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.

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

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

Cite this work as:

Gaussian 09, Revision D.01,

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

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)

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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)

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40 initial guesses have been made.

Convergence on wavefunction: 0.001000000000000

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

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

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

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78 ->249 -0.00106

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79 ->213 -0.00119

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161 <-280 0.00171

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161 <-331 0.00131

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

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72 ->215 -0.00123

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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

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82 ->213 -0.00186

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83 ->217 -0.00195

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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.

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Population analysis using the SCF density.

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Orbital symmetries:

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(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.