 ->177 -0.00144

 135 ->142 0.00764

 135 ->146 0.00921

 135 ->150 -0.00145

 135 ->174 0.00129

 136 ->141 0.04985

 136 ->143 0.00430

 136 ->153 -0.01810

 136 ->168 -0.00349

 136 ->175 -0.00146

 136 ->274 0.00158

 137 ->140 0.65326

 137 ->144 0.00264

 137 ->148 -0.01878

 137 ->165 0.00686

 137 ->176 0.00162

 138 ->140 -0.03424

 138 ->144 0.04979

 66 <-207 -0.00104

 85 <-181 0.00121

 87 <-182 -0.00101

 92 <-139 -0.00235

 92 <-177 0.00110

 93 <-185 -0.00110

 95 <-146 -0.00116

 95 <-174 0.00145

 96 <-141 0.00189

 97 <-180 -0.00103

 97 <-196 0.00101

 97 <-265 -0.00108

 102 <-257 0.00113

 102 <-297 -0.00100

 103 <-179 0.00119

 103 <-198 -0.00109

 103 <-278 -0.00111

 105 <-144 0.00122

 105 <-165 0.00103

 105 <-176 -0.00127

 107 <-139 -0.00175

 109 <-175 -0.00211

 110 <-174 -0.00173

 113 <-139 0.00160

 113 <-164 -0.00135

 113 <-177 0.00174

 115 <-195 -0.00118

 116 <-148 0.00174

 116 <-176 0.00156

 117 <-179 -0.00142

 117 <-188 0.00103

 118 <-191 -0.00123

 119 <-181 -0.00127

 119 <-190 0.00111

 120 <-260 -0.00111

 121 <-211 0.00109

 122 <-142 0.00250

 122 <-150 -0.00166

 123 <-141 -0.00107

 123 <-153 -0.00170

 123 <-168 0.00158

 126 <-210 0.00105

 126 <-271 -0.00103

 127 <-140 -0.00385

 127 <-144 0.00249

 128 <-185 -0.00103

 129 <-196 -0.00134

 130 <-139 0.00238

 130 <-145 0.00268

 131 <-142 -0.00342

 131 <-146 0.00165

 132 <-141 0.00189

 132 <-143 0.00277

 132 <-153 0.00193

 133 <-139 -0.00355

 133 <-145 0.00298

 133 <-147 0.00570

 133 <-164 -0.00104

 134 <-139 -0.00420

 134 <-164 -0.00264

 134 <-177 -0.00102

 135 <-146 0.00551

 135 <-150 0.00180

 135 <-269 -0.00128

 136 <-141 -0.00703

 136 <-143 0.00224

 136 <-153 -0.00220

 136 <-168 -0.00214

 136 <-274 0.00127

 137 <-140 -0.00859

 137 <-148 -0.00426

 137 <-165 0.00186

 137 <-176 0.00101

 138 <-140 0.01554

 138 <-144 0.00155

 138 <-148 0.00106

 Excited State 4: Singlet-E 3.3275 eV 372.60 nm f=0.0370 <S\*\*2>=0.000

 56 ->190 0.00113

 57 ->191 0.00104

 58 ->188 0.00122

 66 ->231 -0.00104

 67 ->207 -0.00145

 69 ->221 0.00101

 71 ->225 -0.00103

 73 ->196 0.00113

 79 ->179 0.00131

 79 ->188 -0.00127

 81 ->181 -0.00118

 82 ->187 0.00103

 84 ->186 0.00117

 85 ->180 -0.00159

 85 ->212 0.00127

 86 ->160 -0.00115

 86 ->185 0.00134

 87 ->187 -0.00108

 87 ->192 0.00142

 87 ->215 0.00108

 88 ->154 0.00101

 88 ->162 0.00131

 88 ->182 0.00170

 92 ->140 -0.00632

 92 ->176 0.00124

 93 ->161 0.00119

 93 ->167 0.00108

 93 ->186 0.00180

 95 ->141 -0.00319

 95 ->175 -0.00104

 96 ->142 -0.00228

 96 ->146 0.00135

 96 ->174 -0.00164

 97 ->181 -0.00152

 97 ->197 0.00142

 97 ->264 -0.00136

 98 ->187 -0.00132

 99 ->159 0.00121

 101 ->186 0.00130

 102 ->179 -0.00183

 102 ->182 -0.00117

 102 ->198 0.00150

 102 ->207 -0.00115

 102 ->271 0.00123

 102 ->278 0.00142

 103 ->157 -0.00117

 103 ->187 0.00139

 103 ->191 0.00102

 103 ->226 0.00117

 103 ->257 -0.00145

 103 ->297 0.00129

 104 ->145 -0.00141

 104 ->180 -0.00140

 104 ->203 -0.00121

 104 ->265 -0.00125

 105 ->145 -0.00218

 105 ->147 -0.00114

 105 ->164 0.00115

 105 ->177 -0.00151

 106 ->209 0.00129

 106 ->233 -0.00112

 107 ->140 0.00387

 107 ->144 0.00110

 107 ->148 -0.00146

 108 ->155 -0.00106

 108 ->160 -0.00105

 108 ->172 -0.00107

 109 ->174 0.00193

 110 ->141 -0.00669

 110 ->153 0.00327

 110 ->175 0.00292

 111 ->157 -0.00105

 111 ->187 0.00107

 111 ->206 -0.00106

 112 ->162 -0.00131

 112 ->182 0.00153

 113 ->140 0.01639

 113 ->144 0.00103

 113 ->148 -0.00195

 113 ->176 0.00235

 114 ->167 -0.00108

 114 ->180 -0.00128

 114 ->186 0.00166

 115 ->181 -0.00142

 115 ->190 0.00123

 115 ->194 0.00181

 115 ->228 -0.00135

 116 ->139 0.02953

 116 ->145 -0.00287

 116 ->147 0.00183

 116 ->164 0.00177

 116 ->177 0.00233

 117 ->163 -0.00107

 117 ->170 0.00111

 117 ->187 -0.00147

 117 ->191 0.00193

 117 ->192 -0.00104

 117 ->231 0.00131

 118 ->179 0.00229

 118 ->188 -0.00165

 118 ->237 -0.00108

 119 ->167 0.00155

 119 ->180 -0.00209

 119 ->189 -0.00180

 119 ->227 0.00110

 119 ->265 -0.00113

 120 ->143 -0.00122

 120 ->182 -0.00117

 120 ->184 0.00111

 120 ->207 -0.00111

 120 ->211 -0.00159

 120 ->225 0.00106

 120 ->229 0.00102

 121 ->142 0.00252

 121 ->150 -0.00236

 121 ->260 0.00150

 122 ->141 0.00761

 122 ->143 -0.00358

 122 ->168 0.00139

 123 ->142 0.00432

 123 ->150 -0.00358

 124 ->151 0.00114

 124 ->160 0.00129

 124 ->181 -0.00101

 124 ->190 0.00130

 124 ->264 -0.00131

 125 ->141 -0.00189

 125 ->154 0.00111

 125 ->159 0.00140

 125 ->188 0.00102

 125 ->207 -0.00105

 125 ->210 0.00158

 125 ->271 0.00143

 126 ->183 -0.00158

 126 ->187 0.00135

 126 ->191 -0.00106

 126 ->192 -0.00120

 126 ->218 0.00119

 126 ->226 0.00100

 127 ->139 0.01533

 127 ->145 0.00282

 127 ->164 -0.00161

 127 ->177 -0.00155

 128 ->139 0.04742

 128 ->147 0.00222

 128 ->186 -0.00180

 128 ->221 0.00135

 129 ->144 0.00108

 129 ->151 -0.00129

 129 ->190 0.00140

 129 ->197 0.00219

 130 ->140 -0.02207

 130 ->144 0.00745

 130 ->165 0.00257

 131 ->141 -0.00668

 131 ->143 -0.00991

 131 ->153 0.00510

 131 ->168 0.00231

 131 ->220 -0.00143

 132 ->142 0.00568

 132 ->146 0.00227

 132 ->219 0.00129

 133 ->140 0.20586

 133 ->144 0.00338

 133 ->148 -0.01284

 133 ->165 0.00355

 134 ->140 0.13849

 134 ->144 -0.00679

 134 ->148 -0.00249

 134 ->165 -0.00452

 134 ->176 -0.00144

 135 ->141 -0.04985

 135 ->143 0.00430

 135 ->153 0.01810

 135 ->168 -0.00349

 135 ->175 0.00146

 135 ->274 -0.00158

 136 ->142 0.00764

 136 ->146 -0.00921

 136 ->150 -0.00145

 136 ->174 -0.00129

 137 ->139 0.65326

 137 ->145 -0.00264

 137 ->147 0.01878

 137 ->164 0.00686

 137 ->177 0.00162

 138 ->139 0.03424

 138 ->145 0.04979

 67 <-207 -0.00104

 85 <-180 -0.00121

 88 <-182 0.00101

 92 <-140 -0.00235

 92 <-176 0.00110

 93 <-186 0.00110

 95 <-141 -0.00189

 96 <-146 0.00116

 96 <-174 -0.00145

 97 <-181 -0.00103

 97 <-197 0.00101

 97 <-264 -0.00108

 102 <-179 -0.00119

 102 <-198 0.00109

 102 <-278 0.00111

 103 <-257 -0.00113

 103 <-297 0.00100

 105 <-145 -0.00122

 105 <-164 0.00103

 105 <-177 -0.00127

 107 <-140 0.00175

 109 <-174 0.00173

 110 <-175 0.00211

 113 <-140 0.00160

 113 <-165 -0.00135

 113 <-176 0.00174

 115 <-194 0.00118

 116 <-147 -0.00174

 116 <-177 0.00156

 117 <-191 0.00123

 118 <-179 0.00142

 118 <-188 -0.00103

 119 <-180 -0.00127

 119 <-189 -0.00111

 120 <-211 -0.00109

 121 <-260 0.00111

 122 <-141 0.00107

 122 <-153 0.00170

 122 <-168 0.00158

 123 <-142 0.00250

 123 <-150 -0.00166

 125 <-210 0.00105

 125 <-271 0.00103

 127 <-139 0.00385

 127 <-145 0.00249

 128 <-186 -0.00103

 129 <-197 0.00134

 130 <-140 -0.00238

 130 <-144 0.00268

 131 <-141 0.00189

 131 <-143 -0.00277

 131 <-153 0.00193

 132 <-142 0.00342

 132 <-146 0.00165

 133 <-140 -0.00355

 133 <-144 -0.00298

 133 <-148 -0.00570

 133 <-165 -0.00104

 134 <-140 -0.00420

 134 <-165 -0.00264

 134 <-176 -0.00102

 135 <-141 0.00703

 135 <-143 0.00224

 135 <-153 0.00220

 135 <-168 -0.00214

 135 <-274 -0.00127

 136 <-146 -0.00551

 136 <-150 0.00180

 136 <-269 0.00128

 137 <-139 -0.00859

 137 <-147 0.00426

 137 <-164 0.00186

 137 <-177 0.00101

 138 <-139 -0.01554

 138 <-145 0.00155

 138 <-147 0.00106

 Excited State 5: Singlet-E 3.3346 eV 371.81 nm f=0.0000 <S\*\*2>=0.000

 56 ->191 -0.00127

 56 ->239 0.00110

 57 ->190 -0.00121

 58 ->189 0.00121

 59 ->188 -0.00155

 64 ->198 -0.00120

 65 ->231 0.00108

 69 ->179 0.00123

 69 ->207 -0.00176

 71 ->196 -0.00102

 71 ->221 -0.00110

 72 ->197 0.00102

 72 ->222 0.00110

 73 ->225 0.00107

 79 ->180 -0.00122

 80 ->181 0.00122

 81 ->163 0.00117

 81 ->187 0.00163

 84 ->188 -0.00137

 86 ->192 0.00114

 86 ->218 -0.00108

 87 ->185 0.00140

 88 ->186 0.00140

 92 ->174 -0.00139

 93 ->162 0.00143

 93 ->182 0.00129

 93 ->225 -0.00121

 95 ->139 0.00575

 95 ->177 -0.00129

 96 ->140 -0.00575

 96 ->176 0.00129

 97 ->187 0.00265

 97 ->191 0.00131

 97 ->226 0.00113

 97 ->239 -0.00100

 97 ->257 -0.00231

 97 ->297 0.00160

 98 ->181 0.00109

 99 ->180 -0.00109

 101 ->259 0.00122

 102 ->180 0.00193

 102 ->189 -0.00116

 102 ->203 0.00123

 102 ->265 0.00174

 103 ->181 -0.00193

 103 ->190 -0.00116

 103 ->204 0.00123

 103 ->264 -0.00174

 104 ->141 -0.00202

 104 ->179 0.00205

 104 ->198 -0.00187

 104 ->271 -0.00133

 104 ->278 -0.00152

 105 ->141 -0.00322

 105 ->175 -0.00178

 105 ->179 -0.00120

 105 ->198 0.00131

 105 ->278 0.00104

 106 ->187 -0.00139

 107 ->150 -0.00142

 108 ->157 -0.00136

 108 ->170 0.00122

 109 ->140 -0.01557

 109 ->148 0.00237

 109 ->176 -0.00273

 110 ->139 0.01557

 110 ->147 0.00237

 110 ->177 0.00273

 111 ->155 -0.00115

 112 ->156 0.00115

 113 ->146 0.00193

 113 ->174 -0.00261

 114 ->158 0.00117

 114 ->162 -0.00114

 114 ->182 0.00121

 115 ->163 0.00106

 115 ->187 0.00229

 115 ->191 -0.00242

 115 ->231 -0.00184

 115 ->257 -0.00113

 115 ->289 -0.00102

 115 ->331 0.00103

 116 ->141 -0.01238

 116 ->153 0.00476

 116 ->175 0.00265

 117 ->181 0.00208

 117 ->190 -0.00144

 117 ->194 -0.00160

 117 ->228 0.00147

 117 ->264 0.00105

 118 ->180 -0.00208

 118 ->189 -0.00144

 118 ->195 -0.00160

 118 ->227 0.00147

 118 ->265 -0.00105

 119 ->169 0.00120

 119 ->179 0.00318

 119 ->188 -0.00192

 119 ->207 -0.00119

 119 ->237 -0.00123

 119 ->258 0.00137

 119 ->271 -0.00106

 120 ->139 -0.00570

 120 ->180 0.00164

 121 ->140 0.00570

 121 ->181 -0.00164

 122 ->139 -0.03506

 122 ->145 0.00125

 122 ->147 -0.00236

 123 ->140 0.03506

 123 ->144 0.00125

 123 ->148 -0.00236

 124 ->187 0.00147

 124 ->226 0.00118

 124 ->257 -0.00148

 125 ->139 0.00888

 125 ->189 0.00127

 125 ->196 -0.00105

 126 ->140 -0.00888

 126 ->190 0.00127

 126 ->197 0.00105

 127 ->143 -0.00498

 127 ->220 -0.00156

 128 ->141 -0.00427

 128 ->179 -0.00149

 128 ->188 0.00109

 128 ->207 -0.00131

 128 ->211 -0.00109

 128 ->271 0.00125

 129 ->142 -0.00227

 129 ->218 0.00112

 130 ->142 -0.00785

 130 ->150 -0.00224

 130 ->219 -0.00170

 131 ->139 0.00460

 131 ->145 0.00960

 131 ->147 0.00146

 131 ->224 -0.00112

 132 ->140 0.00460

 132 ->144 -0.00960

 132 ->148 -0.00146

 132 ->223 -0.00112

 133 ->146 0.01226

 135 ->139 0.49414

 135 ->145 -0.00440

 135 ->147 0.02042

 135 ->164 0.00543

 135 ->177 0.00219

 136 ->140 -0.49414

 136 ->144 -0.00440

 136 ->148 0.02042

 136 ->165 -0.00543

 136 ->176 -0.00219

 137 ->141 -0.05375

 137 ->153 0.02308

 137 ->175 0.00299

 137 ->274 -0.00178

 138 ->143 -0.05930

 138 ->149 0.00252

 56 <-191 -0.00100

 59 <-188 -0.00112

 69 <-207 -0.00133

 81 <-187 0.00114

 92 <-174 -0.00119

 95 <-139 0.00128

 95 <-177 -0.00115

 96 <-140 -0.00128

 96 <-176 0.00115

 97 <-187 0.00184

 97 <-257 -0.00178

 97 <-297 0.00125

 102 <-180 0.00129

 102 <-265 0.00135

 103 <-181 -0.00129

 103 <-264 -0.00135

 104 <-141 -0.00141

 104 <-179 0.00130

 104 <-198 -0.00131

 104 <-278 -0.00117

 105 <-141 -0.00202

 105 <-175 -0.00143

 109 <-176 -0.00196

 110 <-177 0.00196

 113 <-174 -0.00233

 115 <-187 0.00144

 115 <-191 -0.00155

 115 <-231 -0.00135

 116 <-141 -0.00114

 116 <-175 0.00163

 117 <-181 0.00130

 117 <-194 -0.00103

 117 <-228 0.00107

 118 <-180 -0.00130

 118 <-195 -0.00103

 118 <-227 0.00107

 119 <-179 0.00194

 119 <-188 -0.00116

 119 <-258 0.00106

 122 <-139 -0.00282

 122 <-147 0.00103

 123 <-140 0.00282

 123 <-148 0.00103

 124 <-257 -0.00110

 127 <-143 -0.00350

 127 <-149 0.00137

 130 <-142 -0.00421

 130 <-219 -0.00102

 131 <-145 0.00455

 131 <-147 0.00146

 132 <-144 -0.00455

 132 <-148 -0.00146

 133 <-146 0.00730

 133 <-174 -0.00151

 133 <-269 -0.00145

 135 <-139 -0.00777

 135 <-145 0.00126

 135 <-147 0.00626

 135 <-177 0.00149

 136 <-140 0.00777

 136 <-144 0.00126

 136 <-148 0.00626

 136 <-176 -0.00149

 137 <-141 0.00921

 137 <-153 0.00361

 137 <-175 0.00132

 137 <-274 -0.00147

 138 <-143 -0.00215

 138 <-149 -0.00200

 138 <-168 0.00171

 Excited State 6: Singlet-E 3.3391 eV 371.32 nm f=0.0000 <S\*\*2>=0.000

 48 ->207 -0.00119

 56 ->188 0.00158

 57 ->186 0.00123

 58 ->185 0.00123

 59 ->191 0.00132

 59 ->239 -0.00113

 64 ->187 -0.00120

 65 ->169 -0.00100

 65 ->207 -0.00163

 65 ->321 0.00112

 66 ->221 -0.00106

 67 ->222 -0.00106

 68 ->193 0.00102

 68 ->201 0.00106

 69 ->187 -0.00120

 69 ->231 0.00125

 70 ->205 0.00103

 71 ->181 -0.00105

 72 ->180 0.00105

 73 ->183 -0.00114

 73 ->202 -0.00107

 79 ->190 -0.00129

 80 ->189 -0.00129

 81 ->179 -0.00142

 81 ->188 0.00126

 84 ->191 0.00151

 84 ->260 -0.00118

 85 ->183 0.00153

 85 ->218 -0.00131

 86 ->162 0.00146

 86 ->182 0.00184

 87 ->161 0.00120

 87 ->186 0.00153

 87 ->189 0.00135

 87 ->251 0.00106

 88 ->160 -0.00120

 88 ->185 0.00153

 88 ->190 -0.00135

 88 ->252 0.00106

 89 ->179 -0.00118

 92 ->141 -0.00319

 92 ->175 -0.00132

 93 ->157 -0.00132

 93 ->192 0.00179

 93 ->215 0.00150

 95 ->140 -0.00448

 95 ->176 0.00152

 96 ->139 0.00448

 96 ->177 -0.00152

 97 ->179 -0.00199

 97 ->198 0.00190

 97 ->271 0.00153

 97 ->278 0.00188

 101 ->215 0.00106

 102 ->181 -0.00133

 102 ->197 0.00122

 102 ->204 0.00107

 102 ->264 -0.00114

 103 ->180 0.00133

 103 ->196 -0.00122

 103 ->203 0.00107

 103 ->265 0.00114

 104 ->146 0.00110

 104 ->174 -0.00139

 104 ->187 -0.00178

 104 ->226 -0.00157

 104 ->231 -0.00105

 104 ->257 0.00159

 104 ->297 -0.00129

 105 ->146 0.00182

 105 ->174 -0.00216

 105 ->187 0.00118

 105 ->226 0.00102

 105 ->257 -0.00110

 106 ->141 0.00115

 106 ->207 0.00139

 106 ->211 0.00158

 107 ->143 0.00167

 108 ->162 0.00121

 108 ->182 -0.00156

 109 ->139 0.02009

 109 ->145 -0.00144

 109 ->147 0.00224

 109 ->177 0.00276

 110 ->140 -0.02009

 110 ->144 -0.00144

 110 ->148 0.00224

 110 ->176 -0.00276

 111 ->139 0.00141

 111 ->156 -0.00105

 111 ->186 -0.00139

 112 ->140 -0.00141

 112 ->155 0.00105

 112 ->185 0.00139

 113 ->141 0.00883

 113 ->153 -0.00327

 113 ->175 -0.00305

 113 ->296 0.00106

 114 ->170 -0.00152

 114 ->192 0.00145

 114 ->206 0.00130

 115 ->169 -0.00114

 115 ->179 -0.00222

 115 ->188 0.00172

 115 ->211 -0.00116

 115 ->237 0.00153

 116 ->174 0.00166

 117 ->139 0.00170

 117 ->180 -0.00190

 117 ->189 -0.00201

 117 ->195 -0.00134

 117 ->227 0.00110

 118 ->140 -0.00170

 118 ->181 0.00190

 118 ->190 -0.00201

 118 ->194 -0.00134

 118 ->228 0.00110

 119 ->163 -0.00146

 119 ->187 -0.00250

 119 ->191 0.00243

 119 ->231 0.00129

 119 ->257 0.00126

 119 ->260 -0.00113

 119 ->331 -0.00119

 120 ->197 0.00132

 120 ->252 -0.00145

 121 ->196 -0.00132

 121 ->251 0.00145

 122 ->140 0.01583

 123 ->139 -0.01583

 124 ->141 -0.00179

 124 ->159 0.00218

 124 ->188 0.00211

 124 ->207 -0.00101

 124 ->271 0.00124

 125 ->140 -0.00668

 125 ->151 0.00198

 125 ->160 0.00114

 125 ->181 -0.00111

 125 ->185 0.00145

 125 ->197 -0.00147

 125 ->264 -0.00139

 126 ->139 0.00668

 126 ->152 -0.00198

 126 ->161 0.00114

 126 ->180 0.00111

 126 ->186 -0.00145

 126 ->196 0.00147

 126 ->265 0.00139

 127 ->142 0.00892

 127 ->150 -0.00546

 127 ->219 0.00121

 128 ->226 0.00170

 128 ->260 0.00214

 129 ->143 0.00137

 129 ->149 -0.00107

 129 ->154 -0.00192

 129 ->162 0.00109

 129 ->182 -0.00139

 129 ->205 -0.00106

 129 ->210 -0.00178

 129 ->225 0.00104

 129 ->259 -0.00137

 129 ->266 0.00111

 130 ->143 0.00956

 130 ->168 -0.00256

 130 ->220 0.00150

 131 ->140 -0.01171

 131 ->144 -0.01007

 131 ->148 0.00268

 131 ->165 -0.00446

 132 ->139 -0.01171

 132 ->145 0.01007

 132 ->147 -0.00268

 132 ->164 -0.00446

 133 ->141 0.04862

 133 ->153 -0.01986

 133 ->175 -0.00117

 133 ->274 0.00194

 134 ->141 0.00590

 134 ->230 -0.00104

 135 ->140 -0.49606

 135 ->148 0.01711

 135 ->165 -0.00456

 136 ->139 0.49606

 136 ->147 0.01711

 136 ->164 0.00456

 137 ->146 -0.01024

 137 ->174 -0.00175

 138 ->142 0.04491

 138 ->150 0.00799

 56 <-188 0.00114

 59 <-191 0.00103

 65 <-207 -0.00118

 84 <-191 0.00103

 85 <-183 0.00124

 86 <-182 0.00111

 92 <-141 -0.00189

 92 <-175 -0.00122

 93 <-192 0.00109

 93 <-215 0.00109

 95 <-140 -0.00136

 95 <-176 0.00138

 96 <-139 0.00136

 96 <-177 -0.00138

 97 <-179 -0.00134

 97 <-198 0.00141

 97 <-271 0.00115

 97 <-278 0.00148

 104 <-174 -0.00126

 104 <-187 -0.00119

 104 <-226 -0.00108

 104 <-257 0.00121

 104 <-297 -0.00102

 105 <-146 0.00109

 105 <-174 -0.00185

 106 <-211 0.00112

 109 <-139 0.00207

 109 <-177 0.00206

 110 <-140 -0.00207

 110 <-176 -0.00206

 113 <-175 -0.00214

 115 <-179 -0.00137

 115 <-188 0.00107

 115 <-237 0.00113

 116 <-146 0.00179

 116 <-174 0.00158

 117 <-180 -0.00117

 117 <-189 -0.00125

 118 <-181 0.00117

 118 <-190 -0.00125

 119 <-187 -0.00157

 119 <-191 0.00152

 120 <-140 -0.00141

 120 <-252 -0.00103

 121 <-139 0.00141

 121 <-251 0.00103

 122 <-140 -0.00280

 122 <-148 0.00188

 123 <-139 0.00280

 123 <-147 0.00188

 124 <-159 0.00103

 124 <-188 0.00117

 125 <-264 -0.00103

 126 <-265 0.00103

 127 <-142 0.00405

 127 <-150 -0.00114

 128 <-226 0.00109

 128 <-260 0.00151

 129 <-210 -0.00118

 130 <-143 0.00300

 131 <-140 0.00171

 131 <-144 -0.00236

 131 <-148 0.00221

 131 <-165 -0.00120

 132 <-139 0.00171

 132 <-145 0.00236

 132 <-147 -0.00221

 132 <-164 -0.00120

 133 <-141 -0.00777

 133 <-153 -0.00319

 133 <-274 0.00159

 134 <-141 -0.00315

 134 <-153 0.00292

 135 <-140 0.00599

 135 <-144 0.00351

 135 <-148 0.00500

 136 <-139 -0.00599

 136 <-145 0.00351

 136 <-147 0.00500

 137 <-146 -0.00623

 137 <-269 0.00152

 138 <-142 -0.00270

 138 <-150 0.00289

 Excited State 7: Singlet-E 3.5349 eV 350.75 nm f=0.0016 <S\*\*2>=0.000

 41 ->140 0.00138

 43 ->141 0.00113

 43 ->153 -0.00112

 45 ->140 -0.00202

 45 ->165 -0.00123

 47 ->141 0.00126

 47 ->153 -0.00113

 47 ->168 -0.00134

 48 ->140 0.00123

 48 ->165 0.00124

 68 ->140 0.00325

 70 ->140 -0.00389

 70 ->148 0.00164

 71 ->168 -0.00102

 73 ->164 -0.00103

 78 ->140 0.00253

 78 ->148 -0.00105

 79 ->141 -0.00219

 79 ->153 0.00205

 80 ->142 0.00132

 80 ->150 -0.00219

 81 ->165 0.00101

 82 ->150 -0.00104

 83 ->168 -0.00143

 85 ->139 0.00109

 85 ->145 -0.00208

 85 ->164 0.00337

 86 ->165 0.00111

 88 ->168 -0.00133

 97 ->165 0.00166

 98 ->146 0.00108

 98 ->150 -0.00105

 99 ->153 0.00115

 100 ->140 -0.00281

 100 ->148 0.00130

 102 ->141 0.00154

 103 ->150 0.00115

 106 ->140 -0.00274

 106 ->144 -0.00254

 106 ->165 -0.00323

 108 ->140 -0.00588

 108 ->148 0.00213

 111 ->146 -0.00179

 111 ->150 0.00119

 112 ->141 0.00122

 112 ->143 0.00151

 112 ->153 -0.00186

 112 ->168 -0.00121

 114 ->139 0.00188

 114 ->145 -0.00207

 114 ->147 -0.00148

 114 ->164 0.00126

 115 ->144 0.00213

 115 ->165 0.00241

 119 ->139 -0.00103

 120 ->141 0.01625

 120 ->143 0.00166

 120 ->153 -0.00639

 120 ->168 -0.00180

 120 ->175 -0.00138

 121 ->142 -0.00828

 121 ->150 0.00696

 122 ->141 -0.00896

 122 ->153 0.00331

 123 ->142 0.00458

 123 ->150 -0.00352

 124 ->140 0.00201

 124 ->144 -0.01197

 124 ->148 -0.00560

 124 ->165 -0.01052

 124 ->176 -0.00207

 124 ->267 0.00101

 124 ->327 0.00147

 125 ->141 -0.05259

 125 ->143 -0.00567

 125 ->149 -0.00218

 125 ->153 0.01526

 125 ->168 0.00477

 125 ->175 0.00260

 125 ->315 0.00182

 125 ->316 0.00109

 125 ->337 0.00111

 125 ->338 -0.00134

 126 ->142 0.02883

 126 ->146 0.00566

 126 ->150 -0.02068

 126 ->240 -0.00107

 127 ->139 -0.00224

 128 ->139 -0.10417

 128 ->147 -0.00493

 129 ->139 -0.00464

 129 ->140 0.67681

 129 ->144 0.00138

 129 ->148 -0.02399

 129 ->165 0.00171

 129 ->176 0.00282

 129 ->327 -0.00157

 130 ->139 0.00108

 130 ->140 -0.15767

 130 ->148 0.00436

 131 ->141 0.00394

 132 ->142 0.00125

 132 ->150 -0.00130

 133 ->140 -0.00501

 133 ->144 0.00123

 134 ->140 -0.00859

 134 ->160 -0.00109

 134 ->166 -0.00100

 134 ->185 -0.00105

 135 ->141 -0.00111

 135 ->143 -0.00181

 136 ->142 0.00209

 137 ->139 0.00671

 137 ->145 0.00161

 138 ->139 -0.00305

 138 ->145 -0.00392

 138 ->152 -0.00112

 138 ->186 -0.00101

 48 <-140 0.00105

 68 <-140 0.00113

 120 <-141 -0.00119

 122 <-205 0.00135

 122 <-210 0.00110

 122 <-266 -0.00125

 124 <-140 0.00386

 124 <-144 0.00149

 124 <-165 0.00280

 124 <-176 0.00135

 125 <-141 0.00408

 125 <-143 0.00151

 125 <-153 -0.00308

 125 <-168 -0.00254

 125 <-175 -0.00129

 129 <-140 -0.00520

 129 <-144 -0.00129

 129 <-165 -0.00252

 129 <-176 -0.00130

 130 <-140 0.00137

 134 <-181 -0.00242

 134 <-197 -0.00204

 138 <-139 0.00157

 138 <-180 -0.00194

 138 <-189 0.00117

 138 <-196 -0.00210

 138 <-203 0.00104

 Excited State 8: Singlet-E 3.5349 eV 350.75 nm f=0.0016 <S\*\*2>=0.000

 41 ->139 -0.00138

 42 ->141 0.00113

 42 ->153 -0.00112

 45 ->139 -0.00202

 45 ->164 -0.00123

 46 ->141 0.00126

 46 ->153 -0.00113

 46 ->168 0.00134

 48 ->139 -0.00123

 48 ->164 -0.00124

 68 ->139 0.00325

 70 ->139 -0.00389

 70 ->147 -0.00164

 72 ->168 0.00102

 73 ->165 -0.00103

 78 ->139 0.00253

 78 ->147 0.00105

 79 ->142 -0.00132

 79 ->150 0.00219

 80 ->141 -0.00219

 80 ->153 0.00205

 81 ->164 -0.00101

 82 ->168 0.00143

 83 ->150 0.00104

 85 ->140 0.00109

 85 ->144 0.00208

 85 ->165 0.00337

 86 ->164 0.00111

 87 ->168 -0.00133

 97 ->164 -0.00166

 98 ->153 0.00115

 99 ->146 0.00108

 99 ->150 0.00105

 100 ->139 -0.00281

 100 ->147 -0.00130

 102 ->150 -0.00115

 103 ->141 0.00154

 106 ->139 0.00274

 106 ->145 -0.00254

 106 ->164 0.00323

 108 ->139 -0.00588

 108 ->147 -0.00213

 111 ->141 0.00122

 111 ->143 -0.00151

 111 ->153 -0.00186

 111 ->168 0.00121

 112 ->146 -0.00179

 112 ->150 -0.00119

 114 ->140 0.00188

 114 ->144 0.00207

 114 ->148 0.00148

 114 ->165 0.00126

 115 ->145 0.00213

 115 ->164 -0.00241

 119 ->140 0.00103

 120 ->142 0.00828

 120 ->150 -0.00696

 121 ->141 0.01625

 121 ->143 -0.00166

 121 ->153 -0.00639

 121 ->168 0.00180

 121 ->175 -0.00138

 122 ->142 -0.00458

 122 ->150 0.00352

 123 ->141 -0.00896

 123 ->153 0.00331

 124 ->139 -0.00201

 124 ->145 -0.01197

 124 ->147 -0.00560

 124 ->164 0.01052

 124 ->177 0.00207

 124 ->268 -0.00101

 124 ->328 -0.00147

 125 ->142 -0.02883

 125 ->146 0.00566

 125 ->150 0.02068

 125 ->240 0.00107

 126 ->141 -0.05259

 126 ->143 0.00567

 126 ->149 0.00218

 126 ->153 0.01526

 126 ->168 -0.00477

 126 ->175 0.00260

 126 ->315 -0.00182

 126 ->316 -0.00109

 126 ->337 0.00111

 126 ->338 -0.00134

 127 ->140 -0.00224

 128 ->140 0.10417

 128 ->148 -0.00493

 129 ->139 0.67681

 129 ->140 0.00464

 129 ->145 -0.00138

 129 ->147 0.02399

 129 ->164 0.00171

 129 ->177 0.00282

 129 ->328 -0.00157

 130 ->139 -0.15767

 130 ->140 -0.00108

 130 ->147 -0.00436

 131 ->142 0.00125

 131 ->150 -0.00130

 132 ->141 -0.00394

 133 ->139 0.00501

 133 ->145 0.00123

 134 ->139 0.00859

 134 ->161 -0.00109

 134 ->167 -0.00100

 134 ->186 0.00105

 135 ->142 -0.00209

 136 ->141 -0.00111

 136 ->143 0.00181

 137 ->140 -0.00671

 137 ->144 0.00161

 138 ->140 -0.00305

 138 ->144 0.00392

 138 ->151 -0.00112

 138 ->185 -0.00101

 48 <-139 -0.00105

 68 <-139 0.00113

 121 <-141 -0.00119

 123 <-205 -0.00135

 123 <-210 -0.00110

 123 <-266 0.00125

 124 <-139 -0.00386

 124 <-145 0.00149

 124 <-164 -0.00280

 124 <-177 -0.00135

 126 <-141 0.00408

 126 <-143 -0.00151

 126 <-153 -0.00308

 126 <-168 0.00254

 126 <-175 -0.00129

 129 <-139 -0.00520

 129 <-145 0.00129

 129 <-164 -0.00252

 129 <-177 -0.00130

 130 <-139 0.00137

 134 <-180 0.00242

 134 <-196 0.00204

 138 <-140 0.00157

 138 <-181 -0.00194

 138 <-190 -0.00117

 138 <-197 -0.00210

 138 <-204 -0.00104

 Excited State 9: Singlet-E 3.5458 eV 349.67 nm f=0.0002 <S\*\*2>=0.000

 44 ->139 0.00134

 87 ->142 0.00122

 87 ->150 -0.00106

 88 ->141 0.00108

 89 ->148 -0.00124

 89 ->165 0.00127

 90 ->146 -0.00191

 90 ->150 -0.00112

 91 ->153 0.00193

 93 ->145 0.00110

 93 ->164 -0.00152

 94 ->139 -0.00484

 94 ->147 -0.00273

 95 ->178 0.00106

 104 ->139 0.00180

 104 ->147 0.00132

 105 ->139 -0.00213

 105 ->147 -0.00110

 106 ->140 0.00806

 106 ->144 0.00441

 106 ->165 0.00456

 107 ->140 0.00133

 110 ->141 0.00114

 114 ->145 0.00113

 115 ->140 -0.00188

 116 ->139 -0.00560

 117 ->142 0.00284

 117 ->150 -0.00283

 118 ->141 -0.00437

 118 ->153 0.00229

 118 ->184 0.00123

 119 ->139 0.00626

 119 ->147 0.00171

 120 ->141 -0.02308

 120 ->149 0.00162

 120 ->153 0.00890

 120 ->158 -0.00137

 120 ->175 0.00178

 120 ->184 0.00250

 121 ->142 0.01258

 121 ->146 -0.00214

 121 ->150 -0.01046

 122 ->141 0.00828

 122 ->149 -0.00257

 122 ->153 -0.00336

 122 ->178 -0.00101

 122 ->193 -0.00109

 123 ->142 -0.00426

 123 ->150 0.00326

 124 ->140 -0.00513

 124 ->144 -0.00585

 124 ->148 -0.00181

 124 ->165 -0.00519

 124 ->176 -0.00105

 125 ->141 -0.02562

 125 ->143 -0.00350

 125 ->153 0.00796

 125 ->168 0.00253

 125 ->175 0.00131

 125 ->184 0.00208

 126 ->142 0.01344

 126 ->150 -0.00969

 127 ->139 0.00411

 128 ->139 0.69404

 128 ->145 0.00567

 128 ->147 0.02800

 128 ->164 -0.00346

 128 ->177 0.00221

 128 ->313 -0.00115

 129 ->140 0.10414

 129 ->144 0.00115

 129 ->148 -0.00357

 129 ->165 0.00110

 130 ->140 -0.00632

 130 ->144 -0.00116

 131 ->143 0.00145

 133 ->140 -0.01220

 133 ->148 0.00155

 134 ->140 0.03176

 134 ->181 -0.00110

 135 ->141 0.00113

 135 ->149 0.00255

 135 ->153 -0.00122

 135 ->158 0.00155

 135 ->178 0.00149

 135 ->193 0.00100

 135 ->205 -0.00125

 136 ->146 0.00154

 137 ->139 -0.05251

 137 ->147 -0.00150

 137 ->180 0.00118

 138 ->139 0.00364

 138 ->145 -0.01330

 138 ->147 -0.00322

 106 <-140 0.00101

 106 <-165 -0.00131

 120 <-168 -0.00140

 121 <-142 -0.00194

 121 <-150 0.00178

 124 <-140 0.00125

 125 <-141 0.00127

 128 <-139 -0.00402

 128 <-145 -0.00160

 128 <-164 0.00198

 129 <-140 -0.00128

 134 <-140 -0.00149

 134 <-204 -0.00134

 134 <-233 0.00117

 138 <-139 -0.00244

 138 <-147 -0.00103

 138 <-180 0.00147

 138 <-189 0.00124

 138 <-203 0.00104

 138 <-208 -0.00119

 Excited State 10: Singlet-E 3.5458 eV 349.67 nm f=0.0002 <S\*\*2>=0.000

 44 ->140 0.00134

 87 ->141 0.00108

 88 ->142 -0.00122

 88 ->150 0.00106

 89 ->147 0.00124

 89 ->164 0.00127

 90 ->153 -0.00193

 91 ->146 0.00191

 91 ->150 -0.00112

 93 ->144 0.00110

 93 ->165 0.00152

 94 ->140 -0.00484

 94 ->148 0.00273

 96 ->178 0.00106

 104 ->140 0.00180

 104 ->148 -0.00132

 105 ->140 -0.00213

 105 ->148 0.00110

 106 ->139 0.00806

 106 ->145 -0.00441

 106 ->164 0.00456

 107 ->139 -0.00133

 109 ->141 -0.00114

 114 ->144 0.00113

 115 ->139 -0.00188

 116 ->140 -0.00560

 117 ->141 0.00437

 117 ->153 -0.00229

 117 ->184 0.00123

 118 ->142 0.00284

 118 ->150 -0.00283

 119 ->140 0.00626

 119 ->148 -0.00171

 120 ->142 0.01258

 120 ->146 0.00214

 120 ->150 -0.01046

 121 ->141 0.02308

 121 ->149 0.00162

 121 ->153 -0.00890

 121 ->158 -0.00137

 121 ->175 -0.00178

 121 ->184 0.00250

 122 ->142 -0.00426

 122 ->150 0.00326

 123 ->141 -0.00828

 123 ->149 -0.00257

 123 ->153 0.00336

 123 ->178 -0.00101

 123 ->193 -0.00109

 124 ->139 -0.00513

 124 ->145 0.00585

 124 ->147 0.00181

 124 ->164 -0.00519

 124 ->177 -0.00105

 125 ->142 0.01344

 125 ->150 -0.00969

 126 ->141 0.02562

 126 ->143 -0.00350

 126 ->153 -0.00796

 126 ->168 0.00253

 126 ->175 -0.00131

 126 ->184 0.00208

 127 ->140 -0.00411

 128 ->140 0.69404

 128 ->144 -0.00567

 128 ->148 -0.02800

 128 ->165 -0.00346

 128 ->176 0.00221

 128 ->314 -0.00115

 129 ->139 -0.10414

 129 ->145 0.00115

 129 ->147 -0.00357

 129 ->164 -0.00110

 130 ->139 0.00632

 130 ->145 -0.00116

 132 ->143 -0.00145

 133 ->139 -0.01220

 133 ->147 -0.00155

 134 ->139 0.03176

 134 ->180 -0.00110

 135 ->146 -0.00154

 136 ->141 -0.00113

 136 ->149 0.00255

 136 ->153 0.00122

 136 ->158 0.00155

 136 ->178 0.00149

 136 ->193 0.00100

 136 ->205 -0.00125

 137 ->140 -0.05251

 137 ->148 0.00150

 137 ->181 0.00118

 138 ->140 -0.00364

 138 ->144 -0.01330

 138 ->148 -0.00322

 106 <-139 0.00101

 106 <-164 -0.00131

 120 <-142 -0.00194

 120 <-150 0.00178

 121 <-168 -0.00140

 124 <-139 0.00125

 126 <-141 -0.00127

 128 <-140 -0.00402

 128 <-144 0.00160

 128 <-165 0.00198

 129 <-139 0.00128

 134 <-139 -0.00149

 134 <-203 0.00134

 134 <-234 0.00117

 138 <-140 0.00244

 138 <-148 -0.00103

 138 <-181 -0.00147

 138 <-190 0.00124

 138 <-204 0.00104

 138 <-209 0.00119

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

 Leave Link 914 at Thu Sep 19 00:46:15 2019, MaxMem= 1342177280 cpu: 4801.1

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

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

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

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

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

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

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

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

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

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

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

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

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

 (A2)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

 The electronic state is 1-A1.

 Alpha occ. eigenvalues -- -14.32011 -14.32011 -14.32011 -14.32011 -14.31793

 Alpha occ. eigenvalues -- -14.31793 -14.31793 -14.31793 -10.25157 -10.25157

 Alpha occ. eigenvalues -- -10.25157 -10.25157 -10.25155 -10.25155 -10.25155

 Alpha occ. eigenvalues -- -10.25155 -10.18551 -10.18551 -10.18551 -10.18551

 Alpha occ. eigenvalues -- -10.18505 -10.18505 -10.18505 -10.18504 -10.18260

 Alpha occ. eigenvalues -- -10.18260 -10.18260 -10.18260 -10.18259 -10.18259

 Alpha occ. eigenvalues -- -10.18259 -10.18259 -10.17950 -10.17950 -10.17950

 Alpha occ. eigenvalues -- -10.17950 -10.17901 -10.17901 -10.17901 -10.17901

 Alpha occ. eigenvalues -- -1.00961 -0.99581 -0.99581 -0.96815 -0.94779

 Alpha occ. eigenvalues -- -0.90680 -0.90680 -0.87588 -0.85906 -0.85906

 Alpha occ. eigenvalues -- -0.85878 -0.85865 -0.77861 -0.76408 -0.76408

 Alpha occ. eigenvalues -- -0.76324 -0.75974 -0.75974 -0.75851 -0.75822

 Alpha occ. eigenvalues -- -0.72488 -0.69852 -0.69852 -0.64555 -0.63699

 Alpha occ. eigenvalues -- -0.63169 -0.63169 -0.62826 -0.62482 -0.59981

 Alpha occ. eigenvalues -- -0.59901 -0.59901 -0.58975 -0.58274 -0.57166

 Alpha occ. eigenvalues -- -0.56801 -0.56801 -0.55803 -0.55264 -0.55264

 Alpha occ. eigenvalues -- -0.55112 -0.53535 -0.53535 -0.52648 -0.50638

 Alpha occ. eigenvalues -- -0.49939 -0.48319 -0.48319 -0.47362 -0.46698

 Alpha occ. eigenvalues -- -0.46698 -0.46481 -0.46427 -0.46289 -0.44931

 Alpha occ. eigenvalues -- -0.44931 -0.44615 -0.44245 -0.44245 -0.44226

 Alpha occ. eigenvalues -- -0.43244 -0.42800 -0.42800 -0.42202 -0.42142

 Alpha occ. eigenvalues -- -0.39017 -0.38889 -0.37267 -0.37024 -0.37024

 Alpha occ. eigenvalues -- -0.36971 -0.36971 -0.36828 -0.36285 -0.35655

 Alpha occ. eigenvalues -- -0.35156 -0.35132 -0.35132 -0.34557 -0.33269

 Alpha occ. eigenvalues -- -0.33269 -0.32313 -0.32313 -0.31156 -0.28416

 Alpha occ. eigenvalues -- -0.28416 -0.28320 -0.26889 -0.26762 -0.26404

 Alpha occ. eigenvalues -- -0.26300 -0.26300 -0.25918 -0.25488 -0.25356

 Alpha occ. eigenvalues -- -0.25356 -0.25151 -0.18714

 Alpha virt. eigenvalues -- -0.10700 -0.10700 -0.04736 -0.03494 -0.03009

 Alpha virt. eigenvalues -- -0.02732 -0.02732 0.01845 0.02083 0.02083

 Alpha virt. eigenvalues -- 0.02202 0.04724 0.04866 0.04866 0.05327

 Alpha virt. eigenvalues -- 0.05534 0.06745 0.06745 0.06854 0.06937

 Alpha virt. eigenvalues -- 0.07382 0.08784 0.08784 0.09724 0.10512

 Alpha virt. eigenvalues -- 0.10712 0.10712 0.11804 0.11804 0.12159

 Alpha virt. eigenvalues -- 0.12419 0.14372 0.15107 0.15107 0.16021

 Alpha virt. eigenvalues -- 0.16775 0.17290 0.17381 0.17381 0.18513

 Alpha virt. eigenvalues -- 0.19845 0.20176 0.20176 0.20642 0.21210

 Alpha virt. eigenvalues -- 0.22390 0.22898 0.22898 0.23198 0.23844

 Alpha virt. eigenvalues -- 0.24404 0.24404 0.25235 0.25817 0.26464

 Alpha virt. eigenvalues -- 0.26779 0.26779 0.27231 0.27231 0.28057

 Alpha virt. eigenvalues -- 0.28145 0.28145 0.28251 0.28825 0.29517

 Alpha virt. eigenvalues -- 0.29517 0.30265 0.30368 0.31116 0.32284

 Alpha virt. eigenvalues -- 0.32284 0.33460 0.33578 0.34646 0.34646

 Alpha virt. eigenvalues -- 0.35448 0.35513 0.36297 0.36297 0.37176

 Alpha virt. eigenvalues -- 0.37538 0.38145 0.38248 0.38248 0.38977

 Alpha virt. eigenvalues -- 0.38977 0.39341 0.39901 0.40212 0.40212

 Alpha virt. eigenvalues -- 0.40279 0.40525 0.41057 0.41145 0.41580

 Alpha virt. eigenvalues -- 0.41580 0.42203 0.42203 0.42239 0.42280

 Alpha virt. eigenvalues -- 0.42643 0.42854 0.42935 0.42935 0.43046

 Alpha virt. eigenvalues -- 0.43104 0.43104 0.43255 0.43491 0.43527

 Alpha virt. eigenvalues -- 0.44818 0.44818 0.46232 0.46232 0.46401

 Alpha virt. eigenvalues -- 0.46513 0.46962 0.46962 0.47538 0.47680

 Alpha virt. eigenvalues -- 0.47875 0.49632 0.49643 0.49643 0.50346

 Alpha virt. eigenvalues -- 0.50637 0.50637 0.51129 0.51336 0.51336

 Alpha virt. eigenvalues -- 0.51779 0.51855 0.52870 0.53574 0.53574

 Alpha virt. eigenvalues -- 0.54090 0.54434 0.55224 0.55224 0.56392

 Alpha virt. eigenvalues -- 0.58122 0.59182 0.59182 0.60043 0.60098

 Alpha virt. eigenvalues -- 0.60153 0.60153 0.60208 0.60623 0.60623

 Alpha virt. eigenvalues -- 0.60852 0.61319 0.61319 0.61383 0.62508

 Alpha virt. eigenvalues -- 0.62667 0.62667 0.62814 0.63154 0.64290

 Alpha virt. eigenvalues -- 0.64408 0.64429 0.64471 0.64471 0.65624

 Alpha virt. eigenvalues -- 0.66463 0.66463 0.66818 0.67411 0.67411

 Alpha virt. eigenvalues -- 0.69095 0.69573 0.69573 0.69771 0.70220

 Alpha virt. eigenvalues -- 0.70220 0.70363 0.71507 0.72105 0.73316

 Alpha virt. eigenvalues -- 0.73316 0.73460 0.74088 0.74489 0.74489

 Alpha virt. eigenvalues -- 0.75869 0.76700 0.77134 0.77195 0.77195

 Alpha virt. eigenvalues -- 0.77474 0.77474 0.77541 0.78684 0.79440

 Alpha virt. eigenvalues -- 0.79440 0.79673 0.79763 0.79918 0.81388

 Alpha virt. eigenvalues -- 0.81601 0.81781 0.81781 0.82652 0.83338

 Alpha virt. eigenvalues -- 0.83931 0.83931 0.85036 0.86100 0.86568

 Alpha virt. eigenvalues -- 0.86568 0.86637 0.88119 0.88663 0.88663

 Alpha virt. eigenvalues -- 0.89360 0.90215 0.90215 0.90805 0.90805

 Alpha virt. eigenvalues -- 0.91198 0.91342 0.91342 0.91778 0.93597

 Alpha virt. eigenvalues -- 0.94404 0.95577 0.96911 0.98919 0.98919

 Alpha virt. eigenvalues -- 0.98972 0.99369 0.99369 0.99692 0.99791

 Alpha virt. eigenvalues -- 1.00188 1.01868 1.01868 1.02231 1.02561

 Alpha virt. eigenvalues -- 1.02561 1.05092 1.05230 1.05230 1.06917

 Alpha virt. eigenvalues -- 1.09538 1.10027 1.10027 1.10247 1.10255

 Alpha virt. eigenvalues -- 1.10648 1.11628 1.11738 1.11738 1.13364

 Alpha virt. eigenvalues -- 1.13462 1.14074 1.14074 1.14404 1.14448

 Alpha virt. eigenvalues -- 1.15290 1.15290 1.17975 1.18947 1.20253

 Alpha virt. eigenvalues -- 1.20253 1.20383 1.20495 1.20670 1.20762

 Alpha virt. eigenvalues -- 1.20836 1.20836 1.22673 1.22673 1.25084

 Alpha virt. eigenvalues -- 1.25084 1.25337 1.25896 1.26364 1.26801

 Alpha virt. eigenvalues -- 1.26801 1.27799 1.28262 1.28578 1.28655

 Alpha virt. eigenvalues -- 1.31596 1.32937 1.32937 1.33151 1.34024

 Alpha virt. eigenvalues -- 1.34024 1.35216 1.37862 1.38082 1.40601

 Alpha virt. eigenvalues -- 1.40601 1.40649 1.42072 1.42072 1.42413

 Alpha virt. eigenvalues -- 1.44816 1.44816 1.45182 1.45206 1.45206

 Alpha virt. eigenvalues -- 1.45321 1.48087 1.49368 1.50860 1.50860

 Alpha virt. eigenvalues -- 1.51296 1.52273 1.52283 1.52500 1.52500

 Alpha virt. eigenvalues -- 1.52587 1.53062 1.53062 1.54586 1.55280

 Alpha virt. eigenvalues -- 1.57361 1.57361 1.58808 1.61525 1.61525

 Alpha virt. eigenvalues -- 1.62336 1.62554 1.63044 1.64018 1.65160

 Alpha virt. eigenvalues -- 1.65160 1.65481 1.67347 1.68281 1.68281

 Alpha virt. eigenvalues -- 1.71929 1.71929 1.72134 1.73574 1.73725

 Alpha virt. eigenvalues -- 1.73926 1.74588 1.74588 1.75795 1.76085

 Alpha virt. eigenvalues -- 1.76085 1.79924 1.80627 1.80781 1.80781

 Alpha virt. eigenvalues -- 1.81462 1.81503 1.81788 1.82173 1.82173

 Alpha virt. eigenvalues -- 1.82691 1.83872 1.84075 1.84075 1.86248

 Alpha virt. eigenvalues -- 1.86248 1.86562 1.88597 1.89342 1.90532

 Alpha virt. eigenvalues -- 1.90532 1.90590 1.90637 1.90864 1.90864

 Alpha virt. eigenvalues -- 1.91044 1.91119 1.91329 1.91329 1.92162

 Alpha virt. eigenvalues -- 1.92162 1.92221 1.92760 1.93648 1.94590

 Alpha virt. eigenvalues -- 1.94601 1.94601 1.95182 1.98256 1.98611

 Alpha virt. eigenvalues -- 1.98611 1.99500 2.00458 2.02234 2.02234

 Alpha virt. eigenvalues -- 2.02768 2.03595 2.03652 2.05624 2.05624

 Alpha virt. eigenvalues -- 2.08209 2.10522 2.12875 2.12875 2.15268

 Alpha virt. eigenvalues -- 2.15268 2.18130 2.19177 2.21333 2.22229

 Alpha virt. eigenvalues -- 2.22605 2.23289 2.23289 2.24311 2.25080

 Alpha virt. eigenvalues -- 2.25080 2.25931 2.26808 2.27362 2.27362

 Alpha virt. eigenvalues -- 2.27723 2.27723 2.27878 2.28369 2.28726

 Alpha virt. eigenvalues -- 2.30003 2.30389 2.30447 2.30447 2.32618

 Alpha virt. eigenvalues -- 2.32954 2.32954 2.33554 2.36877 2.38447

 Alpha virt. eigenvalues -- 2.38447 2.39415 2.39493 2.39601 2.39601

 Alpha virt. eigenvalues -- 2.41428 2.43012 2.43012 2.43533 2.44865

 Alpha virt. eigenvalues -- 2.45806 2.48400 2.48400 2.51302 2.52273

 Alpha virt. eigenvalues -- 2.53193 2.53193 2.55029 2.55127 2.55127

 Alpha virt. eigenvalues -- 2.56184 2.56575 2.57798 2.58113 2.58113

 Alpha virt. eigenvalues -- 2.59315 2.60992 2.64100 2.64324 2.64324

 Alpha virt. eigenvalues -- 2.65036 2.65619 2.65619 2.67804 2.68529

 Alpha virt. eigenvalues -- 2.68563 2.68563 2.69939 2.73572 2.74057

 Alpha virt. eigenvalues -- 2.74057 2.74101 2.74794 2.74968 2.74968

 Alpha virt. eigenvalues -- 2.75972 2.77247 2.77620 2.78076 2.78076

 Alpha virt. eigenvalues -- 2.78688 2.78991 2.78991 2.81223 2.81846

 Alpha virt. eigenvalues -- 2.82180 2.82261 2.82261 2.84686 2.84686

 Alpha virt. eigenvalues -- 2.85136 2.86455 2.87824 2.87824 2.88142

 Alpha virt. eigenvalues -- 2.88725 2.91359 2.91382 2.91712 2.91716

 Alpha virt. eigenvalues -- 2.91716 2.96836 2.96836 2.99743 3.03722

 Alpha virt. eigenvalues -- 3.04501 3.04644 3.04644 3.07101 3.09169

 Alpha virt. eigenvalues -- 3.09169 3.15919 3.16775 3.16826 3.16826

 Alpha virt. eigenvalues -- 3.17720 3.18605 3.19086 3.19086 3.19925

 Alpha virt. eigenvalues -- 3.21234 3.22072 3.22675 3.22675 3.25266

 Alpha virt. eigenvalues -- 3.25686 3.25686 3.26838 3.27399 3.27424

 Alpha virt. eigenvalues -- 3.27424 3.27648 3.30005 3.30446 3.30446

 Alpha virt. eigenvalues -- 3.30510 3.31028 3.33012 3.33012 3.35867

 Alpha virt. eigenvalues -- 3.37827 3.39959 3.39959 3.41504 3.45948

 Alpha virt. eigenvalues -- 3.46862 3.46862 3.47565 3.47667 3.48191

 Alpha virt. eigenvalues -- 3.48191 3.49669 3.55443 3.60743 3.60743

 Alpha virt. eigenvalues -- 3.65006 3.65006 3.65012 3.65672 3.72516

 Alpha virt. eigenvalues -- 3.72516 3.73163 3.74018 3.75762 3.76324

 Alpha virt. eigenvalues -- 3.76602 3.76602 3.81925 3.83356 3.83356

 Alpha virt. eigenvalues -- 3.84257 3.86940 3.87945 3.89589 3.89589

 Alpha virt. eigenvalues -- 3.89946 3.95365 3.96186 3.96186 3.97166

 Alpha virt. eigenvalues -- 4.10750 4.11744 4.11744 4.17354 4.17835

 Alpha virt. eigenvalues -- 4.17835 4.20617 4.22966 4.33807 4.39313

 Alpha virt. eigenvalues -- 4.39313 4.40260 4.46145 4.53110 4.53171

 Alpha virt. eigenvalues -- 4.53171 4.78690 4.78832 4.78832 4.79132

 Alpha virt. eigenvalues -- 5.12102 5.12102 5.13221 5.16329 5.20802

 Alpha virt. eigenvalues -- 5.36052 5.36052 5.52397 7.83886 7.86323

 Alpha virt. eigenvalues -- 7.86323 7.89915 8.12600 11.11816 23.27409

 Alpha virt. eigenvalues -- 23.30383 23.30383 23.32110 23.76747 23.79126

 Alpha virt. eigenvalues -- 23.79126 23.79265 23.79482 23.79482 23.79650

 Alpha virt. eigenvalues -- 23.81081 23.88431 23.88431 23.88617 23.89182

 Alpha virt. eigenvalues -- 23.89336 23.89623 23.90011 23.90011 24.03275

 Alpha virt. eigenvalues -- 24.03605 24.03605 24.04220 24.05626 24.05640

 Alpha virt. eigenvalues -- 24.05640 24.05724 24.13932 24.14084 24.14084

 Alpha virt. eigenvalues -- 24.14438 35.56481 35.60200 35.60200 35.61455

 Alpha virt. eigenvalues -- 35.68759 35.69653 35.69653 35.69731

 Condensed to atoms (all electrons):

 Mulliken charges:

 1

 1 C 0.383710

 2 N -0.652760

 3 C 0.383710

 4 C -0.062491

 5 C -0.062491

 6 N -0.400169

 7 C 0.383710

 8 N -0.652760

 9 C 0.383710

 10 C -0.062491

 11 C -0.062491

 12 N -0.400169

 13 C -0.062491

 14 C -0.062491

 15 C 0.383710

 16 N -0.652760

 17 C 0.383710

 18 N -0.400169

 19 N -0.652760

 20 C 0.383710

 21 C -0.062491

 22 C -0.062491

 23 C 0.383710

 24 N -0.400169

 25 Zn 1.408722

 26 C -0.206140

 27 C -0.223613

 28 C -0.223613

 29 C -0.206140

 30 C -0.206140

 31 C -0.223613

 32 C -0.223613

 33 C -0.206140

 34 C -0.206140

 35 C -0.223613

 36 C -0.223613

 37 C -0.206140

 38 C -0.206140

 39 C -0.223613

 40 C -0.223613

 41 C -0.206140

 42 H 0.227431

 43 H 0.227431

 44 H 0.227431

 45 H 0.227431

 46 H 0.227431

 47 H 0.227431

 48 H 0.227431

 49 H 0.227431

 50 H 0.231478

 51 H 0.231478

 52 H 0.231478

 53 H 0.231478

 54 H 0.231478

 55 H 0.231478

 56 H 0.231478

 57 H 0.231478

 Sum of Mulliken charges = -0.00000

 Mulliken charges with hydrogens summed into heavy atoms:

 1

 1 C 0.383710

 2 N -0.652760

 3 C 0.383710

 4 C -0.062491

 5 C -0.062491

 6 N -0.400169

 7 C 0.383710

 8 N -0.652760

 9 C 0.383710

 10 C -0.062491

 11 C -0.062491

 12 N -0.400169

 13 C -0.062491

 14 C -0.062491

 15 C 0.383710

 16 N -0.652760

 17 C 0.383710

 18 N -0.400169

 19 N -0.652760

 20 C 0.383710

 21 C -0.062491

 22 C -0.062491

 23 C 0.383710

 24 N -0.400169

 25 Zn 1.408722

 26 C 0.021290

 27 C 0.007865

 28 C 0.007865

 29 C 0.021290

 30 C 0.021290

 31 C 0.007865

 32 C 0.007865

 33 C 0.021290

 34 C 0.021290

 35 C 0.007865

 36 C 0.007865

 37 C 0.021290

 38 C 0.021290

 39 C 0.007865

 40 C 0.007865

 41 C 0.021290

 Electronic spatial extent (au): <R\*\*2>= 22206.6571

 Charge= -0.0000 electrons

 Dipole moment (field-independent basis, Debye):

 X= -0.0000 Y= -0.0000 Z= 2.4723 Tot= 2.4723

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

 XX= -204.7559 YY= -204.7559 ZZ= -242.3486

 XY= -0.0000 XZ= 0.0000 YZ= 0.0000

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

 XX= 12.5309 YY= 12.5309 ZZ= -25.0618

 XY= -0.0000 XZ= 0.0000 YZ= 0.0000

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

 XXX= -0.0000 YYY= -0.0000 ZZZ= 35.5425 XYY= 0.0000

 XXY= -0.0000 XXZ= -9.0862 XZZ= 0.0000 YZZ= -0.0000

 YYZ= -9.0862 XYZ= 0.0000

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

 XXXX= -13405.8961 YYYY= -13405.8961 ZZZZ= -287.8060 XXXY= 0.0000

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

 ZZZY= 0.0000 XXYY= -3942.6006 XXZZ= -2896.0353 YYZZ= -2896.0353

 XXYZ= -0.0000 YYXZ= -0.0000 ZZXY= 0.0000

 N-N= 4.380949706301D+03 E-N=-1.287661455937D+04 KE= 1.776541638178D+03

 Symmetry A1 KE= 5.103287750189D+02

 Symmetry A2 KE= 3.909478542394D+02

 Symmetry B1 KE= 4.376325044598D+02

 Symmetry B2 KE= 4.376325044598D+02

 Leave Link 601 at Thu Sep 19 00:46:35 2019, MaxMem= 1342177280 cpu: 19.2

 (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\C32H16N8Zn1

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

 nt=dmso,smd) empiricaldispersion=gd3bj IOp(9/40=3)\\ZnPC0td\\0,1\C,0,2

 .766507,1.18235,0.019533\N,0,1.424701,1.424701,0.068191\C,0,1.18235,2.

 766507,0.019533\C,0,2.467721,3.466489,-0.047388\C,0,3.466489,2.467721,

 -0.047388\N,0,0.,3.378152,0.00933\C,0,-1.18235,2.766507,0.019533\N,0,-

 1.424701,1.424701,0.068191\C,0,-2.766507,1.18235,0.019533\C,0,-3.46648

 9,2.467721,-0.047388\C,0,-2.467721,3.466489,-0.047388\N,0,3.378152,0.,

 0.00933\C,0,3.466489,-2.467721,-0.047388\C,0,2.467721,-3.466489,-0.047

 388\C,0,1.18235,-2.766507,0.019533\N,0,1.424701,-1.424701,0.068191\C,0

 ,2.766507,-1.18235,0.019533\N,0,0.,-3.378152,0.00933\N,0,-1.424701,-1.

 424701,0.068191\C,0,-1.18235,-2.766507,0.019533\C,0,-2.467721,-3.46648

 9,-0.047388\C,0,-3.466489,-2.467721,-0.047388\C,0,-2.766507,-1.18235,0

 .019533\N,0,-3.378152,0.,0.00933\Zn,0,0.,0.,0.510466\C,0,4.815847,-2.8

 04179,-0.11201\C,0,5.149164,-4.1562,-0.169185\C,0,4.1562,-5.149164,-0.

 169185\C,0,2.804179,-4.815847,-0.11201\C,0,-4.815847,-2.804179,-0.1120

 1\C,0,-5.149164,-4.1562,-0.169185\C,0,-4.1562,-5.149164,-0.169185\C,0,

 -2.804179,-4.815847,-0.11201\C,0,-2.804179,4.815847,-0.11201\C,0,-4.15

 62,5.149164,-0.169185\C,0,-5.149164,4.1562,-0.169185\C,0,-4.815847,2.8

 04179,-0.11201\C,0,4.815847,2.804179,-0.11201\C,0,5.149164,4.1562,-0.1

 69185\C,0,4.1562,5.149164,-0.169185\C,0,2.804179,4.815847,-0.11201\H,0

 ,5.582686,-2.037386,-0.115625\H,0,2.037386,-5.582686,-0.115625\H,0,-5.

 582686,-2.037386,-0.115625\H,0,-2.037386,-5.582686,-0.115625\H,0,-2.03

 7386,5.582686,-0.115625\H,0,-5.582686,2.037386,-0.115625\H,0,5.582686,

 2.037386,-0.115625\H,0,2.037386,5.582686,-0.115625\H,0,-4.449274,6.192

 416,-0.215654\H,0,-6.192416,4.449274,-0.215654\H,0,4.449274,6.192416,-

 0.215654\H,0,6.192416,4.449274,-0.215654\H,0,6.192416,-4.449274,-0.215

 654\H,0,4.449274,-6.192416,-0.215654\H,0,-4.449274,-6.192416,-0.215654

 \H,0,-6.192416,-4.449274,-0.215654\\Version=ES64L-G09RevE.01\State=1-A

 1\HF=-1733.3896474\RMSD=4.996e-09\PG=C04V [C4(Zn1),2SGV(N2),2SGD(N2),X

 (C32H16)]\\@

 VIRTUE IS LEARNED AT YOUR MOTHER'S KNEE,

 VICES ARE PICKED UP AT SOME OTHER JOINT.

 Job cpu time: 0 days 1 hours 36 minutes 44.4 seconds.

 File lengths (MBytes): RWF= 2402 Int= 0 D2E= 0 Chk= 239 Scr= 1

 Normal termination of Gaussian 09 at Thu Sep 19 00:47:29 2019.