Entering Gaussian System, Link 0=g09

 Initial command:

 /apps/gaussian/g09d01/g09/l1.exe "/srv/scratch/z5105842/Gau-19256.inp" -scrdir="/srv/scratch/z5105842/"

 Entering Link 1 = /apps/gaussian/g09d01/g09/l1.exe PID= 19274.

 Copyright (c) 1988,1990,1992,1993,1995,1998,2003,2009,2013,

 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 D.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-G09RevD.01 24-Apr-2013

 5-Sep-2019

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

 %nprocshared=12

 Will use up to 12 processors via shared memory.

 %mem=10GB

 %chk=TPP0td.chk

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

 #p td(root=1,nstates=10) b3lyp/6-311G\* scrf=(solvent=dmso,smd) empiric

 aldispersion=gd3bj IOp(9/40=3)

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

 1/38=1/1;

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

 3/5=4,6=6,7=1,11=9,16=1,25=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=2,107=1,108=10/1;

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

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

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

 Leave Link 1 at Thu Sep 5 21:44:32 2019, MaxMem= 1342177280 cpu: 0.6

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

 ------

 TPP0td

 ------

 Symbolic Z-matrix:

 Charge = 0 Multiplicity = 1

 C -0.68416 4.23797 0.1734

 C -1.13173 2.88312 0.0404

 N 0. 2.10277 -0.02395

 C 1.13173 2.88312 0.0404

 C 0.68416 4.23797 0.1734

 C 2.45874 2.43876 -0.00975

 C 2.8605 1.09096 -0.06504

 N 2.0397 0. 0.00961

 C 2.8605 -1.09096 -0.06504

 C 4.24999 -0.67741 -0.22258

 C 4.24999 0.67741 -0.22258

 C -2.45874 2.43876 -0.00975

 C -2.8605 1.09096 -0.06504

 C -4.24999 0.67741 -0.22258

 C -4.24999 -0.67741 -0.22258

 C -2.8605 -1.09096 -0.06504

 N -2.0397 0. 0.00961

 C -2.45874 -2.43876 -0.00975

 C -1.13173 -2.88312 0.0404

 C -0.68416 -4.23797 0.1734

 C 0.68416 -4.23797 0.1734

 C 1.13173 -2.88312 0.0404

 N 0. -2.10277 -0.02395

 C 2.45874 -2.43876 -0.00975

 C 3.51916 3.48937 0.00178

 C 3.63978 4.39529 -1.05869

 C 4.63245 5.37237 -1.04642

 C 5.51516 5.4605 0.02908

 C 5.40114 4.56435 1.09112

 C 4.41154 3.58452 1.07644

 C -5.51516 5.4605 0.02908

 C -4.63245 5.37237 -1.04642

 C -3.63978 4.39529 -1.05869

 C -3.51916 3.48937 0.00178

 C -4.41154 3.58452 1.07644

 C -5.40114 4.56435 1.09112

 C 3.51916 -3.48937 0.00178

 C 4.41154 -3.58452 1.07644

 C 5.40114 -4.56435 1.09112

 C 5.51516 -5.4605 0.02908

 C 4.63245 -5.37237 -1.04642

 C 3.63978 -4.39529 -1.05869

 C -3.51916 -3.48937 0.00178

 C -4.41154 -3.58452 1.07644

 C -5.40114 -4.56435 1.09112

 C -5.51516 -5.4605 0.02908

 C -4.63245 -5.37237 -1.04642

 C -3.63978 -4.39529 -1.05869

 H -1.33286 5.0936 0.26959

 H 1.33286 5.0936 0.26959

 H 5.09797 -1.33486 -0.33683

 H 5.09797 1.33486 -0.33683

 H -5.09797 1.33486 -0.33683

 H -5.09797 -1.33486 -0.33683

 H -1.33286 -5.0936 0.26959

 H 1.33286 -5.0936 0.26959

 H 2.95811 4.32551 -1.89933

 H 4.71729 6.06291 -1.87896

 H 6.28725 6.22262 0.03949

 H 6.08164 4.62858 1.93371

 H 4.32232 2.89106 1.90541

 H -6.28725 6.22262 0.03949

 H -4.71729 6.06291 -1.87896

 H -2.95811 4.32551 -1.89933

 H -4.32232 2.89106 1.90541

 H -6.08164 4.62858 1.93371

 H 4.32232 -2.89106 1.90541

 H 6.08164 -4.62858 1.93371

 H 6.28725 -6.22262 0.03949

 H 4.71729 -6.06291 -1.87896

 H 2.95811 -4.32551 -1.89933

 H -4.32232 -2.89106 1.90541

 H -6.08164 -4.62858 1.93371

 H -6.28725 -6.22262 0.03949

 H -4.71729 -6.06291 -1.87896

 H -2.95811 -4.32551 -1.89933

 H 0. 1.09244 -0.08272

 H 0. -1.09244 -0.08272

 NAtoms= 78 NQM= 78 NQMF= 0 NMMI= 0 NMMIF= 0

 NMic= 0 NMicF= 0.

 Isotopes and Nuclear Properties:

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

 in nuclear magnetons)

 Atom 1 2 3 4 5 6 7 8 9 10

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

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

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

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

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

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

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

 Atom 11 12 13 14 15 16 17 18 19 20

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

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

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

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

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

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

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

 Atom 21 22 23 24 25 26 27 28 29 30

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

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

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

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

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

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

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

 Atom 31 32 33 34 35 36 37 38 39 40

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

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

 NucSpn= 0 0 0 0 0 0 0 0 0 0

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

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

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

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

 Atom 41 42 43 44 45 46 47 48 49 50

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

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

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

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

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

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

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

 Atom 51 52 53 54 55 56 57 58 59 60

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

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

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

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

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

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

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

 Atom 61 62 63 64 65 66 67 68 69 70

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

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

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

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

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

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

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

 Atom 71 72 73 74 75 76 77 78

 IAtWgt= 1 1 1 1 1 1 1 1

 AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

 NucSpn= 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

 NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

 NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

 AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

 Leave Link 101 at Thu Sep 5 21:44:33 2019, MaxMem= 1342177280 cpu: 1.4

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

 Stoichiometry C44H30N4

 Framework group C2V[SGV(H2N2),SGV'(N2),X(C44H28)]

 Deg. of freedom 59

 Full point group C2V NOp 4

 Largest Abelian subgroup C2V NOp 4

 Largest concise Abelian subgroup C2V NOp 4

 Standard orientation:

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

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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

 1 6 0 -0.684157 4.237971 0.173400

 2 6 0 -1.131729 2.883123 0.040396

 3 7 0 0.000000 2.102773 -0.023951

 4 6 0 1.131729 2.883123 0.040396

 5 6 0 0.684157 4.237971 0.173400

 6 6 0 2.458736 2.438755 -0.009747

 7 6 0 2.860501 1.090959 -0.065036

 8 7 0 2.039697 0.000000 0.009609

 9 6 0 2.860501 -1.090959 -0.065036

 10 6 0 4.249993 -0.677406 -0.222575

 11 6 0 4.249993 0.677406 -0.222575

 12 6 0 -2.458736 2.438755 -0.009747

 13 6 0 -2.860501 1.090959 -0.065036

 14 6 0 -4.249993 0.677406 -0.222575

 15 6 0 -4.249993 -0.677406 -0.222575

 16 6 0 -2.860501 -1.090959 -0.065036

 17 7 0 -2.039697 0.000000 0.009609

 18 6 0 -2.458736 -2.438755 -0.009747

 19 6 0 -1.131729 -2.883123 0.040396

 20 6 0 -0.684157 -4.237971 0.173400

 21 6 0 0.684157 -4.237971 0.173400

 22 6 0 1.131729 -2.883123 0.040396

 23 7 0 0.000000 -2.102773 -0.023951

 24 6 0 2.458736 -2.438755 -0.009747

 25 6 0 3.519159 3.489365 0.001777

 26 6 0 3.639775 4.395294 -1.058689

 27 6 0 4.632445 5.372370 -1.046425

 28 6 0 5.515158 5.460502 0.029084

 29 6 0 5.401135 4.564352 1.091122

 30 6 0 4.411543 3.584521 1.076438

 31 6 0 -5.515158 5.460502 0.029084

 32 6 0 -4.632445 5.372370 -1.046425

 33 6 0 -3.639775 4.395294 -1.058689

 34 6 0 -3.519159 3.489365 0.001777

 35 6 0 -4.411543 3.584521 1.076438

 36 6 0 -5.401135 4.564352 1.091122

 37 6 0 3.519159 -3.489365 0.001777

 38 6 0 4.411543 -3.584521 1.076438

 39 6 0 5.401135 -4.564352 1.091122

 40 6 0 5.515158 -5.460502 0.029084

 41 6 0 4.632445 -5.372370 -1.046425

 42 6 0 3.639775 -4.395294 -1.058689

 43 6 0 -3.519159 -3.489365 0.001777

 44 6 0 -4.411543 -3.584521 1.076438

 45 6 0 -5.401135 -4.564352 1.091122

 46 6 0 -5.515158 -5.460502 0.029084

 47 6 0 -4.632445 -5.372370 -1.046425

 48 6 0 -3.639775 -4.395294 -1.058689

 49 1 0 -1.332862 5.093596 0.269591

 50 1 0 1.332862 5.093596 0.269591

 51 1 0 5.097972 -1.334858 -0.336827

 52 1 0 5.097972 1.334858 -0.336827

 53 1 0 -5.097972 1.334858 -0.336827

 54 1 0 -5.097972 -1.334858 -0.336827

 55 1 0 -1.332862 -5.093596 0.269591

 56 1 0 1.332862 -5.093596 0.269591

 57 1 0 2.958110 4.325512 -1.899332

 58 1 0 4.717290 6.062914 -1.878958

 59 1 0 6.287254 6.222625 0.039493

 60 1 0 6.081643 4.628576 1.933705

 61 1 0 4.322318 2.891059 1.905414

 62 1 0 -6.287254 6.222625 0.039493

 63 1 0 -4.717290 6.062914 -1.878958

 64 1 0 -2.958110 4.325512 -1.899332

 65 1 0 -4.322318 2.891059 1.905414

 66 1 0 -6.081643 4.628576 1.933705

 67 1 0 4.322318 -2.891059 1.905414

 68 1 0 6.081643 -4.628576 1.933705

 69 1 0 6.287254 -6.222625 0.039493

 70 1 0 4.717290 -6.062914 -1.878958

 71 1 0 2.958110 -4.325512 -1.899332

 72 1 0 -4.322318 -2.891059 1.905414

 73 1 0 -6.081643 -4.628576 1.933705

 74 1 0 -6.287254 -6.222625 0.039493

 75 1 0 -4.717290 -6.062914 -1.878958

 76 1 0 -2.958110 -4.325512 -1.899332

 77 1 0 0.000000 1.092438 -0.082721

 78 1 0 0.000000 -1.092438 -0.082721

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

 Rotational constants (GHZ): 0.0588256 0.0580329 0.0301998

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

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

 Standard basis: 6-311G(d) (5D, 7F)

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

 There are 261 symmetry adapted cartesian basis functions of A1 symmetry.

 There are 240 symmetry adapted cartesian basis functions of A2 symmetry.

 There are 249 symmetry adapted cartesian basis functions of B1 symmetry.

 There are 252 symmetry adapted cartesian basis functions of B2 symmetry.

 There are 248 symmetry adapted basis functions of A1 symmetry.

 There are 229 symmetry adapted basis functions of A2 symmetry.

 There are 237 symmetry adapted basis functions of B1 symmetry.

 There are 240 symmetry adapted basis functions of B2 symmetry.

 954 basis functions, 1686 primitive gaussians, 1002 cartesian basis functions

 161 alpha electrons 161 beta electrons

 nuclear repulsion energy 5359.0290093584 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= 78 NActive= 78 NUniq= 21 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T Big=F

 Integral buffers will be 131072 words long.

 Regular integral format.

 Two-electron integral symmetry is turned on.

 R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2121186179 Hartrees.

 Nuclear repulsion after empirical dispersion term = 5358.8168907404 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= 78.

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

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

 Polarization charges: spherical gaussians, with

 point-specific exponents (IZeta= 3).

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

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

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

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

 GePol: Number of generator spheres = 78

 GePol: Total number of spheres = 78

 GePol: Number of exposed spheres = 78 (100.00%)

 GePol: Number of points = 5698

 GePol: Average weight of points = 0.11

 GePol: Minimum weight of points = 0.11D-07

 GePol: Maximum weight of points = 0.17992

 GePol: Number of points with low weight = 294

 GePol: Fraction of low-weight points (<1% of avg) = 5.16%

 GePol: Cavity surface area = 616.128 Ang\*\*2

 GePol: Cavity volume = 627.764 Ang\*\*3

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

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

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

 PCM non-electrostatic energy = -0.0024210678 Hartrees.

 Nuclear repulsion after PCM non-electrostatic terms = 5358.8144696726 Hartrees.

 Leave Link 301 at Thu Sep 5 21:44:33 2019, MaxMem= 1342177280 cpu: 0.9

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

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

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

 One-electron integrals computed using PRISM.

 One-electron integral symmetry used in STVInt

 NBasis= 954 RedAO= T EigKep= 6.24D-05 NBF= 248 229 237 240

 NBsUse= 954 1.00D-06 EigRej= -1.00D+00 NBFU= 248 229 237 240

 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= 939 939 939 939 940 MxSgAt= 78 MxSgA2= 78.

 Leave Link 302 at Thu Sep 5 21:44:34 2019, MaxMem= 1342177280 cpu: 15.2

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

 Leave Link 308 at Thu Sep 5 21:44:34 2019, MaxMem= 1342177280 cpu: 2.7

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

 DipDrv: MaxL=1.

 Leave Link 303 at Thu Sep 5 21:44:35 2019, MaxMem= 1342177280 cpu: 1.8

 (Enter /apps/gaussian/g09d01/g09/l401.exe)

 ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

 Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

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

 ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

 NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

 wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

 NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

 Petite list used in FoFCou.

 Harris En= -1914.36874352971

 JPrj=0 DoOrth=F DoCkMO=F.

 Initial guess orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

 (A1)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

 (B2) (A1) (B1)

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

 Leave Link 401 at Thu Sep 5 21:44:37 2019, MaxMem= 1342177280 cpu: 23.5

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

 Closed shell SCF:

 Using DIIS extrapolation, IDIIS= 1040.

 Integral symmetry usage will be decided dynamically.

 IVT= 3053902 IEndB= 3053902 NGot= 1342177280 MDV= 1340145025

 LenX= 1340145025 LenY= 1339140019

 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= 480000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2000

 NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

 wScrn= 0.000000 ICntrl= 0 IOpCl= 0 I1Cent= 0 NGrid= 0

 NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

 Petite list used in FoFCou.

 Inv3: Mode=1 IEnd= 97401612.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 1.22D-14 for 432.

 Iteration 1 A\*A^-1 deviation from orthogonality is 4.30D-15 for 3915 438.

 Iteration 1 A^-1\*A deviation from unit magnitude is 8.66D-15 for 5695.

 Iteration 1 A^-1\*A deviation from orthogonality is 3.16D-12 for 3412 3402.

 E= -1913.44228163101

 DIIS: error= 4.86D-02 at cycle 1 NSaved= 1.

 NSaved= 1 IEnMin= 1 EnMin= -1913.44228163101 IErMin= 1 ErrMin= 4.86D-02

 ErrMax= 4.86D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.99D-01 BMatP= 9.99D-01

 IDIUse=3 WtCom= 5.14D-01 WtEn= 4.86D-01

 Coeff-Com: 0.100D+01

 Coeff-En: 0.100D+01

 Coeff: 0.100D+01

 Gap= 0.109 Goal= None Shift= 0.000

 GapD= 0.109 DampG=1.000 DampE=0.500 DampFc=0.5000 IDamp=-1.

 Damping current iteration by 5.00D-01

 RMSDP=1.90D-03 MaxDP=9.81D-02 OVMax= 1.73D-01

 Cycle 2 Pass 1 IDiag 1:

 RMSU= 9.42D-04 CP: 9.81D-01

 E= -1913.90374897476 Delta-E= -0.461467343742 Rises=F Damp=T

 DIIS: error= 7.43D-03 at cycle 2 NSaved= 2.

 NSaved= 2 IEnMin= 2 EnMin= -1913.90374897476 IErMin= 2 ErrMin= 7.43D-03

 ErrMax= 7.43D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.28D-02 BMatP= 9.99D-01

 IDIUse=3 WtCom= 9.26D-01 WtEn= 7.43D-02

 Coeff-Com: -0.678D-01 0.107D+01

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

 Coeff: -0.628D-01 0.106D+01

 Gap= 0.107 Goal= None Shift= 0.000

 RMSDP=4.82D-04 MaxDP=2.09D-02 DE=-4.61D-01 OVMax= 1.05D-01

 Cycle 3 Pass 1 IDiag 1:

 RMSU= 4.76D-04 CP: 9.78D-01 9.25D-01

 E= -1914.34221588728 Delta-E= -0.438466912528 Rises=F Damp=F

 DIIS: error= 7.49D-03 at cycle 3 NSaved= 3.

 NSaved= 3 IEnMin= 3 EnMin= -1914.34221588728 IErMin= 2 ErrMin= 7.43D-03

 ErrMax= 7.49D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.31D-02 BMatP= 6.28D-02

 IDIUse=3 WtCom= 9.25D-01 WtEn= 7.49D-02

 Coeff-Com: -0.911D-01 0.508D+00 0.583D+00

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

 Coeff: -0.843D-01 0.470D+00 0.614D+00

 Gap= 0.100 Goal= None Shift= 0.000

 RMSDP=3.12D-04 MaxDP=1.50D-02 DE=-4.38D-01 OVMax= 5.64D-02

 Cycle 4 Pass 1 IDiag 1:

 RMSU= 2.02D-04 CP: 9.81D-01 1.05D+00 5.65D-01

 E= -1914.37356060637 Delta-E= -0.031344719083 Rises=F Damp=F

 DIIS: error= 3.93D-03 at cycle 4 NSaved= 4.

 NSaved= 4 IEnMin= 4 EnMin= -1914.37356060637 IErMin= 4 ErrMin= 3.93D-03

 ErrMax= 3.93D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.11D-02 BMatP= 4.31D-02

 IDIUse=3 WtCom= 9.61D-01 WtEn= 3.93D-02

 Coeff-Com: -0.428D-01 0.155D+00 0.375D+00 0.513D+00

 Coeff-En: 0.000D+00 0.000D+00 0.218D+00 0.782D+00

 Coeff: -0.411D-01 0.149D+00 0.369D+00 0.524D+00

 Gap= 0.098 Goal= None Shift= 0.000

 RMSDP=1.47D-04 MaxDP=8.05D-03 DE=-3.13D-02 OVMax= 2.53D-02

 Cycle 5 Pass 1 IDiag 1:

 RMSU= 7.97D-05 CP: 9.78D-01 1.01D+00 6.63D-01 4.65D-01

 E= -1914.38405543154 Delta-E= -0.010494825171 Rises=F Damp=F

 DIIS: error= 1.06D-03 at cycle 5 NSaved= 5.

 NSaved= 5 IEnMin= 5 EnMin= -1914.38405543154 IErMin= 5 ErrMin= 1.06D-03

 ErrMax= 1.06D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.55D-04 BMatP= 1.11D-02

 IDIUse=3 WtCom= 9.89D-01 WtEn= 1.06D-02

 Coeff-Com: -0.161D-01 0.408D-01 0.154D+00 0.293D+00 0.528D+00

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

 Coeff: -0.160D-01 0.404D-01 0.152D+00 0.290D+00 0.533D+00

 Gap= 0.097 Goal= None Shift= 0.000

 RMSDP=4.40D-05 MaxDP=2.84D-03 DE=-1.05D-02 OVMax= 9.53D-03

 Cycle 6 Pass 1 IDiag 1:

 RMSU= 1.91D-05 CP: 9.78D-01 1.03D+00 6.80D-01 5.41D-01 5.76D-01

 E= -1914.38472900454 Delta-E= -0.000673573007 Rises=F Damp=F

 DIIS: error= 3.47D-04 at cycle 6 NSaved= 6.

 NSaved= 6 IEnMin= 6 EnMin= -1914.38472900454 IErMin= 6 ErrMin= 3.47D-04

 ErrMax= 3.47D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.28D-05 BMatP= 7.55D-04

 IDIUse=3 WtCom= 9.97D-01 WtEn= 3.47D-03

 Coeff-Com: -0.538D-02 0.106D-01 0.519D-01 0.114D+00 0.295D+00 0.534D+00

 Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.320D-02 0.997D+00

 Coeff: -0.536D-02 0.106D-01 0.518D-01 0.114D+00 0.294D+00 0.535D+00

 Gap= 0.098 Goal= None Shift= 0.000

 RMSDP=1.02D-05 MaxDP=6.96D-04 DE=-6.74D-04 OVMax= 2.95D-03

 Cycle 7 Pass 1 IDiag 1:

 RMSU= 4.87D-06 CP: 9.78D-01 1.02D+00 6.81D-01 5.36D-01 6.43D-01

 CP: 6.55D-01

 E= -1914.38478665171 Delta-E= -0.000057647169 Rises=F Damp=F

 DIIS: error= 9.79D-05 at cycle 7 NSaved= 7.

 NSaved= 7 IEnMin= 7 EnMin= -1914.38478665171 IErMin= 7 ErrMin= 9.79D-05

 ErrMax= 9.79D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.08D-06 BMatP= 6.28D-05

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

 Coeff-Com: -0.196D-02 0.316D-02 0.189D-01 0.449D-01 0.132D+00 0.304D+00

 Coeff-Com: 0.499D+00

 Coeff: -0.196D-02 0.316D-02 0.189D-01 0.449D-01 0.132D+00 0.304D+00

 Coeff: 0.499D+00

 Gap= 0.098 Goal= None Shift= 0.000

 RMSDP=2.70D-06 MaxDP=1.23D-04 DE=-5.76D-05 OVMax= 6.03D-04

 Cycle 8 Pass 1 IDiag 1:

 RMSU= 1.41D-06 CP: 9.78D-01 1.02D+00 6.81D-01 5.40D-01 6.39D-01

 CP: 6.82D-01 6.01D-01

 E= -1914.38479113620 Delta-E= -0.000004484486 Rises=F Damp=F

 DIIS: error= 2.05D-05 at cycle 8 NSaved= 8.

 NSaved= 8 IEnMin= 8 EnMin= -1914.38479113620 IErMin= 8 ErrMin= 2.05D-05

 ErrMax= 2.05D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.81D-07 BMatP= 5.08D-06

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

 Coeff-Com: -0.606D-04-0.134D-03 0.800D-03 0.284D-02 0.144D-01 0.530D-01

 Coeff-Com: 0.186D+00 0.743D+00

 Coeff: -0.606D-04-0.134D-03 0.800D-03 0.284D-02 0.144D-01 0.530D-01

 Coeff: 0.186D+00 0.743D+00

 Gap= 0.098 Goal= None Shift= 0.000

 RMSDP=6.00D-07 MaxDP=3.07D-05 DE=-4.48D-06 OVMax= 1.09D-04

 Cycle 9 Pass 1 IDiag 1:

 RMSU= 3.80D-07 CP: 9.78D-01 1.02D+00 6.81D-01 5.40D-01 6.42D-01

 CP: 6.85D-01 6.43D-01 8.24D-01

 E= -1914.38479125946 Delta-E= -0.000000123259 Rises=F Damp=F

 DIIS: error= 9.90D-06 at cycle 9 NSaved= 9.

 NSaved= 9 IEnMin= 9 EnMin= -1914.38479125946 IErMin= 9 ErrMin= 9.90D-06

 ErrMax= 9.90D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.17D-08 BMatP= 1.81D-07

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

 Coeff-Com: 0.773D-04-0.246D-03-0.635D-03-0.115D-02 0.194D-03 0.115D-01

 Coeff-Com: 0.704D-01 0.417D+00 0.503D+00

 Coeff: 0.773D-04-0.246D-03-0.635D-03-0.115D-02 0.194D-03 0.115D-01

 Coeff: 0.704D-01 0.417D+00 0.503D+00

 Gap= 0.098 Goal= None Shift= 0.000

 RMSDP=2.03D-07 MaxDP=1.06D-05 DE=-1.23D-07 OVMax= 3.77D-05

 Cycle 10 Pass 1 IDiag 1:

 RMSU= 1.23D-07 CP: 9.78D-01 1.02D+00 6.81D-01 5.40D-01 6.42D-01

 CP: 6.87D-01 6.48D-01 8.70D-01 6.66D-01

 E= -1914.38479130081 Delta-E= -0.000000041348 Rises=F Damp=F

 DIIS: error= 1.31D-06 at cycle 10 NSaved= 10.

 NSaved=10 IEnMin=10 EnMin= -1914.38479130081 IErMin=10 ErrMin= 1.31D-06

 ErrMax= 1.31D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.28D-09 BMatP= 4.17D-08

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

 Coeff-Com: 0.325D-04-0.773D-04-0.296D-03-0.733D-03-0.104D-02 0.691D-03

 Coeff-Com: 0.111D-01 0.105D+00 0.189D+00 0.697D+00

 Coeff: 0.325D-04-0.773D-04-0.296D-03-0.733D-03-0.104D-02 0.691D-03

 Coeff: 0.111D-01 0.105D+00 0.189D+00 0.697D+00

 Gap= 0.098 Goal= None Shift= 0.000

 RMSDP=4.61D-08 MaxDP=2.17D-06 DE=-4.13D-08 OVMax= 7.31D-06

 Cycle 11 Pass 1 IDiag 1:

 RMSU= 3.13D-08 CP: 9.78D-01 1.02D+00 6.81D-01 5.40D-01 6.42D-01

 CP: 6.87D-01 6.50D-01 8.75D-01 7.18D-01 8.75D-01

 E= -1914.38479130166 Delta-E= -0.000000000849 Rises=F Damp=F

 DIIS: error= 8.46D-07 at cycle 11 NSaved= 11.

 NSaved=11 IEnMin=11 EnMin= -1914.38479130166 IErMin=11 ErrMin= 8.46D-07

 ErrMax= 8.46D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.31D-10 BMatP= 1.28D-09

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

 Coeff-Com: 0.973D-05-0.170D-04-0.962D-04-0.302D-03-0.597D-03-0.854D-03

 Coeff-Com: -0.207D-02 0.131D-01 0.507D-01 0.398D+00 0.542D+00

 Coeff: 0.973D-05-0.170D-04-0.962D-04-0.302D-03-0.597D-03-0.854D-03

 Coeff: -0.207D-02 0.131D-01 0.507D-01 0.398D+00 0.542D+00

 Gap= 0.098 Goal= None Shift= 0.000

 RMSDP=1.88D-08 MaxDP=9.46D-07 DE=-8.49D-10 OVMax= 3.25D-06

 Cycle 12 Pass 1 IDiag 1:

 RMSU= 8.86D-09 CP: 9.78D-01 1.02D+00 6.81D-01 5.40D-01 6.42D-01

 CP: 6.88D-01 6.49D-01 8.80D-01 7.19D-01 9.21D-01

 CP: 6.79D-01

 E= -1914.38479130229 Delta-E= -0.000000000628 Rises=F Damp=F

 DIIS: error= 9.74D-08 at cycle 12 NSaved= 12.

 NSaved=12 IEnMin=12 EnMin= -1914.38479130229 IErMin=12 ErrMin= 9.74D-08

 ErrMax= 9.74D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.36D-12 BMatP= 3.31D-10

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

 Coeff-Com: 0.107D-05-0.906D-06-0.132D-04-0.535D-04-0.114D-03-0.288D-03

 Coeff-Com: -0.116D-02-0.120D-02 0.390D-02 0.631D-01 0.156D+00 0.780D+00

 Coeff: 0.107D-05-0.906D-06-0.132D-04-0.535D-04-0.114D-03-0.288D-03

 Coeff: -0.116D-02-0.120D-02 0.390D-02 0.631D-01 0.156D+00 0.780D+00

 Gap= 0.098 Goal= None Shift= 0.000

 RMSDP=3.69D-09 MaxDP=4.10D-07 DE=-6.28D-10 OVMax= 7.76D-07

 Error on total polarization charges = 0.08279

 SCF Done: E(RB3LYP) = -1914.38479130 A.U. after 12 cycles

 NFock= 12 Conv=0.37D-08 -V/T= 2.0042

 KE= 1.906418097378D+03 PE=-1.516735648768D+04 EE= 5.987739129331D+03

 SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.52

 (included in total energy above)

 Leave Link 502 at Thu Sep 5 21:47:32 2019, MaxMem= 1342177280 cpu: 2036.1

 (Enter /apps/gaussian/g09d01/g09/l801.exe)

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

 ExpMin= 1.03D-01 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

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

 ICtDFT= 12500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

 Largest valence mixing into a core orbital is 4.90D-05

 Largest core mixing into a valence orbital is 2.05D-05

 Range of M.O.s used for correlation: 49 954

 NBasis= 954 NAE= 161 NBE= 161 NFC= 48 NFV= 0

 NROrb= 906 NOA= 113 NOB= 113 NVA= 793 NVB= 793

 \*\*\*\* Warning!!: The largest alpha MO coefficient is 0.10218176D+02

 \*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.97758902D-01

 Leave Link 801 at Thu Sep 5 21:47:33 2019, MaxMem= 1342177280 cpu: 4.0

 (Enter /apps/gaussian/g09d01/g09/l914.exe)

 RHF ground state

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

 Would need an additional 128354500000 words for in-memory AO integral storage.

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

 Inv3: Mode=1 IEnd= 97401612.

 Iteration 1 A\*A^-1 deviation from unit magnitude is 9.33D-15 for 1390.

 Iteration 1 A\*A^-1 deviation from orthogonality is 4.33D-15 for 4531 1414.

 Iteration 1 A^-1\*A deviation from unit magnitude is 8.99D-15 for 900.

 Iteration 1 A^-1\*A deviation from orthogonality is 2.85D-15 for 2136 1051.

 Making orbital integer symmetry assigments:

 Orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

 (A1)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

 (B2) (A1) (B1)

 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: 179218

 Iteration 1 Dimension 40 NMult 0 NNew 40

 CISAX will form 40 AO SS matrices at one time.

 NMat= 40 NSing= 40 JSym2X=-1.

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

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

 New state 3 was old state 4

 New state 4 was old state 5

 New state 5 was old state 3

 New state 6 was old state 7

 New state 7 was old state 10

 New state 8 was old state 9

 New state 9 was old state 8

 New state 10 was old state 12

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.281882846027917

 Root 2 : 2.542139353552912

 Root 3 : 3.439344384081407

 Root 4 : 3.545326077686738

 Root 5 : 3.554914899641028

 Root 6 : 3.712899815358504

 Root 7 : 3.763944339753410

 Root 8 : 3.792419498781949

 Root 9 : 3.793999110633338

 Root 10 : 3.799719545829973

 Root 11 : 3.811545174524036

 Root 12 : 3.845832351236136

 Root 13 : 3.856746171120057

 Root 14 : 3.881363286016283

 Root 15 : 3.952779368520527

 Root 16 : 3.958027834030462

 Root 17 : 3.963206047085432

 Root 18 : 3.980224717731598

 Root 19 : 3.988614479965933

 Root 20 : 4.027186743984631

 Root 21 : 4.040140549260506

 Root 22 : 4.045650629349651

 Root 23 : 4.073684360077699

 Root 24 : 4.111551747548791

 Root 25 : 4.155825904619658

 Root 26 : 4.222884437945212

 Root 27 : 4.262676320640339

 Root 28 : 4.280409187334236

 Root 29 : 4.305271052247103

 Root 30 : 4.383471781791887

 Root 31 : 4.425506834234395

 Root 32 : 4.455357730241539

 Root 33 : 4.517616476072424

 Root 34 : 4.529494351485790

 Root 35 : 4.537633705176518

 Root 36 : 4.567203977005707

 Root 37 : 4.595495917978345

 Root 38 : 4.613798786149834

 Root 39 : 4.641172226573226

 Root 40 : 4.744467368892649

 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 0.038413891666237

 Root 2 not converged, maximum delta is 0.051370199731832

 Root 3 not converged, maximum delta is 0.144376874019650

 New state 4 was old state 5

 Root 4 not converged, maximum delta is 0.151020064549954

 New state 5 was old state 4

 Root 5 not converged, maximum delta is 0.041617537091344

 Root 6 not converged, maximum delta is 0.208301465003569

 New state 7 was old state 9

 Root 7 not converged, maximum delta is 0.276322320072069

 Root 8 not converged, maximum delta is 0.288747010470206

 New state 9 was old state 7

 Root 9 not converged, maximum delta is 0.126055708918905

 Root 10 not converged, maximum delta is 0.119137319083588

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.138895452576175 Change is -0.142987393451742

 Root 2 : 2.276013309490355 Change is -0.266126044062558

 Root 3 : 3.051593061047751 Change is -0.387751323033655

 Root 4 : 3.094495091815169 Change is -0.460419807825859

 Root 5 : 3.356603269713296 Change is -0.188722807973442

 Root 6 : 3.511427861355289 Change is -0.201471954003215

 Root 7 : 3.609086069752045 Change is -0.184913040881292

 Root 8 : 3.669628765557476 Change is -0.122790733224473

 Root 9 : 3.729931428142065 Change is -0.034012911611345

 Root 10 : 3.759701365705830 Change is -0.040018180124143

 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 0.005713248916644

 Root 2 not converged, maximum delta is 0.006000904488782

 Root 3 not converged, maximum delta is 0.019308020383729

 Root 4 not converged, maximum delta is 0.011195836274974

 Root 5 not converged, maximum delta is 0.021238105346059

 Root 6 not converged, maximum delta is 0.022732410273574

 New state 7 was old state 8

 Root 7 not converged, maximum delta is 0.328141763096228

 New state 8 was old state 7

 Root 8 not converged, maximum delta is 0.039096652004294

 Root 9 not converged, maximum delta is 0.016632071307167

 No map to state 10

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.129069611771939 Change is -0.009825840804236

 Root 2 : 2.264653156175020 Change is -0.011360153315334

 Root 3 : 3.025570614812454 Change is -0.026022446235297

 Root 4 : 3.062979924536678 Change is -0.031515167278491

 Root 5 : 3.350532495432520 Change is -0.006070774280776

 Root 6 : 3.496600163928238 Change is -0.014827697427051

 Root 7 : 3.586914263975268 Change is -0.082714501582208

 Root 8 : 3.599501267489476 Change is -0.009584802262569

 Root 9 : 3.727040978064051 Change is -0.002890450078014

 Root 10 : 3.739890589640454

 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 0.003090970144515

 Root 2 not converged, maximum delta is 0.002721127412310

 Root 3 not converged, maximum delta is 0.004489187609046

 Root 4 not converged, maximum delta is 0.007042070114274

 Root 5 not converged, maximum delta is 0.003233070180699

 Root 6 not converged, maximum delta is 0.004508394645966

 Root 7 not converged, maximum delta is 0.076599779406088

 Root 8 not converged, maximum delta is 0.007787759969459

 New state 9 was old state 10

 Root 9 not converged, maximum delta is 0.077594733683599

 New state 10 was old state 9

 Root 10 not converged, maximum delta is 0.010086362909318

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.127789219549580 Change is -0.001280392222360

 Root 2 : 2.263132827165948 Change is -0.001520329009072

 Root 3 : 3.022057403683315 Change is -0.003513211129140

 Root 4 : 3.058926833810305 Change is -0.004053090726373

 Root 5 : 3.349628194081226 Change is -0.000904301351295

 Root 6 : 3.494848614595938 Change is -0.001751549332301

 Root 7 : 3.569819946370251 Change is -0.017094317605017

 Root 8 : 3.597700650057823 Change is -0.001800617431653

 Root 9 : 3.717500419496045 Change is -0.022390170144409

 Root 10 : 3.726498684436079 Change is -0.000542293627972

 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 0.001816721237704

 Root 4 has converged.

 Root 5 has converged.

 Root 6 has converged.

 Root 7 not converged, maximum delta is 0.011049556840326

 Root 8 not converged, maximum delta is 0.001194135785670

 Root 9 not converged, maximum delta is 0.009782817084614

 Root 10 not converged, maximum delta is 0.004181492410070

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.127701633439234 Change is -0.000087586110346

 Root 2 : 2.263019832932872 Change is -0.000112994233076

 Root 3 : 3.021607385944005 Change is -0.000450017739309

 Root 4 : 3.058582660576322 Change is -0.000344173233983

 Root 5 : 3.349507163201091 Change is -0.000121030880134

 Root 6 : 3.494688725955580 Change is -0.000159888640358

 Root 7 : 3.567251700101594 Change is -0.002568246268657

 Root 8 : 3.597469819507925 Change is -0.000230830549898

 Root 9 : 3.714946128365510 Change is -0.002554291130535

 Root 10 : 3.726434671102353 Change is -0.000064013333727

 Iteration 6 Dimension 130 NMult 120 NNew 10

 CISAX will form 10 AO SS matrices at one time.

 NMat= 10 NSing= 10 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 0.001370018443181

 Root 8 has converged.

 Root 9 not converged, maximum delta is 0.002167223114673

 Root 10 not converged, maximum delta is 0.002537715072375

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.127701540753341 Change is -0.000000092685893

 Root 2 : 2.263018634349008 Change is -0.000001198583864

 Root 3 : 3.021582553510585 Change is -0.000024832433420

 Root 4 : 3.058580644785156 Change is -0.000002015791166

 Root 5 : 3.349506651949390 Change is -0.000000511251701

 Root 6 : 3.494687601538981 Change is -0.000001124416598

 Root 7 : 3.566866541817229 Change is -0.000385158284366

 Root 8 : 3.597447653472669 Change is -0.000022166035256

 Root 9 : 3.714617436688497 Change is -0.000328691677013

 Root 10 : 3.726421611234748 Change is -0.000013059867604

 Iteration 7 Dimension 136 NMult 130 NNew 6

 CISAX will form 6 AO SS matrices at one time.

 NMat= 6 NSing= 6 JSym2X=-1.

 Root 1 has converged.

 Root 2 has converged.

 Root 3 has converged.

 Root 4 has converged.

 Root 5 has converged.

 Root 6 has converged.

 Root 7 has converged.

 Root 8 has converged.

 Root 9 has converged.

 Root 10 not converged, maximum delta is 0.001226200890871

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.127701540753341 Change is 0.000000000000000

 Root 2 : 2.263018634349044 Change is 0.000000000000036

 Root 3 : 3.021582553510585 Change is 0.000000000000000

 Root 4 : 3.058580644785129 Change is -0.000000000000027

 Root 5 : 3.349506492403938 Change is -0.000000159545453

 Root 6 : 3.494687601539098 Change is 0.000000000000117

 Root 7 : 3.566830724969183 Change is -0.000035816848045

 Root 8 : 3.597447653472600 Change is -0.000000000000069

 Root 9 : 3.714585606034346 Change is -0.000031830654151

 Root 10 : 3.726418485212985 Change is -0.000003126021763

 Iteration 8 Dimension 138 NMult 136 NNew 2

 CISAX will form 2 AO SS matrices at one time.

 NMat= 2 NSing= 2 JSym2X=-1.

 Root 1 has converged.

 Root 2 has converged.

 Root 3 has converged.

 Root 4 has converged.

 Root 5 has converged.

 Root 6 has converged.

 Root 7 has converged.

 Root 8 has converged.

 Root 9 has converged.

 Root 10 has converged.

 Excitation Energies [eV] at current iteration:

 Root 1 : 2.127701540753418 Change is 0.000000000000077

 Root 2 : 2.263018634349153 Change is 0.000000000000109

 Root 3 : 3.021582553510531 Change is -0.000000000000054

 Root 4 : 3.058580644784995 Change is -0.000000000000134

 Root 5 : 3.349505619549675 Change is -0.000000872854262

 Root 6 : 3.494687601539122 Change is 0.000000000000023

 Root 7 : 3.566830724969275 Change is 0.000000000000092

 Root 8 : 3.597447653472646 Change is 0.000000000000046

 Root 9 : 3.714585606034301 Change is -0.000000000000045

 Root 10 : 3.726417998899535 Change is -0.000000486313451

 Convergence achieved on expansion vectors.

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

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

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

 1PDM for each excited state written to RWF 633

 Ground to excited state transition densities written to RWF 633

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

 state X Y Z Dip. S. Osc.

 1 0.0000 1.0834 0.0000 1.1737 0.0612

 2 -1.0900 0.0000 0.0000 1.1880 0.0659

 3 0.0000 -4.4422 0.0000 19.7330 1.4608

 4 -4.8670 0.0000 0.0000 23.6876 1.7750

 5 0.0000 0.0000 0.0000 0.0000 0.0000

 6 0.0000 2.1493 0.0000 4.6193 0.3955

 7 0.0000 0.0000 -0.0006 0.0000 0.0000

 8 -0.7455 0.0000 0.0000 0.5558 0.0490

 9 0.0000 0.0000 -0.0197 0.0004 0.0000

 10 0.0000 0.0000 0.0000 0.0000 0.0000

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

 state X Y Z Dip. S. Osc.

 1 0.0000 -0.0799 0.0000 0.0064 0.0545

 2 0.0879 0.0000 0.0000 0.0077 0.0619

 3 0.0000 0.4811 0.0000 0.2314 1.3896

 4 0.5389 0.0000 0.0000 0.2904 1.7222

 5 0.0000 0.0000 0.0000 0.0000 0.0000

 6 0.0000 -0.2741 0.0000 0.0751 0.3899

 7 0.0000 0.0000 0.0002 0.0000 0.0000

 8 0.0976 0.0000 0.0000 0.0095 0.0480

 9 0.0000 0.0000 0.0033 0.0000 0.0001

 10 0.0000 0.0000 0.0000 0.0000 0.0000

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

 state X Y Z

 1 0.0302 0.0000 0.0000

 2 0.0000 -0.0170 0.0000

 3 0.0332 0.0000 0.0000

 4 0.0000 0.0557 0.0000

 5 0.0000 0.0000 -1.8480

 6 -0.1214 0.0000 0.0000

 7 0.0000 0.0000 0.0000

 8 0.0000 -0.1241 0.0000

 9 0.0000 0.0000 0.0000

 10 0.0000 0.0000 0.2592

 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 0.0340

 2 0.0000 0.0000 0.0000 0.0000 0.0604 0.0000

 3 0.0000 0.0000 0.0000 0.0000 0.0000 0.0465

 4 0.0000 0.0000 0.0000 0.0000 -0.0343 0.0000

 5 0.0000 0.0000 0.0000 -0.0239 0.0000 0.0000

 6 0.0000 0.0000 0.0000 0.0000 0.0000 0.0251

 7 0.0147 -0.0087 -0.0076 0.0000 0.0000 0.0000

 8 0.0000 0.0000 0.0000 0.0000 0.0156 0.0000

 9 -0.6391 -1.0593 -0.0422 0.0000 0.0000 0.0000

 10 0.0000 0.0000 0.0000 1.0968 0.0000 0.0000

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

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

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

 1 0.0000 0.0000 0.0000 0.0000 90.00

 2 0.0000 0.0000 0.0000 0.0000 90.00

 3 0.0000 0.0000 0.0000 0.0000 90.00

 4 0.0000 0.0000 0.0000 0.0000 90.00

 5 0.0000 0.0000 0.0000 0.0000 90.00

 6 0.0000 0.0000 0.0000 0.0000 90.00

 7 0.0000 0.0000 0.0000 0.0000 90.00

 8 0.0000 0.0000 0.0000 0.0000 90.00

 9 0.0000 0.0000 0.0000 0.0000 90.00

 10 0.0000 0.0000 0.0000 0.0000 90.00

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

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

 state XX YY ZZ R(length)

 1 0.0000 0.0000 0.0000 0.0000

 2 0.0000 0.0000 0.0000 0.0000

 3 0.0000 0.0000 0.0000 0.0000

 4 0.0000 0.0000 0.0000 0.0000

 5 0.0000 0.0000 0.0000 0.0000

 6 0.0000 0.0000 0.0000 0.0000

 7 0.0000 0.0000 0.0000 0.0000

 8 0.0000 0.0000 0.0000 0.0000

 9 0.0000 0.0000 0.0000 0.0000

 10 0.0000 0.0000 0.0000 0.0000

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

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

 1 0.0000 -0.0866 0.0000 0.0866 0.0577

 2 -0.0958 0.0000 0.0000 0.0958 0.0639

 3 0.0000 -2.1371 0.0000 2.1371 1.4247

 4 -2.6226 0.0000 0.0000 2.6226 1.7484

 5 0.0000 0.0000 0.0000 0.0000 0.0000

 6 0.0000 -0.5890 0.0000 0.5890 0.3927

 7 0.0000 0.0000 0.0000 0.0000 0.0000

 8 -0.0727 0.0000 0.0000 0.0727 0.0485

 9 0.0000 0.0000 -0.0001 0.0001 0.0000

 10 0.0000 0.0000 0.0000 0.0000 0.0000

 Excitation energies and oscillator strengths:

 Excited State 1: Singlet-B2 2.1277 eV 582.71 nm f=0.0612 <S\*\*2>=0.000

 59 ->219 0.00132

 62 ->224 0.00136

 72 ->216 -0.00116

 72 ->220 -0.00140

 73 ->224 -0.00139

 74 ->217 -0.00145

 74 ->221 0.00104

 74 ->249 -0.00148

 74 ->266 0.00135

 75 ->219 -0.00130

 75 ->229 -0.00120

 75 ->306 0.00134

 75 ->313 0.00102

 76 ->220 -0.00102

 76 ->232 0.00106

 77 ->312 -0.00116

 84 ->257 -0.00129

 85 ->195 0.00157

 87 ->215 -0.00104

 87 ->312 0.00172

 87 ->317 -0.00146

 87 ->342 -0.00114

 87 ->387 -0.00130

 88 ->217 0.00131

 89 ->220 0.00193

 92 ->332 -0.00169

 92 ->339 0.00120

 97 ->178 -0.00102

 97 ->220 0.00145

 98 ->217 0.00163

 98 ->332 -0.00144

 98 ->339 0.00105

 99 ->222 -0.00110

 100 ->215 -0.00101

 101 ->163 0.00138

 101 ->243 -0.00124

 101 ->307 -0.00129

 102 ->162 -0.00222

 102 ->174 0.00102

 102 ->194 0.00190

 103 ->173 -0.00114

 104 ->164 0.00204

 104 ->189 0.00108

 105 ->165 -0.00101

 105 ->190 -0.00105

 106 ->164 -0.00135

 106 ->221 -0.00102

 107 ->163 -0.00195

 107 ->307 -0.00122

 109 ->163 0.00137

 109 ->250 -0.00151

 109 ->252 -0.00113

 111 ->162 -0.00345

 111 ->194 0.00124

 113 ->215 -0.00116

 114 ->165 -0.00110

 114 ->222 0.00129

 115 ->221 0.00212

 116 ->164 0.00144

 116 ->185 -0.00110

 119 ->162 0.00139

 119 ->182 0.00109

 120 ->183 -0.00114

 121 ->216 0.00105

 121 ->220 0.00149

 121 ->250 -0.00161

 121 ->307 -0.00118

 122 ->164 0.00428

 122 ->189 0.00158

 122 ->249 -0.00111

 123 ->164 0.00590

 123 ->169 0.00208

 123 ->185 0.00106

 123 ->189 0.00237

 123 ->214 -0.00127

 124 ->165 0.00123

 124 ->229 0.00120

 124 ->306 -0.00115

 125 ->163 0.00112

 125 ->167 -0.00140

 125 ->220 0.00139

 126 ->162 -0.00925

 126 ->171 -0.00110

 126 ->174 0.00246

 126 ->194 0.00304

 126 ->211 -0.00143

 127 ->162 0.00116

 127 ->215 -0.00105

 127 ->218 -0.00106

 127 ->312 0.00144

 127 ->317 -0.00108

 128 ->163 0.00140

 129 ->269 -0.00134

 129 ->332 -0.00114

 130 ->165 0.00125

 131 ->162 0.00134

 131 ->166 -0.00124

 132 ->169 -0.00113

 133 ->210 0.00112

 133 ->229 0.00135

 134 ->163 -0.00320

 135 ->192 0.00143

 135 ->211 0.00111

 135 ->215 0.00136

 136 ->163 -0.00591

 136 ->196 0.00137

 137 ->179 0.00107

 137 ->191 -0.00110

 137 ->221 -0.00239

 138 ->173 0.00148

 138 ->197 -0.00103

 140 ->162 -0.00134

 140 ->194 -0.00110

 141 ->165 -0.00166

 141 ->190 -0.00122

 141 ->197 -0.00105

 141 ->210 -0.00111

 141 ->322 -0.00109

 142 ->167 -0.00156

 142 ->178 0.00101

 142 ->193 0.00112

 142 ->216 0.00102

 142 ->220 0.00144

 142 ->232 0.00217

 142 ->250 -0.00161

 143 ->163 0.01435

 143 ->167 0.00199

 143 ->175 -0.00168

 143 ->204 0.00133

 143 ->212 0.00147

 144 ->164 0.00799

 144 ->169 0.00120

 144 ->180 -0.00103

 145 ->165 0.00156

 145 ->170 -0.00408

 145 ->173 -0.01539

 145 ->195 -0.00197

 145 ->197 0.00324

 145 ->201 0.00337

 145 ->210 -0.00320

 145 ->262 -0.00112

 146 ->164 0.00106

 146 ->217 -0.00201

 146 ->231 0.00119

 146 ->249 0.00101

 147 ->162 -0.00639

 147 ->174 -0.00156

 147 ->194 -0.00110

 147 ->215 0.00108

 147 ->218 0.00186

 147 ->230 0.00226

 147 ->265 0.00136

 148 ->162 0.00777

 148 ->166 0.00207

 148 ->174 0.00641

 148 ->194 0.00414

 148 ->203 -0.00113

 148 ->211 -0.00156

 149 ->165 0.00144

 149 ->170 -0.00143

 149 ->173 -0.00689

 149 ->197 0.00164

 149 ->210 -0.00126

 150 ->162 -0.00326

 150 ->166 0.00388

 150 ->171 0.00146

 150 ->174 0.00222

 150 ->194 0.00196

 150 ->203 -0.00114

 151 ->163 -0.01065

 151 ->167 -0.00188

 151 ->172 0.00167

 151 ->175 0.00126

 152 ->164 0.00130

 152 ->168 -0.00261

 153 ->162 -0.01019

 153 ->166 -0.00111

 153 ->171 0.00178

 154 ->165 0.00230

 154 ->170 0.00225

 154 ->173 -0.00246

 155 ->167 -0.00541

 155 ->172 -0.00148

 155 ->175 0.00111

 155 ->196 -0.00105

 156 ->164 -0.01022

 156 ->168 -0.00125

 156 ->169 0.00379

 156 ->189 -0.00127

 156 ->202 0.00110

 157 ->165 -0.00423

 157 ->170 -0.00256

 157 ->173 -0.00969

 157 ->210 -0.00145

 157 ->229 0.00131

 158 ->162 -0.04186

 158 ->166 -0.00338

 158 ->171 -0.00294

 159 ->164 0.02090

 159 ->168 -0.00230

 159 ->169 0.00354

 159 ->180 -0.00212

 159 ->189 0.00208

 160 ->163 0.38051

 160 ->167 0.00436

 160 ->172 0.00744

 160 ->175 -0.01040

 160 ->178 0.00213

 160 ->196 -0.00320

 160 ->204 0.00198

 160 ->212 0.00259

 160 ->243 0.00128

 161 ->162 0.59382

 161 ->166 0.00266

 161 ->171 0.00398

 161 ->174 0.00996

 161 ->194 0.00633

 161 ->203 -0.00216

 161 ->211 -0.00399

 161 ->215 0.00129

 161 ->258 0.00166

 161 ->327 0.00125

 161 ->340 0.00106

 59 <-219 0.00113

 62 <-224 0.00116

 72 <-220 -0.00120

 73 <-224 -0.00117

 74 <-217 -0.00120

 74 <-249 -0.00128

 74 <-266 0.00117

 75 <-219 -0.00106

 75 <-229 -0.00103

 75 <-306 0.00117

 77 <-312 -0.00101

 84 <-257 -0.00108

 85 <-195 0.00123

 87 <-312 0.00151

 87 <-317 -0.00125

 87 <-387 -0.00114

 88 <-217 0.00107

 89 <-220 0.00155

 92 <-332 -0.00146

 92 <-339 0.00103

 97 <-220 0.00115

 98 <-217 0.00127

 98 <-332 -0.00123

 101 <-307 -0.00107

 102 <-162 -0.00182

 102 <-194 0.00157

 104 <-164 0.00161

 107 <-163 -0.00114

 107 <-307 -0.00101

 109 <-250 -0.00122

 111 <-162 -0.00169

 111 <-194 0.00128

 114 <-222 0.00102

 115 <-221 0.00162

 116 <-164 0.00103

 121 <-220 0.00115

 121 <-250 -0.00129

 122 <-164 0.00250

 122 <-189 0.00112

 123 <-164 0.00344

 123 <-169 0.00123

 123 <-189 0.00167

 125 <-220 0.00109

 126 <-162 -0.00368

 126 <-194 0.00177

 127 <-312 0.00117

 129 <-269 -0.00106

 133 <-229 0.00101

 134 <-163 -0.00186

 136 <-163 -0.00322

 136 <-196 0.00139

 137 <-221 -0.00175

 142 <-220 0.00110

 142 <-232 0.00165

 142 <-250 -0.00125

 143 <-163 0.00789

 143 <-196 -0.00163

 143 <-204 0.00129

 143 <-212 0.00149

 144 <-164 -0.00191

 144 <-180 -0.00109

 145 <-170 -0.00118

 145 <-173 -0.00486

 145 <-195 -0.00143

 145 <-197 0.00276

 145 <-201 0.00262

 145 <-210 -0.00250

 146 <-217 -0.00142

 147 <-162 -0.00233

 147 <-218 0.00132

 147 <-230 0.00166

 147 <-265 0.00105

 148 <-162 0.00653

 148 <-166 0.00102

 148 <-174 0.00384

 148 <-194 0.00228

 149 <-173 -0.00487

 150 <-162 -0.00160

 150 <-166 0.00165

 151 <-163 -0.00310

 153 <-171 0.00107

 154 <-165 0.00101

 154 <-173 -0.00119

 155 <-163 -0.00130

 155 <-167 -0.00193

 156 <-169 0.00190

 157 <-165 -0.00183

 157 <-173 -0.00228

 157 <-210 -0.00125

 158 <-162 -0.00289

 158 <-166 -0.00116

 160 <-163 0.03853

 160 <-167 0.00157

 160 <-172 0.00264

 160 <-175 -0.00517

 160 <-178 0.00112

 160 <-196 -0.00266

 160 <-204 0.00133

 160 <-212 0.00230

 161 <-162 -0.00630

 161 <-174 0.00364

 161 <-194 0.00387

 161 <-203 -0.00174

 161 <-211 -0.00237

 161 <-258 0.00145

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

 Total Energy, E(TD-HF/TD-KS) = -1914.30659971

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

 Excited State 2: Singlet-B1 2.2630 eV 547.87 nm f=0.0659 <S\*\*2>=0.000

 51 ->222 -0.00108

 51 ->229 0.00103

 52 ->216 -0.00111

 52 ->228 0.00100

 53 ->224 0.00112

 57 ->224 0.00152

 57 ->256 0.00129

 57 ->263 0.00118

 58 ->219 0.00180

 58 ->225 -0.00138

 58 ->254 0.00119

 58 ->264 -0.00139

 59 ->217 0.00129

 59 ->249 0.00131

 59 ->266 -0.00131

 59 ->277 0.00111

 60 ->220 -0.00126

 62 ->232 0.00129

 62 ->274 0.00126

 64 ->220 -0.00116

 72 ->224 -0.00121

 73 ->220 0.00143

 73 ->232 -0.00127

 73 ->274 -0.00130

 74 ->229 0.00203

 74 ->306 -0.00133

 74 ->313 -0.00120

 74 ->396 -0.00107

 75 ->217 -0.00131

 75 ->231 0.00106

 75 ->239 -0.00116

 75 ->249 -0.00147

 75 ->266 0.00137

 75 ->267 0.00112

 75 ->269 0.00111

 75 ->289 -0.00105

 76 ->224 0.00116

 76 ->227 -0.00124

 84 ->227 -0.00128

 84 ->256 0.00144

 84 ->312 -0.00116

 87 ->167 -0.00114

 87 ->228 0.00103

 87 ->252 -0.00136

 87 ->307 0.00168

 87 ->314 0.00158

 87 ->321 0.00113

 87 ->341 0.00160

 88 ->222 0.00113

 89 ->224 -0.00136

 90 ->217 -0.00112

 90 ->231 0.00101

 90 ->277 0.00157

 91 ->199 -0.00127

 91 ->224 -0.00162

 91 ->230 0.00103

 91 ->304 0.00105

 92 ->253 0.00103

 92 ->306 -0.00112

 93 ->269 0.00120

 93 ->332 0.00142

 93 ->339 -0.00122

 95 ->188 -0.00120

 95 ->195 0.00136

 95 ->219 -0.00105

 96 ->184 -0.00115

 96 ->187 -0.00115

 96 ->193 0.00104

 96 ->220 0.00111

 96 ->250 -0.00109

 97 ->177 0.00150

 97 ->224 -0.00164

 97 ->227 0.00119

 98 ->165 0.00114

 98 ->176 -0.00113

 98 ->188 -0.00108

 98 ->195 0.00134

 98 ->210 0.00113

 98 ->219 0.00171

 98 ->229 0.00102

 98 ->306 -0.00108

 99 ->179 0.00109

 99 ->217 -0.00261

 99 ->231 0.00105

 99 ->332 -0.00208

 99 ->339 0.00133

 100 ->216 0.00119

 100 ->333 -0.00126

 101 ->162 0.00144

 101 ->230 -0.00178

 101 ->237 -0.00231

 101 ->312 -0.00104

 101 ->317 0.00127

 101 ->342 0.00173

 101 ->362 0.00124

 101 ->387 0.00145

 102 ->163 -0.00347

 102 ->196 0.00292

 102 ->212 -0.00155

 103 ->164 -0.00330

 103 ->189 -0.00215

 104 ->197 -0.00137

 105 ->164 0.00132

 105 ->217 0.00160

 105 ->221 -0.00105

 105 ->231 -0.00110

 105 ->332 0.00163

 106 ->165 0.00127

 106 ->197 0.00122

 106 ->219 0.00116

 107 ->162 -0.00190

 107 ->166 0.00121

 107 ->224 -0.00104

 107 ->237 -0.00124

 107 ->247 0.00142

 109 ->162 0.00144

 109 ->224 -0.00127

 109 ->230 0.00199

 109 ->309 0.00127

 109 ->312 0.00141

 109 ->317 -0.00156

 109 ->342 -0.00180

 109 ->362 -0.00114

 109 ->387 -0.00101

 111 ->163 -0.00630

 111 ->196 0.00300

 111 ->204 -0.00127

 111 ->212 -0.00199

 111 ->243 -0.00106

 112 ->164 -0.00468

 112 ->168 0.00110

 112 ->180 0.00142

 112 ->189 -0.00292

 112 ->214 0.00150

 113 ->178 0.00109

 113 ->216 0.00143

 113 ->220 0.00200

 113 ->228 -0.00106

 113 ->333 -0.00140

 114 ->217 0.00104

 114 ->221 -0.00241

 114 ->269 -0.00151

 114 ->335 -0.00135

 115 ->165 -0.00114

 115 ->219 -0.00160

 115 ->253 -0.00108

 115 ->322 0.00140

 116 ->183 0.00142

 117 ->186 -0.00145

 118 ->184 0.00146

 118 ->220 0.00144

 119 ->163 0.00227

 119 ->187 -0.00140

 119 ->196 -0.00104

 120 ->164 0.00138

 120 ->185 0.00192

 121 ->199 -0.00110

 121 ->224 -0.00131

 121 ->227 0.00188

 121 ->237 -0.00137

 121 ->247 0.00140

 121 ->309 0.00109

 121 ->312 0.00148

 121 ->317 -0.00101

 122 ->181 0.00117

 122 ->197 -0.00143

 122 ->210 0.00150

 122 ->242 -0.00100

 122 ->301 0.00133

 123 ->197 -0.00252

 123 ->201 -0.00141

 123 ->210 0.00117

 124 ->231 0.00239

 124 ->249 0.00117

 124 ->303 -0.00100

 124 ->332 -0.00115

 124 ->339 0.00105

 125 ->218 0.00138

 125 ->224 -0.00138

 125 ->230 0.00128

 125 ->317 -0.00107

 126 ->196 0.00113

 127 ->243 0.00102

 127 ->250 -0.00183

 127 ->261 -0.00105

 127 ->274 -0.00119

 127 ->307 0.00115

 127 ->321 0.00141

 127 ->341 0.00137

 127 ->344 0.00125

 128 ->162 0.00154

 128 ->166 -0.00171

 128 ->256 -0.00104

 128 ->265 -0.00129

 128 ->304 -0.00103

 129 ->181 0.00102

 129 ->222 -0.00134

 129 ->242 -0.00116

 129 ->251 0.00110

 129 ->264 0.00111

 129 ->306 -0.00131

 129 ->313 -0.00145

 129 ->354 0.00130

 129 ->396 -0.00110

 130 ->164 -0.00115

 130 ->169 0.00108

 130 ->217 0.00148

 130 ->269 -0.00141

 130 ->277 -0.00169

 131 ->163 0.00197

 131 ->167 -0.00118

 131 ->250 -0.00104

 132 ->165 -0.00117

 132 ->188 -0.00106

 132 ->229 0.00112

 133 ->164 0.00106

 133 ->202 -0.00103

 133 ->269 -0.00118

 133 ->277 -0.00150

 133 ->332 -0.00153

 133 ->339 0.00130

 134 ->162 -0.00398

 134 ->199 -0.00103

 134 ->211 -0.00201

 134 ->237 0.00106

 134 ->312 0.00119

 134 ->317 -0.00148

 134 ->342 -0.00102

 135 ->178 -0.00114

 135 ->193 -0.00173

 135 ->216 -0.00192

 135 ->232 -0.00144

 136 ->162 -0.00650

 136 ->194 0.00258

 137 ->176 0.00102

 137 ->190 -0.00169

 137 ->213 0.00144

 137 ->242 -0.00129

 137 ->251 -0.00138

 137 ->301 0.00125

 137 ->322 -0.00103

 138 ->164 0.00105

 138 ->189 0.00122

 138 ->221 0.00144

 138 ->231 0.00108

 139 ->197 0.00178

 140 ->196 -0.00149

 141 ->179 0.00116

 141 ->191 -0.00120

 141 ->221 -0.00215

 141 ->231 -0.00153

 141 ->236 -0.00129

 142 ->166 0.00140

 142 ->177 -0.00126

 142 ->192 -0.00146

 142 ->218 0.00140

 142 ->230 0.00158

 142 ->237 -0.00255

 142 ->247 0.00198

 143 ->162 0.01912

 143 ->166 0.00150

 143 ->174 -0.00133

 143 ->194 -0.00336

 143 ->203 0.00187

 143 ->211 0.00220

 144 ->170 0.00370

 144 ->173 0.00955

 144 ->195 -0.00215

 144 ->197 0.00498

 144 ->201 0.00410

 144 ->210 -0.00380

 144 ->213 -0.00154

 144 ->262 -0.00108

 144 ->328 0.00103

 144 ->343 -0.00103

 145 ->180 0.00178

 145 ->189 -0.00116

 145 ->209 -0.00103

 145 ->214 0.00107

 145 ->487 -0.00104

 146 ->165 0.00128

 146 ->181 -0.00317

 146 ->188 0.00203

 146 ->190 0.00159

 146 ->195 -0.00506

 146 ->197 -0.00194

 146 ->210 0.00135

 146 ->229 0.00248

 146 ->238 0.00141

 146 ->242 0.00145

 146 ->245 0.00166

 146 ->251 -0.00114

 146 ->262 -0.00111

 146 ->264 0.00119

 146 ->271 -0.00143

 146 ->306 -0.00135

 146 ->354 -0.00201

 146 ->360 -0.00110

 146 ->385 -0.00132

 146 ->463 -0.00120

 147 ->163 0.00254

 147 ->184 0.00130

 147 ->216 0.00207

 147 ->228 0.00213

 147 ->252 -0.00149

 147 ->257 0.00187

 147 ->307 0.00213

 147 ->333 -0.00126

 147 ->341 -0.00153

 147 ->359 -0.00113

 147 ->407 -0.00125

 148 ->163 -0.01481

 148 ->167 -0.00171

 148 ->175 -0.00459

 148 ->178 0.00138

 149 ->164 -0.00383

 149 ->169 -0.00347

 149 ->180 -0.00348

 149 ->189 0.00240

 149 ->214 -0.00104

 150 ->163 0.00415

 150 ->167 0.00505

 150 ->172 0.00153

 150 ->175 -0.00319

 150 ->187 -0.00106

 150 ->193 0.00108

 150 ->196 0.00399

 150 ->204 -0.00204

 150 ->212 -0.00190

 151 ->162 0.00727

 151 ->166 0.00182

 151 ->171 -0.00254

 151 ->174 0.00181

 152 ->165 0.00234

 152 ->170 -0.00328

 152 ->173 -0.00157

 153 ->163 0.00155

 153 ->172 -0.00326

 153 ->175 -0.00258

 153 ->196 0.00127

 154 ->164 -0.00100

 154 ->168 0.00203

 154 ->169 0.00137

 154 ->180 -0.00193

 154 ->198 0.00117

 155 ->162 -0.00670

 155 ->166 -0.00626

 155 ->171 -0.00108

 155 ->199 0.00140

 156 ->165 0.00559

 156 ->170 -0.00140

 156 ->173 -0.00672

 156 ->197 -0.00173

 156 ->210 0.00176

 156 ->213 0.00105

 156 ->229 -0.00171

 157 ->164 0.01048

 157 ->168 0.00416

 157 ->169 -0.00246

 157 ->180 0.00196

 157 ->202 -0.00123

 158 ->163 0.01909

 158 ->167 0.00104

 158 ->175 -0.00626

 158 ->178 0.00202

 158 ->196 0.00709

 158 ->204 -0.00249

 158 ->212 -0.00443

 158 ->259 -0.00120

 158 ->261 -0.00116

 159 ->165 -0.00299

 159 ->173 -0.00708

 159 ->195 0.00130

 159 ->197 -0.00424

 159 ->201 -0.00270

 159 ->210 0.00263

 159 ->213 0.00133

 160 ->162 -0.40857

 160 ->166 -0.00241

 160 ->171 -0.00481

 160 ->174 -0.01028

 160 ->177 -0.00116

 160 ->194 0.00362

 160 ->203 -0.00119

 160 ->211 -0.00183

 161 ->163 0.57587

 161 ->175 -0.00441

 161 ->178 0.00132

 161 ->196 0.00637

 161 ->204 -0.00280

 161 ->207 0.00108

 161 ->212 -0.00514

 161 ->259 -0.00121

 161 ->261 -0.00142

 161 ->326 -0.00156

 161 ->388 -0.00128

 57 <-224 0.00132

 57 <-256 0.00112

 57 <-263 0.00103

 58 <-219 0.00156

 58 <-225 -0.00119

 58 <-254 0.00104

 58 <-264 -0.00121

 59 <-217 0.00109

 59 <-249 0.00114

 59 <-266 -0.00114

 60 <-220 -0.00107

 62 <-232 0.00111

 62 <-274 0.00111

 72 <-224 -0.00101

 73 <-220 0.00119

 73 <-232 -0.00109

 73 <-274 -0.00116

 74 <-229 0.00167

 74 <-306 -0.00111

 74 <-313 -0.00100

 75 <-217 -0.00106

 75 <-249 -0.00125

 75 <-266 0.00117

 76 <-227 -0.00101

 84 <-227 -0.00104

 84 <-256 0.00124

 87 <-252 -0.00111

 87 <-307 0.00140

 87 <-314 0.00138

 87 <-341 0.00136

 89 <-224 -0.00108

 90 <-277 0.00133

 91 <-224 -0.00129

 93 <-332 0.00121

 93 <-339 -0.00103

 95 <-195 0.00100

 97 <-177 0.00106

 97 <-224 -0.00130

 98 <-219 0.00136

 99 <-217 -0.00199

 99 <-332 -0.00175

 99 <-339 0.00112

 100 <-333 -0.00105

 101 <-230 -0.00140

 101 <-237 -0.00180

 101 <-317 0.00106

 101 <-342 0.00146

 101 <-362 0.00106

 101 <-387 0.00124

 102 <-163 -0.00249

 102 <-196 0.00234

 102 <-212 -0.00128

 103 <-164 -0.00247

 103 <-189 -0.00171

 104 <-197 -0.00116

 105 <-217 0.00120

 105 <-332 0.00136

 107 <-162 -0.00124

 107 <-237 -0.00101

 107 <-247 0.00110

 109 <-230 0.00153

 109 <-309 0.00106

 109 <-312 0.00117

 109 <-317 -0.00127

 109 <-342 -0.00152

 111 <-163 -0.00312

 111 <-196 0.00244

 111 <-204 -0.00103

 111 <-212 -0.00168

 112 <-164 -0.00282

 112 <-180 0.00143

 112 <-189 -0.00224

 112 <-214 0.00119

 113 <-216 0.00108

 113 <-220 0.00152

 113 <-333 -0.00116

 114 <-221 -0.00182

 114 <-269 -0.00122

 114 <-335 -0.00112

 115 <-219 -0.00124

 115 <-322 0.00116

 118 <-220 0.00109

 120 <-185 0.00132

 121 <-224 -0.00101

 121 <-227 0.00143

 121 <-237 -0.00106

 121 <-247 0.00109

 121 <-312 0.00120

 122 <-197 -0.00130

 122 <-210 0.00126

 122 <-301 0.00107

 123 <-197 -0.00225

 123 <-201 -0.00132

 123 <-210 0.00114

 124 <-231 0.00181

 125 <-218 0.00101

 125 <-224 -0.00106

 126 <-175 -0.00130

 126 <-196 0.00148

 127 <-250 -0.00140

 127 <-321 0.00116

 127 <-341 0.00113

 127 <-344 0.00104

 128 <-166 -0.00100

 128 <-265 -0.00103

 129 <-222 -0.00101

 129 <-306 -0.00108

 129 <-313 -0.00118

 129 <-354 0.00107

 130 <-217 0.00109

 130 <-269 -0.00114

 130 <-277 -0.00136

 133 <-277 -0.00121

 133 <-332 -0.00127

 133 <-339 0.00107

 134 <-162 -0.00204

 134 <-211 -0.00148

 134 <-317 -0.00121

 135 <-193 -0.00112

 135 <-216 -0.00134

 135 <-232 -0.00107

 136 <-162 -0.00360

 136 <-174 0.00112

 136 <-194 0.00224

 137 <-190 -0.00109

 137 <-251 -0.00104

 138 <-164 0.00114

 138 <-221 0.00101

 139 <-197 0.00124

 141 <-221 -0.00153

 141 <-231 -0.00112

 142 <-230 0.00114

 142 <-237 -0.00191

 142 <-247 0.00149

 143 <-162 0.01006

 143 <-174 -0.00313

 143 <-194 -0.00363

 143 <-203 0.00164

 143 <-211 0.00194

 144 <-170 0.00105

 144 <-173 0.00156

 144 <-195 -0.00165

 144 <-197 0.00367

 144 <-201 0.00304

 144 <-210 -0.00282

 144 <-213 -0.00110

 145 <-164 -0.00733

 145 <-169 -0.00115

 145 <-180 0.00149

 145 <-189 -0.00160

 146 <-181 -0.00185

 146 <-188 0.00124

 146 <-195 -0.00310

 146 <-197 -0.00129

 146 <-229 0.00175

 146 <-238 0.00103

 146 <-242 0.00105

 146 <-245 0.00121

 146 <-271 -0.00111

 146 <-306 -0.00106

 146 <-354 -0.00164

 146 <-385 -0.00110

 146 <-463 -0.00103

 147 <-216 0.00137

 147 <-228 0.00151

 147 <-252 -0.00109

 147 <-257 0.00140

 147 <-307 0.00165

 147 <-333 -0.00101

 147 <-341 -0.00124

 147 <-407 -0.00102

 148 <-175 -0.00355

 149 <-169 -0.00130

 149 <-180 -0.00221

 149 <-189 0.00212

 150 <-167 0.00201

 150 <-175 -0.00172

 150 <-196 0.00238

 150 <-204 -0.00128

 150 <-212 -0.00113

 151 <-162 0.00175

 152 <-170 -0.00128

 152 <-173 -0.00132

 153 <-163 0.00221

 153 <-172 -0.00101

 153 <-175 -0.00214

 153 <-196 0.00103

 154 <-180 -0.00120

 155 <-162 -0.00333

 155 <-166 -0.00189

 156 <-165 0.00168

 156 <-173 -0.00144

 156 <-197 -0.00134

 156 <-210 0.00135

 156 <-229 -0.00121

 157 <-164 -0.00254

 157 <-168 0.00183

 157 <-169 -0.00186

 157 <-180 0.00141

 158 <-163 0.00785

 158 <-175 -0.00426

 158 <-178 0.00129

 158 <-196 0.00466

 158 <-204 -0.00158

 158 <-212 -0.00296

 159 <-173 -0.00690

 159 <-197 -0.00237

 159 <-201 -0.00144

 159 <-210 0.00148

 160 <-162 -0.02339

 160 <-171 -0.00121

 160 <-174 -0.00572

 160 <-194 0.00255

 160 <-211 -0.00148

 161 <-163 -0.01646

 161 <-172 -0.00143

 161 <-196 0.00335

 161 <-204 -0.00206

 161 <-212 -0.00273

 161 <-259 -0.00108

 161 <-261 -0.00113

 161 <-326 -0.00128

 161 <-388 -0.00111

 Excited State 3: Singlet-B2 3.0216 eV 410.33 nm f=1.4608 <S\*\*2>=0.000

 57 ->216 -0.00112

 58 ->217 -0.00118

 59 ->213 0.00116

 61 ->195 -0.00157

 62 ->215 0.00149

 63 ->221 0.00120

 64 ->199 0.00115

 64 ->256 -0.00102

 70 ->231 0.00106

 74 ->277 0.00122

 75 ->213 -0.00155

 75 ->229 -0.00128

 76 ->193 -0.00101

 76 ->216 -0.00116

 76 ->252 -0.00108

 76 ->259 -0.00101

 77 ->162 -0.00153

 77 ->182 -0.00104

 77 ->218 0.00155

 78 ->198 0.00121

 78 ->217 0.00104

 78 ->249 -0.00106

 79 ->181 0.00101

 79 ->213 -0.00119

 80 ->172 0.00109

 81 ->182 -0.00286

 81 ->186 0.00182

 81 ->192 0.00164

 81 ->218 0.00247

 81 ->227 -0.00249

 81 ->230 0.00137

 81 ->248 0.00120

 81 ->263 -0.00123

 82 ->198 0.00132

 82 ->249 -0.00105

 82 ->277 0.00108

 83 ->165 -0.00147

 83 ->181 0.00321

 83 ->188 -0.00161

 83 ->190 -0.00186

 83 ->195 0.00185

 83 ->246 -0.00150

 84 ->200 0.00248

 84 ->220 0.00130

 84 ->274 -0.00120

 84 ->321 0.00118

 85 ->176 0.00269

 85 ->181 -0.00540

 85 ->188 0.00201

 85 ->190 0.00105

 85 ->195 -0.00303

 85 ->197 -0.00109

 85 ->210 -0.00112

 85 ->213 0.00227

 85 ->246 0.00132

 86 ->166 -0.00123

 86 ->182 -0.00106

 86 ->227 -0.00101

 87 ->166 -0.00144

 87 ->182 -0.00155

 87 ->215 0.00133

 87 ->224 0.00260

 87 ->227 -0.00187

 87 ->265 0.00123

 88 ->179 -0.00102

 88 ->191 0.00149

 88 ->198 0.00181

 88 ->202 -0.00142

 88 ->209 -0.00112

 88 ->239 -0.00136

 88 ->249 -0.00180

 89 ->178 -0.00123

 89 ->200 0.00199

 89 ->216 -0.00161

 89 ->228 -0.00121

 89 ->232 0.00164

 89 ->243 -0.00113

 89 ->257 -0.00123

 89 ->259 0.00102

 89 ->307 -0.00143

 90 ->165 -0.00164

 90 ->181 -0.00316

 90 ->188 0.00165

 90 ->190 0.00149

 90 ->195 -0.00211

 90 ->197 -0.00125

 90 ->213 -0.00456

 90 ->219 -0.00227

 90 ->222 0.00112

 90 ->245 -0.00131

 90 ->264 0.00125

 91 ->167 0.00183

 91 ->200 -0.00262

 91 ->212 0.00116

 91 ->216 0.00572

 91 ->232 -0.00111

 91 ->257 0.00144

 92 ->169 0.00114

 92 ->198 -0.00114

 92 ->217 0.00222

 92 ->221 -0.00165

 93 ->165 -0.00131

 93 ->181 -0.00253

 93 ->195 -0.00106

 93 ->219 -0.00211

 93 ->222 -0.00101

 93 ->225 0.00234

 93 ->246 -0.00115

 93 ->253 -0.00140

 93 ->254 -0.00111

 93 ->264 0.00122

 94 ->177 0.00131

 94 ->211 -0.00115

 94 ->215 -0.00182

 95 ->202 0.00117

 95 ->209 0.00103

 95 ->217 -0.00285

 95 ->221 -0.00210

 95 ->226 0.00108

 95 ->239 0.00138

 95 ->249 0.00227

 95 ->332 0.00161

 96 ->182 -0.00216

 96 ->186 0.00134

 96 ->211 0.00127

 96 ->215 0.00290

 96 ->230 0.00242

 96 ->237 0.00133

 96 ->256 0.00205

 96 ->312 -0.00117

 96 ->325 0.00101

 97 ->167 0.00150

 97 ->178 0.00235

 97 ->216 0.00232

 97 ->223 0.00145

 97 ->252 0.00145

 97 ->268 0.00122

 98 ->179 0.00159

 98 ->221 -0.00201

 98 ->226 0.00181

 98 ->266 -0.00108

 98 ->277 0.00116

 99 ->176 -0.00244

 99 ->213 -0.00231

 99 ->219 0.00106

 99 ->222 0.00479

 99 ->225 -0.00169

 99 ->229 -0.00196

 99 ->245 -0.00138

 99 ->254 0.00149

 99 ->306 0.00116

 100 ->177 0.00209

 100 ->182 0.00183

 100 ->186 -0.00140

 100 ->211 0.00253

 100 ->215 0.00163

 100 ->263 -0.00116

 100 ->265 0.00169

 101 ->163 -0.00125

 101 ->200 -0.00107

 101 ->212 -0.00149

 101 ->216 -0.00172

 101 ->220 0.00423

 101 ->243 0.00151

 101 ->250 -0.00157

 101 ->252 -0.00105

 101 ->259 -0.00117

 101 ->268 0.00114

 101 ->274 -0.00140

 101 ->278 -0.00106

 102 ->162 0.00619

 102 ->166 0.00106

 102 ->237 -0.00108

 102 ->240 0.00103

 102 ->247 -0.00125

 102 ->258 -0.00111

 103 ->165 0.00131

 103 ->173 -0.00187

 103 ->210 0.00102

 103 ->242 0.00124

 103 ->245 -0.00135

 104 ->164 -0.00268

 104 ->226 -0.00110

 104 ->244 -0.00104

 105 ->165 0.00116

 105 ->173 0.00205

 105 ->181 -0.00102

 105 ->183 -0.00139

 105 ->188 -0.00128

 105 ->190 0.00240

 105 ->195 -0.00575

 105 ->197 -0.00103

 105 ->205 -0.00193

 105 ->210 0.00188

 105 ->213 0.00169

 105 ->222 -0.00300

 105 ->225 0.00103

 105 ->229 0.00130

 105 ->242 0.00151

 105 ->245 0.00269

 105 ->251 0.00182

 105 ->264 0.00131

 105 ->320 0.00127

 106 ->164 0.00175

 106 ->168 -0.00114

 106 ->169 0.00160

 106 ->208 0.00157

 106 ->214 -0.00132

 106 ->217 0.00134

 106 ->244 0.00119

 107 ->163 0.00176

 107 ->167 0.00170

 107 ->207 0.00120

 107 ->220 0.00181

 107 ->232 -0.00158

 107 ->268 0.00104

 108 ->166 -0.00110

 108 ->177 0.00178

 108 ->182 0.00419

 108 ->186 -0.00267

 108 ->192 -0.00293

 108 ->206 0.00108

 108 ->215 0.00105

 108 ->218 0.00195

 108 ->227 -0.00156

 108 ->230 0.00196

 108 ->237 0.00107

 108 ->265 0.00277

 108 ->270 -0.00134

 108 ->302 -0.00127

 108 ->304 -0.00119

 109 ->163 -0.00116

 109 ->184 -0.00107

 109 ->187 -0.00101

 109 ->196 0.00162

 109 ->207 0.00176

 109 ->212 0.00217

 109 ->216 0.00264

 109 ->220 -0.00360

 109 ->228 -0.00195

 109 ->241 -0.00141

 109 ->250 0.00343

 109 ->252 0.00146

 109 ->274 0.00119

 109 ->278 0.00119

 109 ->314 -0.00118

 109 ->333 0.00126

 110 ->165 -0.00136

 110 ->176 -0.00150

 110 ->183 -0.00278

 110 ->188 -0.00323

 110 ->190 0.00104

 110 ->195 -0.00833

 110 ->197 -0.00223

 110 ->225 -0.00157

 110 ->238 0.00162

 110 ->251 0.00118

 110 ->264 0.00130

 110 ->285 -0.00107

 110 ->298 0.00126

 111 ->162 0.00314

 111 ->171 0.00196

 111 ->174 0.00229

 111 ->182 -0.00110

 111 ->186 -0.00112

 111 ->194 0.00371

 111 ->258 -0.00219

 111 ->275 -0.00154

 111 ->290 -0.00152

 111 ->296 -0.00104

 111 ->315 0.00107

 112 ->165 0.00144

 112 ->170 0.00107

 112 ->173 -0.00332

 112 ->183 0.00131

 112 ->188 -0.00101

 112 ->195 -0.00183

 112 ->197 0.00348

 112 ->210 -0.00119

 112 ->225 0.00119

 112 ->253 -0.00155

 112 ->262 0.00174

 112 ->271 -0.00198

 112 ->288 0.00180

 112 ->310 0.00118

 113 ->182 -0.00443

 113 ->186 0.00260

 113 ->192 0.00162

 113 ->199 -0.00104

 113 ->215 0.00223

 113 ->218 -0.00262

 113 ->275 0.00100

 114 ->165 0.00203

 114 ->170 0.00125

 114 ->181 -0.00431

 114 ->183 0.00101

 114 ->188 0.00106

 114 ->195 0.00203

 114 ->210 0.00124

 114 ->213 -0.00231

 114 ->222 -0.00225

 114 ->242 0.00126

 114 ->264 -0.00112

 114 ->301 -0.00125

 114 ->320 0.00111

 115 ->179 0.00269

 115 ->180 -0.00142

 115 ->198 -0.00323

 115 ->202 0.00196

 115 ->209 0.00139

 115 ->214 0.00101

 115 ->217 -0.00133

 115 ->221 -0.00243

 115 ->267 0.00114

 115 ->277 0.00130

 116 ->179 0.00140

 116 ->185 0.00273

 117 ->184 0.00197

 117 ->187 -0.00206

 118 ->166 -0.00139

 118 ->174 -0.00122

 118 ->177 -0.00229

 118 ->192 0.00132

 118 ->211 -0.00134

 118 ->224 0.00250

 118 ->230 0.00192

 118 ->248 -0.00201

 119 ->174 -0.00115

 119 ->177 0.00185

 119 ->182 -0.00112

 119 ->186 -0.00185

 119 ->194 -0.00102

 119 ->224 -0.00161

 119 ->258 0.00143

 120 ->165 -0.00105

 120 ->173 0.00112

 120 ->176 -0.00114

 120 ->183 0.00183

 120 ->188 -0.00146

 120 ->190 0.00109

 120 ->197 -0.00168

 120 ->253 0.00101

 120 ->262 -0.00121

 121 ->167 0.00168

 121 ->172 0.00101

 121 ->178 -0.00215

 121 ->184 0.00121

 121 ->200 0.00496

 121 ->204 -0.00107

 121 ->207 0.00181

 121 ->212 0.00276

 121 ->220 -0.00136

 121 ->223 0.00191

 121 ->228 -0.00224

 121 ->232 -0.00248

 121 ->250 0.00298

 121 ->252 0.00130

 121 ->314 -0.00152

 121 ->321 -0.00140

 121 ->364 0.00105

 122 ->164 -0.00209

 122 ->179 -0.00100

 122 ->180 0.00119

 122 ->189 0.00239

 122 ->191 -0.00231

 122 ->198 -0.00336

 122 ->202 0.00199

 122 ->217 0.00166

 122 ->231 -0.00106

 122 ->266 -0.00219

 122 ->269 -0.00103

 122 ->277 0.00164

 122 ->300 0.00119

 123 ->168 0.00168

 123 ->169 -0.00357

 123 ->180 0.00247

 123 ->189 0.00394

 123 ->191 0.00104

 123 ->198 0.00211

 123 ->202 -0.00169

 123 ->214 -0.00134

 123 ->266 0.00152

 123 ->277 -0.00104

 123 ->303 0.00118

 124 ->165 -0.00310

 124 ->176 0.00249

 124 ->181 -0.00254

 124 ->190 0.00225

 124 ->195 -0.00206

 124 ->197 -0.00150

 124 ->201 -0.00147

 124 ->210 -0.00132

 124 ->213 -0.00290

 124 ->219 -0.00322

 124 ->222 0.00426

 124 ->229 -0.00287

 124 ->242 0.00111

 124 ->246 -0.00161

 124 ->251 -0.00136

 124 ->254 0.00172

 124 ->262 -0.00141

 124 ->285 -0.00177

 124 ->298 0.00118

 124 ->301 0.00159

 124 ->322 -0.00184

 124 ->324 -0.00120

 124 ->336 0.00109

 125 ->163 -0.00203

 125 ->167 0.00307

 125 ->172 0.00137

 125 ->175 -0.00106

 125 ->187 0.00114

 125 ->193 0.00176

 125 ->200 -0.00473

 125 ->207 0.00109

 125 ->216 0.00186

 125 ->220 -0.00224

 125 ->243 -0.00127

 125 ->250 0.00262

 125 ->252 0.00161

 125 ->268 0.00221

 125 ->274 0.00107

 125 ->291 0.00127

 125 ->297 0.00150

 125 ->305 -0.00174

 125 ->333 0.00147

 126 ->166 0.00204

 126 ->171 -0.00104

 126 ->174 -0.00635

 126 ->186 0.00129

 126 ->194 0.00202

 126 ->203 -0.00112

 126 ->211 -0.00115

 126 ->215 0.00115

 127 ->162 0.00292

 127 ->166 -0.00307

 127 ->171 -0.00214

 127 ->174 0.00121

 127 ->177 0.00124

 127 ->186 -0.00109

 127 ->194 -0.00152

 127 ->199 -0.00174

 127 ->215 0.00317

 127 ->224 0.00210

 127 ->227 -0.00288

 127 ->247 -0.00134

 127 ->248 0.00231

 127 ->256 0.00460

 127 ->263 0.00146

 127 ->275 -0.00105

 127 ->302 0.00126

 127 ->312 -0.00239

 128 ->163 -0.00211

 128 ->167 0.00131

 128 ->193 -0.00164

 128 ->212 -0.00139

 128 ->216 -0.00745

 128 ->220 -0.00345

 128 ->223 -0.00106

 128 ->232 0.00231

 128 ->243 -0.00116

 128 ->257 -0.00220

 128 ->274 0.00131

 128 ->278 0.00123

 128 ->307 -0.00181

 129 ->169 0.00186

 129 ->202 -0.00363

 129 ->209 -0.00303

 129 ->214 -0.00192

 129 ->217 0.00181

 129 ->221 -0.00407

 129 ->226 0.00176

 129 ->239 0.00327

 129 ->249 0.00511

 129 ->260 -0.00147

 129 ->267 -0.00171

 129 ->289 0.00195

 129 ->300 -0.00202

 129 ->323 -0.00102

 129 ->332 0.00101

 130 ->165 -0.00259

 130 ->176 0.00179

 130 ->183 0.00116

 130 ->188 0.00144

 130 ->190 -0.00150

 130 ->210 -0.00181

 130 ->213 0.00509

 130 ->219 0.00277

 130 ->222 -0.00157

 130 ->229 -0.00381

 130 ->238 0.00229

 130 ->242 0.00232

 130 ->245 0.00142

 130 ->254 0.00133

 130 ->264 -0.00320

 130 ->271 0.00142

 130 ->276 -0.00113

 130 ->281 0.00112

 130 ->288 0.00110

 130 ->306 0.00132

 131 ->162 -0.00515

 131 ->166 0.00324

 131 ->171 -0.00177

 131 ->177 0.00210

 131 ->182 0.00184

 131 ->186 -0.00179

 131 ->199 -0.00325

 131 ->227 -0.00196

 131 ->230 -0.00131

 131 ->248 0.00140

 131 ->256 0.00146

 131 ->275 -0.00138

 132 ->164 -0.00449

 132 ->168 -0.00351

 132 ->169 0.00129

 132 ->179 -0.00164

 132 ->191 0.00181

 132 ->198 0.00376

 132 ->209 -0.00103

 132 ->260 -0.00156

 132 ->267 -0.00114

 133 ->165 0.00161

 133 ->170 -0.00101

 133 ->173 0.00155

 133 ->176 -0.00143

 133 ->181 0.00280

 133 ->183 0.00135

 133 ->188 0.00173

 133 ->190 -0.00169

 133 ->195 -0.00275

 133 ->210 -0.00221

 133 ->213 0.00550

 133 ->219 0.00415

 133 ->225 -0.00231

 133 ->229 -0.00420

 133 ->238 0.00103

 133 ->253 0.00109

 133 ->254 0.00132

 133 ->264 -0.00240

 133 ->306 0.00167

 133 ->313 0.00132

 134 ->163 0.00325

 134 ->172 -0.00247

 134 ->175 0.00265

 134 ->178 0.00116

 134 ->184 0.00256

 134 ->187 0.00316

 134 ->193 -0.00172

 134 ->200 -0.00272

 134 ->216 -0.00606

 134 ->220 -0.00450

 134 ->228 -0.00323

 134 ->232 0.00145

 134 ->241 -0.00100

 134 ->257 -0.00179

 134 ->259 0.00115

 134 ->274 0.00272

 134 ->278 0.00139

 134 ->291 0.00128

 134 ->333 0.00117

 135 ->166 -0.00109

 135 ->177 -0.00138

 135 ->192 -0.00301

 135 ->203 -0.00131

 135 ->206 -0.00178

 135 ->211 -0.00234

 135 ->215 -0.00273

 135 ->218 0.00117

 135 ->224 0.00155

 135 ->230 0.00219

 135 ->248 -0.00122

 136 ->163 0.00335

 136 ->167 0.00223

 136 ->175 0.00253

 136 ->184 -0.00119

 136 ->193 0.00147

 136 ->200 0.00111

 136 ->204 -0.00141

 136 ->216 0.00243

 136 ->220 0.00157

 136 ->234 0.00164

 136 ->261 0.00103

 136 ->274 -0.00120

 136 ->293 -0.00120

 137 ->179 -0.00191

 137 ->191 0.00242

 137 ->198 -0.00242

 137 ->208 -0.00125

 137 ->217 0.00198

 137 ->221 0.00412

 137 ->226 -0.00129

 137 ->239 0.00100

 137 ->266 -0.00154

 138 ->165 -0.00243

 138 ->183 -0.00157

 138 ->195 -0.00102

 138 ->201 -0.00150

 138 ->205 -0.00161

 138 ->210 -0.00167

 138 ->219 -0.00254

 138 ->222 0.00193

 138 ->225 0.00122

 138 ->233 -0.00174

 138 ->301 0.00107

 139 ->164 0.00376

 139 ->169 0.00201

 139 ->180 0.00172

 139 ->189 0.00228

 139 ->209 -0.00125

 139 ->236 -0.00178

 140 ->162 -0.00624

 140 ->194 0.00231

 140 ->206 -0.00139

 140 ->235 -0.00163

 140 ->237 0.00101

 141 ->165 0.00263

 141 ->176 -0.00177

 141 ->190 0.00225

 141 ->195 0.00122

 141 ->197 0.00275

 141 ->205 0.00123

 141 ->210 0.00217

 141 ->213 -0.00102

 141 ->219 0.00241

 141 ->222 -0.00246

 141 ->229 0.00126

 141 ->238 -0.00110

 141 ->242 0.00115

 141 ->245 0.00145

 141 ->246 0.00151

 141 ->251 0.00185

 141 ->285 0.00121

 141 ->301 -0.00115

 141 ->306 -0.00125

 141 ->322 0.00145

 142 ->167 0.00353

 142 ->172 0.00137

 142 ->178 -0.00163

 142 ->184 -0.00125

 142 ->193 -0.00195

 142 ->200 -0.00275

 142 ->204 -0.00118

 142 ->212 0.00191

 142 ->223 0.00177

 142 ->228 0.00124

 142 ->232 -0.00397

 142 ->234 0.00150

 142 ->250 0.00365

 142 ->259 -0.00124

 142 ->268 0.00180

 142 ->291 0.00141

 142 ->293 0.00116

 142 ->305 -0.00149

 142 ->333 0.00149

 142 ->384 -0.00106

 143 ->167 -0.00557

 143 ->172 0.00168

 143 ->175 -0.00615

 143 ->178 0.00137

 143 ->196 -0.00380

 143 ->204 -0.00150

 143 ->216 -0.00106

 143 ->259 -0.00196

 143 ->261 -0.00178

 143 ->268 -0.00140

 143 ->278 -0.00180

 143 ->291 -0.00133

 143 ->337 -0.00114

 144 ->164 0.01093

 144 ->168 0.00555

 144 ->169 0.00637

 144 ->179 0.00301

 144 ->180 0.01132

 144 ->198 -0.00107

 144 ->202 -0.00225

 144 ->209 0.00250

 144 ->214 -0.00157

 144 ->221 -0.00120

 144 ->260 0.00317

 144 ->267 -0.00182

 144 ->269 0.00111

 144 ->284 -0.00151

 144 ->294 0.00190

 144 ->318 -0.00149

 144 ->339 0.00134

 145 ->165 0.00354

 145 ->170 0.00168

 145 ->173 -0.00497

 145 ->195 0.00116

 145 ->201 -0.00204

 145 ->213 0.00122

 145 ->245 0.00221

 145 ->251 -0.00103

 145 ->262 0.00122

 145 ->271 0.00149

 145 ->276 0.00165

 145 ->285 0.00209

 145 ->328 0.00112

 146 ->164 -0.00295

 146 ->169 0.00186

 146 ->217 0.00902

 146 ->221 -0.00365

 146 ->231 -0.00269

 146 ->249 -0.00273

 146 ->255 -0.00323

 146 ->260 -0.00146

 146 ->266 -0.00342

 146 ->267 -0.00230

 146 ->269 -0.00166

 146 ->273 0.00301

 146 ->277 0.00122

 146 ->284 0.00170

 146 ->286 0.00158

 146 ->300 0.00170

 146 ->323 -0.00150

 146 ->332 0.00231

 146 ->335 0.00206

 146 ->339 -0.00124

 146 ->356 -0.00108

 147 ->162 0.00849

 147 ->166 -0.00329

 147 ->174 -0.00121

 147 ->182 0.00174

 147 ->186 -0.00101

 147 ->199 0.00281

 147 ->206 -0.00116

 147 ->211 -0.00169

 147 ->215 -0.00303

 147 ->218 -0.00905

 147 ->224 0.00384

 147 ->227 0.00173

 147 ->230 -0.00625

 147 ->247 -0.00142

 147 ->248 0.00210

 147 ->256 0.00176

 147 ->258 -0.00172

 147 ->263 0.00177

 147 ->265 -0.00518

 147 ->272 -0.00212

 147 ->275 -0.00181

 147 ->296 0.00181

 147 ->304 -0.00120

 147 ->309 -0.00199

 147 ->312 -0.00220

 147 ->317 0.00102

 147 ->342 0.00181

 147 ->362 0.00109

 148 ->162 0.04382

 148 ->171 -0.00117

 148 ->174 0.00425

 148 ->177 0.00162

 148 ->186 0.00131

 148 ->192 0.00178

 148 ->199 0.00170

 148 ->203 -0.00161

 148 ->211 -0.00197

 148 ->218 -0.00230

 148 ->230 -0.00226

 148 ->256 0.00137

 148 ->258 0.00171

 148 ->265 -0.00328

 148 ->270 -0.00308

 148 ->275 0.00103

 148 ->280 0.00197

 148 ->292 0.00187

 148 ->296 -0.00178

 148 ->302 -0.00161

 148 ->304 0.00254

 148 ->309 -0.00173

 148 ->317 -0.00118

 148 ->331 0.00151

 149 ->165 0.00106

 149 ->170 -0.00351

 149 ->173 -0.00286

 149 ->183 -0.00128

 149 ->188 0.00187

 149 ->190 0.00103

 149 ->201 0.00312

 149 ->210 -0.00269

 149 ->219 0.00129

 149 ->253 0.00158

 149 ->254 -0.00105

 149 ->262 -0.00126

 149 ->264 0.00132

 149 ->271 0.00234

 149 ->279 0.00111

 149 ->285 0.00298

 149 ->295 0.00400

 149 ->298 0.00171

 149 ->320 0.00147

 149 ->324 -0.00220

 149 ->336 -0.00125

 149 ->380 0.00148

 150 ->162 0.09172

 150 ->166 -0.01118

 150 ->171 0.00306

 150 ->177 -0.00113

 150 ->182 -0.00164

 150 ->186 0.00135

 150 ->194 -0.00276

 150 ->199 0.00269

 150 ->203 0.00239

 150 ->227 0.00134

 150 ->230 0.00254

 150 ->237 0.00206

 150 ->248 -0.00163

 150 ->258 -0.00113

 150 ->270 -0.00112

 150 ->309 0.00109

 151 ->163 0.02859

 151 ->167 0.00707

 151 ->172 -0.00620

 151 ->184 -0.00130

 151 ->200 -0.00158

 151 ->220 0.00106

 151 ->261 0.00105

 152 ->164 0.00975

 152 ->168 0.00989

 152 ->169 0.00577

 152 ->180 0.00103

 152 ->189 0.00113

 152 ->191 -0.00106

 152 ->209 0.00143

 152 ->260 0.00135

 152 ->266 0.00134

 153 ->162 0.01769

 153 ->166 0.00472

 153 ->171 -0.01003

 153 ->177 0.00121

 153 ->182 0.00206

 153 ->258 0.00115

 153 ->280 0.00100

 153 ->302 -0.00117

 154 ->165 -0.00574

 154 ->170 -0.00998

 154 ->173 -0.00302

 154 ->183 -0.00233

 154 ->190 0.00112

 154 ->210 -0.00134

 154 ->229 0.00154

 154 ->253 0.00102

 154 ->276 0.00109

 154 ->285 0.00126

 154 ->298 0.00109

 155 ->163 -0.03436

 155 ->167 0.01462

 155 ->172 0.00891

 155 ->184 -0.00206

 155 ->187 -0.00247

 155 ->193 0.00100

 155 ->196 0.00424

 155 ->200 0.00146

 155 ->204 -0.00228

 155 ->207 0.00143

 155 ->212 0.00126

 155 ->216 0.00151

 155 ->228 0.00307

 155 ->241 0.00121

 155 ->268 0.00158

 155 ->316 0.00109

 155 ->333 -0.00135

 155 ->357 0.00109

 156 ->164 0.01216

 156 ->168 0.00816

 156 ->169 -0.01426

 156 ->180 -0.00457

 156 ->185 0.00132

 156 ->189 0.00260

 156 ->191 -0.00237

 156 ->198 -0.00286

 156 ->202 -0.00159

 156 ->214 0.00230

 156 ->217 0.00175

 156 ->255 0.00165

 156 ->260 -0.00101

 156 ->266 0.00119

 156 ->267 0.00134

 156 ->269 0.00117

 156 ->303 0.00119

 156 ->323 0.00123

 156 ->356 -0.00102

 157 ->165 0.01865

 157 ->170 -0.00513

 157 ->173 0.00206

 157 ->176 -0.00194

 157 ->181 0.00295

 157 ->195 -0.00255

 157 ->197 0.00160

 157 ->201 0.00128

 157 ->210 0.00117

 157 ->213 0.00228

 157 ->219 0.00149

 157 ->222 0.00145

 157 ->225 -0.00147

 157 ->242 -0.00159

 157 ->246 0.00152

 157 ->281 0.00131

 157 ->310 -0.00128

 157 ->329 0.00137

 157 ->336 0.00130

 158 ->162 0.15684

 158 ->166 0.01111

 158 ->171 0.00496

 158 ->174 -0.01002

 158 ->177 -0.00101

 158 ->199 -0.00181

 158 ->211 0.00138

 158 ->215 -0.00103

 158 ->296 0.00131

 158 ->302 0.00128

 158 ->309 0.00169

 158 ->492 -0.00104

 159 ->164 -0.04405

 159 ->168 0.00966

 159 ->169 -0.00587

 159 ->179 0.00248

 159 ->180 0.01023

 159 ->244 0.00113

 159 ->303 -0.00138

 159 ->318 -0.00217

 160 ->163 0.58001

 160 ->172 -0.01301

 160 ->175 0.00884

 160 ->196 0.00536

 160 ->200 0.00149

 160 ->207 -0.00106

 160 ->212 -0.00194

 160 ->243 -0.00177

 160 ->252 -0.00156

 160 ->259 0.00108

 160 ->268 0.00181

 160 ->293 -0.00122

 160 ->314 -0.00156

 160 ->316 -0.00120

 160 ->326 0.00259

 160 ->330 0.00195

 160 ->337 0.00172

 160 ->341 -0.00109

 161 ->162 -0.36317

 161 ->166 0.02140

 161 ->171 0.02166

 161 ->174 0.02790

 161 ->177 0.00321

 161 ->186 -0.00208

 161 ->192 0.00104

 161 ->194 -0.00432

 161 ->203 0.00364

 161 ->206 -0.00179

 161 ->211 0.00464

 161 ->215 -0.00347

 161 ->218 0.00101

 161 ->258 -0.00221

 161 ->263 0.00150

 161 ->270 -0.00248

 161 ->272 0.00133

 161 ->280 0.00207

 161 ->290 -0.00172

 161 ->296 -0.00159

 161 ->302 -0.00110

 161 ->304 0.00104

 61 <-195 -0.00117

 62 <-215 0.00114

 74 <-277 0.00122

 75 <-213 -0.00113

 75 <-229 -0.00102

 77 <-162 -0.00115

 77 <-218 0.00114

 81 <-182 -0.00197

 81 <-186 0.00125

 81 <-192 0.00114

 81 <-218 0.00181

 81 <-227 -0.00183

 83 <-181 0.00221

 83 <-188 -0.00112

 83 <-190 -0.00130

 83 <-195 0.00131

 83 <-246 -0.00112

 84 <-200 0.00178

 85 <-176 0.00183

 85 <-181 -0.00369

 85 <-188 0.00138

 85 <-195 -0.00212

 85 <-213 0.00163

 87 <-166 -0.00101

 87 <-182 -0.00107

 87 <-224 0.00206

 87 <-227 -0.00142

 88 <-191 0.00105

 88 <-198 0.00128

 88 <-239 -0.00105

 88 <-249 -0.00145

 89 <-200 0.00134

 89 <-216 -0.00119

 89 <-232 0.00124

 89 <-307 -0.00117

 90 <-165 -0.00105

 90 <-181 -0.00216

 90 <-188 0.00111

 90 <-190 0.00104

 90 <-195 -0.00149

 90 <-213 -0.00326

 90 <-219 -0.00172

 90 <-245 -0.00101

 91 <-167 0.00115

 91 <-200 -0.00185

 91 <-216 0.00413

 91 <-257 0.00109

 92 <-217 0.00163

 92 <-221 -0.00115

 93 <-181 -0.00168

 93 <-219 -0.00159

 93 <-225 0.00175

 93 <-253 -0.00109

 94 <-215 -0.00128

 95 <-217 -0.00200

 95 <-221 -0.00151

 95 <-239 0.00101

 95 <-249 0.00167

 95 <-332 0.00128

 96 <-182 -0.00142

 96 <-215 0.00199

 96 <-230 0.00174

 96 <-256 0.00154

 97 <-178 0.00146

 97 <-216 0.00165

 97 <-223 0.00107

 97 <-252 0.00110

 98 <-221 -0.00139

 98 <-226 0.00132

 99 <-176 -0.00153

 99 <-213 -0.00163

 99 <-222 0.00357

 99 <-225 -0.00127

 99 <-229 -0.00158

 99 <-245 -0.00107

 99 <-254 0.00118

 99 <-306 0.00102

 100 <-177 0.00128

 100 <-182 0.00115

 100 <-211 0.00169

 100 <-215 0.00108

 100 <-265 0.00126

 101 <-212 -0.00104

 101 <-216 -0.00120

 101 <-220 0.00307

 101 <-243 0.00113

 101 <-250 -0.00124

 101 <-274 -0.00114

 102 <-162 0.00375

 103 <-173 -0.00153

 104 <-164 -0.00160

 105 <-173 0.00127

 105 <-190 0.00152

 105 <-195 -0.00368

 105 <-205 -0.00126

 105 <-210 0.00132

 105 <-213 0.00122

 105 <-222 -0.00221

 105 <-229 0.00102

 105 <-242 0.00109

 105 <-245 0.00199

 105 <-251 0.00130

 105 <-320 0.00101

 106 <-164 0.00112

 106 <-169 0.00101

 106 <-208 0.00101

 107 <-167 0.00102

 107 <-220 0.00129

 107 <-232 -0.00113

 108 <-177 0.00108

 108 <-182 0.00258

 108 <-186 -0.00167

 108 <-192 -0.00185

 108 <-218 0.00133

 108 <-227 -0.00109

 108 <-230 0.00138

 108 <-265 0.00201

 109 <-196 0.00108

 109 <-207 0.00118

 109 <-212 0.00152

 109 <-216 0.00187

 109 <-220 -0.00265

 109 <-228 -0.00149

 109 <-241 -0.00107

 109 <-250 0.00260

 109 <-252 0.00118

 109 <-333 0.00107

 110 <-183 -0.00174

 110 <-188 -0.00201

 110 <-195 -0.00533

 110 <-197 -0.00140

 110 <-225 -0.00109

 110 <-238 0.00114

 111 <-194 0.00268

 111 <-258 -0.00153

 111 <-275 -0.00115

 111 <-290 -0.00115

 112 <-173 -0.00216

 112 <-195 -0.00128

 112 <-197 0.00243

 112 <-253 -0.00108

 112 <-262 0.00121

 112 <-271 -0.00149

 112 <-288 0.00132

 113 <-182 -0.00269

 113 <-186 0.00159

 113 <-192 0.00101

 113 <-215 0.00146

 113 <-218 -0.00174

 114 <-165 0.00102

 114 <-181 -0.00257

 114 <-195 0.00127

 114 <-213 -0.00146

 114 <-222 -0.00157

 115 <-179 0.00156

 115 <-198 -0.00202

 115 <-202 0.00122

 115 <-221 -0.00164

 115 <-277 0.00101

 116 <-185 0.00165

 117 <-184 0.00118

 117 <-187 -0.00126

 118 <-177 -0.00135

 118 <-224 0.00167

 118 <-230 0.00131

 118 <-248 -0.00144

 119 <-177 0.00108

 119 <-186 -0.00112

 119 <-224 -0.00107

 119 <-258 0.00103

 120 <-183 0.00110

 120 <-197 -0.00114

 121 <-178 -0.00127

 121 <-200 0.00306

 121 <-207 0.00116

 121 <-212 0.00180

 121 <-220 -0.00101

 121 <-223 0.00131

 121 <-228 -0.00159

 121 <-232 -0.00179

 121 <-250 0.00214

 121 <-314 -0.00119

 121 <-321 -0.00107

 122 <-164 -0.00189

 122 <-180 0.00118

 122 <-189 0.00141

 122 <-191 -0.00138

 122 <-198 -0.00211

 122 <-202 0.00131

 122 <-217 0.00109

 122 <-266 -0.00162

 122 <-277 0.00120

 123 <-164 -0.00128

 123 <-168 0.00112

 123 <-169 -0.00188

 123 <-180 0.00239

 123 <-189 0.00228

 123 <-198 0.00123

 123 <-266 0.00108

 124 <-165 -0.00154

 124 <-176 0.00139

 124 <-181 -0.00150

 124 <-190 0.00137

 124 <-195 -0.00127

 124 <-213 -0.00192

 124 <-219 -0.00213

 124 <-222 0.00306

 124 <-229 -0.00213

 124 <-246 -0.00112

 124 <-254 0.00133

 124 <-262 -0.00101

 124 <-285 -0.00134

 124 <-301 0.00119

 124 <-322 -0.00140

 125 <-163 -0.00111

 125 <-167 0.00148

 125 <-193 0.00106

 125 <-200 -0.00291

 125 <-216 0.00127

 125 <-220 -0.00161

 125 <-250 0.00195

 125 <-252 0.00122

 125 <-268 0.00160

 125 <-297 0.00108

 125 <-305 -0.00132

 125 <-333 0.00117

 126 <-174 -0.00507

 127 <-162 0.00125

 127 <-166 -0.00147

 127 <-174 0.00116

 127 <-199 -0.00110

 127 <-215 0.00201

 127 <-224 0.00154

 127 <-227 -0.00200

 127 <-248 0.00163

 127 <-256 0.00336

 127 <-263 0.00109

 127 <-312 -0.00182

 128 <-193 -0.00103

 128 <-216 -0.00480

 128 <-220 -0.00229

 128 <-232 0.00162

 128 <-257 -0.00161

 128 <-307 -0.00131

 129 <-169 0.00102

 129 <-202 -0.00220

 129 <-209 -0.00187

 129 <-214 -0.00120

 129 <-217 0.00120

 129 <-221 -0.00275

 129 <-226 0.00120

 129 <-239 0.00233

 129 <-249 0.00368

 129 <-260 -0.00101

 129 <-267 -0.00124

 129 <-289 0.00150

 129 <-300 -0.00152

 130 <-165 -0.00123

 130 <-210 -0.00110

 130 <-213 0.00322

 130 <-219 0.00186

 130 <-229 -0.00260

 130 <-238 0.00159

 130 <-242 0.00162

 130 <-264 -0.00235

 130 <-271 0.00105

 131 <-162 -0.00139

 131 <-166 0.00153

 131 <-177 0.00112

 131 <-182 0.00106

 131 <-186 -0.00103

 131 <-199 -0.00190

 131 <-227 -0.00132

 131 <-256 0.00106

 131 <-275 -0.00101

 132 <-168 -0.00191

 132 <-191 0.00104

 132 <-198 0.00221

 132 <-260 -0.00107

 133 <-181 0.00159

 133 <-195 -0.00159

 133 <-210 -0.00138

 133 <-213 0.00343

 133 <-219 0.00278

 133 <-225 -0.00160

 133 <-229 -0.00285

 133 <-254 0.00101

 133 <-264 -0.00177

 133 <-306 0.00128

 133 <-313 0.00101

 134 <-172 -0.00131

 134 <-175 0.00128

 134 <-184 0.00144

 134 <-187 0.00182

 134 <-200 -0.00159

 134 <-216 -0.00387

 134 <-220 -0.00302

 134 <-228 -0.00218

 134 <-232 0.00101

 134 <-257 -0.00130

 134 <-274 0.00204

 134 <-278 0.00102

 135 <-192 -0.00170

 135 <-206 -0.00106

 135 <-211 -0.00137

 135 <-215 -0.00171

 135 <-224 0.00100

 135 <-230 0.00142

 136 <-175 0.00135

 136 <-216 0.00149

 136 <-220 0.00103

 136 <-234 0.00111

 137 <-179 -0.00102

 137 <-191 0.00136

 137 <-198 -0.00141

 137 <-217 0.00128

 137 <-221 0.00265

 137 <-266 -0.00106

 138 <-165 -0.00119

 138 <-210 -0.00101

 138 <-219 -0.00164

 138 <-222 0.00127

 138 <-233 -0.00117

 139 <-164 0.00107

 139 <-180 0.00118

 139 <-189 0.00129

 139 <-236 -0.00117

 140 <-162 -0.00344

 140 <-194 0.00136

 140 <-235 -0.00108

 141 <-165 0.00129

 141 <-190 0.00127

 141 <-197 0.00166

 141 <-210 0.00126

 141 <-219 0.00157

 141 <-222 -0.00172

 141 <-245 0.00104

 141 <-246 0.00105

 141 <-251 0.00125

 141 <-322 0.00105

 142 <-167 0.00177

 142 <-193 -0.00109

 142 <-200 -0.00158

 142 <-212 0.00117

 142 <-223 0.00116

 142 <-232 -0.00267

 142 <-234 0.00100

 142 <-250 0.00255

 142 <-268 0.00129

 142 <-291 0.00104

 142 <-305 -0.00111

 142 <-333 0.00113

 143 <-163 0.00100

 143 <-167 -0.00188

 143 <-175 -0.00254

 143 <-196 -0.00196

 143 <-204 -0.00105

 143 <-259 -0.00139

 143 <-261 -0.00126

 143 <-268 -0.00105

 143 <-278 -0.00134

 144 <-168 0.00289

 144 <-169 0.00127

 144 <-179 0.00145

 144 <-180 0.00525

 144 <-202 -0.00122

 144 <-209 0.00108

 144 <-260 0.00200

 144 <-267 -0.00103

 144 <-294 0.00128

 145 <-165 0.00143

 145 <-173 -0.00152

 145 <-195 0.00101

 145 <-201 -0.00172

 145 <-245 0.00150

 145 <-262 0.00104

 145 <-271 0.00101

 145 <-276 0.00126

 145 <-285 0.00147

 146 <-217 0.00543

 146 <-221 -0.00229

 146 <-231 -0.00163

 146 <-249 -0.00174

 146 <-255 -0.00220

 146 <-266 -0.00241

 146 <-267 -0.00155

 146 <-269 -0.00112

 146 <-273 0.00211

 146 <-277 0.00101

 146 <-284 0.00116

 146 <-286 0.00108

 146 <-300 0.00115

 146 <-323 -0.00113

 146 <-332 0.00174

 146 <-335 0.00153

 147 <-162 0.00134

 147 <-166 -0.00117

 147 <-199 0.00147

 147 <-215 -0.00172

 147 <-218 -0.00546

 147 <-224 0.00240

 147 <-227 0.00105

 147 <-230 -0.00388

 147 <-248 0.00141

 147 <-256 0.00127

 147 <-258 -0.00113

 147 <-263 0.00127

 147 <-265 -0.00348

 147 <-272 -0.00156

 147 <-275 -0.00124

 147 <-296 0.00131

 147 <-309 -0.00144

 147 <-312 -0.00166

 147 <-342 0.00137

 148 <-162 0.00601

 148 <-174 0.00245

 148 <-211 -0.00120

 148 <-218 -0.00139

 148 <-230 -0.00135

 148 <-258 0.00113

 148 <-265 -0.00220

 148 <-270 -0.00219

 148 <-280 0.00131

 148 <-292 0.00138

 148 <-296 -0.00129

 148 <-302 -0.00110

 148 <-304 0.00186

 148 <-309 -0.00127

 148 <-331 0.00104

 149 <-170 -0.00150

 149 <-173 -0.00150

 149 <-201 0.00186

 149 <-210 -0.00164

 149 <-253 0.00108

 149 <-271 0.00162

 149 <-285 0.00211

 149 <-295 0.00288

 149 <-298 0.00125

 149 <-320 0.00107

 149 <-324 -0.00159

 149 <-380 0.00120

 150 <-162 0.01534

 150 <-166 -0.00296

 150 <-171 0.00171

 150 <-174 0.00152

 150 <-199 0.00148

 150 <-203 0.00115

 150 <-230 0.00160

 150 <-237 0.00138

 151 <-163 0.00686

 151 <-167 0.00251

 152 <-164 0.00227

 152 <-168 0.00256

 152 <-169 0.00203

 153 <-162 -0.00213

 153 <-171 -0.00321

 154 <-165 -0.00201

 154 <-170 -0.00243

 154 <-173 -0.00146

 154 <-183 -0.00106

 155 <-163 -0.00245

 155 <-167 0.00326

 155 <-172 0.00285

 155 <-184 -0.00105

 155 <-187 -0.00107

 155 <-196 0.00185

 155 <-228 0.00197

 155 <-268 0.00103

 156 <-164 0.00398

 156 <-168 0.00256

 156 <-169 -0.00297

 156 <-180 -0.00127

 156 <-189 0.00172

 156 <-191 -0.00122

 156 <-198 -0.00150

 156 <-214 0.00103

 156 <-217 0.00104

 156 <-255 0.00107

 157 <-165 0.00440

 157 <-170 -0.00159

 157 <-173 0.00193

 157 <-181 0.00133

 157 <-213 0.00116

 157 <-242 -0.00102

 157 <-329 0.00112

 158 <-162 0.00288

 158 <-166 0.00322

 158 <-174 -0.00378

 158 <-194 0.00204

 158 <-302 0.00105

 158 <-309 0.00130

 158 <-492 -0.00110

 159 <-164 -0.00416

 159 <-168 0.00313

 159 <-179 0.00107

 159 <-180 0.00397

 159 <-189 0.00235

 159 <-266 -0.00100

 159 <-318 -0.00123

 160 <-163 -0.07698

 160 <-167 -0.00298

 160 <-172 -0.00642

 160 <-175 0.00600

 160 <-196 0.00245

 160 <-204 -0.00114

 160 <-212 -0.00133

 160 <-243 -0.00186

 160 <-252 -0.00109

 160 <-268 0.00120

 160 <-293 -0.00102

 160 <-314 -0.00140

 160 <-326 0.00172

 160 <-330 0.00176

 161 <-162 0.09031

 161 <-166 0.00367

 161 <-171 0.00728

 161 <-174 0.01282

 161 <-177 0.00121

 161 <-194 -0.00335

 161 <-203 0.00244

 161 <-211 0.00246

 161 <-215 -0.00205

 161 <-258 -0.00161

 161 <-270 -0.00150

 161 <-280 0.00171

 161 <-290 -0.00105

 161 <-331 0.00131

 Excited State 4: Singlet-B1 3.0586 eV 405.37 nm f=1.7750 <S\*\*2>=0.000

 52 ->216 -0.00101

 59 ->217 0.00112

 59 ->221 0.00108

 59 ->226 -0.00129

 60 ->216 0.00118

 64 ->216 0.00119

 71 ->226 -0.00122

 72 ->166 -0.00105

 72 ->215 -0.00123

 74 ->165 -0.00124

 74 ->210 -0.00134

 74 ->213 0.00170

 74 ->229 -0.00123

 74 ->306 0.00101

 75 ->249 -0.00129

 76 ->192 -0.00122

 76 ->211 -0.00107

 76 ->215 -0.00174

 76 ->230 0.00160

 76 ->248 -0.00115

 76 ->263 0.00119

 77 ->163 0.00155

 77 ->220 0.00174

 78 ->210 0.00105

 78 ->213 -0.00196

 78 ->219 0.00107

 79 ->169 0.00104

 80 ->171 -0.00111

 81 ->220 0.00234

 81 ->243 -0.00102

 82 ->190 0.00109

 82 ->213 -0.00186

 83 ->198 -0.00100

 83 ->217 -0.00195

 83 ->249 0.00167

 84 ->199 0.00101

 84 ->211 0.00108

 84 ->215 0.00178

 84 ->224 0.00114

 85 ->217 0.00246

 85 ->249 -0.00141

 86 ->167 -0.00163

 86 ->193 -0.00111

 86 ->220 0.00107

 86 ->252 -0.00103

 87 ->167 0.00163

 87 ->216 -0.00244

 87 ->228 -0.00175

 87 ->252 0.00175

 87 ->257 -0.00126

 87 ->274 0.00122

 88 ->165 0.00255

 88 ->210 0.00279

 88 ->213 -0.00440

 88 ->219 0.00116

 88 ->222 -0.00153

 88 ->229 0.00132

 88 ->246 0.00149

 88 ->264 0.00103

 89 ->166 0.00232

 89 ->199 -0.00303

 89 ->211 0.00307

 89 ->215 0.00504

 89 ->230 -0.00123

 89 ->237 -0.00161

 89 ->247 0.00115

 89 ->248 0.00169

 90 ->179 -0.00123

 90 ->191 0.00122

 90 ->198 0.00209

 90 ->202 0.00159

 90 ->209 0.00109

 90 ->217 0.00212

 90 ->239 -0.00171

 90 ->249 -0.00306

 90 ->255 -0.00107

 91 ->177 -0.00128

 91 ->192 -0.00114

 91 ->199 0.00309

 91 ->215 -0.00228

 91 ->224 -0.00105

 91 ->227 0.00103

 91 ->230 -0.00196

 91 ->256 -0.00145

 91 ->263 -0.00120

 92 ->176 0.00121

 92 ->188 -0.00163

 92 ->190 0.00122

 92 ->219 0.00362

 92 ->225 -0.00293

 92 ->229 -0.00121

 92 ->251 0.00135

 92 ->253 0.00116

 92 ->254 0.00248

 92 ->264 -0.00128

 92 ->271 0.00106

 93 ->179 0.00104

 93 ->191 0.00120

 93 ->198 0.00152

 93 ->202 0.00113

 93 ->209 0.00110

 93 ->221 0.00185

 93 ->231 0.00106

 93 ->267 0.00102

 94 ->178 0.00107

 94 ->184 -0.00150

 94 ->187 -0.00102

 94 ->216 -0.00176

 94 ->223 0.00105

 94 ->252 -0.00163

 95 ->165 -0.00121

 95 ->176 -0.00134

 95 ->181 0.00578

 95 ->183 0.00322

 95 ->188 0.00321

 95 ->190 -0.00244

 95 ->195 0.00157

 95 ->210 -0.00196

 95 ->219 -0.00260

 95 ->222 0.00185

 95 ->238 0.00116

 95 ->242 0.00198

 95 ->251 -0.00128

 95 ->253 -0.00101

 95 ->262 -0.00119

 95 ->320 0.00100

 96 ->178 0.00230

 96 ->184 0.00484

 96 ->187 0.00396

 96 ->193 -0.00329

 96 ->220 0.00124

 96 ->228 0.00172

 96 ->232 0.00254

 96 ->243 -0.00216

 96 ->250 0.00247

 97 ->166 0.00136

 97 ->177 0.00232

 97 ->211 0.00210

 97 ->215 0.00181

 97 ->224 -0.00101

 97 ->227 0.00163

 97 ->230 -0.00177

 97 ->237 -0.00168

 97 ->247 0.00137

 97 ->248 0.00112

 97 ->256 -0.00138

 98 ->176 -0.00374

 98 ->181 0.00259

 98 ->183 0.00172

 98 ->188 0.00161

 98 ->190 -0.00175

 98 ->210 0.00106

 98 ->213 -0.00188

 98 ->219 0.00525

 98 ->225 -0.00139

 98 ->238 0.00137

 98 ->246 0.00149

 98 ->254 0.00145

 98 ->281 0.00111

 99 ->179 0.00170

 99 ->217 0.00100

 99 ->249 -0.00111

 99 ->273 0.00128

 100 ->167 0.00128

 100 ->178 0.00117

 100 ->193 0.00115

 100 ->204 -0.00111

 100 ->207 -0.00100

 100 ->212 0.00171

 100 ->216 0.00266

 100 ->232 0.00132

 100 ->243 -0.00108

 100 ->252 0.00156

 100 ->307 -0.00151

 101 ->162 0.00123

 101 ->206 0.00183

 101 ->211 0.00292

 101 ->215 0.00182

 101 ->218 0.00215

 101 ->224 -0.00311

 101 ->227 0.00151

 101 ->237 -0.00274

 101 ->247 0.00142

 101 ->256 -0.00134

 101 ->265 0.00150

 101 ->272 0.00114

 101 ->325 0.00116

 102 ->163 -0.00397

 102 ->243 0.00141

 103 ->164 -0.00241

 103 ->169 -0.00108

 103 ->226 0.00111

 103 ->244 -0.00136

 104 ->165 0.00162

 104 ->173 0.00174

 104 ->205 0.00101

 104 ->210 0.00153

 104 ->219 0.00132

 104 ->222 -0.00115

 104 ->229 0.00149

 104 ->245 -0.00107

 105 ->168 -0.00119

 105 ->169 0.00167

 105 ->208 -0.00119

 105 ->221 -0.00251

 105 ->226 0.00182

 105 ->249 -0.00105

 105 ->255 -0.00160

 105 ->332 -0.00153

 106 ->165 0.00212

 106 ->173 -0.00124

 106 ->181 0.00107

 106 ->190 -0.00187

 106 ->205 0.00176

 106 ->210 0.00190

 106 ->219 0.00307

 106 ->222 -0.00139

 106 ->225 -0.00158

 106 ->229 0.00103

 106 ->242 -0.00146

 106 ->301 0.00140

 107 ->162 -0.00131

 107 ->166 0.00134

 107 ->192 -0.00114

 107 ->194 0.00159

 107 ->206 0.00192

 107 ->211 0.00216

 107 ->215 0.00129

 107 ->224 -0.00237

 107 ->230 -0.00128

 107 ->237 -0.00223

 107 ->247 0.00270

 107 ->265 0.00101

 108 ->212 -0.00114

 108 ->220 0.00254

 108 ->232 0.00131

 108 ->261 -0.00126

 108 ->268 0.00142

 108 ->307 -0.00151

 108 ->333 0.00148

 109 ->162 0.00130

 109 ->166 0.00182

 109 ->174 -0.00104

 109 ->199 -0.00119

 109 ->215 -0.00231

 109 ->218 -0.00170

 109 ->224 0.00193

 109 ->227 -0.00138

 109 ->247 -0.00147

 109 ->263 0.00127

 109 ->265 -0.00112

 110 ->208 0.00102

 110 ->217 0.00160

 110 ->221 -0.00148

 110 ->249 -0.00214

 110 ->255 -0.00165

 110 ->266 -0.00116

 110 ->277 0.00146

 110 ->335 0.00101

 111 ->163 0.00303

 111 ->167 -0.00119

 111 ->175 -0.00253

 111 ->196 -0.00356

 111 ->212 0.00171

 112 ->164 0.00123

 112 ->169 -0.00152

 112 ->179 -0.00107

 112 ->180 -0.00242

 112 ->185 0.00170

 112 ->189 0.00378

 112 ->214 -0.00130

 113 ->178 0.00105

 113 ->184 -0.00378

 113 ->187 -0.00273

 113 ->193 0.00165

 113 ->200 -0.00108

 113 ->216 0.00421

 113 ->220 0.00373

 113 ->307 -0.00167

 114 ->168 0.00120

 114 ->179 0.00261

 114 ->180 -0.00167

 114 ->198 -0.00296

 114 ->202 -0.00197

 114 ->209 -0.00129

 114 ->221 -0.00433

 114 ->226 0.00144

 114 ->231 0.00102

 114 ->239 0.00174

 114 ->267 -0.00169

 114 ->269 -0.00134

 114 ->273 0.00108

 115 ->165 -0.00253

 115 ->181 -0.00361

 115 ->183 -0.00231

 115 ->188 -0.00187

 115 ->195 0.00211

 115 ->213 -0.00409

 115 ->219 -0.00334

 115 ->229 -0.00113

 115 ->251 0.00110

 115 ->301 -0.00141

 116 ->183 0.00234

 116 ->188 -0.00221

 117 ->177 -0.00120

 117 ->182 -0.00162

 117 ->186 -0.00263

 118 ->167 -0.00172

 118 ->178 -0.00310

 118 ->187 -0.00138

 118 ->193 0.00127

 118 ->212 -0.00169

 118 ->220 0.00415

 118 ->223 0.00117

 118 ->228 0.00159

 118 ->241 0.00108

 118 ->252 -0.00235

 118 ->333 0.00121

 119 ->163 -0.00154

 119 ->167 0.00114

 119 ->184 0.00210

 119 ->187 -0.00186

 119 ->193 -0.00126

 119 ->196 0.00122

 119 ->220 -0.00176

 120 ->164 -0.00104

 120 ->179 -0.00119

 120 ->180 0.00133

 120 ->185 0.00249

 120 ->189 -0.00210

 121 ->166 0.00229

 121 ->177 -0.00232

 121 ->182 0.00199

 121 ->199 0.00330

 121 ->206 0.00140

 121 ->215 -0.00406

 121 ->218 0.00352

 121 ->230 -0.00213

 121 ->237 -0.00247

 121 ->247 0.00221

 121 ->256 -0.00165

 121 ->312 -0.00155

 122 ->165 0.00258

 122 ->173 0.00127

 122 ->176 0.00139

 122 ->188 -0.00152

 122 ->190 0.00220

 122 ->197 0.00361

 122 ->201 0.00112

 122 ->210 0.00235

 122 ->213 -0.00346

 122 ->219 0.00291

 122 ->222 -0.00261

 122 ->229 0.00197

 122 ->251 -0.00212

 122 ->262 0.00261

 122 ->288 0.00174

 122 ->301 0.00110

 122 ->322 -0.00171

 123 ->170 -0.00215

 123 ->173 0.00248

 123 ->176 -0.00188

 123 ->195 -0.00271

 123 ->197 0.00315

 123 ->205 -0.00140

 123 ->210 -0.00295

 123 ->213 0.00184

 123 ->219 -0.00159

 123 ->222 0.00218

 123 ->225 -0.00211

 123 ->238 0.00105

 123 ->242 0.00137

 123 ->245 -0.00123

 123 ->253 -0.00187

 123 ->254 0.00133

 123 ->262 0.00139

 123 ->264 0.00139

 123 ->271 0.00118

 123 ->281 -0.00177

 123 ->285 0.00158

 123 ->288 0.00101

 123 ->306 -0.00103

 123 ->324 0.00156

 124 ->164 0.00200

 124 ->168 0.00309

 124 ->169 -0.00233

 124 ->179 -0.00125

 124 ->191 -0.00230

 124 ->198 -0.00320

 124 ->202 -0.00309

 124 ->208 0.00151

 124 ->217 0.00508

 124 ->221 -0.00102

 124 ->226 0.00149

 124 ->231 0.00233

 124 ->266 -0.00344

 124 ->273 0.00265

 124 ->300 0.00178

 124 ->303 0.00109

 124 ->335 0.00103

 125 ->166 0.00286

 125 ->171 0.00101

 125 ->177 -0.00113

 125 ->192 0.00234

 125 ->199 -0.00393

 125 ->206 0.00144

 125 ->211 0.00263

 125 ->215 0.00452

 125 ->218 -0.00169

 125 ->224 0.00239

 125 ->237 -0.00262

 125 ->240 0.00155

 125 ->247 0.00240

 125 ->263 0.00263

 125 ->304 -0.00156

 126 ->163 -0.00517

 126 ->167 0.00192

 126 ->172 -0.00212

 126 ->175 0.00644

 126 ->187 -0.00163

 126 ->193 0.00142

 126 ->196 -0.00253

 126 ->204 -0.00170

 126 ->220 -0.00167

 126 ->223 -0.00118

 126 ->250 0.00209

 126 ->259 -0.00190

 126 ->261 -0.00246

 126 ->282 -0.00102

 126 ->283 -0.00161

 126 ->291 -0.00150

 126 ->293 0.00122

 126 ->308 0.00217

 126 ->316 -0.00147

 127 ->163 -0.00359

 127 ->167 0.00295

 127 ->172 0.00321

 127 ->178 -0.00169

 127 ->184 -0.00258

 127 ->187 -0.00240

 127 ->216 -0.00245

 127 ->220 -0.00332

 127 ->223 -0.00204

 127 ->228 0.00301

 127 ->241 0.00133

 127 ->243 -0.00218

 127 ->250 0.00305

 127 ->252 0.00174

 127 ->257 -0.00439

 127 ->259 0.00147

 127 ->274 0.00145

 127 ->291 0.00117

 127 ->307 0.00167

 127 ->314 0.00134

 127 ->321 0.00115

 128 ->162 0.00331

 128 ->166 -0.00248

 128 ->171 -0.00114

 128 ->174 -0.00124

 128 ->186 0.00113

 128 ->199 0.00391

 128 ->211 0.00316

 128 ->215 0.00388

 128 ->224 0.00404

 128 ->227 -0.00360

 128 ->256 0.00143

 128 ->272 -0.00108

 128 ->287 0.00101

 128 ->296 -0.00104

 128 ->304 0.00114

 128 ->309 0.00108

 129 ->181 0.00353

 129 ->183 -0.00228

 129 ->188 -0.00432

 129 ->190 -0.00193

 129 ->195 0.00507

 129 ->197 0.00143

 129 ->210 -0.00200

 129 ->213 0.00525

 129 ->222 0.00534

 129 ->225 -0.00211

 129 ->229 0.00428

 129 ->238 0.00118

 129 ->245 0.00162

 129 ->253 0.00205

 129 ->262 0.00117

 129 ->264 -0.00371

 129 ->276 0.00109

 129 ->285 -0.00143

 129 ->306 -0.00112

 129 ->320 0.00101

 130 ->164 -0.00326

 130 ->168 0.00147

 130 ->169 0.00129

 130 ->202 0.00335

 130 ->209 0.00199

 130 ->214 0.00208

 130 ->217 0.00514

 130 ->221 -0.00417

 130 ->226 0.00119

 130 ->239 0.00244

 130 ->249 0.00340

 130 ->255 -0.00117

 130 ->289 0.00158

 130 ->300 -0.00144

 130 ->332 -0.00109

 131 ->163 0.00619

 131 ->167 -0.00325

 131 ->172 0.00141

 131 ->178 -0.00211

 131 ->184 -0.00225

 131 ->187 -0.00253

 131 ->200 0.00254

 131 ->220 -0.00169

 131 ->223 -0.00123

 131 ->228 0.00259

 131 ->232 0.00116

 131 ->257 -0.00161

 131 ->274 0.00112

 131 ->283 -0.00124

 132 ->165 -0.00360

 132 ->170 -0.00141

 132 ->173 0.00136

 132 ->176 -0.00227

 132 ->181 0.00379

 132 ->190 -0.00127

 132 ->213 0.00254

 132 ->219 0.00179

 132 ->222 0.00217

 132 ->225 -0.00172

 132 ->242 -0.00103

 132 ->254 0.00100

 133 ->164 0.00389

 133 ->168 0.00143

 133 ->169 -0.00355

 133 ->179 -0.00158

 133 ->189 0.00129

 133 ->191 0.00139

 133 ->198 0.00421

 133 ->202 0.00224

 133 ->209 0.00246

 133 ->214 0.00200

 133 ->217 0.00303

 133 ->221 -0.00319

 133 ->226 0.00129

 133 ->239 0.00180

 133 ->249 0.00221

 133 ->255 -0.00177

 133 ->260 0.00237

 133 ->266 -0.00127

 133 ->267 0.00138

 133 ->273 0.00162

 133 ->289 0.00182

 133 ->300 -0.00135

 134 ->162 -0.00163

 134 ->166 0.00130

 134 ->171 0.00270

 134 ->174 0.00257

 134 ->177 -0.00182

 134 ->182 -0.00253

 134 ->186 0.00283

 134 ->199 0.00398

 134 ->206 0.00165

 134 ->211 0.00305

 134 ->215 0.00382

 134 ->218 -0.00298

 134 ->224 0.00506

 134 ->227 -0.00187

 134 ->230 0.00109

 134 ->256 0.00113

 134 ->258 0.00146

 134 ->270 -0.00150

 134 ->272 -0.00159

 134 ->275 -0.00165

 134 ->280 -0.00101

 134 ->287 0.00131

 135 ->167 -0.00136

 135 ->172 -0.00106

 135 ->178 -0.00142

 135 ->193 -0.00326

 135 ->204 -0.00127

 135 ->207 -0.00200

 135 ->212 -0.00184

 135 ->216 -0.00389

 135 ->228 0.00194

 135 ->232 -0.00170

 135 ->252 -0.00185

 136 ->162 -0.00429

 136 ->166 -0.00269

 136 ->174 0.00322

 136 ->182 0.00125

 136 ->192 -0.00123

 136 ->199 -0.00125

 136 ->203 0.00163

 136 ->211 -0.00124

 136 ->215 -0.00174

 136 ->224 -0.00170

 136 ->235 -0.00180

 136 ->270 0.00127

 137 ->165 0.00352

 137 ->176 0.00120

 137 ->183 0.00131

 137 ->190 -0.00249

 137 ->201 0.00106

 137 ->205 -0.00201

 137 ->210 0.00269

 137 ->219 0.00273

 137 ->222 -0.00405

 137 ->225 0.00213

 137 ->229 0.00175

 137 ->233 0.00132

 137 ->242 -0.00188

 137 ->251 -0.00152

 137 ->288 0.00105

 137 ->301 0.00115

 138 ->164 0.00307

 138 ->179 -0.00190

 138 ->180 -0.00163

 138 ->189 0.00192

 138 ->191 0.00156

 138 ->198 -0.00201

 138 ->209 -0.00180

 138 ->217 0.00157

 138 ->221 0.00305

 138 ->226 -0.00107

 138 ->231 0.00155

 138 ->294 0.00106

 139 ->173 -0.00136

 139 ->190 -0.00174

 139 ->197 0.00285

 139 ->201 -0.00110

 139 ->233 -0.00148

 139 ->242 -0.00116

 140 ->163 0.00668

 140 ->184 -0.00108

 140 ->196 -0.00231

 140 ->204 -0.00120

 140 ->207 0.00133

 140 ->234 0.00196

 141 ->164 0.00195

 141 ->168 -0.00293

 141 ->169 0.00212

 141 ->179 0.00105

 141 ->180 -0.00152

 141 ->185 -0.00117

 141 ->191 -0.00179

 141 ->198 0.00183

 141 ->202 0.00139

 141 ->208 0.00159

 141 ->214 -0.00126

 141 ->217 -0.00329

 141 ->221 -0.00255

 141 ->236 -0.00210

 141 ->266 0.00250

 141 ->273 -0.00104

 142 ->166 0.00481

 142 ->171 0.00110

 142 ->177 -0.00193

 142 ->192 -0.00240

 142 ->199 -0.00322

 142 ->203 -0.00124

 142 ->206 -0.00106

 142 ->211 0.00220

 142 ->224 0.00123

 142 ->227 0.00111

 142 ->237 -0.00549

 142 ->247 0.00343

 142 ->263 0.00269

 142 ->292 -0.00124

 142 ->304 -0.00137

 142 ->342 0.00105

 143 ->162 0.00416

 143 ->166 0.00550

 143 ->171 -0.00239

 143 ->174 -0.00641

 143 ->194 0.00527

 143 ->203 0.00170

 143 ->206 -0.00110

 143 ->215 0.00115

 143 ->258 -0.00281

 143 ->270 -0.00134

 143 ->272 0.00116

 143 ->290 -0.00133

 144 ->165 -0.00316

 144 ->173 -0.00324

 144 ->181 -0.00125

 144 ->190 0.00120

 144 ->201 0.00201

 144 ->210 -0.00128

 144 ->242 0.00190

 144 ->246 -0.00118

 144 ->253 0.00109

 144 ->262 -0.00103

 144 ->271 0.00211

 144 ->276 -0.00143

 144 ->281 -0.00146

 144 ->306 -0.00109

 144 ->328 -0.00136

 145 ->164 -0.01194

 145 ->168 0.00886

 145 ->169 0.00335

 145 ->179 0.00350

 145 ->180 0.01290

 145 ->185 0.00105

 145 ->189 0.00331

 145 ->198 -0.00139

 145 ->202 0.00216

 145 ->209 -0.00255

 145 ->221 -0.00116

 145 ->260 -0.00313

 145 ->267 0.00182

 145 ->269 -0.00127

 145 ->277 -0.00117

 145 ->284 0.00111

 145 ->286 -0.00123

 145 ->289 -0.00114

 145 ->294 -0.00185

 145 ->318 0.00197

 145 ->339 -0.00119

 146 ->165 0.00429

 146 ->173 0.00553

 146 ->176 0.00585

 146 ->181 -0.01808

 146 ->188 0.00596

 146 ->190 0.00661

 146 ->195 -0.02604

 146 ->197 -0.00818

 146 ->205 -0.00266

 146 ->210 0.00147

 146 ->213 0.00178

 146 ->225 -0.00107

 146 ->229 0.00157

 146 ->238 0.00329

 146 ->242 0.00265

 146 ->245 0.00289

 146 ->246 0.00164

 146 ->253 0.00284

 146 ->262 0.00112

 146 ->281 0.00145

 146 ->354 0.00124

 146 ->360 0.00107

 146 ->447 0.00121

 146 ->456 0.00132

 146 ->463 -0.00224

 147 ->163 -0.00127

 147 ->167 0.00285

 147 ->175 0.00401

 147 ->184 0.00200

 147 ->187 0.00199

 147 ->193 -0.00195

 147 ->196 0.00112

 147 ->200 -0.00185

 147 ->207 0.00120

 147 ->212 0.00182

 147 ->216 0.00277

 147 ->220 -0.00780

 147 ->223 0.00138

 147 ->232 -0.00230

 147 ->243 0.00239

 147 ->252 -0.00422

 147 ->268 -0.00332

 147 ->274 0.00109

 147 ->291 -0.00106

 147 ->307 0.00251

 147 ->326 -0.00104

 147 ->333 -0.00230

 147 ->341 0.00107

 147 ->352 0.00108

 147 ->357 0.00148

 147 ->359 0.00113

 147 ->364 0.00243

 147 ->373 0.00138

 147 ->381 -0.00133

 147 ->384 -0.00251

 147 ->388 0.00106

 147 ->395 -0.00113

 147 ->407 -0.00164

 147 ->424 0.00210

 147 ->440 0.00102

 148 ->163 -0.03849

 148 ->167 -0.00410

 148 ->172 0.00308

 148 ->175 -0.01035

 148 ->178 0.00194

 148 ->187 0.00173

 148 ->193 -0.00110

 148 ->196 -0.00209

 148 ->204 0.00122

 148 ->212 0.00252

 148 ->220 -0.00207

 148 ->232 -0.00100

 148 ->252 -0.00114

 148 ->268 -0.00146

 149 ->164 -0.00894

 149 ->168 -0.00192

 149 ->169 -0.01094

 149 ->179 -0.00281

 149 ->180 -0.01083

 149 ->189 0.00528

 149 ->209 0.00166

 149 ->214 -0.00159

 149 ->260 0.00108

 149 ->318 -0.00151

 150 ->163 -0.08229

 150 ->167 0.01345

 150 ->172 -0.00380

 150 ->175 0.00544

 150 ->184 0.00163

 150 ->187 0.00135

 150 ->196 0.00275

 150 ->200 -0.00222

 150 ->204 -0.00226

 150 ->207 0.00110

 150 ->220 0.00146

 150 ->228 -0.00259

 150 ->232 -0.00150

 150 ->252 0.00265

 150 ->259 -0.00150

 150 ->278 -0.00141

 150 ->293 0.00116

 150 ->305 -0.00173

 150 ->344 0.00102

 151 ->162 0.03333

 151 ->166 0.00838

 151 ->171 -0.00648

 151 ->182 -0.00146

 151 ->199 -0.00120

 152 ->165 0.00971

 152 ->170 -0.00689

 152 ->173 -0.00298

 152 ->183 0.00101

 152 ->195 0.00155

 152 ->197 0.00147

 152 ->201 0.00146

 152 ->219 -0.00106

 152 ->222 -0.00121

 152 ->271 -0.00104

 152 ->298 0.00125

 153 ->167 -0.00461

 153 ->172 -0.00857

 153 ->175 -0.00179

 153 ->200 0.00198

 153 ->220 -0.00105

 153 ->268 -0.00149

 153 ->308 0.00116

 154 ->164 -0.01613

 154 ->168 0.01090

 154 ->180 -0.00231

 154 ->202 -0.00141

 154 ->209 -0.00104

 154 ->260 -0.00117

 154 ->300 0.00114

 154 ->303 -0.00110

 155 ->162 0.01967

 155 ->166 -0.01783

 155 ->171 -0.00932

 155 ->174 -0.00181

 155 ->182 0.00201

 155 ->186 -0.00195

 155 ->194 -0.00499

 155 ->199 -0.00139

 155 ->203 0.00221

 155 ->206 -0.00161

 155 ->211 -0.00160

 155 ->218 0.00195

 155 ->224 -0.00122

 155 ->230 -0.00265

 155 ->265 0.00104

 155 ->270 0.00148

 155 ->296 0.00117

 155 ->317 -0.00147

 155 ->325 0.00170

 156 ->165 0.01597

 156 ->170 0.00954

 156 ->173 -0.00395

 156 ->176 0.00192

 156 ->181 -0.00129

 156 ->183 -0.00211

 156 ->195 0.00178

 156 ->197 0.00239

 156 ->201 0.00203

 156 ->210 0.00106

 156 ->219 -0.00243

 156 ->225 0.00143

 156 ->245 0.00153

 156 ->279 -0.00122

 156 ->285 0.00177

 156 ->310 0.00163

 156 ->329 0.00134

 157 ->164 0.02120

 157 ->168 0.01363

 157 ->169 -0.01146

 157 ->179 0.00159

 157 ->180 0.00959

 157 ->185 0.00176

 157 ->189 0.00506

 157 ->198 0.00237

 157 ->214 0.00255

 157 ->217 -0.00221

 157 ->255 -0.00151

 157 ->260 -0.00107

 157 ->266 -0.00195

 157 ->267 0.00106

 157 ->303 0.00215

 157 ->323 0.00125

 157 ->355 0.00100

 158 ->163 -0.02856

 158 ->167 -0.00258

 158 ->172 0.00680

 158 ->175 0.01113

 158 ->178 -0.00409

 158 ->184 -0.00139

 158 ->193 -0.00142

 158 ->196 0.00188

 158 ->250 -0.00136

 158 ->259 0.00100

 158 ->268 -0.00278

 158 ->278 -0.00278

 158 ->283 0.00132

 158 ->291 -0.00196

 158 ->293 0.00174

 158 ->297 -0.00149

 158 ->305 -0.00362

 158 ->308 0.00369

 158 ->330 0.00139

 158 ->333 -0.00102

 158 ->407 0.00139

 159 ->165 -0.01036

 159 ->170 0.00703

 159 ->173 0.00482

 159 ->183 -0.00157

 159 ->190 -0.00121

 159 ->195 -0.00182

 159 ->197 -0.00108

 159 ->201 0.00151

 159 ->210 -0.00286

 159 ->251 0.00165

 159 ->264 -0.00157

 159 ->271 -0.00299

 159 ->285 0.00283

 159 ->295 0.00395

 159 ->298 0.00231

 159 ->301 0.00171

 159 ->320 -0.00156

 159 ->322 -0.00193

 159 ->324 0.00321

 159 ->338 -0.00175

 159 ->380 0.00133

 160 ->162 0.57285

 160 ->166 0.00529

 160 ->171 -0.01655

 160 ->174 -0.01636

 160 ->182 -0.00117

 160 ->194 0.00982

 160 ->199 0.00109

 160 ->206 -0.00110

 160 ->211 -0.00189

 160 ->215 0.00207

 160 ->247 -0.00169

 160 ->248 -0.00158

 160 ->258 -0.00124

 160 ->270 -0.00194

 160 ->272 0.00173

 160 ->290 -0.00107

 160 ->309 0.00111

 160 ->312 -0.00112

 160 ->317 -0.00156

 160 ->327 -0.00243

 160 ->331 -0.00200

 160 ->340 -0.00229

 161 ->163 0.41057

 161 ->167 -0.02624

 161 ->172 -0.02694

 161 ->175 0.02141

 161 ->178 -0.00492

 161 ->187 -0.00253

 161 ->200 0.00125

 161 ->204 -0.00375

 161 ->207 0.00154

 161 ->212 -0.00583

 161 ->216 0.00248

 161 ->243 -0.00183

 161 ->259 -0.00158

 161 ->261 -0.00254

 161 ->268 -0.00118

 161 ->278 -0.00230

 161 ->291 -0.00120

 161 ->308 -0.00146

 161 ->316 0.00110

 161 ->359 -0.00109

 161 ->395 0.00129

 161 ->407 -0.00118

 59 <-226 -0.00105

 74 <-210 -0.00104

 74 <-213 0.00115

 74 <-229 -0.00110

 75 <-249 -0.00110

 76 <-215 -0.00127

 76 <-230 0.00122

 77 <-163 0.00116

 77 <-220 0.00135

 78 <-213 -0.00143

 81 <-220 0.00173

 82 <-213 -0.00138

 83 <-217 -0.00146

 83 <-249 0.00124

 84 <-215 0.00131

 85 <-217 0.00182

 85 <-249 -0.00109

 86 <-167 -0.00105

 87 <-167 0.00113

 87 <-216 -0.00173

 87 <-228 -0.00141

 87 <-252 0.00142

 87 <-274 0.00110

 88 <-165 0.00161

 88 <-210 0.00204

 88 <-213 -0.00313

 88 <-222 -0.00120

 88 <-229 0.00102

 88 <-246 0.00112

 89 <-166 0.00147

 89 <-199 -0.00215

 89 <-211 0.00228

 89 <-215 0.00362

 89 <-237 -0.00129

 89 <-248 0.00131

 90 <-198 0.00144

 90 <-202 0.00107

 90 <-217 0.00152

 90 <-239 -0.00130

 90 <-249 -0.00236

 91 <-199 0.00209

 91 <-215 -0.00166

 91 <-230 -0.00148

 91 <-256 -0.00115

 92 <-188 -0.00107

 92 <-219 0.00276

 92 <-225 -0.00222

 92 <-251 0.00100

 92 <-254 0.00197

 92 <-264 -0.00105

 93 <-198 0.00104

 93 <-221 0.00126

 94 <-216 -0.00123

 94 <-252 -0.00121

 95 <-181 0.00372

 95 <-183 0.00206

 95 <-188 0.00207

 95 <-190 -0.00160

 95 <-195 0.00101

 95 <-210 -0.00137

 95 <-219 -0.00189

 95 <-222 0.00137

 95 <-242 0.00145

 96 <-178 0.00146

 96 <-184 0.00313

 96 <-187 0.00256

 96 <-193 -0.00214

 96 <-228 0.00120

 96 <-232 0.00184

 96 <-243 -0.00157

 96 <-250 0.00181

 97 <-177 0.00146

 97 <-211 0.00150

 97 <-215 0.00128

 97 <-227 0.00120

 97 <-230 -0.00132

 97 <-237 -0.00131

 97 <-247 0.00105

 97 <-256 -0.00107

 98 <-176 -0.00236

 98 <-181 0.00163

 98 <-183 0.00115

 98 <-188 0.00104

 98 <-190 -0.00113

 98 <-213 -0.00128

 98 <-219 0.00393

 98 <-225 -0.00111

 98 <-238 0.00104

 98 <-246 0.00112

 98 <-254 0.00120

 99 <-179 0.00104

 100 <-212 0.00113

 100 <-216 0.00180

 100 <-252 0.00114

 100 <-307 -0.00116

 101 <-206 0.00121

 101 <-211 0.00200

 101 <-215 0.00130

 101 <-218 0.00156

 101 <-224 -0.00235

 101 <-227 0.00111

 101 <-237 -0.00200

 101 <-247 0.00107

 101 <-256 -0.00107

 101 <-265 0.00113

 102 <-163 -0.00298

 103 <-164 -0.00170

 104 <-173 0.00136

 104 <-229 0.00107

 105 <-169 0.00101

 105 <-221 -0.00176

 105 <-226 0.00127

 105 <-255 -0.00118

 105 <-332 -0.00122

 106 <-165 0.00123

 106 <-190 -0.00118

 106 <-205 0.00115

 106 <-210 0.00138

 106 <-219 0.00225

 106 <-225 -0.00115

 106 <-242 -0.00104

 106 <-301 0.00107

 107 <-194 0.00103

 107 <-206 0.00129

 107 <-211 0.00154

 107 <-224 -0.00176

 107 <-237 -0.00167

 107 <-247 0.00198

 108 <-220 0.00177

 108 <-268 0.00108

 108 <-307 -0.00117

 108 <-333 0.00116

 109 <-166 0.00105

 109 <-215 -0.00160

 109 <-218 -0.00118

 109 <-224 0.00143

 109 <-227 -0.00100

 109 <-247 -0.00105

 109 <-263 0.00101

 110 <-217 0.00110

 110 <-221 -0.00101

 110 <-249 -0.00155

 110 <-255 -0.00122

 110 <-277 0.00112

 111 <-163 0.00156

 111 <-175 -0.00239

 111 <-196 -0.00215

 111 <-212 0.00110

 112 <-169 -0.00121

 112 <-180 -0.00217

 112 <-189 0.00211

 113 <-184 -0.00228

 113 <-187 -0.00166

 113 <-193 0.00102

 113 <-216 0.00284

 113 <-220 0.00254

 113 <-307 -0.00134

 114 <-179 0.00152

 114 <-180 -0.00101

 114 <-198 -0.00191

 114 <-202 -0.00119

 114 <-221 -0.00296

 114 <-226 0.00102

 114 <-239 0.00128

 114 <-267 -0.00121

 114 <-269 -0.00109

 115 <-165 -0.00128

 115 <-181 -0.00213

 115 <-183 -0.00141

 115 <-188 -0.00115

 115 <-195 0.00130

 115 <-213 -0.00264

 115 <-219 -0.00233

 115 <-301 -0.00106

 116 <-183 0.00139

 116 <-188 -0.00136

 117 <-186 -0.00160

 118 <-178 -0.00183

 118 <-212 -0.00101

 118 <-220 0.00287

 118 <-228 0.00107

 118 <-252 -0.00172

 119 <-163 -0.00112

 119 <-184 0.00126

 119 <-187 -0.00114

 119 <-220 -0.00121

 120 <-180 0.00103

 120 <-185 0.00153

 120 <-189 -0.00119

 121 <-166 0.00122

 121 <-177 -0.00134

 121 <-182 0.00115

 121 <-199 0.00202

 121 <-215 -0.00260

 121 <-218 0.00243

 121 <-230 -0.00147

 121 <-237 -0.00180

 121 <-247 0.00159

 121 <-256 -0.00123

 121 <-312 -0.00124

 122 <-165 0.00115

 122 <-190 0.00134

 122 <-197 0.00234

 122 <-210 0.00140

 122 <-213 -0.00232

 122 <-219 0.00212

 122 <-222 -0.00179

 122 <-229 0.00142

 122 <-251 -0.00150

 122 <-262 0.00182

 122 <-288 0.00129

 122 <-322 -0.00134

 123 <-173 0.00143

 123 <-176 -0.00105

 123 <-195 -0.00172

 123 <-197 0.00213

 123 <-210 -0.00213

 123 <-213 0.00119

 123 <-219 -0.00106

 123 <-222 0.00145

 123 <-225 -0.00138

 123 <-253 -0.00127

 123 <-281 -0.00133

 123 <-285 0.00112

 123 <-324 0.00122

 124 <-168 0.00156

 124 <-169 -0.00109

 124 <-191 -0.00139

 124 <-198 -0.00198

 124 <-202 -0.00187

 124 <-217 0.00342

 124 <-226 0.00102

 124 <-231 0.00163

 124 <-266 -0.00252

 124 <-273 0.00198

 124 <-300 0.00132

 125 <-166 0.00141

 125 <-192 0.00143

 125 <-199 -0.00243

 125 <-211 0.00174

 125 <-215 0.00299

 125 <-218 -0.00115

 125 <-224 0.00158

 125 <-237 -0.00186

 125 <-240 0.00107

 125 <-247 0.00170

 125 <-263 0.00190

 125 <-304 -0.00114

 126 <-167 0.00125

 126 <-175 0.00387

 126 <-196 -0.00195

 126 <-220 -0.00106

 126 <-250 0.00142

 126 <-259 -0.00114

 126 <-261 -0.00154

 126 <-283 -0.00116

 126 <-308 0.00166

 126 <-316 -0.00120

 127 <-163 -0.00179

 127 <-167 0.00137

 127 <-172 0.00148

 127 <-184 -0.00148

 127 <-187 -0.00140

 127 <-216 -0.00161

 127 <-220 -0.00240

 127 <-223 -0.00138

 127 <-228 0.00193

 127 <-243 -0.00159

 127 <-250 0.00226

 127 <-252 0.00128

 127 <-257 -0.00323

 127 <-259 0.00115

 127 <-274 0.00111

 127 <-307 0.00129

 127 <-314 0.00101

 128 <-166 -0.00108

 128 <-199 0.00232

 128 <-211 0.00191

 128 <-215 0.00252

 128 <-224 0.00274

 128 <-227 -0.00246

 128 <-256 0.00113

 129 <-181 0.00205

 129 <-183 -0.00129

 129 <-188 -0.00252

 129 <-190 -0.00118

 129 <-195 0.00298

 129 <-210 -0.00126

 129 <-213 0.00337

 129 <-222 0.00365

 129 <-225 -0.00152

 129 <-229 0.00287

 129 <-245 0.00109

 129 <-253 0.00150

 129 <-264 -0.00277

 129 <-285 -0.00108

 130 <-202 0.00198

 130 <-209 0.00128

 130 <-214 0.00129

 130 <-217 0.00336

 130 <-221 -0.00285

 130 <-239 0.00178

 130 <-249 0.00250

 130 <-289 0.00116

 130 <-300 -0.00102

 131 <-163 0.00171

 131 <-167 -0.00157

 131 <-178 -0.00111

 131 <-184 -0.00128

 131 <-187 -0.00145

 131 <-200 0.00150

 131 <-220 -0.00113

 131 <-228 0.00171

 131 <-257 -0.00118

 132 <-165 -0.00160

 132 <-176 -0.00122

 132 <-181 0.00212

 132 <-213 0.00161

 132 <-219 0.00121

 132 <-222 0.00148

 132 <-225 -0.00121

 133 <-164 0.00114

 133 <-169 -0.00190

 133 <-198 0.00241

 133 <-202 0.00139

 133 <-209 0.00139

 133 <-214 0.00126

 133 <-217 0.00199

 133 <-221 -0.00216

 133 <-239 0.00130

 133 <-249 0.00165

 133 <-255 -0.00122

 133 <-260 0.00163

 133 <-267 0.00100

 133 <-273 0.00124

 133 <-289 0.00138

 134 <-171 0.00139

 134 <-174 0.00119

 134 <-177 -0.00101

 134 <-182 -0.00144

 134 <-186 0.00161

 134 <-199 0.00228

 134 <-211 0.00189

 134 <-215 0.00245

 134 <-218 -0.00201

 134 <-224 0.00345

 134 <-227 -0.00127

 134 <-258 0.00102

 134 <-270 -0.00106

 134 <-272 -0.00119

 134 <-275 -0.00128

 135 <-193 -0.00183

 135 <-207 -0.00117

 135 <-212 -0.00106

 135 <-216 -0.00242

 135 <-228 0.00126

 135 <-232 -0.00112

 135 <-252 -0.00129

 136 <-166 -0.00114

 136 <-174 0.00181

 136 <-215 -0.00109

 136 <-224 -0.00112

 136 <-235 -0.00123

 137 <-165 0.00169

 137 <-190 -0.00136

 137 <-205 -0.00119

 137 <-210 0.00160

 137 <-219 0.00182

 137 <-222 -0.00266

 137 <-225 0.00135

 137 <-229 0.00118

 137 <-242 -0.00129

 137 <-251 -0.00105

 138 <-164 0.00106

 138 <-179 -0.00105

 138 <-180 -0.00101

 138 <-189 0.00101

 138 <-198 -0.00116

 138 <-209 -0.00107

 138 <-217 0.00103

 138 <-221 0.00194

 138 <-231 0.00105

 139 <-197 0.00170

 139 <-233 -0.00100

 140 <-163 0.00382

 140 <-196 -0.00133

 140 <-234 0.00130

 141 <-168 -0.00150

 141 <-198 0.00106

 141 <-217 -0.00208

 141 <-221 -0.00159

 141 <-236 -0.00140

 141 <-266 0.00178

 142 <-166 0.00225

 142 <-192 -0.00132

 142 <-199 -0.00184

 142 <-211 0.00136

 142 <-237 -0.00370

 142 <-247 0.00238

 142 <-263 0.00188

 143 <-166 0.00182

 143 <-171 -0.00107

 143 <-174 -0.00278

 143 <-194 0.00280

 143 <-203 0.00110

 143 <-258 -0.00189

 143 <-270 -0.00109

 144 <-165 -0.00147

 144 <-173 -0.00109

 144 <-201 0.00159

 144 <-242 0.00131

 144 <-271 0.00120

 144 <-276 -0.00118

 144 <-281 -0.00122

 145 <-168 0.00284

 145 <-169 0.00229

 145 <-179 0.00165

 145 <-180 0.00581

 145 <-189 0.00243

 145 <-202 0.00121

 145 <-209 -0.00109

 145 <-260 -0.00184

 145 <-294 -0.00120

 145 <-318 0.00127

 146 <-165 0.00147

 146 <-173 0.00217

 146 <-176 0.00259

 146 <-181 -0.00847

 146 <-188 0.00296

 146 <-190 0.00327

 146 <-195 -0.01317

 146 <-197 -0.00425

 146 <-205 -0.00140

 146 <-213 0.00104

 146 <-238 0.00210

 146 <-242 0.00170

 146 <-245 0.00187

 146 <-246 0.00108

 146 <-253 0.00191

 146 <-456 0.00104

 146 <-463 -0.00178

 147 <-163 -0.00116

 147 <-167 0.00105

 147 <-175 0.00233

 147 <-184 0.00101

 147 <-200 -0.00100

 147 <-216 0.00154

 147 <-220 -0.00486

 147 <-232 -0.00145

 147 <-243 0.00145

 147 <-252 -0.00276

 147 <-268 -0.00230

 147 <-307 0.00177

 147 <-333 -0.00168

 147 <-357 0.00110

 147 <-364 0.00183

 147 <-373 0.00103

 147 <-384 -0.00189

 147 <-407 -0.00125

 147 <-424 0.00166

 148 <-163 -0.00490

 148 <-167 -0.00155

 148 <-172 0.00129

 148 <-175 -0.00615

 148 <-178 0.00119

 148 <-187 0.00100

 148 <-196 -0.00170

 148 <-204 0.00102

 148 <-212 0.00194

 148 <-220 -0.00115

 149 <-164 -0.00346

 149 <-169 -0.00435

 149 <-179 -0.00161

 149 <-180 -0.00649

 149 <-189 0.00355

 149 <-209 0.00111

 149 <-214 -0.00129

 149 <-318 -0.00107

 150 <-163 -0.01651

 150 <-167 0.00345

 150 <-172 -0.00217

 150 <-175 0.00364

 150 <-196 0.00125

 150 <-200 -0.00121

 150 <-204 -0.00120

 150 <-228 -0.00165

 150 <-232 -0.00105

 150 <-252 0.00167

 150 <-259 -0.00105

 150 <-305 -0.00117

 151 <-162 0.00761

 151 <-166 0.00272

 152 <-165 0.00285

 152 <-170 -0.00115

 152 <-173 -0.00122

 153 <-163 0.00182

 153 <-167 -0.00173

 153 <-172 -0.00159

 153 <-175 -0.00120

 153 <-200 0.00103

 154 <-164 -0.00329

 154 <-168 0.00288

 154 <-180 -0.00121

 155 <-166 -0.00396

 155 <-171 -0.00303

 155 <-194 -0.00193

 155 <-218 0.00110

 155 <-230 -0.00169

 155 <-270 0.00102

 155 <-325 0.00115

 156 <-165 0.00364

 156 <-170 0.00266

 156 <-173 -0.00198

 156 <-219 -0.00141

 156 <-285 0.00127

 156 <-310 0.00105

 156 <-329 0.00107

 157 <-164 0.00507

 157 <-168 0.00274

 157 <-169 -0.00259

 157 <-180 0.00343

 157 <-189 0.00237

 157 <-198 0.00122

 157 <-214 0.00116

 157 <-217 -0.00130

 157 <-266 -0.00136

 157 <-303 0.00137

 158 <-163 -0.00186

 158 <-172 0.00200

 158 <-175 0.00441

 158 <-178 -0.00161

 158 <-196 0.00128

 158 <-268 -0.00185

 158 <-278 -0.00179

 158 <-291 -0.00132

 158 <-293 0.00125

 158 <-305 -0.00252

 158 <-308 0.00267

 158 <-407 0.00112

 159 <-165 -0.00278

 159 <-170 0.00193

 159 <-173 0.00145

 159 <-195 -0.00101

 159 <-201 0.00111

 159 <-210 -0.00156

 159 <-251 0.00113

 159 <-264 -0.00109

 159 <-271 -0.00209

 159 <-285 0.00183

 159 <-295 0.00272

 159 <-298 0.00156

 159 <-301 0.00122

 159 <-320 -0.00114

 159 <-322 -0.00133

 159 <-324 0.00228

 159 <-338 -0.00127

 159 <-380 0.00118

 160 <-162 -0.08544

 160 <-166 -0.00224

 160 <-171 -0.00690

 160 <-174 -0.00885

 160 <-194 0.00525

 160 <-203 -0.00121

 160 <-211 -0.00143

 160 <-215 0.00163

 160 <-247 -0.00139

 160 <-248 -0.00129

 160 <-312 -0.00109

 160 <-317 -0.00131

 160 <-327 -0.00171

 160 <-331 -0.00195

 160 <-340 -0.00151

 161 <-163 -0.09563

 161 <-167 -0.00482

 161 <-172 -0.00801

 161 <-175 0.01158

 161 <-178 -0.00240

 161 <-187 -0.00102

 161 <-204 -0.00238

 161 <-212 -0.00262

 161 <-216 0.00134

 161 <-243 -0.00175

 161 <-259 -0.00122

 161 <-261 -0.00173

 161 <-278 -0.00173

 161 <-291 -0.00110

 161 <-308 -0.00110

 161 <-330 0.00129

 Excited State 5: Singlet-A2 3.3495 eV 370.16 nm f=0.0000 <S\*\*2>=0.000

 63 ->199 0.00189

 63 ->256 -0.00132

 63 ->287 0.00120

 64 ->198 0.00145

 64 ->202 0.00119

 64 ->209 0.00103

 64 ->249 -0.00117

 64 ->277 -0.00138

 64 ->415 0.00115

 74 ->224 0.00149

 75 ->184 -0.00103

 84 ->183 0.00113

 84 ->188 0.00141

 84 ->213 -0.00221

 84 ->219 -0.00116

 84 ->264 0.00112

 85 ->216 -0.00135

 87 ->217 0.00181

 87 ->231 -0.00185

 88 ->215 0.00104

 89 ->188 -0.00104

 89 ->219 0.00185

 90 ->178 0.00118

 90 ->184 0.00198

 90 ->187 0.00160

 90 ->216 0.00281

 90 ->220 0.00122

 90 ->257 0.00103

 90 ->307 0.00106

 91 ->176 -0.00104

 91 ->183 0.00129

 91 ->188 0.00147

 91 ->213 -0.00197

 91 ->219 -0.00117

 91 ->222 0.00112

 92 ->230 -0.00228

 92 ->272 0.00100

 93 ->184 0.00109

 93 ->216 0.00146

 95 ->199 0.00185

 95 ->211 0.00106

 95 ->230 0.00148

 95 ->256 0.00156

 95 ->304 0.00116

 95 ->377 0.00105

 96 ->198 0.00161

 96 ->202 0.00135

 96 ->217 -0.00109

 96 ->221 -0.00127

 96 ->231 0.00103

 96 ->249 0.00166

 96 ->277 0.00110

 96 ->303 -0.00108

 96 ->332 0.00102

 96 ->379 0.00147

 96 ->394 -0.00140

 97 ->213 -0.00104

 98 ->211 0.00112

 98 ->215 0.00136

 101 ->213 -0.00121

 102 ->164 -0.00196

 104 ->162 0.00303

 106 ->162 -0.00242

 109 ->213 0.00104

 111 ->169 -0.00124

 111 ->189 0.00150

 112 ->163 0.00325

 112 ->175 -0.00113

 112 ->196 -0.00130

 113 ->217 -0.00146

 113 ->231 0.00207

 113 ->269 -0.00120

 113 ->286 0.00104

 113 ->335 0.00124

 113 ->356 -0.00115

 113 ->379 -0.00134

 114 ->184 -0.00104

 114 ->257 0.00102

 115 ->215 0.00120

 115 ->224 -0.00114

 115 ->227 0.00108

 115 ->230 0.00162

 115 ->272 -0.00113

 115 ->377 -0.00122

 116 ->162 0.00353

 116 ->174 -0.00106

 118 ->164 -0.00120

 118 ->231 0.00155

 118 ->269 -0.00110

 118 ->335 0.00108

 120 ->163 -0.00154

 121 ->195 -0.00107

 121 ->213 0.00126

 122 ->162 0.01108

 122 ->174 -0.00253

 122 ->199 -0.00126

 122 ->215 0.00157

 122 ->230 0.00136

 122 ->272 -0.00128

 122 ->325 0.00111

 122 ->377 -0.00105

 123 ->162 0.01739

 123 ->166 0.00154

 123 ->171 0.00137

 123 ->174 -0.00411

 123 ->211 -0.00113

 123 ->230 -0.00107

 123 ->317 0.00108

 124 ->257 0.00113

 126 ->164 -0.01124

 126 ->168 0.00229

 126 ->169 -0.00306

 126 ->180 0.00521

 127 ->164 0.00112

 127 ->180 -0.00109

 127 ->217 -0.00288

 127 ->231 0.00243

 127 ->236 0.00121

 127 ->244 0.00103

 127 ->269 -0.00170

 127 ->286 0.00102

 127 ->289 0.00112

 127 ->323 -0.00107

 127 ->335 0.00159

 127 ->356 -0.00149

 127 ->379 -0.00132

 127 ->415 0.00128

 128 ->195 -0.00140

 128 ->253 0.00105

 128 ->262 0.00171

 128 ->264 -0.00117

 128 ->365 -0.00106

 129 ->162 -0.00112

 129 ->199 -0.00169

 129 ->218 0.00103

 129 ->224 -0.00264

 129 ->227 0.00123

 129 ->230 0.00263

 129 ->237 0.00106

 129 ->256 0.00108

 129 ->272 -0.00181

 129 ->275 -0.00100

 129 ->312 -0.00140

 129 ->325 0.00164

 129 ->345 -0.00159

 129 ->348 0.00168

 129 ->377 -0.00183

 129 ->411 -0.00134

 129 ->438 -0.00115

 130 ->216 -0.00135

 130 ->252 -0.00108

 130 ->257 -0.00148

 130 ->307 -0.00163

 131 ->198 -0.00106

 131 ->202 -0.00105

 132 ->166 -0.00102

 132 ->199 0.00105

 133 ->163 0.00106

 133 ->184 0.00173

 133 ->187 0.00136

 133 ->193 -0.00124

 133 ->216 -0.00171

 133 ->257 -0.00147

 133 ->307 -0.00115

 133 ->359 0.00108

 133 ->368 -0.00102

 134 ->183 0.00103

 134 ->188 0.00137

 134 ->195 -0.00151

 134 ->213 0.00112

 134 ->222 -0.00114

 134 ->262 0.00106

 134 ->365 -0.00109

 138 ->163 0.00209

 139 ->162 0.00252

 141 ->163 0.00148

 143 ->165 0.00159

 143 ->173 0.00128

 144 ->162 0.00422

 144 ->171 -0.00110

 144 ->174 -0.00659

 144 ->194 0.00198

 144 ->203 -0.00120

 144 ->211 -0.00189

 145 ->163 -0.02774

 145 ->167 -0.00191

 145 ->175 0.00136

 146 ->162 -0.00697

 146 ->215 0.00129

 146 ->230 0.00109

 146 ->256 0.00202

 146 ->265 -0.00126

 146 ->296 0.00106

 146 ->309 -0.00121

 146 ->312 -0.00115

 146 ->342 0.00146

 146 ->345 -0.00101

 146 ->366 0.00103

 147 ->164 0.00309

 147 ->217 -0.00119

 147 ->221 -0.00144

 147 ->255 -0.00103

 147 ->260 -0.00112

 147 ->267 -0.00129

 147 ->269 -0.00107

 147 ->323 -0.00136

 147 ->332 0.00173

 147 ->335 0.00150

 148 ->164 -0.00800

 148 ->169 -0.00155

 148 ->180 -0.00316

 148 ->189 -0.00191

 149 ->163 0.00603

 149 ->175 -0.00207

 150 ->164 -0.01329

 150 ->168 -0.00221

 150 ->180 -0.00297

 150 ->185 -0.00125

 150 ->189 -0.00492

 150 ->191 0.00144

 150 ->198 0.00158

 150 ->202 0.00154

 150 ->214 0.00198

 151 ->165 -0.00120

 152 ->162 0.05182

 152 ->174 0.00251

 152 ->194 -0.00202

 153 ->164 -0.01310

 153 ->180 -0.00304

 153 ->185 -0.00129

 153 ->189 -0.00417

 153 ->214 0.00146

 154 ->167 0.00131

 154 ->172 0.00105

 155 ->165 -0.00274

 155 ->173 -0.00185

 155 ->188 -0.00116

 155 ->195 0.00101

 156 ->162 0.02805

 156 ->166 0.00261

 156 ->174 0.00366

 156 ->194 -0.00127

 156 ->199 -0.00134

 156 ->215 -0.00115

 157 ->163 -0.03350

 157 ->167 -0.00241

 157 ->172 -0.00294

 157 ->175 0.00196

 158 ->164 -0.05242

 158 ->169 -0.00626

 158 ->179 -0.00169

 158 ->180 -0.00943

 158 ->185 -0.00367

 158 ->189 -0.01484

 158 ->191 0.00234

 158 ->198 0.00127

 158 ->209 -0.00328

 158 ->214 0.00578

 158 ->244 0.00152

 158 ->260 -0.00141

 158 ->303 -0.00102

 158 ->318 -0.00204

 158 ->323 0.00124

 158 ->487 -0.00114

 159 ->162 0.69718

 159 ->171 0.01111

 159 ->174 0.01397

 159 ->194 -0.01314

 159 ->199 0.00101

 159 ->203 0.00442

 159 ->211 0.00609

 159 ->215 -0.00303

 159 ->237 0.00188

 159 ->240 -0.00106

 159 ->258 -0.00101

 159 ->280 0.00120

 159 ->296 0.00146

 159 ->309 0.00189

 159 ->331 0.00126

 160 ->170 0.00206

 160 ->173 0.01016

 160 ->197 -0.00121

 160 ->324 0.00116

 161 ->164 0.05971

 161 ->168 0.00160

 161 ->169 0.00237

 161 ->180 -0.00210

 161 ->185 0.00105

 161 ->189 0.00115

 63 <-199 0.00137

 63 <-287 0.00100

 64 <-198 0.00108

 64 <-415 0.00101

 74 <-224 0.00112

 84 <-213 -0.00150

 87 <-217 0.00128

 87 <-231 -0.00134

 89 <-219 0.00131

 90 <-184 0.00127

 90 <-187 0.00103

 90 <-216 0.00195

 91 <-213 -0.00135

 92 <-230 -0.00160

 95 <-199 0.00126

 95 <-256 0.00107

 96 <-198 0.00108

 96 <-249 0.00112

 96 <-379 0.00114

 96 <-394 -0.00109

 102 <-164 -0.00123

 104 <-162 0.00110

 111 <-189 0.00114

 113 <-231 0.00144

 113 <-379 -0.00108

 115 <-230 0.00112

 116 <-162 0.00110

 118 <-231 0.00106

 122 <-162 0.00258

 122 <-174 -0.00207

 122 <-215 0.00106

 123 <-162 0.00389

 123 <-174 -0.00323

 126 <-164 -0.00438

 126 <-168 0.00119

 126 <-169 -0.00116

 126 <-180 0.00363

 126 <-189 0.00100

 127 <-217 -0.00186

 127 <-231 0.00163

 127 <-269 -0.00129

 127 <-335 0.00121

 127 <-356 -0.00116

 127 <-379 -0.00106

 127 <-415 0.00105

 128 <-262 0.00113

 129 <-224 -0.00180

 129 <-230 0.00172

 129 <-272 -0.00138

 129 <-312 -0.00101

 129 <-325 0.00122

 129 <-345 -0.00124

 129 <-348 0.00132

 129 <-377 -0.00146

 129 <-411 -0.00108

 130 <-307 -0.00113

 144 <-174 -0.00444

 145 <-163 -0.00596

 146 <-256 0.00125

 146 <-342 0.00108

 147 <-332 0.00124

 147 <-335 0.00108

 148 <-164 0.00121

 148 <-180 -0.00227

 149 <-196 -0.00104

 150 <-164 0.00184

 150 <-168 -0.00113

 150 <-180 -0.00200

 150 <-189 -0.00150

 152 <-162 -0.00198

 152 <-174 0.00163

 153 <-164 0.00261

 153 <-169 0.00114

 153 <-180 -0.00225

 156 <-174 0.00226

 157 <-163 -0.00321

 157 <-172 -0.00102

 158 <-164 0.00934

 158 <-168 -0.00218

 158 <-169 0.00271

 158 <-179 -0.00109

 158 <-180 -0.00692

 158 <-189 -0.00349

 158 <-198 0.00109

 158 <-209 -0.00114

 158 <-214 0.00217

 158 <-266 -0.00123

 158 <-289 -0.00115

 158 <-303 -0.00108

 158 <-319 -0.00112

 158 <-323 0.00119

 159 <-162 -0.01387

 159 <-166 -0.00156

 159 <-174 0.00881

 159 <-177 0.00105

 159 <-186 -0.00104

 159 <-194 -0.00299

 159 <-203 0.00115

 159 <-211 0.00241

 159 <-215 -0.00116

 159 <-296 0.00123

 159 <-309 0.00147

 159 <-342 0.00103

 160 <-173 0.00466

 160 <-210 0.00106

 161 <-164 -0.00584

 161 <-168 0.00172

 161 <-169 -0.00159

 Excited State 6: Singlet-B2 3.4947 eV 354.78 nm f=0.3955 <S\*\*2>=0.000

 61 ->195 0.00112

 63 ->198 0.00118

 63 ->277 -0.00133

 63 ->415 0.00102

 64 ->199 0.00177

 64 ->256 -0.00135

 64 ->263 -0.00113

 64 ->287 0.00131

 75 ->213 0.00143

 81 ->218 -0.00136

 83 ->181 -0.00155

 83 ->190 0.00109

 83 ->195 -0.00132

 84 ->184 0.00136

 84 ->187 0.00121

 84 ->216 0.00156

 84 ->307 0.00103

 85 ->181 0.00131

 85 ->188 -0.00124

 85 ->195 0.00227

 85 ->219 0.00105

 87 ->230 -0.00188

 87 ->272 0.00104

 88 ->231 0.00109

 89 ->184 -0.00121

 90 ->176 -0.00189

 90 ->181 0.00234

 90 ->183 0.00164

 90 ->188 0.00155

 90 ->229 0.00108

 91 ->178 0.00108

 91 ->184 0.00179

 91 ->187 0.00122

 91 ->228 0.00135

 92 ->217 0.00123

 92 ->231 -0.00143

 93 ->181 0.00171

 93 ->188 0.00107

 93 ->213 -0.00114

 94 ->177 -0.00113

 95 ->198 0.00177

 95 ->202 0.00116

 95 ->379 0.00103

 95 ->394 -0.00123

 96 ->199 0.00231

 96 ->256 0.00102

 96 ->304 0.00112

 96 ->377 0.00110

 97 ->178 -0.00111

 97 ->184 0.00103

 98 ->179 -0.00110

 98 ->379 0.00107

 99 ->176 0.00135

 99 ->213 0.00112

 99 ->222 -0.00174

 101 ->216 0.00153

 102 ->162 0.00159

 105 ->195 0.00233

 105 ->205 0.00113

 105 ->222 0.00135

 105 ->245 -0.00131

 106 ->208 -0.00111

 108 ->182 -0.00121

 108 ->192 0.00104

 108 ->265 -0.00116

 109 ->216 -0.00165

 109 ->250 -0.00116

 110 ->195 0.00294

 111 ->162 0.00324

 111 ->174 -0.00126

 113 ->182 0.00135

 113 ->186 -0.00111

 113 ->218 0.00110

 113 ->224 -0.00245

 113 ->227 0.00166

 113 ->230 0.00189

 113 ->272 -0.00102

 113 ->345 -0.00100

 113 ->348 0.00119

 113 ->377 -0.00136

 114 ->165 -0.00108

 114 ->181 0.00144

 114 ->183 -0.00114

 114 ->188 -0.00114

 114 ->213 0.00101

 114 ->222 0.00118

 115 ->217 -0.00124

 115 ->231 0.00203

 115 ->239 -0.00104

 115 ->244 0.00104

 115 ->269 -0.00138

 115 ->335 0.00101

 115 ->356 -0.00107

 115 ->379 -0.00105

 116 ->185 -0.00179

 117 ->184 -0.00120

 117 ->187 0.00146

 118 ->162 0.00190

 118 ->177 0.00106

 118 ->224 -0.00227

 118 ->227 0.00116

 118 ->230 0.00125

 118 ->272 -0.00101

 118 ->377 -0.00106

 119 ->162 -0.00124

 119 ->182 0.00107

 119 ->186 0.00123

 119 ->224 0.00139

 120 ->183 -0.00119

 120 ->188 0.00123

 121 ->178 0.00122

 121 ->200 -0.00105

 121 ->228 0.00119

 121 ->250 -0.00150

 121 ->252 -0.00104

 122 ->164 -0.00287

 122 ->168 0.00109

 122 ->169 -0.00181

 122 ->179 0.00112

 122 ->180 0.00185

 122 ->202 -0.00128

 122 ->217 -0.00127

 122 ->231 0.00249

 122 ->236 0.00107

 122 ->379 -0.00108

 123 ->164 -0.00556

 123 ->180 0.00277

 123 ->231 -0.00156

 124 ->165 0.00134

 124 ->190 -0.00155

 124 ->195 0.00217

 124 ->197 0.00108

 124 ->213 0.00152

 124 ->219 0.00150

 124 ->222 -0.00148

 124 ->229 0.00114

 124 ->246 0.00107

 125 ->167 -0.00149

 125 ->200 0.00157

 125 ->216 -0.00128

 125 ->220 0.00151

 126 ->162 0.01860

 126 ->171 0.00139

 126 ->174 -0.00258

 126 ->194 0.00130

 126 ->211 -0.00105

 127 ->162 -0.00554

 127 ->224 -0.00314

 127 ->227 0.00260

 127 ->230 0.00307

 127 ->272 -0.00195

 127 ->287 0.00136

 127 ->317 -0.00165

 127 ->325 0.00117

 127 ->345 -0.00150

 127 ->348 0.00135

 127 ->377 -0.00163

 127 ->411 -0.00105

 128 ->163 0.00186

 128 ->167 -0.00126

 128 ->216 0.00165

 128 ->232 -0.00121

 128 ->243 0.00116

 128 ->252 -0.00126

 128 ->257 -0.00151

 128 ->359 0.00103

 129 ->217 -0.00406

 129 ->221 0.00115

 129 ->231 0.00342

 129 ->236 0.00148

 129 ->239 -0.00131

 129 ->244 0.00145

 129 ->249 -0.00132

 129 ->269 -0.00255

 129 ->286 0.00176

 129 ->335 0.00219

 129 ->355 -0.00113

 129 ->356 -0.00190

 129 ->379 -0.00160

 129 ->415 0.00112

 130 ->165 0.00157

 130 ->195 -0.00121

 130 ->229 0.00115

 130 ->253 0.00100

 130 ->254 -0.00125

 130 ->262 0.00150

 130 ->365 -0.00103

 131 ->162 0.00772

 131 ->224 -0.00141

 131 ->227 0.00111

 131 ->230 0.00173

 131 ->272 -0.00114

 131 ->377 -0.00103

 132 ->164 0.00444

 133 ->210 0.00104

 133 ->229 0.00170

 133 ->254 -0.00142

 133 ->262 0.00142

 133 ->322 0.00108

 133 ->365 -0.00122

 134 ->163 -0.00303

 134 ->220 0.00151

 134 ->252 -0.00138

 134 ->257 -0.00117

 135 ->162 0.00167

 135 ->192 0.00165

 135 ->206 0.00103

 136 ->163 -0.00221

 137 ->191 -0.00127

 137 ->198 0.00113

 137 ->221 -0.00169

 138 ->201 0.00107

 139 ->164 -0.00202

 139 ->209 0.00114

 140 ->162 0.00284

 140 ->203 -0.00109

 141 ->165 -0.00148

 141 ->197 -0.00127

 141 ->222 0.00123

 142 ->167 -0.00172

 142 ->193 0.00116

 142 ->200 0.00115

 142 ->220 0.00110

 142 ->232 0.00190

 142 ->250 -0.00111

 143 ->163 0.00654

 143 ->167 0.00215

 143 ->175 0.00277

 144 ->164 -0.00578

 144 ->169 -0.00384

 144 ->189 0.00410

 144 ->214 -0.00141

 144 ->318 0.00135

 145 ->197 0.00138

 145 ->201 0.00180

 145 ->210 -0.00111

 146 ->164 0.00490

 146 ->168 -0.00109

 146 ->180 -0.00156

 146 ->217 -0.00518

 146 ->231 0.00283

 146 ->236 0.00131

 146 ->249 0.00204

 146 ->303 -0.00122

 146 ->335 0.00101

 147 ->162 -0.02674

 147 ->182 -0.00118

 147 ->199 -0.00143

 147 ->211 0.00163

 147 ->215 0.00299

 147 ->218 0.00319

 147 ->224 -0.00238

 147 ->230 0.00470

 147 ->237 0.00154

 147 ->256 0.00160

 147 ->265 0.00123

 148 ->162 -0.00943

 148 ->171 0.00140

 148 ->174 0.00413

 148 ->211 0.00111

 148 ->230 0.00160

 148 ->296 0.00131

 149 ->173 -0.00180

 149 ->285 -0.00120

 149 ->295 -0.00137

 149 ->380 -0.00100

 150 ->162 -0.01870

 150 ->166 0.00247

 150 ->171 0.00289

 150 ->174 0.00639

 150 ->194 -0.00203

 150 ->211 0.00160

 150 ->215 -0.00124

 150 ->230 -0.00133

 151 ->163 -0.00954

 151 ->167 -0.00327

 151 ->172 0.00323

 151 ->175 0.00118

 152 ->164 -0.01062

 152 ->168 -0.00419

 152 ->169 -0.00275

 152 ->180 -0.00224

 152 ->189 -0.00357

 153 ->162 0.08858

 153 ->166 -0.00232

 153 ->171 0.00676

 153 ->174 0.00591

 153 ->194 -0.00409

 153 ->203 0.00158

 153 ->211 0.00139

 154 ->165 0.00270

 154 ->170 0.00600

 154 ->173 0.00217

 155 ->163 0.03492

 155 ->167 -0.00717

 155 ->175 0.00114

 155 ->196 -0.00250

 155 ->204 0.00123

 156 ->164 -0.02708

 156 ->169 0.00545

 156 ->185 -0.00122

 156 ->189 -0.00538

 156 ->191 0.00101

 156 ->209 -0.00143

 157 ->165 -0.00636

 157 ->170 -0.00241

 157 ->173 -0.00379

 157 ->197 -0.00101

 157 ->222 -0.00104

 158 ->162 0.67740

 158 ->166 -0.00637

 158 ->171 0.00811

 158 ->174 0.02187

 158 ->177 0.00160

 158 ->186 -0.00131

 158 ->192 0.00121

 158 ->194 -0.01427

 158 ->199 0.00131

 158 ->203 0.00462

 158 ->206 -0.00114

 158 ->211 0.00621

 158 ->215 -0.00313

 158 ->237 0.00143

 158 ->258 -0.00105

 158 ->309 0.00129

 159 ->164 -0.03948

 159 ->168 -0.00754

 159 ->169 -0.00358

 159 ->179 -0.00367

 159 ->180 -0.01733

 159 ->185 -0.00407

 159 ->189 -0.01710

 159 ->191 0.00282

 159 ->198 0.00226

 159 ->202 0.00154

 159 ->209 -0.00336

 159 ->214 0.00634

 159 ->244 0.00118

 159 ->260 -0.00155

 159 ->318 -0.00125

 159 ->323 0.00115

 160 ->163 -0.10896

 160 ->172 0.00571

 160 ->175 -0.00734

 160 ->196 -0.00414

 160 ->204 0.00127

 160 ->212 0.00236

 160 ->268 -0.00100

 160 ->305 -0.00123

 161 ->162 0.12118

 161 ->166 -0.00557

 161 ->171 -0.02042

 161 ->174 -0.01079

 161 ->194 0.00534

 161 ->203 -0.00233

 161 ->211 -0.00313

 161 ->215 0.00152

 64 <-199 0.00127

 64 <-256 -0.00100

 64 <-287 0.00108

 84 <-216 0.00103

 85 <-195 0.00151

 87 <-230 -0.00137

 90 <-176 -0.00119

 90 <-181 0.00148

 90 <-183 0.00104

 91 <-184 0.00113

 92 <-231 -0.00100

 93 <-181 0.00106

 95 <-198 0.00114

 96 <-199 0.00152

 99 <-222 -0.00116

 105 <-195 0.00141

 109 <-216 -0.00101

 110 <-195 0.00175

 111 <-162 0.00135

 113 <-224 -0.00166

 113 <-227 0.00112

 113 <-230 0.00129

 113 <-377 -0.00108

 115 <-231 0.00139

 115 <-269 -0.00104

 118 <-224 -0.00150

 122 <-164 -0.00104

 122 <-180 0.00135

 122 <-231 0.00171

 123 <-164 -0.00210

 123 <-180 0.00211

 123 <-189 0.00104

 124 <-195 0.00120

 126 <-162 0.00321

 126 <-174 -0.00273

 126 <-194 0.00111

 127 <-162 -0.00102

 127 <-224 -0.00212

 127 <-227 0.00173

 127 <-230 0.00201

 127 <-272 -0.00142

 127 <-287 0.00104

 127 <-317 -0.00125

 127 <-345 -0.00113

 127 <-348 0.00107

 127 <-377 -0.00128

 128 <-216 0.00109

 129 <-217 -0.00257

 129 <-231 0.00227

 129 <-249 -0.00100

 129 <-269 -0.00188

 129 <-286 0.00130

 129 <-335 0.00165

 129 <-356 -0.00145

 129 <-379 -0.00127

 131 <-230 0.00111

 133 <-229 0.00120

 133 <-254 -0.00101

 134 <-220 0.00106

 137 <-221 -0.00102

 139 <-164 -0.00103

 140 <-162 0.00148

 142 <-232 0.00118

 143 <-163 0.00125

 143 <-175 0.00154

 144 <-164 -0.00493

 144 <-169 -0.00142

 144 <-189 0.00160

 146 <-217 -0.00279

 146 <-231 0.00155

 146 <-249 0.00116

 147 <-162 -0.00174

 147 <-211 0.00102

 147 <-215 0.00148

 147 <-218 0.00173

 147 <-224 -0.00130

 147 <-230 0.00265

 148 <-162 -0.00104

 148 <-174 0.00339

 149 <-173 -0.00173

 150 <-162 -0.00888

 150 <-174 0.00259

 151 <-163 -0.00188

 152 <-164 0.00115

 152 <-180 -0.00142

 152 <-189 -0.00104

 153 <-162 -0.00251

 153 <-174 0.00342

 153 <-194 -0.00110

 156 <-164 0.00190

 156 <-169 0.00142

 156 <-189 -0.00127

 158 <-162 -0.01522

 158 <-166 -0.00234

 158 <-174 0.01092

 158 <-177 0.00124

 158 <-182 -0.00104

 158 <-186 -0.00111

 158 <-194 -0.00386

 158 <-203 0.00136

 158 <-211 0.00262

 158 <-215 -0.00128

 158 <-309 0.00110

 158 <-317 -0.00111

 158 <-342 0.00103

 159 <-164 0.01161

 159 <-168 -0.00438

 159 <-169 0.00335

 159 <-179 -0.00189

 159 <-180 -0.01015

 159 <-189 -0.00478

 159 <-198 0.00162

 159 <-209 -0.00120

 159 <-214 0.00252

 159 <-260 -0.00102

 159 <-266 -0.00106

 159 <-323 0.00107

 160 <-163 0.02405

 160 <-172 0.00118

 160 <-175 -0.00400

 160 <-196 -0.00169

 160 <-212 0.00103

 161 <-162 -0.02822

 161 <-166 0.00125

 161 <-171 -0.00214

 161 <-174 -0.00537

 161 <-194 0.00226

 161 <-203 -0.00111

 161 <-211 -0.00118

 Excited State 7: Singlet-A1 3.5668 eV 347.60 nm f=0.0000 <S\*\*2>=0.000

 51 ->216 0.00196

 51 ->232 -0.00120

 52 ->213 -0.00137

 52 ->222 0.00169

 58 ->216 0.00104

 63 ->216 -0.00111

 63 ->223 -0.00109

 63 ->228 0.00149

 63 ->232 0.00128

 63 ->341 -0.00101

 64 ->181 0.00168

 64 ->195 0.00123

 64 ->222 -0.00102

 64 ->229 0.00133

 70 ->216 -0.00106

 73 ->213 0.00101

 74 ->216 -0.00105

 75 ->224 0.00121

 76 ->217 -0.00112

 81 ->181 -0.00168

 82 ->216 -0.00106

 84 ->198 0.00120

 84 ->249 -0.00144

 85 ->218 0.00109

 85 ->227 -0.00103

 85 ->230 0.00149

 87 ->222 -0.00116

 89 ->217 0.00117

 90 ->199 0.00167

 90 ->224 0.00147

 90 ->227 -0.00120

 90 ->230 -0.00118

 90 ->263 -0.00157

 90 ->270 -0.00109

 90 ->304 -0.00101

 91 ->202 0.00139

 91 ->221 -0.00128

 91 ->231 -0.00224

 91 ->236 -0.00118

 91 ->269 -0.00107

 91 ->277 -0.00204

 92 ->220 0.00218

 95 ->187 0.00105

 95 ->220 -0.00194

 95 ->228 -0.00124

 95 ->252 -0.00108

 96 ->181 -0.00190

 96 ->188 0.00171

 96 ->195 -0.00389

 96 ->197 -0.00123

 96 ->219 0.00101

 96 ->229 -0.00173

 97 ->217 0.00114

 99 ->224 0.00139

 99 ->227 -0.00103

 99 ->230 -0.00234

 99 ->263 -0.00111

 99 ->265 -0.00123

 100 ->213 0.00104

 101 ->231 0.00199

 101 ->277 0.00121

 101 ->332 -0.00102

 102 ->197 0.00126

 103 ->174 0.00135

 105 ->218 0.00130

 105 ->230 0.00204

 105 ->265 0.00187

 108 ->181 -0.00105

 108 ->195 -0.00275

 109 ->221 -0.00123

 109 ->231 -0.00274

 109 ->236 -0.00137

 109 ->277 -0.00191

 109 ->332 0.00116

 110 ->218 0.00109

 110 ->227 -0.00119

 111 ->197 0.00194

 112 ->174 0.00172

 113 ->213 0.00131

 113 ->245 0.00110

 113 ->264 -0.00108

 114 ->256 -0.00114

 115 ->216 -0.00193

 115 ->232 0.00112

 118 ->181 -0.00113

 121 ->198 0.00125

 121 ->221 -0.00157

 121 ->249 0.00103

 122 ->163 -0.00114

 122 ->175 0.00110

 122 ->196 -0.00221

 123 ->163 -0.00187

 123 ->175 0.00202

 123 ->196 -0.00350

 123 ->212 0.00167

 124 ->166 -0.00174

 124 ->224 0.00251

 124 ->227 -0.00154

 124 ->230 -0.00288

 124 ->237 0.00106

 124 ->240 -0.00114

 124 ->247 -0.00131

 124 ->263 -0.00195

 124 ->304 -0.00149

 125 ->169 0.00105

 125 ->217 0.00161

 125 ->231 -0.00246

 125 ->236 -0.00113

 125 ->249 -0.00131

 125 ->277 -0.00115

 126 ->173 0.00587

 126 ->197 0.00281

 126 ->201 0.00138

 126 ->210 -0.00114

 127 ->173 -0.00145

 127 ->195 -0.00153

 127 ->197 -0.00108

 127 ->222 -0.00122

 127 ->245 0.00104

 127 ->313 0.00116

 127 ->354 -0.00115

 128 ->164 0.00111

 128 ->217 -0.00218

 128 ->231 0.00243

 128 ->236 0.00122

 128 ->277 0.00189

 129 ->163 0.00115

 129 ->252 -0.00117

 129 ->268 -0.00106

 129 ->321 -0.00161

 129 ->341 -0.00121

 130 ->224 -0.00129

 130 ->230 0.00190

 132 ->163 0.00332

 133 ->162 0.00114

 133 ->224 -0.00130

 133 ->230 0.00146

 134 ->217 -0.00164

 134 ->231 0.00126

 136 ->180 0.00183

 137 ->216 0.00101

 138 ->230 -0.00104

 139 ->163 -0.00134

 140 ->173 0.00114

 141 ->162 -0.00194

 141 ->166 0.00113

 141 ->224 -0.00103

 141 ->230 0.00144

 141 ->237 -0.00105

 141 ->263 0.00107

 142 ->164 -0.00146

 142 ->169 0.00124

 142 ->217 0.00129

 142 ->221 -0.00148

 142 ->231 -0.00223

 142 ->236 -0.00103

 142 ->277 -0.00139

 143 ->168 -0.00270

 143 ->179 -0.00121

 143 ->180 -0.00542

 143 ->189 -0.00214

 144 ->163 -0.02284

 144 ->172 -0.00205

 144 ->175 0.00386

 145 ->162 0.01693

 145 ->166 -0.00156

 145 ->171 0.00172

 145 ->174 0.01123

 145 ->177 0.00111

 145 ->194 -0.00274

 145 ->211 0.00120

 146 ->163 -0.01771

 146 ->172 -0.00130

 146 ->175 0.00223

 146 ->178 -0.00223

 146 ->184 -0.00302

 146 ->187 -0.00300

 146 ->193 0.00189

 146 ->196 -0.00196

 146 ->216 -0.00462

 146 ->220 0.00209

 146 ->228 -0.00372

 146 ->232 -0.00170

 146 ->250 -0.00205

 146 ->252 0.00350

 146 ->257 -0.00280

 146 ->261 -0.00112

 146 ->268 0.00131

 146 ->282 -0.00158

 146 ->283 -0.00108

 146 ->305 -0.00160

 146 ->307 -0.00397

 146 ->321 0.00258

 146 ->333 0.00171

 146 ->337 0.00153

 146 ->341 0.00306

 146 ->347 0.00130

 146 ->357 0.00100

 146 ->359 0.00184

 146 ->368 -0.00142

 146 ->375 -0.00104

 146 ->384 0.00155

 146 ->395 0.00178

 146 ->407 0.00185

 146 ->478 0.00100

 147 ->165 -0.00219

 147 ->173 0.00238

 147 ->176 -0.00128

 147 ->181 0.00645

 147 ->183 -0.00179

 147 ->188 -0.00466

 147 ->190 -0.00235

 147 ->195 0.01045

 147 ->197 0.00378

 147 ->205 0.00103

 147 ->210 -0.00100

 147 ->213 0.00214

 147 ->219 0.00115

 147 ->229 -0.00348

 147 ->238 -0.00299

 147 ->242 -0.00336

 147 ->245 -0.00239

 147 ->246 -0.00166

 147 ->251 0.00309

 147 ->254 -0.00140

 147 ->262 0.00197

 147 ->264 -0.00101

 147 ->271 0.00149

 147 ->322 0.00171

 147 ->324 0.00140

 147 ->336 0.00130

 147 ->338 0.00145

 147 ->351 -0.00116

 147 ->354 0.00332

 147 ->360 0.00155

 147 ->365 -0.00148

 147 ->385 0.00162

 147 ->463 0.00166

 148 ->165 0.00195

 148 ->170 -0.00241

 148 ->173 -0.00635

 148 ->181 0.00164

 148 ->183 -0.00132

 148 ->195 0.00217

 148 ->197 0.00419

 148 ->201 0.00253

 148 ->210 -0.00290

 148 ->285 0.00101

 148 ->295 0.00120

 148 ->354 0.00103

 149 ->162 0.02776

 149 ->166 0.00169

 149 ->174 0.00312

 149 ->194 0.00263

 149 ->211 -0.00136

 150 ->165 0.00193

 150 ->170 -0.00211

 150 ->173 -0.00403

 150 ->188 0.00166

 150 ->195 -0.00223

 150 ->197 0.00118

 150 ->201 0.00144

 151 ->164 -0.00796

 151 ->168 0.00122

 151 ->180 0.00109

 152 ->163 0.00995

 152 ->175 0.00129

 152 ->196 -0.00209

 153 ->165 0.00177

 153 ->173 0.00210

 153 ->195 -0.00156

 153 ->197 0.00294

 153 ->201 0.00188

 153 ->210 -0.00164

 154 ->162 0.02760

 155 ->164 0.00650

 155 ->168 0.00225

 155 ->169 0.00131

 155 ->180 0.00192

 155 ->189 0.00166

 155 ->202 -0.00119

 156 ->163 0.03801

 156 ->172 0.00227

 156 ->196 -0.00112

 157 ->162 0.06498

 157 ->166 -0.00292

 157 ->171 0.00271

 157 ->174 0.00607

 157 ->194 -0.00337

 157 ->203 0.00102

 157 ->211 0.00158

 158 ->165 0.00752

 158 ->170 -0.00102

 158 ->173 0.00387

 158 ->183 -0.00112

 158 ->188 0.00111

 158 ->195 -0.00383

 158 ->197 0.00894

 158 ->201 0.00567

 158 ->210 -0.00527

 158 ->213 -0.00213

 158 ->262 -0.00144

 158 ->271 -0.00106

 159 ->163 0.69887

 159 ->167 -0.00223

 159 ->172 0.00132

 159 ->175 0.00586

 159 ->178 -0.00190

 159 ->184 0.00103

 159 ->193 -0.00161

 159 ->196 -0.01279

 159 ->204 0.00504

 159 ->207 -0.00189

 159 ->212 0.00642

 159 ->259 0.00182

 159 ->261 0.00153

 159 ->283 0.00113

 159 ->291 0.00121

 159 ->308 -0.00116

 159 ->326 -0.00115

 159 ->407 -0.00130

 160 ->164 0.00991

 160 ->168 -0.00813

 160 ->169 0.00569

 160 ->179 -0.00221

 160 ->180 -0.01243

 160 ->185 -0.00218

 160 ->189 -0.00970

 160 ->191 0.00124

 160 ->198 0.00171

 160 ->209 -0.00134

 160 ->214 0.00302

 161 ->165 -0.00826

 161 ->170 -0.00364

 161 ->173 -0.03900

 161 ->176 0.00174

 161 ->195 0.00102

 161 ->197 -0.00852

 161 ->201 -0.00354

 161 ->210 0.00278

 161 ->213 0.00188

 161 ->295 0.00119

 161 ->409 0.00106

 51 <-216 0.00154

 52 <-213 -0.00106

 52 <-222 0.00136

 63 <-228 0.00115

 64 <-181 0.00118

 64 <-229 0.00107

 81 <-181 -0.00108

 84 <-249 -0.00108

 85 <-230 0.00106

 90 <-199 0.00110

 90 <-224 0.00105

 90 <-263 -0.00113

 91 <-231 -0.00159

 91 <-277 -0.00155

 92 <-220 0.00151

 95 <-220 -0.00131

 96 <-181 -0.00113

 96 <-188 0.00106

 96 <-195 -0.00242

 96 <-229 -0.00122

 99 <-230 -0.00161

 101 <-231 0.00136

 103 <-174 0.00104

 105 <-230 0.00136

 105 <-265 0.00132

 108 <-195 -0.00162

 109 <-231 -0.00185

 109 <-277 -0.00139

 111 <-197 0.00140

 112 <-174 0.00122

 115 <-216 -0.00121

 122 <-163 -0.00221

 122 <-175 0.00112

 122 <-196 -0.00153

 123 <-163 -0.00339

 123 <-175 0.00176

 123 <-196 -0.00226

 123 <-212 0.00103

 124 <-224 0.00159

 124 <-230 -0.00187

 124 <-263 -0.00135

 124 <-304 -0.00107

 125 <-217 0.00101

 125 <-231 -0.00160

 126 <-173 0.00377

 126 <-197 0.00183

 128 <-217 -0.00133

 128 <-231 0.00157

 128 <-277 0.00133

 129 <-321 -0.00116

 130 <-230 0.00119

 136 <-180 0.00110

 139 <-163 -0.00101

 142 <-231 -0.00140

 143 <-164 0.00314

 143 <-168 -0.00127

 143 <-180 -0.00303

 143 <-189 -0.00111

 144 <-163 -0.00590

 145 <-162 0.00180

 145 <-174 0.00612

 145 <-194 -0.00202

 145 <-211 0.00107

 146 <-184 -0.00135

 146 <-187 -0.00131

 146 <-216 -0.00246

 146 <-220 0.00119

 146 <-228 -0.00212

 146 <-250 -0.00130

 146 <-252 0.00222

 146 <-257 -0.00174

 146 <-282 -0.00100

 146 <-305 -0.00111

 146 <-307 -0.00266

 146 <-321 0.00171

 146 <-333 0.00120

 146 <-337 0.00108

 146 <-341 0.00228

 146 <-359 0.00137

 146 <-368 -0.00105

 146 <-384 0.00108

 146 <-395 0.00119

 146 <-407 0.00152

 147 <-181 0.00257

 147 <-188 -0.00205

 147 <-195 0.00467

 147 <-197 0.00136

 147 <-213 0.00122

 147 <-229 -0.00199

 147 <-238 -0.00176

 147 <-242 -0.00194

 147 <-245 -0.00140

 147 <-251 0.00195

 147 <-262 0.00123

 147 <-322 0.00114

 147 <-338 0.00106

 147 <-354 0.00246

 147 <-360 0.00112

 147 <-365 -0.00108

 147 <-385 0.00114

 147 <-463 0.00128

 148 <-195 0.00107

 148 <-197 0.00179

 148 <-201 0.00105

 148 <-210 -0.00131

 149 <-162 0.00235

 149 <-194 0.00103

 152 <-163 -0.00256

 152 <-175 0.00178

 152 <-196 -0.00137

 153 <-173 0.00328

 153 <-197 0.00182

 153 <-201 0.00100

 153 <-210 -0.00103

 154 <-162 0.00101

 155 <-164 -0.00121

 156 <-163 0.00101

 157 <-174 0.00327

 157 <-194 -0.00149

 158 <-165 0.00107

 158 <-170 0.00159

 158 <-173 0.01003

 158 <-195 -0.00124

 158 <-197 0.00498

 158 <-201 0.00266

 158 <-210 -0.00282

 158 <-213 -0.00164

 159 <-163 -0.01651

 159 <-167 -0.00212

 159 <-172 -0.00230

 159 <-175 0.00784

 159 <-178 -0.00194

 159 <-196 -0.00696

 159 <-204 0.00187

 159 <-212 0.00351

 159 <-407 -0.00116

 160 <-168 -0.00163

 160 <-179 -0.00110

 160 <-180 -0.00630

 160 <-185 -0.00115

 160 <-189 -0.00510

 160 <-214 0.00193

 161 <-170 -0.00148

 161 <-173 -0.01162

 161 <-197 -0.00326

 161 <-201 -0.00121

 161 <-210 0.00127

 Excited State 8: Singlet-B1 3.5974 eV 344.64 nm f=0.0490 <S\*\*2>=0.000

 51 ->213 -0.00113

 51 ->222 0.00133

 52 ->216 0.00176

 52 ->232 -0.00112

 63 ->181 0.00156

 63 ->229 0.00120

 64 ->184 0.00102

 64 ->216 -0.00104

 64 ->228 0.00138

 64 ->232 0.00120

 74 ->222 -0.00118

 90 ->198 0.00102

 90 ->202 0.00128

 90 ->231 -0.00167

 90 ->277 -0.00146

 91 ->199 0.00160

 91 ->230 -0.00181

 91 ->263 -0.00153

 91 ->265 -0.00100

 92 ->195 0.00158

 92 ->229 0.00108

 95 ->188 0.00159

 95 ->195 -0.00268

 95 ->213 0.00100

 95 ->229 -0.00108

 96 ->184 0.00128

 96 ->187 0.00120

 96 ->193 -0.00102

 96 ->220 -0.00182

 96 ->228 -0.00149

 97 ->230 -0.00100

 98 ->195 -0.00136

 99 ->217 0.00111

 99 ->221 -0.00153

 99 ->231 -0.00194

 99 ->277 -0.00165

 101 ->224 -0.00137

 101 ->227 0.00106

 101 ->230 0.00109

 102 ->163 -0.00262

 105 ->164 0.00132

 105 ->231 0.00106

 105 ->277 0.00117

 109 ->224 0.00178

 109 ->227 -0.00117

 109 ->230 -0.00171

 109 ->247 -0.00119

 109 ->263 -0.00102

 109 ->265 -0.00109

 111 ->163 -0.00531

 111 ->196 -0.00101

 112 ->164 -0.00243

 112 ->180 -0.00118

 113 ->163 0.00127

 113 ->228 0.00115

 119 ->163 0.00168

 122 ->173 0.00289

 122 ->197 0.00143

 123 ->173 0.00490

 123 ->197 0.00238

 123 ->210 -0.00115

 124 ->217 0.00129

 124 ->221 -0.00139

 124 ->231 -0.00333

 124 ->236 -0.00174

 124 ->277 -0.00222

 125 ->224 0.00128

 125 ->230 -0.00216

 126 ->175 0.00375

 126 ->196 -0.00349

 126 ->212 0.00112

 127 ->212 -0.00106

 127 ->216 -0.00203

 127 ->232 0.00106

 127 ->274 0.00127

 128 ->162 0.00109

 128 ->211 0.00105

 128 ->224 -0.00123

 128 ->230 0.00235

 128 ->256 0.00130

 128 ->304 0.00108

 129 ->195 -0.00148

 129 ->213 0.00232

 129 ->229 0.00101

 129 ->242 0.00116

 129 ->245 0.00144

 129 ->264 -0.00126

 130 ->217 -0.00157

 130 ->231 0.00110

 130 ->249 0.00127

 131 ->163 0.00368

 133 ->164 0.00156

 133 ->217 -0.00174

 133 ->249 0.00108

 134 ->162 -0.00232

 134 ->215 0.00139

 134 ->230 0.00139

 134 ->256 0.00125

 136 ->174 -0.00107

 139 ->173 0.00111

 140 ->163 -0.00127

 141 ->231 0.00162

 141 ->277 0.00116

 142 ->162 0.00139

 142 ->224 0.00126

 142 ->230 -0.00167

 143 ->162 0.00397

 143 ->174 0.00354

 143 ->194 -0.00256

 143 ->203 0.00106

 143 ->211 0.00143

 144 ->170 0.00181

 144 ->173 0.00605

 144 ->197 0.00185

 145 ->168 -0.00235

 145 ->169 0.00259

 145 ->180 -0.00378

 145 ->189 -0.00563

 145 ->209 -0.00147

 145 ->214 0.00221

 146 ->165 -0.00118

 146 ->173 0.00195

 146 ->181 0.00515

 146 ->183 -0.00172

 146 ->188 -0.00385

 146 ->190 -0.00189

 146 ->195 0.00841

 146 ->197 0.00399

 146 ->201 0.00102

 146 ->210 -0.00148

 146 ->213 0.00220

 146 ->219 0.00132

 146 ->229 -0.00292

 146 ->238 -0.00266

 146 ->242 -0.00303

 146 ->245 -0.00212

 146 ->246 -0.00134

 146 ->251 0.00292

 146 ->254 -0.00116

 146 ->262 0.00172

 146 ->264 -0.00108

 146 ->271 0.00183

 146 ->322 0.00169

 146 ->324 0.00119

 146 ->336 0.00115

 146 ->338 0.00133

 146 ->351 -0.00106

 146 ->354 0.00311

 146 ->360 0.00136

 146 ->365 -0.00143

 146 ->385 0.00161

 146 ->463 0.00171

 147 ->163 -0.01156

 147 ->172 -0.00108

 147 ->178 -0.00149

 147 ->184 -0.00213

 147 ->187 -0.00206

 147 ->193 0.00125

 147 ->196 -0.00160

 147 ->216 -0.00429

 147 ->220 0.00102

 147 ->228 -0.00274

 147 ->232 -0.00119

 147 ->250 -0.00167

 147 ->252 0.00252

 147 ->257 -0.00244

 147 ->282 -0.00119

 147 ->305 -0.00112

 147 ->307 -0.00269

 147 ->321 0.00216

 147 ->333 0.00103

 147 ->337 0.00115

 147 ->341 0.00257

 147 ->347 0.00107

 147 ->359 0.00144

 147 ->368 -0.00125

 147 ->384 0.00134

 147 ->395 0.00147

 147 ->407 0.00144

 148 ->163 -0.04485

 148 ->172 -0.00174

 148 ->175 0.00474

 148 ->178 -0.00144

 148 ->216 -0.00119

 149 ->164 -0.00861

 149 ->180 0.00320

 149 ->189 -0.00180

 150 ->163 0.02476

 150 ->167 0.00230

 150 ->172 -0.00239

 150 ->175 -0.00143

 150 ->184 0.00100

 151 ->162 0.02652

 151 ->166 0.00172

 151 ->174 -0.00267

 152 ->165 0.00263

 152 ->173 0.00228

 152 ->197 0.00188

 152 ->201 0.00127

 153 ->163 0.02104

 153 ->167 -0.00251

 153 ->175 0.00151

 153 ->196 -0.00309

 153 ->204 0.00116

 153 ->212 0.00109

 154 ->164 -0.01827

 154 ->168 0.00342

 154 ->169 -0.00267

 154 ->189 -0.00155

 155 ->162 0.04169

 155 ->171 -0.00430

 155 ->174 -0.00347

 155 ->194 -0.00103

 156 ->165 0.00243

 156 ->170 0.00272

 156 ->173 -0.00582

 156 ->181 -0.00107

 156 ->197 0.00153

 156 ->201 0.00130

 156 ->210 -0.00104

 157 ->164 0.01697

 157 ->168 -0.00583

 157 ->180 -0.00286

 157 ->189 -0.00158

 157 ->198 0.00121

 157 ->214 0.00117

 158 ->163 0.70058

 158 ->172 0.00566

 158 ->175 0.00211

 158 ->178 -0.00123

 158 ->193 -0.00139

 158 ->196 -0.00961

 158 ->204 0.00421

 158 ->207 -0.00142

 158 ->212 0.00525

 158 ->259 0.00155

 158 ->261 0.00139

 158 ->326 -0.00105

 159 ->165 0.00744

 159 ->170 -0.00225

 159 ->173 0.00411

 159 ->183 -0.00119

 159 ->188 0.00129

 159 ->195 -0.00429

 159 ->197 0.00963

 159 ->201 0.00616

 159 ->210 -0.00579

 159 ->213 -0.00222

 159 ->262 -0.00156

 159 ->313 -0.00108

 159 ->409 -0.00100

 160 ->162 0.03448

 160 ->166 -0.00792

 160 ->171 0.00216

 160 ->174 0.01342

 160 ->177 0.00107

 160 ->182 -0.00111

 160 ->186 -0.00130

 160 ->194 -0.00650

 160 ->203 0.00210

 160 ->211 0.00333

 160 ->215 -0.00130

 161 ->167 0.00910

 161 ->172 0.01112

 161 ->175 -0.00900

 161 ->178 0.00203

 161 ->196 0.01226

 161 ->204 -0.00363

 161 ->207 0.00162

 161 ->212 -0.00555

 51 <-222 0.00107

 52 <-216 0.00138

 63 <-181 0.00110

 64 <-228 0.00105

 90 <-231 -0.00117

 90 <-277 -0.00111

 91 <-199 0.00105

 91 <-230 -0.00128

 91 <-263 -0.00111

 95 <-195 -0.00166

 96 <-220 -0.00124

 96 <-228 -0.00103

 99 <-221 -0.00101

 99 <-231 -0.00136

 99 <-277 -0.00121

 102 <-163 -0.00172

 109 <-224 0.00119

 109 <-230 -0.00115

 111 <-163 -0.00230

 122 <-173 0.00182

 122 <-197 0.00102

 123 <-173 0.00276

 123 <-197 0.00143

 124 <-231 -0.00216

 124 <-236 -0.00114

 124 <-277 -0.00157

 125 <-230 -0.00140

 126 <-163 -0.00399

 126 <-175 0.00271

 126 <-196 -0.00223

 127 <-216 -0.00121

 128 <-230 0.00149

 129 <-213 0.00128

 133 <-217 -0.00104

 141 <-231 0.00103

 142 <-230 -0.00103

 143 <-174 0.00226

 143 <-194 -0.00186

 143 <-211 0.00107

 145 <-164 0.00196

 145 <-168 -0.00113

 145 <-169 0.00171

 145 <-180 -0.00259

 145 <-189 -0.00320

 145 <-214 0.00137

 146 <-181 0.00205

 146 <-188 -0.00171

 146 <-195 0.00379

 146 <-197 0.00133

 146 <-213 0.00125

 146 <-229 -0.00165

 146 <-238 -0.00156

 146 <-242 -0.00174

 146 <-245 -0.00125

 146 <-251 0.00185

 146 <-262 0.00107

 146 <-271 0.00114

 146 <-322 0.00110

 146 <-354 0.00232

 146 <-365 -0.00105

 146 <-385 0.00110

 146 <-463 0.00132

 147 <-184 -0.00100

 147 <-216 -0.00229

 147 <-228 -0.00156

 147 <-250 -0.00106

 147 <-252 0.00154

 147 <-257 -0.00150

 147 <-307 -0.00176

 147 <-321 0.00148

 147 <-341 0.00187

 147 <-359 0.00107

 147 <-407 0.00123

 148 <-163 0.00110

 148 <-175 0.00277

 149 <-164 0.00187

 149 <-180 0.00206

 150 <-163 -0.00264

 150 <-172 -0.00149

 150 <-175 0.00110

 151 <-166 0.00109

 152 <-165 0.00102

 152 <-173 0.00176

 152 <-197 0.00115

 153 <-163 -0.00302

 153 <-167 -0.00122

 153 <-175 0.00228

 153 <-196 -0.00207

 155 <-171 -0.00121

 156 <-170 0.00130

 157 <-164 0.00108

 157 <-168 -0.00171

 157 <-180 -0.00179

 157 <-189 -0.00158

 158 <-163 -0.01157

 158 <-167 -0.00148

 158 <-172 -0.00107

 158 <-175 0.00577

 158 <-178 -0.00153

 158 <-196 -0.00544

 158 <-204 0.00156

 158 <-212 0.00290

 159 <-165 0.00102

 159 <-170 0.00122

 159 <-173 0.00986

 159 <-195 -0.00143

 159 <-197 0.00529

 159 <-201 0.00291

 159 <-210 -0.00311

 159 <-213 -0.00167

 160 <-162 -0.00947

 160 <-166 -0.00196

 160 <-174 0.00575

 160 <-194 -0.00308

 160 <-211 0.00166

 161 <-163 0.00182

 161 <-167 0.00211

 161 <-172 0.00121

 161 <-175 -0.00371

 161 <-196 0.00499

 161 <-204 -0.00151

 161 <-212 -0.00241

 Excited State 9: Singlet-A1 3.7146 eV 333.78 nm f=0.0000 <S\*\*2>=0.000

 74 ->220 -0.00123

 87 ->165 -0.00112

 87 ->229 -0.00134

 90 ->199 0.00128

 92 ->228 -0.00118

 93 ->162 -0.00125

 93 ->177 -0.00126

 94 ->176 0.00144

 95 ->178 0.00130

 95 ->184 0.00123

 95 ->187 0.00121

 95 ->250 0.00109

 96 ->181 0.00180

 96 ->183 0.00140

 96 ->188 0.00152

 96 ->190 -0.00105

 96 ->251 -0.00102

 97 ->179 -0.00138

 98 ->184 0.00119

 99 ->162 0.00130

 105 ->162 -0.00126

 109 ->168 0.00106

 109 ->169 -0.00116

 110 ->182 0.00103

 111 ->197 0.00116

 112 ->162 -0.00223

 112 ->194 0.00105

 113 ->195 0.00112

 114 ->192 0.00112

 114 ->199 -0.00112

 115 ->193 0.00147

 115 ->216 0.00115

 116 ->163 0.00111

 116 ->184 -0.00105

 117 ->185 -0.00146

 118 ->190 -0.00114

 119 ->183 -0.00104

 119 ->188 0.00102

 120 ->186 0.00120

 121 ->164 -0.00128

 121 ->191 0.00145

 121 ->198 0.00130

 121 ->217 0.00153

 122 ->163 0.00279

 122 ->196 -0.00162

 123 ->163 0.00336

 123 ->196 -0.00167

 124 ->162 0.00139

 124 ->166 0.00129

 124 ->199 -0.00170

 124 ->263 0.00109

 125 ->164 0.00106

 125 ->198 -0.00162

 126 ->170 -0.00124

 126 ->173 -0.00154

 126 ->197 0.00192

 126 ->210 -0.00105

 127 ->173 0.00119

 127 ->183 -0.00104

 127 ->195 0.00104

 127 ->210 -0.00153

 127 ->222 0.00124

 128 ->164 0.00277

 128 ->189 0.00111

 128 ->202 0.00111

 128 ->231 -0.00156

 129 ->184 -0.00124

 129 ->187 -0.00120

 129 ->250 0.00139

 130 ->162 -0.00619

 130 ->199 0.00102

 130 ->224 0.00139

 131 ->173 -0.00112

 131 ->188 -0.00144

 131 ->210 0.00116

 132 ->163 0.00726

 132 ->175 0.00114

 132 ->212 0.00183

 133 ->162 0.01753

 133 ->171 0.00142

 133 ->199 0.00181

 133 ->211 0.00238

 133 ->224 0.00119

 133 ->317 0.00125

 134 ->164 -0.00610

 134 ->169 -0.00146

 134 ->185 -0.00112

 134 ->189 -0.00144

 134 ->202 0.00143

 134 ->209 0.00137

 134 ->214 0.00199

 135 ->190 0.00108

 135 ->213 0.00108

 136 ->164 0.00266

 136 ->168 -0.00141

 136 ->169 0.00160

 136 ->189 -0.00125

 136 ->214 -0.00124

 137 ->212 -0.00112

 137 ->216 -0.00102

 138 ->162 -0.00211

 139 ->163 0.00455

 139 ->204 0.00105

 140 ->201 0.00118

 141 ->162 -0.00616

 141 ->166 -0.00176

 142 ->168 0.00115

 143 ->164 0.00210

 143 ->168 0.00158

 143 ->180 0.00167

 143 ->189 0.00425

 143 ->209 0.00109

 143 ->214 -0.00138

 144 ->163 0.01412

 144 ->167 0.00182

 144 ->175 -0.00190

 144 ->196 0.00304

 144 ->204 -0.00133

 144 ->212 -0.00156

 145 ->162 -0.01923

 145 ->166 0.00307

 145 ->171 -0.00229

 145 ->194 0.00713

 145 ->203 -0.00176

 145 ->211 -0.00261

 146 ->163 0.01416

 146 ->184 0.00102

 146 ->187 0.00111

 146 ->193 -0.00111

 146 ->220 -0.00125

 146 ->252 -0.00113

 147 ->181 -0.00275

 147 ->188 0.00170

 147 ->195 -0.00523

 147 ->197 -0.00122

 148 ->181 -0.00126

 148 ->188 0.00130

 148 ->195 -0.00156

 149 ->162 0.01645

 149 ->194 -0.00117

 150 ->165 -0.00197

 150 ->170 0.00195

 150 ->173 0.00617

 150 ->188 0.00154

 150 ->195 -0.00108

 150 ->197 0.00399

 150 ->201 0.00279

 150 ->210 -0.00261

 150 ->229 -0.00161

 150 ->328 0.00111

 151 ->164 -0.00435

 151 ->168 0.00431

 151 ->169 -0.00203

 151 ->198 -0.00131

 152 ->163 -0.02554

 152 ->167 -0.00250

 152 ->172 -0.00413

 152 ->175 -0.00179

 152 ->196 0.00238

 152 ->200 -0.00101

 152 ->212 -0.00140

 153 ->165 0.00374

 153 ->170 -0.00321

 153 ->173 -0.00447

 153 ->197 -0.00146

 154 ->162 -0.01740

 154 ->166 0.00346

 154 ->171 -0.00236

 154 ->174 0.00116

 154 ->194 0.00109

 154 ->211 -0.00107

 155 ->164 0.05665

 155 ->168 -0.00854

 155 ->169 0.01279

 155 ->180 -0.00179

 155 ->185 0.00107

 155 ->189 0.00414

 155 ->191 -0.00112

 155 ->202 -0.00169

 155 ->214 -0.00174

 155 ->231 -0.00116

 156 ->163 -0.25643

 156 ->167 -0.00463

 156 ->172 -0.00237

 156 ->175 -0.00329

 156 ->187 -0.00111

 156 ->196 0.00330

 156 ->204 -0.00140

 156 ->212 -0.00172

 157 ->162 0.64958

 157 ->166 0.01109

 157 ->171 0.00430

 157 ->174 -0.00310

 157 ->199 0.00111

 157 ->270 -0.00137

 158 ->165 -0.00252

 158 ->170 0.00436

 158 ->173 0.00167

 158 ->197 -0.00116

 158 ->271 -0.00149

 159 ->163 -0.04500

 159 ->167 0.00284

 159 ->172 0.00392

 159 ->175 0.00256

 159 ->178 -0.00103

 159 ->305 -0.00105

 159 ->308 0.00122

 160 ->164 0.04943

 160 ->168 0.01338

 160 ->169 0.00779

 160 ->179 0.00217

 160 ->180 0.00607

 160 ->185 0.00203

 160 ->189 0.00614

 160 ->191 -0.00132

 160 ->214 -0.00141

 161 ->165 0.02511

 161 ->170 -0.00149

 161 ->173 0.00571

 161 ->183 -0.00111

 161 ->195 -0.00138

 161 ->197 0.00580

 161 ->201 0.00260

 161 ->210 -0.00229

 161 ->213 -0.00140

 96 <-181 0.00105

 122 <-163 0.00134

 123 <-163 0.00228

 123 <-196 -0.00136

 126 <-197 0.00107

 133 <-211 0.00115

 134 <-214 0.00102

 136 <-189 -0.00111

 143 <-164 0.00365

 143 <-189 0.00260

 144 <-163 0.00164

 144 <-167 0.00137

 144 <-175 -0.00125

 144 <-196 0.00134

 145 <-162 -0.00620

 145 <-171 -0.00124

 145 <-194 0.00323

 145 <-211 -0.00137

 147 <-181 -0.00108

 147 <-195 -0.00214

 149 <-162 0.00288

 151 <-168 0.00102

 152 <-163 0.00172

 152 <-167 -0.00104

 153 <-165 0.00124

 154 <-162 0.00147

 155 <-164 -0.00276

 155 <-169 0.00194

 156 <-167 -0.00250

 157 <-162 -0.00591

 157 <-166 0.00291

 157 <-194 0.00171

 158 <-170 0.00113

 159 <-163 0.00134

 159 <-167 0.00110

 159 <-172 0.00111

 160 <-164 0.00504

 160 <-169 0.00214

 160 <-189 0.00260

 160 <-214 -0.00118

 161 <-165 0.00595

 161 <-173 0.00389

 161 <-197 0.00316

 161 <-201 0.00174

 161 <-210 -0.00117

 161 <-328 0.00101

 Excited State 10: Singlet-A2 3.7264 eV 332.72 nm f=0.0000 <S\*\*2>=0.000

 93 ->163 -0.00110

 93 ->178 0.00103

 94 ->179 0.00106

 99 ->163 0.00126

 112 ->163 -0.00329

 117 ->183 0.00111

 119 ->185 0.00111

 120 ->163 0.00118

 122 ->162 -0.00196

 122 ->194 0.00110

 123 ->162 -0.00451

 123 ->194 0.00174

 123 ->211 -0.00104

 124 ->163 0.00166

 124 ->193 0.00112

 124 ->216 0.00191

 125 ->190 0.00106

 125 ->213 -0.00111

 126 ->164 0.00611

 126 ->169 0.00116

 126 ->189 0.00245

 127 ->164 -0.00442

 127 ->189 -0.00139

 128 ->213 0.00104

 128 ->219 0.00100

 130 ->163 -0.00725

 131 ->164 0.00479

 131 ->169 0.00120

 131 ->214 -0.00109

 132 ->162 0.00451

 132 ->174 -0.00117

 132 ->194 -0.00142

 132 ->211 0.00110

 133 ->163 0.01362

 134 ->173 -0.00129

 136 ->173 0.00144

 138 ->163 -0.00373

 141 ->163 -0.00522

 142 ->213 -0.00110

 143 ->165 -0.00113

 143 ->170 -0.00102

 143 ->173 -0.00256

 144 ->162 -0.03361

 144 ->166 0.00197

 144 ->174 0.00298

 144 ->194 0.00306

 144 ->203 -0.00100

 145 ->163 0.01855

 145 ->167 0.00214

 145 ->172 0.00183

 145 ->175 -0.00362

 146 ->162 0.00476

 147 ->164 -0.00372

 148 ->164 -0.00628

 148 ->189 -0.00109

 149 ->163 -0.02736

 149 ->175 0.00181

 150 ->164 -0.03604

 150 ->169 -0.00826

 150 ->180 -0.00129

 150 ->185 -0.00109

 150 ->189 -0.00408

 150 ->202 0.00110

 151 ->165 0.00369

 152 ->162 -0.07053

 152 ->166 0.00350

 152 ->174 0.00303

 152 ->194 0.00251

 152 ->211 -0.00102

 153 ->164 0.02408

 153 ->169 0.00120

 153 ->189 0.00189

 154 ->163 -0.02773

 154 ->167 -0.00458

 154 ->175 0.00121

 155 ->170 0.00702

 155 ->173 0.01164

 155 ->188 -0.00118

 155 ->195 0.00119

 155 ->197 -0.00233

 155 ->201 -0.00197

 155 ->210 0.00134

 156 ->162 -0.00260

 156 ->166 -0.00167

 156 ->171 -0.00513

 156 ->174 0.00299

 156 ->194 0.00349

 156 ->203 -0.00113

 156 ->211 -0.00113

 157 ->163 0.65637

 157 ->167 0.00776

 157 ->172 0.00426

 157 ->175 -0.00292

 157 ->196 -0.00198

 157 ->204 0.00137

 157 ->212 0.00125

 158 ->164 0.01001

 158 ->169 0.00423

 158 ->189 0.00202

 159 ->162 0.05911

 159 ->166 0.00198

 159 ->194 0.00103

 160 ->165 0.00471

 160 ->173 -0.00735

 160 ->195 -0.00154

 160 ->197 0.00276

 160 ->201 0.00163

 160 ->210 -0.00143

 161 ->164 -0.23329

 161 ->168 0.00202

 161 ->169 0.00450

 161 ->180 0.00191

 161 ->185 -0.00104

 161 ->189 -0.00187

 123 <-162 -0.00151

 124 <-216 0.00116

 126 <-180 0.00109

 126 <-189 0.00117

 144 <-162 -0.00265

 144 <-194 0.00106

 155 <-165 0.00176

 156 <-162 0.00133

 156 <-166 -0.00142

 157 <-163 -0.00110

 157 <-167 0.00168

 159 <-162 -0.00176

 160 <-165 -0.00127

 160 <-197 0.00129

 161 <-164 -0.00479

 161 <-168 -0.00237

 161 <-169 0.00215

 161 <-189 -0.00152

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

 Leave Link 914 at Thu Sep 5 22:04:02 2019, MaxMem= 1342177280 cpu: 11740.4

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

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

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

 Population analysis using the SCF density.

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

 Orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

 (A1)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

 (B2) (A1) (B1)

 The electronic state is 1-A1.

 Alpha occ. eigenvalues -- -14.35658 -14.35658 -14.29084 -14.29084 -10.22606

 Alpha occ. eigenvalues -- -10.22606 -10.22606 -10.22606 -10.20738 -10.20738

 Alpha occ. eigenvalues -- -10.20738 -10.20738 -10.20006 -10.20006 -10.20006

 Alpha occ. eigenvalues -- -10.20006 -10.18874 -10.18873 -10.18873 -10.18873

 Alpha occ. eigenvalues -- -10.17945 -10.17945 -10.17880 -10.17880 -10.17480

 Alpha occ. eigenvalues -- -10.17480 -10.17480 -10.17480 -10.17461 -10.17461

 Alpha occ. eigenvalues -- -10.17461 -10.17461 -10.17393 -10.17393 -10.17393

 Alpha occ. eigenvalues -- -10.17393 -10.17355 -10.17355 -10.17355 -10.17355

 Alpha occ. eigenvalues -- -10.17320 -10.17320 -10.17320 -10.17320 -10.16737

 Alpha occ. eigenvalues -- -10.16737 -10.16666 -10.16666 -0.99575 -0.99418

 Alpha occ. eigenvalues -- -0.94996 -0.94707 -0.87257 -0.86831 -0.86785

 Alpha occ. eigenvalues -- -0.86606 -0.83020 -0.81590 -0.81158 -0.80311

 Alpha occ. eigenvalues -- -0.79680 -0.78607 -0.76666 -0.76237 -0.75106

 Alpha occ. eigenvalues -- -0.75011 -0.74986 -0.74969 -0.74622 -0.74114

 Alpha occ. eigenvalues -- -0.73659 -0.72613 -0.71454 -0.67132 -0.66631

 Alpha occ. eigenvalues -- -0.62519 -0.61352 -0.61197 -0.60978 -0.60826

 Alpha occ. eigenvalues -- -0.60781 -0.60424 -0.60325 -0.60170 -0.59824

 Alpha occ. eigenvalues -- -0.59667 -0.58199 -0.57453 -0.56323 -0.55519

 Alpha occ. eigenvalues -- -0.54944 -0.53097 -0.52463 -0.52312 -0.51253

 Alpha occ. eigenvalues -- -0.51171 -0.50384 -0.50218 -0.49071 -0.46739

 Alpha occ. eigenvalues -- -0.46506 -0.46215 -0.46035 -0.45934 -0.45597

 Alpha occ. eigenvalues -- -0.45509 -0.45376 -0.45111 -0.44641 -0.44477

 Alpha occ. eigenvalues -- -0.43566 -0.43215 -0.43060 -0.42727 -0.42703

 Alpha occ. eigenvalues -- -0.42368 -0.42318 -0.42310 -0.42211 -0.42189

 Alpha occ. eigenvalues -- -0.41764 -0.40901 -0.40525 -0.39767 -0.39706

 Alpha occ. eigenvalues -- -0.39698 -0.38746 -0.38510 -0.38343 -0.37863

 Alpha occ. eigenvalues -- -0.37011 -0.37008 -0.36482 -0.36072 -0.35345

 Alpha occ. eigenvalues -- -0.34969 -0.34967 -0.34822 -0.34757 -0.34742

 Alpha occ. eigenvalues -- -0.34669 -0.34275 -0.32545 -0.29546 -0.28849

 Alpha occ. eigenvalues -- -0.27958 -0.27945 -0.27411 -0.27328 -0.26489

 Alpha occ. eigenvalues -- -0.26063 -0.26021 -0.26003 -0.25900 -0.25463

 Alpha occ. eigenvalues -- -0.25456 -0.25239 -0.24832 -0.24613 -0.20800

 Alpha occ. eigenvalues -- -0.19523

 Alpha virt. eigenvalues -- -0.09747 -0.09606 -0.03870 -0.01545 -0.01504

 Alpha virt. eigenvalues -- -0.01446 -0.01249 -0.01194 -0.01148 -0.01073

 Alpha virt. eigenvalues -- -0.01039 0.02921 0.04902 0.05309 0.05360

 Alpha virt. eigenvalues -- 0.05619 0.05645 0.05783 0.06897 0.07573

 Alpha virt. eigenvalues -- 0.08347 0.08389 0.08537 0.09115 0.09372

 Alpha virt. eigenvalues -- 0.09395 0.09907 0.10051 0.10172 0.10308

 Alpha virt. eigenvalues -- 0.10403 0.10420 0.11120 0.11127 0.11844

 Alpha virt. eigenvalues -- 0.12172 0.12518 0.12778 0.12827 0.13099

 Alpha virt. eigenvalues -- 0.13214 0.13397 0.13405 0.13748 0.13958

 Alpha virt. eigenvalues -- 0.13965 0.14046 0.14133 0.14655 0.15155

 Alpha virt. eigenvalues -- 0.15553 0.15844 0.16062 0.17217 0.18163

 Alpha virt. eigenvalues -- 0.21081 0.21319 0.22553 0.22596 0.23271

 Alpha virt. eigenvalues -- 0.23580 0.23954 0.24150 0.24425 0.25094

 Alpha virt. eigenvalues -- 0.25300 0.25625 0.26247 0.26263 0.27308

 Alpha virt. eigenvalues -- 0.27793 0.27913 0.27960 0.27966 0.28154

 Alpha virt. eigenvalues -- 0.28339 0.28825 0.28910 0.29493 0.29503

 Alpha virt. eigenvalues -- 0.29549 0.29837 0.29970 0.30204 0.30569

 Alpha virt. eigenvalues -- 0.30726 0.30824 0.31517 0.31671 0.32859

 Alpha virt. eigenvalues -- 0.33646 0.34324 0.34900 0.35207 0.35349

 Alpha virt. eigenvalues -- 0.35361 0.35728 0.35902 0.36139 0.36284

 Alpha virt. eigenvalues -- 0.36485 0.36494 0.36986 0.37160 0.37458

 Alpha virt. eigenvalues -- 0.37850 0.38315 0.38421 0.39116 0.39411

 Alpha virt. eigenvalues -- 0.39602 0.39603 0.39639 0.40198 0.40391

 Alpha virt. eigenvalues -- 0.40536 0.40765 0.40963 0.40972 0.41083

 Alpha virt. eigenvalues -- 0.41187 0.41458 0.41676 0.41715 0.41904

 Alpha virt. eigenvalues -- 0.41942 0.42288 0.42298 0.42783 0.42834

 Alpha virt. eigenvalues -- 0.43052 0.43080 0.43504 0.43523 0.43822

 Alpha virt. eigenvalues -- 0.44266 0.44450 0.44560 0.44678 0.44785

 Alpha virt. eigenvalues -- 0.45019 0.45256 0.45520 0.45571 0.45636

 Alpha virt. eigenvalues -- 0.46119 0.46591 0.46689 0.46989 0.47421

 Alpha virt. eigenvalues -- 0.47553 0.47723 0.48195 0.48422 0.48609

 Alpha virt. eigenvalues -- 0.49416 0.49798 0.49836 0.49922 0.50808

 Alpha virt. eigenvalues -- 0.50846 0.50865 0.51371 0.51977 0.52825

 Alpha virt. eigenvalues -- 0.53095 0.53172 0.53675 0.54043 0.54097

 Alpha virt. eigenvalues -- 0.54758 0.54956 0.55932 0.56424 0.57386

 Alpha virt. eigenvalues -- 0.57496 0.57558 0.57614 0.57632 0.58106

 Alpha virt. eigenvalues -- 0.58445 0.59122 0.59579 0.59884 0.60300

 Alpha virt. eigenvalues -- 0.60314 0.60378 0.60408 0.60784 0.61020

 Alpha virt. eigenvalues -- 0.61024 0.61046 0.61213 0.61379 0.61465

 Alpha virt. eigenvalues -- 0.61509 0.61656 0.62089 0.62125 0.62330

 Alpha virt. eigenvalues -- 0.62470 0.63680 0.63966 0.64073 0.64362

 Alpha virt. eigenvalues -- 0.64549 0.64737 0.64836 0.64850 0.65114

 Alpha virt. eigenvalues -- 0.65437 0.65581 0.65751 0.66268 0.66642

 Alpha virt. eigenvalues -- 0.66909 0.66934 0.67990 0.68849 0.69144

 Alpha virt. eigenvalues -- 0.69249 0.69425 0.70127 0.70528 0.70572

 Alpha virt. eigenvalues -- 0.71029 0.72194 0.72445 0.72569 0.72664

 Alpha virt. eigenvalues -- 0.72898 0.73176 0.73404 0.73984 0.74306

 Alpha virt. eigenvalues -- 0.74389 0.74522 0.75246 0.75270 0.75349

 Alpha virt. eigenvalues -- 0.75581 0.75959 0.76118 0.76467 0.76959

 Alpha virt. eigenvalues -- 0.77498 0.77923 0.78183 0.78634 0.79344

 Alpha virt. eigenvalues -- 0.79557 0.79570 0.79738 0.80096 0.80625

 Alpha virt. eigenvalues -- 0.80720 0.80950 0.81380 0.81710 0.81782

 Alpha virt. eigenvalues -- 0.82101 0.82255 0.83434 0.84277 0.84823

 Alpha virt. eigenvalues -- 0.85213 0.85701 0.85864 0.86890 0.87042

 Alpha virt. eigenvalues -- 0.87078 0.87165 0.89004 0.89056 0.89128

 Alpha virt. eigenvalues -- 0.89230 0.89324 0.89877 0.90761 0.91742

 Alpha virt. eigenvalues -- 0.92020 0.92257 0.92279 0.92916 0.92934

 Alpha virt. eigenvalues -- 0.94908 0.95028 0.95528 0.96231 0.96819

 Alpha virt. eigenvalues -- 0.96829 0.97387 0.98343 0.98739 0.99324

 Alpha virt. eigenvalues -- 0.99650 1.00443 1.01276 1.01347 1.01369

 Alpha virt. eigenvalues -- 1.02472 1.02565 1.02697 1.04495 1.04867

 Alpha virt. eigenvalues -- 1.05090 1.05805 1.06061 1.07875 1.07956

 Alpha virt. eigenvalues -- 1.08411 1.09102 1.09103 1.10024 1.10399

 Alpha virt. eigenvalues -- 1.10752 1.11391 1.13073 1.13346 1.13634

 Alpha virt. eigenvalues -- 1.13729 1.14669 1.14756 1.14982 1.15549

 Alpha virt. eigenvalues -- 1.16354 1.16580 1.16896 1.17126 1.17806

 Alpha virt. eigenvalues -- 1.18455 1.19170 1.19652 1.19962 1.20010

 Alpha virt. eigenvalues -- 1.20629 1.20834 1.20873 1.20919 1.20932

 Alpha virt. eigenvalues -- 1.21694 1.22584 1.23156 1.23299 1.23875

 Alpha virt. eigenvalues -- 1.24366 1.24614 1.24723 1.24814 1.25218

 Alpha virt. eigenvalues -- 1.25383 1.25777 1.25857 1.26374 1.26584

 Alpha virt. eigenvalues -- 1.27261 1.28399 1.28622 1.29417 1.30259

 Alpha virt. eigenvalues -- 1.31147 1.31201 1.31757 1.32953 1.33367

 Alpha virt. eigenvalues -- 1.37543 1.38053 1.38527 1.39784 1.40096

 Alpha virt. eigenvalues -- 1.40656 1.40718 1.42348 1.42476 1.42606

 Alpha virt. eigenvalues -- 1.43189 1.44606 1.44728 1.44972 1.47104

 Alpha virt. eigenvalues -- 1.47136 1.47422 1.47586 1.47724 1.47860

 Alpha virt. eigenvalues -- 1.48492 1.48907 1.48945 1.49041 1.49415

 Alpha virt. eigenvalues -- 1.49543 1.51426 1.53123 1.53555 1.53639

 Alpha virt. eigenvalues -- 1.54100 1.54231 1.54469 1.54776 1.56750

 Alpha virt. eigenvalues -- 1.57614 1.57791 1.58803 1.61250 1.61366

 Alpha virt. eigenvalues -- 1.61904 1.61981 1.62439 1.63366 1.65374

 Alpha virt. eigenvalues -- 1.65450 1.67222 1.67222 1.67704 1.68192

 Alpha virt. eigenvalues -- 1.68684 1.69495 1.70039 1.70425 1.70756

 Alpha virt. eigenvalues -- 1.71388 1.71845 1.73553 1.74274 1.74346

 Alpha virt. eigenvalues -- 1.75123 1.75368 1.75886 1.76065 1.76155

 Alpha virt. eigenvalues -- 1.76172 1.76795 1.77531 1.77595 1.78887

 Alpha virt. eigenvalues -- 1.79511 1.79561 1.80063 1.80607 1.80757

 Alpha virt. eigenvalues -- 1.81225 1.81431 1.82046 1.82374 1.83011

 Alpha virt. eigenvalues -- 1.83274 1.83757 1.84561 1.84607 1.84673

 Alpha virt. eigenvalues -- 1.84993 1.85609 1.87052 1.87310 1.87686

 Alpha virt. eigenvalues -- 1.87981 1.88155 1.88394 1.89109 1.89693

 Alpha virt. eigenvalues -- 1.90938 1.91087 1.91314 1.91433 1.91731

 Alpha virt. eigenvalues -- 1.92311 1.92336 1.92501 1.92508 1.92691

 Alpha virt. eigenvalues -- 1.93276 1.93746 1.93975 1.94008 1.94288

 Alpha virt. eigenvalues -- 1.94402 1.94430 1.95693 1.95865 1.95875

 Alpha virt. eigenvalues -- 1.96478 1.96645 1.97072 1.97868 1.98007

 Alpha virt. eigenvalues -- 1.99344 1.99636 2.00035 2.00303 2.00437

 Alpha virt. eigenvalues -- 2.03048 2.07151 2.07382 2.07489 2.07491

 Alpha virt. eigenvalues -- 2.08203 2.08310 2.08863 2.10377 2.12978

 Alpha virt. eigenvalues -- 2.13404 2.13472 2.17681 2.19174 2.21824

 Alpha virt. eigenvalues -- 2.23438 2.23859 2.23933 2.25284 2.25333

 Alpha virt. eigenvalues -- 2.25815 2.26433 2.26624 2.26678 2.27037

 Alpha virt. eigenvalues -- 2.27051 2.27481 2.27996 2.28021 2.28101

 Alpha virt. eigenvalues -- 2.28369 2.28379 2.29195 2.29629 2.29726

 Alpha virt. eigenvalues -- 2.29757 2.31396 2.31528 2.32016 2.32234

 Alpha virt. eigenvalues -- 2.32750 2.32987 2.33568 2.34026 2.35345

 Alpha virt. eigenvalues -- 2.35467 2.35553 2.35918 2.36100 2.36732

 Alpha virt. eigenvalues -- 2.37000 2.37843 2.38687 2.38832 2.38991

 Alpha virt. eigenvalues -- 2.40581 2.41014 2.41308 2.42920 2.43653

 Alpha virt. eigenvalues -- 2.44707 2.47096 2.47452 2.48989 2.49695

 Alpha virt. eigenvalues -- 2.52398 2.52787 2.53319 2.53783 2.54240

 Alpha virt. eigenvalues -- 2.54651 2.55681 2.57367 2.57582 2.57622

 Alpha virt. eigenvalues -- 2.58647 2.58851 2.59549 2.60326 2.60701

 Alpha virt. eigenvalues -- 2.61037 2.61206 2.61299 2.62324 2.62504

 Alpha virt. eigenvalues -- 2.64183 2.64712 2.64906 2.65436 2.67197

 Alpha virt. eigenvalues -- 2.67573 2.68991 2.69552 2.69598 2.70326

 Alpha virt. eigenvalues -- 2.70370 2.71923 2.73203 2.73258 2.74115

 Alpha virt. eigenvalues -- 2.74377 2.75064 2.75099 2.76207 2.76784

 Alpha virt. eigenvalues -- 2.76984 2.78747 2.79301 2.79357 2.79405

 Alpha virt. eigenvalues -- 2.80030 2.80500 2.81960 2.82515 2.83509

 Alpha virt. eigenvalues -- 2.84671 2.85288 2.85539 2.85555 2.86852

 Alpha virt. eigenvalues -- 2.89050 2.89333 2.89879 2.90265 2.92594

 Alpha virt. eigenvalues -- 2.95020 2.95859 2.95951 2.96537 2.98199

 Alpha virt. eigenvalues -- 2.98366 2.98899 2.99550 3.02035 3.02565

 Alpha virt. eigenvalues -- 3.03066 3.04450 3.05067 3.05404 3.06324

 Alpha virt. eigenvalues -- 3.07417 3.07772 3.07782 3.08007 3.08555

 Alpha virt. eigenvalues -- 3.10685 3.10899 3.11725 3.11931 3.13307

 Alpha virt. eigenvalues -- 3.14603 3.14629 3.16061 3.16250 3.18381

 Alpha virt. eigenvalues -- 3.19567 3.19692 3.21842 3.22380 3.22539

 Alpha virt. eigenvalues -- 3.25412 3.25949 3.26133 3.26171 3.27217

 Alpha virt. eigenvalues -- 3.28125 3.29192 3.29324 3.29385 3.29742

 Alpha virt. eigenvalues -- 3.29857 3.30137 3.30397 3.30590 3.30983

 Alpha virt. eigenvalues -- 3.31194 3.31256 3.31322 3.31934 3.32540

 Alpha virt. eigenvalues -- 3.34251 3.34344 3.34988 3.35713 3.36939

 Alpha virt. eigenvalues -- 3.37342 3.38618 3.38729 3.40457 3.40986

 Alpha virt. eigenvalues -- 3.41404 3.42131 3.42631 3.44686 3.45037

 Alpha virt. eigenvalues -- 3.50314 3.51635 3.51718 3.52395 3.56581

 Alpha virt. eigenvalues -- 3.56816 3.57891 3.58071 3.58099 3.59636

 Alpha virt. eigenvalues -- 3.60089 3.61591 3.63046 3.65752 3.65948

 Alpha virt. eigenvalues -- 3.67489 3.72104 3.72307 3.73349 3.75789

 Alpha virt. eigenvalues -- 3.77196 3.79054 3.81002 3.81324 3.81705

 Alpha virt. eigenvalues -- 3.83653 3.86811 3.89004 3.92430 3.94963

 Alpha virt. eigenvalues -- 3.95089 3.95367 3.95735 3.95957 3.96158

 Alpha virt. eigenvalues -- 3.96227 3.99000 3.99248 4.03615 4.11350

 Alpha virt. eigenvalues -- 4.29064 4.30966 4.36449 4.40213 4.45794

 Alpha virt. eigenvalues -- 4.51004 4.54806 4.56910 4.64588 4.64805

 Alpha virt. eigenvalues -- 4.67551 4.69689 4.78711 4.78721 4.78727

 Alpha virt. eigenvalues -- 4.78736 5.09503 5.15911 5.18695 5.31535

 Alpha virt. eigenvalues -- 23.25230 23.28748 23.29078 23.30639 23.45400

 Alpha virt. eigenvalues -- 23.51877 23.52521 23.57705 23.73503 23.74464

 Alpha virt. eigenvalues -- 23.76961 23.77913 23.80983 23.81139 23.81139

 Alpha virt. eigenvalues -- 23.81388 23.85064 23.85960 23.86041 23.86751

 Alpha virt. eigenvalues -- 23.93330 23.93795 23.95590 23.97525 23.98908

 Alpha virt. eigenvalues -- 23.99343 23.99923 24.00387 24.04694 24.04815

 Alpha virt. eigenvalues -- 24.04905 24.05026 24.09209 24.09434 24.10323

 Alpha virt. eigenvalues -- 24.10516 24.12426 24.12525 24.16146 24.16392

 Alpha virt. eigenvalues -- 24.16722 24.16753 24.16836 24.16849 35.56014

 Alpha virt. eigenvalues -- 35.56966 35.63681 35.64307

 Condensed to atoms (all electrons):

 Mulliken charges:

 1

 1 C -0.255723

 2 C 0.357654

 3 N -0.707694

 4 C 0.357654

 5 C -0.255723

 6 C -0.115784

 7 C 0.223782

 8 N -0.508618

 9 C 0.223782

 10 C -0.248628

 11 C -0.248628

 12 C -0.115784

 13 C 0.223782

 14 C -0.248628

 15 C -0.248628

 16 C 0.223782

 17 N -0.508618

 18 C -0.115784

 19 C 0.357654

 20 C -0.255723

 21 C -0.255723

 22 C 0.357654

 23 N -0.707694

 24 C -0.115784

 25 C -0.123021

 26 C -0.207475

 27 C -0.216992

 28 C -0.219972

 29 C -0.217102

 30 C -0.205184

 31 C -0.219972

 32 C -0.216992

 33 C -0.207475

 34 C -0.123021

 35 C -0.205184

 36 C -0.217102

 37 C -0.123021

 38 C -0.205184

 39 C -0.217102

 40 C -0.219972

 41 C -0.216992

 42 C -0.207475

 43 C -0.123021

 44 C -0.205184

 45 C -0.217102

 46 C -0.219972

 47 C -0.216992

 48 C -0.207475

 49 H 0.253275

 50 H 0.253275

 51 H 0.239735

 52 H 0.239735

 53 H 0.239735

 54 H 0.239735

 55 H 0.253275

 56 H 0.253275

 57 H 0.226139

 58 H 0.227044

 59 H 0.226742

 60 H 0.227080

 61 H 0.225412

 62 H 0.226742

 63 H 0.227044

 64 H 0.226139

 65 H 0.225412

 66 H 0.227080

 67 H 0.225412

 68 H 0.227080

 69 H 0.226742

 70 H 0.227044

 71 H 0.226139

 72 H 0.225412

 73 H 0.227080

 74 H 0.226742

 75 H 0.227044

 76 H 0.226139

 77 H 0.422348

 78 H 0.422348

 Sum of Mulliken charges = 0.00000

 Mulliken charges with hydrogens summed into heavy atoms:

 1

 1 C -0.002449

 2 C 0.357654

 3 N -0.285346

 4 C 0.357654

 5 C -0.002449

 6 C -0.115784

 7 C 0.223782

 8 N -0.508618

 9 C 0.223782

 10 C -0.008893

 11 C -0.008893

 12 C -0.115784

 13 C 0.223782

 14 C -0.008893

 15 C -0.008893

 16 C 0.223782

 17 N -0.508618

 18 C -0.115784

 19 C 0.357654

 20 C -0.002449

 21 C -0.002449

 22 C 0.357654

 23 N -0.285346

 24 C -0.115784

 25 C -0.123021

 26 C 0.018664

 27 C 0.010053

 28 C 0.006770

 29 C 0.009978

 30 C 0.020228

 31 C 0.006770

 32 C 0.010053

 33 C 0.018664

 34 C -0.123021

 35 C 0.020228

 36 C 0.009978

 37 C -0.123021

 38 C 0.020228

 39 C 0.009978

 40 C 0.006770

 41 C 0.010053

 42 C 0.018664

 43 C -0.123021

 44 C 0.020228

 45 C 0.009978

 46 C 0.006770

 47 C 0.010053

 48 C 0.018664

 Electronic spatial extent (au): <R\*\*2>= 33191.7128

 Charge= 0.0000 electrons

 Dipole moment (field-independent basis, Debye):

 X= 0.0000 Y= 0.0000 Z= -0.2505 Tot= 0.2505

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

 XX= -232.1233 YY= -216.2209 ZZ= -268.3449

 XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

 XX= 6.7730 YY= 22.6755 ZZ= -29.4485

 XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

 XXX= 0.0000 YYY= 0.0000 ZZZ= 1.1866 XYY= 0.0000

 XXY= 0.0000 XXZ= 90.6823 XZZ= 0.0000 YZZ= 0.0000

 YYZ= -88.5713 XYZ= 0.0000

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

 XXXX= -21381.0892 YYYY= -20766.5731 ZZZZ= -1069.4300 XXXY= 0.0000

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

 ZZZY= 0.0000 XXYY= -5575.8830 XXZZ= -3820.0642 YYZZ= -3769.7830

 XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

 N-N= 5.358814469673D+03 E-N=-1.516735647859D+04 KE= 1.906418097378D+03

 Symmetry A1 KE= 5.317595982114D+02

 Symmetry A2 KE= 4.227694071419D+02

 Symmetry B1 KE= 4.760245638238D+02

 Symmetry B2 KE= 4.758645282011D+02

 Leave Link 601 at Thu Sep 5 22:04:06 2019, MaxMem= 1342177280 cpu: 44.7

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

 Test job not archived.

 1\1\GINC-K212\SP\RB3LYP TD-FC\6-311G(d)\C44H30N4\Z5105842\05-Sep-2019\

 0\\#p td(root=1,nstates=10) b3lyp/6-311G\* scrf=(solvent=dmso,smd) empi

 ricaldispersion=gd3bj IOp(9/40=3)\\TPP0td\\0,1\C,0,-0.684157,4.237971,

 0.1734\C,0,-1.131729,2.883123,0.040396\N,0,0.,2.102773,-0.023951\C,0,1

 .131729,2.883123,0.040396\C,0,0.684157,4.237971,0.1734\C,0,2.458736,2.

 438755,-0.009747\C,0,2.860501,1.090959,-0.065036\N,0,2.039697,0.,0.009

 609\C,0,2.860501,-1.090959,-0.065036\C,0,4.249993,-0.677406,-0.222575\

 C,0,4.249993,0.677406,-0.222575\C,0,-2.458736,2.438755,-0.009747\C,0,-

 2.860501,1.090959,-0.065036\C,0,-4.249993,0.677406,-0.222575\C,0,-4.24

 9993,-0.677406,-0.222575\C,0,-2.860501,-1.090959,-0.065036\N,0,-2.0396

 97,0.,0.009609\C,0,-2.458736,-2.438755,-0.009747\C,0,-1.131729,-2.8831

 23,0.040396\C,0,-0.684157,-4.237971,0.1734\C,0,0.684157,-4.237971,0.17

 34\C,0,1.131729,-2.883123,0.040396\N,0,0.,-2.102773,-0.023951\C,0,2.45

 8736,-2.438755,-0.009747\C,0,3.519159,3.489365,0.001777\C,0,3.639775,4

 .395294,-1.058689\C,0,4.632445,5.37237,-1.046425\C,0,5.515158,5.460502

 ,0.029084\C,0,5.401135,4.564352,1.091122\C,0,4.411543,3.584521,1.07643

 8\C,0,-5.515158,5.460502,0.029084\C,0,-4.632445,5.37237,-1.046425\C,0,

 -3.639775,4.395294,-1.058689\C,0,-3.519159,3.489365,0.001777\C,0,-4.41

 1543,3.584521,1.076438\C,0,-5.401135,4.564352,1.091122\C,0,3.519159,-3

 .489365,0.001777\C,0,4.411543,-3.584521,1.076438\C,0,5.401135,-4.56435

 2,1.091122\C,0,5.515158,-5.460502,0.029084\C,0,4.632445,-5.37237,-1.04

 6425\C,0,3.639775,-4.395294,-1.058689\C,0,-3.519159,-3.489365,0.001777

 \C,0,-4.411543,-3.584521,1.076438\C,0,-5.401135,-4.564352,1.091122\C,0

 ,-5.515158,-5.460502,0.029084\C,0,-4.632445,-5.37237,-1.046425\C,0,-3.

 639775,-4.395294,-1.058689\H,0,-1.332862,5.093596,0.269591\H,0,1.33286

 2,5.093596,0.269591\H,0,5.097972,-1.334858,-0.336827\H,0,5.097972,1.33

 4858,-0.336827\H,0,-5.097972,1.334858,-0.336827\H,0,-5.097972,-1.33485

 8,-0.336827\H,0,-1.332862,-5.093596,0.269591\H,0,1.332862,-5.093596,0.

 269591\H,0,2.95811,4.325512,-1.899332\H,0,4.71729,6.062914,-1.878958\H

 ,0,6.287254,6.222625,0.039493\H,0,6.081643,4.628576,1.933705\H,0,4.322

 318,2.891059,1.905414\H,0,-6.287254,6.222625,0.039493\H,0,-4.71729,6.0

 62914,-1.878958\H,0,-2.95811,4.325512,-1.899332\H,0,-4.322318,2.891059

 ,1.905414\H,0,-6.081643,4.628576,1.933705\H,0,4.322318,-2.891059,1.905

 414\H,0,6.081643,-4.628576,1.933705\H,0,6.287254,-6.222625,0.039493\H,

 0,4.71729,-6.062914,-1.878958\H,0,2.95811,-4.325512,-1.899332\H,0,-4.3

 22318,-2.891059,1.905414\H,0,-6.081643,-4.628576,1.933705\H,0,-6.28725

 4,-6.222625,0.039493\H,0,-4.71729,-6.062914,-1.878958\H,0,-2.95811,-4.

 325512,-1.899332\H,0,0.,1.092438,-0.082721\H,0,0.,-1.092438,-0.082721\

 \Version=ES64L-G09RevD.01\State=1-A1\HF=-1914.3847913\RMSD=3.693e-09\P

 G=C02V [SGV(H2N2),SGV'(N2),X(C44H28)]\\@

 I FIND THAT THE THREE TRULY GREAT TIMES FOR THINKING THOUGHTS

 ARE WHEN I AM STANDING IN THE SHOWER, SITTING ON THE JOHN, OR WALKING.

 -- COLIN FLETCHER

 Job cpu time: 0 days 3 hours 51 minutes 21.6 seconds.

 File lengths (MBytes): RWF= 3578 Int= 0 D2E= 0 Chk= 328 Scr= 2

 Normal termination of Gaussian 09 at Thu Sep 5 22:04:11 2019.