Entering Gaussian System, Link 0=g09

Input=ZnPC0td.com

Output=ZnPC0td.log

Initial command:

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

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

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

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

Cite this work as:

Gaussian 09, Revision E.01,

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

19-Sep-2019

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

%nprocshared=9

Will use up to 9 processors via shared memory.

%mem=10GB

%chk=ZnPC0td.chk

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

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

ldispersion=gd3bj IOp(9/40=3)

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

1/38=1/1;

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

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

4//1;

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

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

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

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

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

Leave Link 1 at Thu Sep 19 00:35:27 2019, MaxMem= 1342177280 cpu: 0.6

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

-------

ZnPC0td

-------

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C 2.76651 1.18235 0.01953

N 1.4247 1.4247 0.06819

C 1.18235 2.76651 0.01953

C 2.46772 3.46649 -0.04739

C 3.46649 2.46772 -0.04739

N 0. 3.37815 0.00933

C -1.18235 2.76651 0.01953

N -1.4247 1.4247 0.06819

C -2.76651 1.18235 0.01953

C -3.46649 2.46772 -0.04739

C -2.46772 3.46649 -0.04739

N 3.37815 0. 0.00933

C 3.46649 -2.46772 -0.04739

C 2.46772 -3.46649 -0.04739

C 1.18235 -2.76651 0.01953

N 1.4247 -1.4247 0.06819

C 2.76651 -1.18235 0.01953

N 0. -3.37815 0.00933

N -1.4247 -1.4247 0.06819

C -1.18235 -2.76651 0.01953

C -2.46772 -3.46649 -0.04739

C -3.46649 -2.46772 -0.04739

C -2.76651 -1.18235 0.01953

N -3.37815 0. 0.00933

Zn 0. 0. 0.51047

C 4.81585 -2.80418 -0.11201

C 5.14916 -4.1562 -0.16919

C 4.1562 -5.14916 -0.16919

C 2.80418 -4.81585 -0.11201

C -4.81585 -2.80418 -0.11201

C -5.14916 -4.1562 -0.16919

C -4.1562 -5.14916 -0.16919

C -2.80418 -4.81585 -0.11201

C -2.80418 4.81585 -0.11201

C -4.1562 5.14916 -0.16919

C -5.14916 4.1562 -0.16919

C -4.81585 2.80418 -0.11201

C 4.81585 2.80418 -0.11201

C 5.14916 4.1562 -0.16919

C 4.1562 5.14916 -0.16919

C 2.80418 4.81585 -0.11201

H 5.58269 -2.03739 -0.11563

H 2.03739 -5.58269 -0.11563

H -5.58269 -2.03739 -0.11563

H -2.03739 -5.58269 -0.11563

H -2.03739 5.58269 -0.11563

H -5.58269 2.03739 -0.11563

H 5.58269 2.03739 -0.11563

H 2.03739 5.58269 -0.11563

H -4.44927 6.19242 -0.21565

H -6.19242 4.44927 -0.21565

H 4.44927 6.19242 -0.21565

H 6.19242 4.44927 -0.21565

H 6.19242 -4.44927 -0.21565

H 4.44927 -6.19242 -0.21565

H -4.44927 -6.19242 -0.21565

H -6.19242 -4.44927 -0.21565

NAtoms= 57 NQM= 57 NQMF= 0 NMMI= 0 NMMIF= 0

NMic= 0 NMicF= 0.

Isotopes and Nuclear Properties:

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

in nuclear magnetons)

Atom 1 2 3 4 5 6 7 8 9 10

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

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

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

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

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

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

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

Atom 11 12 13 14 15 16 17 18 19 20

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

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

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

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

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

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

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

Atom 21 22 23 24 25 26 27 28 29 30

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

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

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

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

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

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

AtZNuc= 6.0000000 6.0000000 6.0000000 7.0000000 30.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000

Atom 31 32 33 34 35 36 37 38 39 40

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

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

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

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

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

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

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

Atom 41 42 43 44 45 46 47 48 49 50

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

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

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

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

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

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

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

Atom 51 52 53 54 55 56 57

IAtWgt= 1 1 1 1 1 1 1

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 1 1 1 1 1 1 1

AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

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

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

Stoichiometry C32H16N8Zn

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

Deg. of freedom 22

Full point group C4V NOp 8

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 2.766507 1.182350 0.019533

2 7 0 1.424701 1.424701 0.068191

3 6 0 1.182350 2.766507 0.019533

4 6 0 2.467721 3.466489 -0.047388

5 6 0 3.466489 2.467721 -0.047388

6 7 0 0.000000 3.378152 0.009330

7 6 0 -1.182350 2.766507 0.019533

8 7 0 -1.424701 1.424701 0.068191

9 6 0 -2.766507 1.182350 0.019533

10 6 0 -3.466489 2.467721 -0.047388

11 6 0 -2.467721 3.466489 -0.047388

12 7 0 3.378152 -0.000000 0.009330

13 6 0 3.466489 -2.467721 -0.047388

14 6 0 2.467721 -3.466489 -0.047388

15 6 0 1.182350 -2.766507 0.019533

16 7 0 1.424701 -1.424701 0.068191

17 6 0 2.766507 -1.182350 0.019533

18 7 0 -0.000000 -3.378152 0.009330

19 7 0 -1.424701 -1.424701 0.068191

20 6 0 -1.182350 -2.766507 0.019533

21 6 0 -2.467721 -3.466489 -0.047388

22 6 0 -3.466489 -2.467721 -0.047388

23 6 0 -2.766507 -1.182350 0.019533

24 7 0 -3.378152 0.000000 0.009330

25 30 0 0.000000 0.000000 0.510466

26 6 0 4.815847 -2.804179 -0.112010

27 6 0 5.149164 -4.156200 -0.169185

28 6 0 4.156200 -5.149164 -0.169185

29 6 0 2.804179 -4.815847 -0.112010

30 6 0 -4.815847 -2.804179 -0.112010

31 6 0 -5.149164 -4.156200 -0.169185

32 6 0 -4.156200 -5.149164 -0.169185

33 6 0 -2.804179 -4.815847 -0.112010

34 6 0 -2.804179 4.815847 -0.112010

35 6 0 -4.156200 5.149164 -0.169185

36 6 0 -5.149164 4.156200 -0.169185

37 6 0 -4.815847 2.804179 -0.112010

38 6 0 4.815847 2.804179 -0.112010

39 6 0 5.149164 4.156200 -0.169185

40 6 0 4.156200 5.149164 -0.169185

41 6 0 2.804179 4.815847 -0.112010

42 1 0 5.582686 -2.037386 -0.115625

43 1 0 2.037386 -5.582686 -0.115625

44 1 0 -5.582686 -2.037386 -0.115625

45 1 0 -2.037386 -5.582686 -0.115625

46 1 0 -2.037386 5.582686 -0.115625

47 1 0 -5.582686 2.037386 -0.115625

48 1 0 5.582686 2.037386 -0.115625

49 1 0 2.037386 5.582686 -0.115625

50 1 0 -4.449274 6.192416 -0.215654

51 1 0 -6.192416 4.449274 -0.215654

52 1 0 4.449274 6.192416 -0.215654

53 1 0 6.192416 4.449274 -0.215654

54 1 0 6.192416 -4.449274 -0.215654

55 1 0 4.449274 -6.192416 -0.215654

56 1 0 -4.449274 -6.192416 -0.215654

57 1 0 -6.192416 -4.449274 -0.215654

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

Rotational constants (GHZ): 0.0882342 0.0882342 0.0442839

Leave Link 202 at Thu Sep 19 00:35:27 2019, MaxMem= 1342177280 cpu: 0.1

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

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

Centers: 25

S 1 1.00

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

S 1 1.00

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

S 1 1.00

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

P 1 1.00

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

P 1 1.00

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

D 3 1.00

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

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

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

D 1 1.00

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

D 1 1.00

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

\*\*\*\*

Centers: 42 43 44 45 46 47 48 49 50 51

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

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

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

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

Centers: 8 12 16 18 19 24

6-311G\*

\*\*\*\*

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

Pseudopotential Parameters

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

Center Atomic Valence Angular Power

Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

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

1 6

No pseudopotential on this center.

2 7

No pseudopotential on this center.

3 6

No pseudopotential on this center.

4 6

No pseudopotential on this center.

5 6

No pseudopotential on this center.

6 7

No pseudopotential on this center.

7 6

No pseudopotential on this center.

8 7

No pseudopotential on this center.

9 6

No pseudopotential on this center.

10 6

No pseudopotential on this center.

11 6

No pseudopotential on this center.

12 7

No pseudopotential on this center.

13 6

No pseudopotential on this center.

14 6

No pseudopotential on this center.

15 6

No pseudopotential on this center.

16 7

No pseudopotential on this center.

17 6

No pseudopotential on this center.

18 7

No pseudopotential on this center.

19 7

No pseudopotential on this center.

20 6

No pseudopotential on this center.

21 6

No pseudopotential on this center.

22 6

No pseudopotential on this center.

23 6

No pseudopotential on this center.

24 7

No pseudopotential on this center.

25 30 12

F and up

1 386.7379660 -18.00000000 0.00000000

2 72.8587359 -124.35274030 0.00000000

2 15.9066170 -30.66018220 0.00000000

2 4.3502340 -10.63589890 0.00000000

2 1.2842199 -0.76836230 0.00000000

S - F

0 19.0867858 3.00000000 0.00000000

1 5.0231080 22.52342250 0.00000000

2 1.2701744 48.44659420 0.00000000

2 1.0671287 -44.55601190 0.00000000

2 0.9264190 12.99839580 0.00000000

P - F

0 43.4927750 5.00000000 0.00000000

1 20.8692669 20.74355890 0.00000000

2 21.7118378 90.30271580 0.00000000

2 6.3616915 74.66103160 0.00000000

2 1.2291195 9.88944240 0.00000000

D - F

2 13.5851800 -4.84903590 0.00000000

2 9.8373050 3.69133790 0.00000000

2 0.8373113 -0.50373190 0.00000000

26 6

No pseudopotential on this center.

27 6

No pseudopotential on this center.

28 6

No pseudopotential on this center.

29 6

No pseudopotential on this center.

30 6

No pseudopotential on this center.

31 6

No pseudopotential on this center.

32 6

No pseudopotential on this center.

33 6

No pseudopotential on this center.

34 6

No pseudopotential on this center.

35 6

No pseudopotential on this center.

36 6

No pseudopotential on this center.

37 6

No pseudopotential on this center.

38 6

No pseudopotential on this center.

39 6

No pseudopotential on this center.

40 6

No pseudopotential on this center.

41 6

No pseudopotential on this center.

42 1

No pseudopotential on this center.

43 1

No pseudopotential on this center.

44 1

No pseudopotential on this center.

45 1

No pseudopotential on this center.

46 1

No pseudopotential on this center.

47 1

No pseudopotential on this center.

48 1

No pseudopotential on this center.

49 1

No pseudopotential on this center.

50 1

No pseudopotential on this center.

51 1

No pseudopotential on this center.

52 1

No pseudopotential on this center.

53 1

No pseudopotential on this center.

54 1

No pseudopotential on this center.

55 1

No pseudopotential on this center.

56 1

No pseudopotential on this center.

57 1

No pseudopotential on this center.

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

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

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

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

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

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

There are 211 symmetry adapted basis functions of A1 symmetry.

There are 187 symmetry adapted basis functions of A2 symmetry.

There are 197 symmetry adapted basis functions of B1 symmetry.

There are 197 symmetry adapted basis functions of B2 symmetry.

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

138 alpha electrons 138 beta electrons

nuclear repulsion energy 4381.1283324348 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 57 NActive= 57 NUniq= 9 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1642256700 Hartrees.

Nuclear repulsion after empirical dispersion term = 4380.9641067648 Hartrees.

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

Polarizable Continuum Model (PCM)

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

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 57.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

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

GePol: Number of generator spheres = 57

GePol: Total number of spheres = 57

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

GePol: Number of points = 4638

GePol: Average weight of points = 0.10

GePol: Minimum weight of points = 0.18D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 288

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

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

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

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

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

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

PCM non-electrostatic energy = -0.0144004639 Hartrees.

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

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

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

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

LDataN: DoStor=T MaxTD1= 5 Len= 102

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

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

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

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

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

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

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

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

DipDrv: MaxL=1.

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

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

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -1733.63499390998

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

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

LenX= 1340763889 LenY= 1340065829

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

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

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 64533132.

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

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

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

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

E= -1732.57712527219

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

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

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

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

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.102 Goal= None Shift= 0.000

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

Damping current iteration by 2.50D-01

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

Cycle 2 Pass 1 IDiag 1:

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

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

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

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

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

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

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

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

Coeff: -0.558D+00 0.156D+01

Gap= 0.093 Goal= None Shift= 0.000

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

Cycle 3 Pass 1 IDiag 1:

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

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

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

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

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

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

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

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

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

Gap= 0.080 Goal= None Shift= 0.000

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

Cycle 4 Pass 1 IDiag 1:

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

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

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

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

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

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

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

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

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

Gap= 0.080 Goal= None Shift= 0.000

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

Cycle 5 Pass 1 IDiag 1:

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

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

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

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

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

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

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

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

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

Gap= 0.080 Goal= None Shift= 0.000

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

Cycle 6 Pass 1 IDiag 1:

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

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

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

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

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

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

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

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

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

Gap= 0.080 Goal= None Shift= 0.000

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

Cycle 7 Pass 1 IDiag 1:

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

CP: 6.95D-01

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

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

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

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

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

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

Coeff-Com: 0.469D+00

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

Coeff-En: 0.955D+00

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

Coeff: 0.470D+00

Gap= 0.080 Goal= None Shift= 0.000

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

Cycle 8 Pass 1 IDiag 1:

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

CP: 7.38D-01 5.59D-01

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

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

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

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

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

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

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

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

Coeff: 0.227D+00 0.654D+00

Gap= 0.080 Goal= None Shift= 0.000

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

Cycle 9 Pass 1 IDiag 1:

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

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

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

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

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

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

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

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

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

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

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

Gap= 0.080 Goal= None Shift= 0.000

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

Cycle 10 Pass 1 IDiag 1:

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

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

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

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

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

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

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

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

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

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

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

Gap= 0.080 Goal= None Shift= 0.000

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

Cycle 11 Pass 1 IDiag 1:

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

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

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

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

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

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

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

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

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

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

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

Gap= 0.080 Goal= None Shift= 0.000

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

Cycle 12 Pass 1 IDiag 1:

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

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

CP: 7.11D-01

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

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

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

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

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

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

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

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

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

Gap= 0.080 Goal= None Shift= 0.000

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

Error on total polarization charges = 0.07181

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

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

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

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

(included in total energy above)

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

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

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

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

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

ICtDFT= 12500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

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

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

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

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

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

RHF ground state

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

Would need an additional 60292500000 words for in-memory AO integral storage.

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

Inv3: Mode=1 IEnd= 64533132.

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

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

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

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

Making orbital integer symmetry assigments:

Orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

(A2)

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

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

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

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

40 initial guesses have been made.

Convergence on wavefunction: 0.001000000000000

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

Max sub-space: 200 roots to seek: 40 dimension of matrix: 128184

Iteration 1 Dimension 40 NMult 0 NNew 40

CISAX will form 40 AO SS matrices at one time.

NMat= 40 NSing= 40 JSym2X=-1.

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

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

New state 1 was old state 2

New state 2 was old state 1

New state 3 was old state 5

New state 5 was old state 7

New state 6 was old state 9

New state 7 was old state 26

New state 8 was old state 27

New state 9 was old state 25

New state 10 was old state 24

Excitation Energies [eV] at current iteration:

Root 1 : 2.260807998217566

Root 2 : 2.260807998224620

Root 3 : 3.457428761343296

Root 4 : 3.457428761346411

Root 5 : 3.468717621705896

Root 6 : 3.489833386634942

Root 7 : 3.579469781343652

Root 8 : 3.579469781358811

Root 9 : 3.590696141983564

Root 10 : 3.590696141989334

Root 11 : 3.618743841667010

Root 12 : 3.676359187609923

Root 13 : 3.704616573459891

Root 14 : 3.729453254352031

Root 15 : 3.735579215217723

Root 16 : 3.755248424184478

Root 17 : 3.755248424190279

Root 18 : 3.848660248869227

Root 19 : 3.848660248878092

Root 20 : 3.945378968962145

Root 21 : 4.008267469238258

Root 22 : 4.008267469245128

Root 23 : 4.023658395473614

Root 24 : 4.034464615116606

Root 25 : 4.038310244438326

Root 26 : 4.062343964567411

Root 27 : 4.066978394101302

Root 28 : 4.083618928872398

Root 29 : 4.111250622589590

Root 30 : 4.168743718125652

Root 31 : 4.168743718125692

Root 32 : 4.830614947804804

Root 33 : 4.830614947808276

Root 34 : 4.862426119805578

Root 35 : 4.862426119813643

Root 36 : 5.272471588444855

Root 37 : 5.315989537378972

Root 38 : 5.315989537382929

Root 39 : 5.531889283617966

Root 40 : 5.725020830369886

Iteration 2 Dimension 60 NMult 40 NNew 20

CISAX will form 20 AO SS matrices at one time.

NMat= 20 NSing= 20 JSym2X=-1.

Root 1 not converged, maximum delta is 0.051794436019275

Root 2 not converged, maximum delta is 0.051794436019433

Root 3 not converged, maximum delta is 0.046754364880017

Root 4 not converged, maximum delta is 0.046754364880358

Root 5 not converged, maximum delta is 0.106984290190375

Root 6 not converged, maximum delta is 0.036229801857750

New state 7 was old state 9

Root 7 not converged, maximum delta is 0.438241206409545

New state 8 was old state 10

Root 8 not converged, maximum delta is 0.438241205662629

New state 9 was old state 7

Root 9 not converged, maximum delta is 0.429824601382394

New state 10 was old state 8

Root 10 not converged, maximum delta is 0.429824600655773

Excitation Energies [eV] at current iteration:

Root 1 : 2.012194999998586 Change is -0.248612998218980

Root 2 : 2.012195000006430 Change is -0.248612998218190

Root 3 : 3.335838681312229 Change is -0.121590080031067

Root 4 : 3.335838681313757 Change is -0.121590080032654

Root 5 : 3.341778660155455 Change is -0.126938961550441

Root 6 : 3.346703459191904 Change is -0.143129927443038

Root 7 : 3.536556122233153 Change is -0.054140019750411

Root 8 : 3.536556122246961 Change is -0.054140019742373

Root 9 : 3.547240293331287 Change is -0.032229488012365

Root 10 : 3.547240293337429 Change is -0.032229488021381

Iteration 3 Dimension 80 NMult 60 NNew 20

CISAX will form 20 AO SS matrices at one time.

NMat= 20 NSing= 20 JSym2X=-1.

Root 1 not converged, maximum delta is 0.025594509613801

Root 2 not converged, maximum delta is 0.025594509615225

Root 3 not converged, maximum delta is 0.029011773416201

Root 4 not converged, maximum delta is 0.029011773415995

Root 5 not converged, maximum delta is 0.008125897073670

Root 6 not converged, maximum delta is 0.004421255593668

Root 7 not converged, maximum delta is 0.005007772400976

Root 8 not converged, maximum delta is 0.005007772403527

Root 9 not converged, maximum delta is 0.003860706353288

Root 10 not converged, maximum delta is 0.003860706358977

Excitation Energies [eV] at current iteration:

Root 1 : 1.991459156606346 Change is -0.020735843392240

Root 2 : 1.991459156612579 Change is -0.020735843393851

Root 3 : 3.328534804325345 Change is -0.007303876986884

Root 4 : 3.328534804326258 Change is -0.007303876987499

Root 5 : 3.335654475723512 Change is -0.006124184431943

Root 6 : 3.340330632719558 Change is -0.006372826472346

Root 7 : 3.535068983313655 Change is -0.001487138919498

Root 8 : 3.535068983327003 Change is -0.001487138919958

Root 9 : 3.546052810293530 Change is -0.001187483037757

Root 10 : 3.546052810299882 Change is -0.001187483037547

Iteration 4 Dimension 100 NMult 80 NNew 20

CISAX will form 20 AO SS matrices at one time.

NMat= 20 NSing= 20 JSym2X=-1.

Root 1 not converged, maximum delta is 0.002671964295458

Root 2 not converged, maximum delta is 0.002671964295560

Root 3 not converged, maximum delta is 0.002789337360566

Root 4 not converged, maximum delta is 0.002789337360924

Root 5 not converged, maximum delta is 0.003142960503575

Root 6 not converged, maximum delta is 0.004415172495125

Root 7 not converged, maximum delta is 0.003394898050984

Root 8 not converged, maximum delta is 0.003394898059712

Root 9 not converged, maximum delta is 0.003136249529189

Root 10 not converged, maximum delta is 0.003136249537544

Excitation Energies [eV] at current iteration:

Root 1 : 1.989283700182521 Change is -0.002175456423825

Root 2 : 1.989283700188844 Change is -0.002175456423735

Root 3 : 3.327597607736869 Change is -0.000937196588476

Root 4 : 3.327597607737758 Change is -0.000937196588501

Root 5 : 3.334669440577445 Change is -0.000985035146067

Root 6 : 3.339212294070485 Change is -0.001118338649073

Root 7 : 3.534902582323987 Change is -0.000166400989667

Root 8 : 3.534902582337150 Change is -0.000166400989852

Root 9 : 3.545810180691952 Change is -0.000242629601579

Root 10 : 3.545810180698420 Change is -0.000242629601463

Iteration 5 Dimension 120 NMult 100 NNew 20

CISAX will form 20 AO SS matrices at one time.

NMat= 20 NSing= 20 JSym2X=-1.

Root 1 has converged.

Root 2 has converged.

Root 3 not converged, maximum delta is 0.001703385137473

Root 4 not converged, maximum delta is 0.001703385139258

Root 5 has converged.

Root 6 has converged.

Root 7 has converged.

Root 8 has converged.

Root 9 has converged.

Root 10 has converged.

Excitation Energies [eV] at current iteration:

Root 1 : 1.989116946614429 Change is -0.000166753568092

Root 2 : 1.989116946620918 Change is -0.000166753567926

Root 3 : 3.327515090394606 Change is -0.000082517342262

Root 4 : 3.327515090395348 Change is -0.000082517342410

Root 5 : 3.334587553711279 Change is -0.000081886866166

Root 6 : 3.339056369279984 Change is -0.000155924790501

Root 7 : 3.534878973849753 Change is -0.000023608474234

Root 8 : 3.534878973863056 Change is -0.000023608474095

Root 9 : 3.545792620846008 Change is -0.000017559845944

Root 10 : 3.545792620852522 Change is -0.000017559845897

Iteration 6 Dimension 124 NMult 120 NNew 4

CISAX will form 4 AO SS matrices at one time.

NMat= 4 NSing= 4 JSym2X=-1.

Root 1 has converged.

Root 2 has converged.

Root 3 has converged.

Root 4 has converged.

Root 5 has converged.

Root 6 has converged.

Root 7 not converged, maximum delta is 0.004609101758526

Root 8 not converged, maximum delta is 0.004609101757096

Root 9 has converged.

Root 10 has converged.

Excitation Energies [eV] at current iteration:

Root 1 : 1.989116913943556 Change is -0.000000032670873

Root 2 : 1.989116913949756 Change is -0.000000032671162

Root 3 : 3.327509834292781 Change is -0.000005256101826

Root 4 : 3.327509834293497 Change is -0.000005256101851

Root 5 : 3.334587553711304 Change is 0.000000000000025

Root 6 : 3.339056369279910 Change is -0.000000000000074

Root 7 : 3.534878966542337 Change is -0.000000007307417

Root 8 : 3.534878966555523 Change is -0.000000007307533

Root 9 : 3.545792610120685 Change is -0.000000010725323

Root 10 : 3.545792610127269 Change is -0.000000010725253

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

Convergence on expansion vectors.

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

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

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

1PDM for each excited state written to RWF 633

Ground to excited state transition densities written to RWF 633

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

state X Y Z Dip. S. Osc.

1 0.0000 3.6174 -0.0000 13.0858 0.6377

2 -3.6174 0.0000 0.0000 13.0858 0.6377

3 0.0000 -0.6734 -0.0000 0.4535 0.0370

4 -0.6734 -0.0000 0.0000 0.4535 0.0370

5 0.0000 0.0000 0.0000 0.0000 0.0000

6 -0.0000 -0.0000 -0.0000 0.0000 0.0000

7 0.1364 0.0009 -0.0000 0.0186 0.0016

8 0.0009 -0.1364 -0.0000 0.0186 0.0016

9 -0.0533 -0.0000 -0.0000 0.0028 0.0002

10 0.0000 -0.0533 -0.0000 0.0028 0.0002

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

state X Y Z Dip. S. Osc.

1 -0.0000 -0.2631 -0.0000 0.0692 0.6314

2 0.2631 -0.0000 0.0000 0.0692 0.6314

3 -0.0000 0.0761 0.0000 0.0058 0.0316

4 0.0761 0.0000 -0.0000 0.0058 0.0316

5 -0.0000 -0.0000 -0.0000 0.0000 0.0000

6 0.0000 0.0000 0.0000 0.0000 0.0000

7 -0.0177 -0.0001 -0.0000 0.0003 0.0016

8 -0.0001 0.0177 -0.0000 0.0003 0.0016

9 0.0098 0.0000 0.0000 0.0001 0.0005

10 -0.0000 0.0098 0.0000 0.0001 0.0005

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

state X Y Z

1 0.0256 -0.0000 0.0000

2 0.0000 0.0256 -0.0000

3 -0.1166 -0.0000 0.0000

4 -0.0000 0.1166 -0.0000

5 0.0000 -0.0000 1.8419

6 -0.0000 0.0000 0.0000

7 -0.0029 0.4202 0.0000

8 0.4202 0.0029 -0.0000

9 -0.0000 0.4162 0.0000

10 -0.4162 -0.0000 0.0000

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

state XX YY ZZ XY XZ YZ

1 -0.0000 0.0000 -0.0000 0.0000 0.0000 0.0457

2 0.0000 -0.0000 -0.0000 0.0000 -0.0457 0.0000

3 0.0000 -0.0000 -0.0000 -0.0000 0.0000 -0.0131

4 -0.0000 0.0000 -0.0000 0.0000 -0.0131 -0.0000

5 0.0000 -0.0000 0.0000 -0.0000 0.0000 0.0000

6 -0.4336 0.4336 0.0000 -0.0000 -0.0000 0.0000

7 0.0000 -0.0000 -0.0000 0.0000 -0.1166 -0.0008

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

9 -0.0000 0.0000 -0.0000 0.0000 0.0125 0.0000

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

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

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

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

1 0.0000 -0.0000 -0.0000 0.0000 90.00

2 -0.0000 0.0000 -0.0000 0.0000 90.00

3 -0.0000 0.0000 -0.0000 -0.0000 90.00

4 0.0000 -0.0000 -0.0000 -0.0000 90.00

5 -0.0000 -0.0000 0.0000 -0.0000 90.00

6 0.0000 0.0000 0.0000 0.0000 90.00

7 -0.1776 0.1776 0.0000 -0.0000 90.00

8 0.1776 -0.1776 -0.0000 -0.0000 90.00

9 0.0000 -0.0000 0.0000 0.0000 90.00

10 -0.0000 0.0000 -0.0000 -0.0000 90.00

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

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

state XX YY ZZ R(length)

1 -0.0000 0.0000 0.0000 0.0000

2 0.0000 -0.0000 0.0000 0.0000

3 0.0000 -0.0000 0.0000 -0.0000

4 -0.0000 0.0000 0.0000 -0.0000

5 -0.0000 0.0000 -0.0000 -0.0000

6 -0.0000 0.0000 0.0000 0.0000

7 0.2781 -0.2781 0.0000 0.0000

8 -0.2781 0.2781 -0.0000 -0.0000

9 -0.0000 0.0000 0.0000 0.0000

10 0.0000 -0.0000 0.0000 -0.0000

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

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

1 -0.0000 -0.9518 0.0000 0.9518 0.6345

2 -0.9518 -0.0000 0.0000 0.9518 0.6345

3 -0.0000 -0.0512 -0.0000 0.0512 0.0342

4 -0.0512 -0.0000 -0.0000 0.0512 0.0342

5 -0.0000 -0.0000 -0.0000 0.0000 0.0000

6 -0.0000 -0.0000 -0.0000 0.0000 0.0000

7 -0.0024 -0.0000 0.0000 0.0024 0.0016

8 -0.0000 -0.0024 0.0000 0.0024 0.0016

9 -0.0005 -0.0000 -0.0000 0.0005 0.0003

10 -0.0000 -0.0005 -0.0000 0.0005 0.0003

Excitation energies and oscillator strengths:

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

41 ->186 0.00106

42 ->207 0.00107

44 ->181 0.00107

45 ->186 0.00143

46 ->178 -0.00103

46 ->182 0.00105

46 ->207 0.00152

47 ->214 0.00111

48 ->186 0.00114

48 ->195 0.00104

48 ->212 -0.00119

53 ->181 -0.00114

61 ->181 -0.00174

62 ->179 -0.00136

63 ->183 -0.00195

63 ->187 -0.00144

63 ->218 0.00107

63 ->232 -0.00130

63 ->239 -0.00104

64 ->181 0.00114

64 ->185 0.00170

64 ->327 -0.00102

68 ->196 0.00122

69 ->185 0.00146

69 ->197 0.00103

70 ->189 0.00137

70 ->195 0.00120

70 ->196 -0.00170

70 ->203 0.00133

70 ->212 -0.00109

70 ->216 -0.00110

70 ->234 0.00116

70 ->249 0.00114

71 ->163 -0.00106

71 ->183 0.00173

71 ->214 0.00111

72 ->169 -0.00104

72 ->182 -0.00172

72 ->210 -0.00123

72 ->211 -0.00111

73 ->166 -0.00125

73 ->181 0.00163

73 ->185 -0.00121

73 ->194 0.00117

73 ->197 0.00140

77 ->149 0.00106

78 ->180 -0.00111

78 ->189 -0.00143

78 ->196 0.00104

78 ->203 -0.00131

78 ->234 -0.00103

79 ->157 0.00125

79 ->183 0.00239

79 ->187 0.00160

79 ->257 -0.00146

79 ->260 -0.00199

79 ->297 -0.00168

80 ->178 -0.00109

80 ->179 0.00314

80 ->193 0.00187

80 ->205 -0.00159

80 ->211 -0.00190

80 ->259 -0.00105

81 ->152 0.00143

81 ->156 -0.00110

81 ->186 -0.00137

82 ->154 0.00236

82 ->162 -0.00140

82 ->169 0.00115

82 ->178 -0.00249

82 ->179 0.00246

82 ->184 0.00101

82 ->193 0.00111

82 ->205 -0.00133

82 ->207 -0.00176

82 ->211 -0.00205

82 ->266 0.00120

83 ->157 -0.00157

83 ->257 -0.00126

83 ->260 -0.00106

83 ->282 0.00109

83 ->297 -0.00189

83 ->320 0.00125

84 ->151 -0.00208

84 ->155 0.00198

84 ->185 -0.00109

84 ->190 -0.00149

84 ->194 0.00102

85 ->151 -0.00216

85 ->166 -0.00137

85 ->172 0.00108

85 ->181 -0.00534

85 ->197 -0.00114

85 ->199 -0.00170

85 ->204 -0.00114

85 ->209 0.00184

85 ->213 0.00152

85 ->241 0.00105

85 ->250 0.00170

85 ->252 0.00135

85 ->280 -0.00100

85 ->290 0.00160

85 ->302 -0.00125

85 ->327 -0.00108

86 ->167 -0.00109

86 ->186 0.00251

86 ->203 0.00102

86 ->261 0.00110

86 ->272 -0.00104

87 ->154 0.00205

87 ->158 -0.00107

87 ->169 -0.00159

87 ->178 -0.00212

87 ->182 0.00398

87 ->207 -0.00123

87 ->258 -0.00137

87 ->271 -0.00149

88 ->173 0.00189

88 ->183 0.00127

88 ->192 0.00133

88 ->214 0.00140

89 ->156 0.00185

89 ->180 0.00112

89 ->195 0.00141

89 ->203 0.00110

90 ->149 0.00129

90 ->154 0.00207

90 ->162 0.00140

90 ->179 0.00216

90 ->193 0.00189

91 ->157 -0.00220

91 ->187 -0.00118

91 ->192 0.00101

91 ->206 -0.00114

92 ->139 -0.00119

92 ->145 0.00344

92 ->164 -0.00454

92 ->177 -0.00178

92 ->212 0.00102

92 ->216 -0.00198

93 ->160 -0.00168

93 ->172 0.00273

93 ->185 0.00332

93 ->194 -0.00204

93 ->197 -0.00106

93 ->209 -0.00117

94 ->151 -0.00107

94 ->155 0.00145

94 ->181 -0.00144

94 ->197 0.00154

95 ->142 0.00438

95 ->150 -0.00355

95 ->219 -0.00139

96 ->141 0.00408

96 ->143 -0.00423

96 ->149 -0.00355

96 ->153 -0.00401

96 ->158 0.00169

96 ->168 0.00325

96 ->175 -0.00195

96 ->220 0.00135

96 ->230 -0.00101

96 ->243 0.00158

97 ->152 -0.00106

97 ->156 0.00277

97 ->161 -0.00150

97 ->186 -0.00184

98 ->154 0.00226

98 ->159 0.00386

98 ->182 0.00134

99 ->157 -0.00103

99 ->163 -0.00216

99 ->173 0.00254

100 ->161 -0.00307

100 ->171 0.00245

100 ->227 -0.00117

101 ->151 0.00218

101 ->155 -0.00164

101 ->160 0.00288

101 ->185 0.00344

101 ->194 -0.00180

101 ->197 -0.00100

102 ->157 0.00340

102 ->163 -0.00206

102 ->183 -0.00128

102 ->192 -0.00147

102 ->206 -0.00155

102 ->226 0.00141

103 ->149 -0.00117

103 ->158 -0.00126

103 ->159 0.00172

103 ->162 -0.00261

103 ->178 -0.00296

103 ->182 0.00104

103 ->188 0.00198

103 ->207 -0.00260

103 ->210 0.00159

104 ->140 0.00546

104 ->144 -0.00138

104 ->148 -0.00124

104 ->155 -0.00252

104 ->160 -0.00109

104 ->166 -0.00130

104 ->190 -0.00163

104 ->213 0.00171

104 ->217 -0.00160

105 ->140 0.00796

105 ->144 -0.00221

105 ->148 -0.00180

105 ->155 0.00133

105 ->166 0.00102

105 ->190 0.00158

105 ->194 -0.00105

105 ->204 0.00148

105 ->217 -0.00132

106 ->156 -0.00159

106 ->186 0.00121

106 ->234 0.00103

106 ->281 0.00103

107 ->139 -0.01027

107 ->145 -0.00152

107 ->147 -0.00425

107 ->177 -0.00190

107 ->216 -0.00151

107 ->234 0.00108

108 ->161 0.00162

108 ->167 -0.00269

108 ->171 0.00157

108 ->186 -0.00249

108 ->195 0.00163

108 ->235 0.00103

109 ->141 -0.00219

109 ->149 -0.00264

109 ->153 -0.00213

109 ->168 0.00265

109 ->220 -0.00186

109 ->230 -0.00126

109 ->243 0.00119

110 ->142 0.00237

110 ->150 -0.00475

110 ->219 0.00205

111 ->159 0.00115

111 ->162 0.00106

111 ->169 -0.00314

111 ->178 0.00141

111 ->182 -0.00338

111 ->188 0.00111

111 ->207 0.00117

111 ->237 -0.00106

112 ->163 -0.00288

112 ->173 -0.00136

112 ->191 0.00243

112 ->192 0.00186

113 ->139 -0.00627

113 ->145 0.00111

113 ->164 0.00315

113 ->224 0.00202

114 ->160 -0.00165

114 ->166 0.00263

114 ->185 0.00402

114 ->190 -0.00246

114 ->194 -0.00221

115 ->161 0.00119

115 ->167 0.00231

115 ->171 0.00344

115 ->186 -0.00180

115 ->189 -0.00135

116 ->140 0.00964

116 ->144 -0.00144

116 ->148 -0.00550

116 ->165 -0.00168

116 ->176 0.00103

116 ->223 -0.00205

116 ->244 0.00115

117 ->149 0.00255

117 ->154 0.00185

117 ->158 0.00238

117 ->159 0.00128

117 ->162 -0.00308

117 ->178 0.00385

117 ->184 -0.00121

117 ->207 0.00254

117 ->211 -0.00111

118 ->170 -0.00385

118 ->173 -0.00112

118 ->192 0.00250

119 ->151 0.00134

119 ->160 0.00253

119 ->166 0.00242

119 ->172 0.00144

119 ->190 -0.00207

119 ->194 0.00273

119 ->222 0.00182

119 ->233 -0.00103

119 ->241 0.00116

120 ->142 0.00237

120 ->146 -0.00231

120 ->150 -0.00139

120 ->157 0.00155

120 ->170 0.00180

120 ->183 -0.00264

120 ->192 -0.00140

120 ->214 -0.00106

120 ->260 0.00115

120 ->282 -0.00104

121 ->141 -0.00220

121 ->143 0.00283

121 ->149 0.00632

121 ->153 0.00155

121 ->158 0.00597

121 ->162 0.00104

121 ->175 0.00101

121 ->178 0.00360

121 ->179 0.00404

121 ->182 0.00202

121 ->193 0.00195

121 ->201 0.00206

121 ->205 -0.00315

121 ->207 -0.00221

121 ->211 -0.00296

121 ->229 0.00155

121 ->298 0.00113

122 ->142 0.00392

122 ->146 -0.00577

122 ->150 -0.00146

122 ->174 0.00171

122 ->183 0.00115

122 ->240 0.00153

122 ->246 0.00154

123 ->141 -0.00543

123 ->143 0.00559

123 ->153 0.00394

123 ->158 -0.00332

123 ->168 -0.00152

123 ->175 0.00125

123 ->178 -0.00121

123 ->179 -0.00161

123 ->184 0.00238

123 ->205 0.00121

123 ->211 0.00100

123 ->230 -0.00230

124 ->152 -0.00132

124 ->171 -0.00106

124 ->180 -0.00359

124 ->186 -0.00109

124 ->189 0.00171

124 ->196 -0.00221

124 ->203 0.00111

124 ->216 -0.00137

124 ->251 0.00100

125 ->170 -0.00220

125 ->173 -0.00129

125 ->183 0.00796

125 ->187 -0.00172

125 ->191 -0.00119

125 ->192 0.00120

125 ->215 0.00218

125 ->218 -0.00147

125 ->226 0.00217

125 ->257 -0.00100

126 ->149 0.00393

126 ->158 0.00449

126 ->169 0.00123

126 ->178 0.00170

126 ->179 0.00466

126 ->182 -0.00159

126 ->193 0.00129

126 ->201 0.00119

126 ->205 -0.00179

126 ->207 -0.00125

126 ->211 -0.00310

126 ->229 0.00128

126 ->278 0.00115

127 ->140 0.01459

127 ->144 0.00761

127 ->148 0.00165

127 ->165 -0.00112

127 ->176 -0.00173

127 ->241 -0.00104

127 ->244 0.00260

128 ->140 -0.00308

128 ->151 0.00281

128 ->155 0.00267

128 ->160 -0.00158

128 ->172 -0.00128

128 ->181 0.00665

128 ->185 0.00127

128 ->190 -0.00315

128 ->194 0.00281

128 ->199 0.00268

128 ->204 -0.00135

128 ->209 -0.00254

128 ->213 -0.00190

128 ->217 -0.00139

128 ->222 -0.00205

128 ->223 -0.00107

128 ->233 0.00181

128 ->273 -0.00121

128 ->276 -0.00103

128 ->290 -0.00144

128 ->295 0.00138

128 ->302 0.00125

129 ->147 -0.00160

129 ->156 0.00219

129 ->171 0.00288

129 ->180 0.00331

129 ->186 -0.00181

129 ->189 -0.00310

129 ->195 -0.00153

129 ->196 0.00369

129 ->203 -0.00164

129 ->208 0.00120

129 ->212 0.00124

129 ->216 0.00201

129 ->281 -0.00137

130 ->139 -0.00635

130 ->145 -0.00117

130 ->147 -0.01102

130 ->164 0.00393

130 ->177 -0.00229

130 ->245 0.00225

131 ->142 0.00526

131 ->146 -0.01001

131 ->150 -0.01159

131 ->174 0.00304

131 ->246 -0.00246

132 ->141 0.02370

132 ->143 0.00175

132 ->175 0.00209

132 ->230 -0.00103

132 ->253 -0.00215

133 ->139 -0.01412

133 ->145 0.00437

133 ->147 0.00177

133 ->164 0.00213

133 ->177 0.00284

133 ->245 0.00104

133 ->249 -0.00119

133 ->255 -0.00132

134 ->139 0.15135

134 ->147 0.01571

134 ->164 -0.00186

134 ->177 0.00224

134 ->434 0.00120

135 ->142 -0.00171

135 ->146 0.00869

135 ->150 -0.00164

135 ->174 -0.00375

135 ->240 0.00158

135 ->279 0.00149

136 ->143 -0.00313

136 ->149 -0.00718

136 ->153 -0.00383

136 ->154 0.00111

136 ->158 0.00239

136 ->168 0.00536

136 ->175 -0.00295

136 ->184 -0.00219

136 ->243 -0.00136

136 ->263 0.00142

137 ->140 0.00789

137 ->144 -0.00297

137 ->148 -0.00888

137 ->165 -0.00419

137 ->176 0.00267

137 ->250 -0.00164

137 ->256 0.00151

138 ->140 0.69448

138 ->144 -0.00891

138 ->148 0.00537

138 ->165 -0.00138

138 ->176 -0.00199

138 ->209 0.00118

138 ->223 -0.00106

138 ->250 -0.00127

138 ->256 0.00158

138 ->262 0.00192

138 ->267 -0.00206

138 ->288 -0.00197

138 ->305 -0.00117

138 ->314 -0.00102

45 <-186 0.00125

46 <-207 0.00133

47 <-214 0.00112

48 <-186 0.00100

48 <-212 -0.00111

61 <-181 -0.00148

62 <-179 -0.00111

63 <-183 -0.00173

63 <-187 -0.00116

63 <-232 -0.00117

64 <-185 0.00149

68 <-196 0.00109

69 <-185 0.00128

70 <-189 0.00112

70 <-195 0.00103

70 <-196 -0.00149

70 <-203 0.00115

70 <-234 0.00103

71 <-183 0.00144

72 <-182 -0.00144

72 <-210 -0.00104

73 <-181 0.00134

73 <-185 -0.00102

73 <-194 0.00101

73 <-197 0.00117

78 <-189 -0.00116

78 <-203 -0.00111

79 <-183 0.00206

79 <-187 0.00129

79 <-257 -0.00126

79 <-260 -0.00173

79 <-297 -0.00147

80 <-179 0.00253

80 <-193 0.00159

80 <-205 -0.00137

80 <-211 -0.00159

81 <-152 0.00109

81 <-186 -0.00110

82 <-154 0.00182

82 <-162 -0.00111

82 <-178 -0.00206

82 <-179 0.00200

82 <-205 -0.00116

82 <-207 -0.00153

82 <-211 -0.00172

82 <-266 0.00108

83 <-157 -0.00118

83 <-257 -0.00107

83 <-297 -0.00164

83 <-320 0.00109

84 <-151 -0.00158

84 <-155 0.00148

84 <-190 -0.00122

85 <-151 -0.00167

85 <-166 -0.00107

85 <-181 -0.00434

85 <-199 -0.00144

85 <-204 -0.00102

85 <-209 0.00154

85 <-213 0.00128

85 <-250 0.00145

85 <-252 0.00112

85 <-290 0.00141

85 <-302 -0.00112

86 <-186 0.00199

87 <-154 0.00152

87 <-169 -0.00120

87 <-178 -0.00170

87 <-182 0.00317

87 <-207 -0.00108

87 <-258 -0.00113

87 <-271 -0.00127

88 <-173 0.00145

88 <-192 0.00108

88 <-214 0.00119

89 <-156 0.00135

89 <-195 0.00111

90 <-154 0.00150

90 <-162 0.00102

90 <-179 0.00170

90 <-193 0.00150

91 <-157 -0.00160

92 <-145 0.00242

92 <-164 -0.00364

92 <-177 -0.00161

92 <-216 -0.00171

93 <-160 -0.00124

93 <-172 0.00209

93 <-185 0.00272

93 <-194 -0.00166

94 <-155 0.00105

94 <-181 -0.00111

94 <-197 0.00123

95 <-142 0.00304

95 <-150 -0.00276

95 <-219 -0.00123

96 <-141 0.00235

96 <-143 -0.00306

96 <-149 -0.00253

96 <-153 -0.00272

96 <-158 0.00121

96 <-168 0.00298

96 <-175 -0.00145

96 <-220 0.00112

96 <-243 0.00131

97 <-156 0.00200

97 <-161 -0.00109

97 <-186 -0.00144

98 <-154 0.00161

98 <-159 0.00278

98 <-182 0.00104

99 <-163 -0.00158

99 <-173 0.00192

100 <-161 -0.00223

100 <-171 0.00183

101 <-151 0.00156

101 <-155 -0.00118

101 <-160 0.00208

101 <-185 0.00275

101 <-194 -0.00144

102 <-157 0.00242

102 <-163 -0.00150

102 <-183 -0.00100

102 <-192 -0.00115

102 <-206 -0.00123

102 <-226 0.00116

103 <-159 0.00124

103 <-162 -0.00192

103 <-178 -0.00233

103 <-188 0.00160

103 <-207 -0.00214

103 <-210 0.00129

104 <-140 0.00266

104 <-144 -0.00111

104 <-155 -0.00178

104 <-166 -0.00100

104 <-190 -0.00131

104 <-213 0.00138

104 <-217 -0.00128

105 <-140 0.00384

105 <-144 -0.00174

105 <-148 -0.00138

105 <-165 -0.00132

105 <-190 0.00121

105 <-204 0.00114

105 <-217 -0.00103

106 <-156 -0.00109

107 <-139 -0.00721

107 <-147 -0.00258

107 <-164 -0.00167

107 <-177 -0.00147

107 <-216 -0.00116

108 <-161 0.00112

108 <-167 -0.00191

108 <-171 0.00112

108 <-186 -0.00190

108 <-195 0.00127

109 <-149 -0.00162

109 <-153 -0.00195

109 <-168 0.00219

109 <-220 -0.00150

109 <-230 -0.00101

109 <-243 0.00103

110 <-142 0.00142

110 <-150 -0.00301

110 <-219 0.00158

111 <-169 -0.00222

111 <-178 0.00107

111 <-182 -0.00256

112 <-163 -0.00201

112 <-191 0.00184

112 <-192 0.00145

113 <-139 -0.00447

113 <-164 0.00246

113 <-224 0.00164

114 <-160 -0.00114

114 <-166 0.00184

114 <-185 0.00311

114 <-190 -0.00185

114 <-194 -0.00169

115 <-167 0.00161

115 <-171 0.00248

115 <-186 -0.00135

115 <-189 -0.00103

116 <-140 0.00365

116 <-144 -0.00162

116 <-148 -0.00409

116 <-165 -0.00209

116 <-223 -0.00158

116 <-244 0.00102

117 <-149 0.00162

117 <-154 0.00121

117 <-158 0.00157

117 <-162 -0.00211

117 <-178 0.00287

117 <-207 0.00202

118 <-170 -0.00273

118 <-192 0.00191

119 <-160 0.00173

119 <-166 0.00169

119 <-172 0.00101

119 <-190 -0.00156

119 <-194 0.00211

119 <-222 0.00146

120 <-146 -0.00174

120 <-157 0.00102

120 <-170 0.00127

120 <-183 -0.00194

120 <-192 -0.00105

121 <-143 0.00158

121 <-149 0.00400

121 <-158 0.00386

121 <-178 0.00258

121 <-179 0.00300

121 <-182 0.00155

121 <-193 0.00154

121 <-201 0.00158

121 <-205 -0.00243

121 <-207 -0.00178

121 <-211 -0.00233

121 <-229 0.00122

122 <-146 -0.00444

122 <-174 0.00130

122 <-240 0.00119

122 <-246 0.00136

123 <-141 0.00128

123 <-143 0.00314

123 <-158 -0.00227

123 <-168 -0.00125

123 <-179 -0.00113

123 <-184 0.00192

123 <-230 -0.00167

124 <-180 -0.00259

124 <-189 0.00128

124 <-196 -0.00164

124 <-216 -0.00110

125 <-170 -0.00152

125 <-183 0.00575

125 <-187 -0.00123

125 <-215 0.00175

125 <-218 -0.00115

125 <-226 0.00171

126 <-149 0.00225

126 <-158 0.00279

126 <-178 0.00114

126 <-179 0.00333

126 <-182 -0.00111

126 <-193 0.00101

126 <-205 -0.00137

126 <-211 -0.00239

126 <-229 0.00102

127 <-140 0.01115

127 <-144 0.00372

127 <-148 -0.00100

127 <-165 -0.00104

127 <-244 0.00214

128 <-151 0.00166

128 <-155 0.00160

128 <-181 0.00468

128 <-190 -0.00227

128 <-194 0.00204

128 <-199 0.00199

128 <-209 -0.00196

128 <-213 -0.00143

128 <-217 -0.00106

128 <-222 -0.00162

128 <-233 0.00141

128 <-290 -0.00121

128 <-295 0.00115

128 <-302 0.00106

129 <-156 0.00134

129 <-171 0.00196

129 <-180 0.00237

129 <-186 -0.00129

129 <-189 -0.00230

129 <-195 -0.00113

129 <-196 0.00273

129 <-203 -0.00125

129 <-216 0.00158

129 <-281 -0.00114

130 <-139 -0.00598

130 <-145 0.00133

130 <-147 -0.00502

130 <-164 0.00196

130 <-177 -0.00136

130 <-245 0.00169

131 <-142 0.00111

131 <-146 -0.00494

131 <-150 -0.00616

131 <-174 0.00180

131 <-246 -0.00192

132 <-141 0.00502

132 <-143 0.00194

132 <-175 0.00133

132 <-253 -0.00176

133 <-139 -0.00641

133 <-145 0.00129

133 <-147 0.00132

133 <-164 0.00154

133 <-177 0.00231

133 <-255 -0.00107

134 <-139 0.05392

134 <-147 0.01116

134 <-164 -0.00149

134 <-177 0.00209

134 <-434 0.00129

135 <-146 0.00596

135 <-150 -0.00152

135 <-174 -0.00309

135 <-240 0.00127

135 <-279 0.00121

136 <-141 -0.00249

136 <-143 -0.00199

136 <-149 -0.00386

136 <-153 -0.00229

136 <-158 0.00147

136 <-168 0.00345

136 <-175 -0.00237

136 <-184 -0.00154

136 <-243 -0.00104

136 <-263 0.00120

137 <-140 0.00293

137 <-144 -0.00243

137 <-148 -0.00548

137 <-165 -0.00281

137 <-176 0.00218

137 <-250 -0.00129

137 <-256 0.00122

138 <-140 -0.07206

138 <-144 -0.00240

138 <-148 0.00640

138 <-176 -0.00111

138 <-256 0.00118

138 <-262 0.00153

138 <-267 -0.00167

138 <-288 -0.00166

138 <-305 -0.00101

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

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

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

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

41 ->185 -0.00106

43 ->207 0.00107

44 ->180 -0.00107

45 ->185 0.00143

46 ->214 0.00111

47 ->178 0.00103

47 ->182 -0.00105

47 ->207 0.00152

48 ->185 -0.00114

48 ->194 0.00104

48 ->213 0.00119

53 ->180 -0.00114

61 ->180 -0.00174

62 ->183 0.00195

62 ->187 -0.00144

62 ->218 -0.00107

62 ->232 0.00130

62 ->239 -0.00104

63 ->179 -0.00136

64 ->180 -0.00114

64 ->186 -0.00170

64 ->328 0.00102

68 ->197 0.00122

69 ->186 -0.00146

69 ->196 -0.00103

70 ->190 -0.00137

70 ->194 -0.00120

70 ->197 -0.00170

70 ->204 -0.00133

70 ->213 -0.00109

70 ->217 -0.00110

70 ->233 0.00116

70 ->250 -0.00114

71 ->169 -0.00104

71 ->182 0.00172

71 ->210 0.00123

71 ->211 -0.00111

72 ->163 -0.00106

72 ->183 -0.00173

72 ->214 0.00111

73 ->167 0.00125

73 ->180 0.00163

73 ->186 -0.00121

73 ->195 -0.00117

73 ->196 0.00140

76 ->149 -0.00106

78 ->181 -0.00111

78 ->190 0.00143

78 ->197 0.00104

78 ->204 0.00131

78 ->233 -0.00103

79 ->178 0.00109

79 ->179 0.00314

79 ->193 -0.00187

79 ->205 0.00159

79 ->211 -0.00190

79 ->259 0.00105

80 ->157 -0.00125

80 ->183 -0.00239

80 ->187 0.00160

80 ->257 -0.00146

80 ->260 -0.00199

80 ->297 -0.00168

81 ->151 -0.00143

81 ->155 0.00110

81 ->185 0.00137

82 ->157 0.00157

82 ->257 -0.00126

82 ->260 -0.00106

82 ->282 -0.00109

82 ->297 -0.00189

82 ->320 -0.00125

83 ->154 -0.00236

83 ->162 0.00140

83 ->169 0.00115

83 ->178 0.00249

83 ->179 0.00246

83 ->184 -0.00101

83 ->193 -0.00111

83 ->205 0.00133

83 ->207 -0.00176

83 ->211 -0.00205

83 ->266 -0.00120

84 ->152 0.00208

84 ->156 -0.00198

84 ->186 0.00109

84 ->189 -0.00149

84 ->195 0.00102

85 ->152 -0.00216

85 ->167 0.00137

85 ->171 -0.00108

85 ->180 -0.00534

85 ->196 -0.00114

85 ->200 -0.00170

85 ->203 0.00114

85 ->208 0.00184

85 ->212 0.00152

85 ->242 -0.00105

85 ->249 -0.00170

85 ->251 0.00135

85 ->281 -0.00100

85 ->291 0.00160

85 ->301 -0.00125

85 ->328 -0.00108

86 ->166 0.00109

86 ->185 0.00251

86 ->204 -0.00102

86 ->262 0.00110

86 ->273 -0.00104

87 ->173 -0.00189

87 ->183 0.00127

87 ->192 0.00133

87 ->214 -0.00140

88 ->154 0.00205

88 ->158 -0.00107

88 ->169 0.00159

88 ->178 -0.00212

88 ->182 0.00398

88 ->207 0.00123

88 ->258 0.00137

88 ->271 0.00149

89 ->155 -0.00185

89 ->181 -0.00112

89 ->194 0.00141

89 ->204 0.00110

90 ->157 0.00220

90 ->187 -0.00118

90 ->192 -0.00101

90 ->206 0.00114

91 ->149 -0.00129

91 ->154 -0.00207

91 ->162 -0.00140

91 ->179 0.00216

91 ->193 -0.00189

92 ->140 0.00119

92 ->144 0.00344

92 ->165 0.00454

92 ->176 0.00178

92 ->213 -0.00102

92 ->217 0.00198

93 ->161 0.00168

93 ->171 -0.00273

93 ->186 0.00332

93 ->195 0.00204

93 ->196 -0.00106

93 ->208 -0.00117

94 ->152 0.00107

94 ->156 -0.00145

94 ->180 0.00144

94 ->196 -0.00154

95 ->141 0.00408

95 ->143 0.00423

95 ->149 0.00355

95 ->153 -0.00401

95 ->158 -0.00169

95 ->168 -0.00325

95 ->175 -0.00195

95 ->220 -0.00135

95 ->230 -0.00101

95 ->243 -0.00158

96 ->142 -0.00438

96 ->150 0.00355

96 ->219 0.00139

97 ->151 0.00106

97 ->155 -0.00277

97 ->160 -0.00150

97 ->185 0.00184

98 ->157 0.00103

98 ->163 -0.00216

98 ->173 0.00254

99 ->154 -0.00226

99 ->159 0.00386

99 ->182 -0.00134

100 ->160 0.00307

100 ->172 -0.00245

100 ->228 0.00117

101 ->152 0.00218

101 ->156 -0.00164

101 ->161 -0.00288

101 ->186 0.00344

101 ->195 0.00180

101 ->196 -0.00100

102 ->149 0.00117

102 ->158 0.00126

102 ->159 0.00172

102 ->162 0.00261

102 ->178 0.00296

102 ->182 -0.00104

102 ->188 0.00198

102 ->207 -0.00260

102 ->210 -0.00159

103 ->157 -0.00340

103 ->163 -0.00206

103 ->183 0.00128

103 ->192 0.00147

103 ->206 0.00155

103 ->226 0.00141

104 ->139 -0.00546

104 ->145 -0.00138

104 ->147 -0.00124

104 ->156 0.00252

104 ->161 -0.00109

104 ->167 -0.00130

104 ->189 -0.00163

104 ->212 -0.00171

104 ->216 0.00160

105 ->139 -0.00796

105 ->145 -0.00221

105 ->147 -0.00180

105 ->156 -0.00133

105 ->167 0.00102

105 ->189 0.00158

105 ->195 -0.00105

105 ->203 0.00148

105 ->216 0.00132

106 ->155 0.00159

106 ->185 -0.00121

106 ->233 -0.00103

106 ->280 -0.00103

107 ->140 -0.01027

107 ->144 0.00152

107 ->148 0.00425

107 ->176 -0.00190

107 ->217 -0.00151

107 ->233 0.00108

108 ->160 -0.00162

108 ->166 0.00269

108 ->172 -0.00157

108 ->185 -0.00249

108 ->194 -0.00163

108 ->236 -0.00103

109 ->142 -0.00237

109 ->150 0.00475

109 ->219 -0.00205

110 ->141 -0.00219

110 ->149 0.00264

110 ->153 -0.00213

110 ->168 -0.00265

110 ->220 0.00186

110 ->230 -0.00126

110 ->243 -0.00119

111 ->163 -0.00288

111 ->173 -0.00136

111 ->191 0.00243

111 ->192 -0.00186

112 ->159 0.00115

112 ->162 -0.00106

112 ->169 -0.00314

112 ->178 -0.00141

112 ->182 0.00338

112 ->188 0.00111

112 ->207 0.00117

112 ->237 -0.00106

113 ->140 0.00627

113 ->144 0.00111

113 ->165 -0.00315

113 ->223 -0.00202

114 ->161 0.00165

114 ->167 -0.00263

114 ->186 0.00402

114 ->189 0.00246

114 ->195 0.00221

115 ->160 0.00119

115 ->166 0.00231

115 ->172 0.00344

115 ->185 0.00180

115 ->190 -0.00135

116 ->139 -0.00964

116 ->145 -0.00144

116 ->147 -0.00550

116 ->164 0.00168

116 ->177 -0.00103

116 ->224 0.00205

116 ->245 -0.00115

117 ->170 0.00385

117 ->173 -0.00112

117 ->192 -0.00250

118 ->149 -0.00255

118 ->154 -0.00185

118 ->158 -0.00238

118 ->159 0.00128

118 ->162 0.00308

118 ->178 -0.00385

118 ->184 0.00121

118 ->207 0.00254

118 ->211 -0.00111

119 ->152 -0.00134

119 ->161 0.00253

119 ->167 0.00242

119 ->171 0.00144

119 ->189 -0.00207

119 ->195 0.00273

119 ->221 -0.00182

119 ->234 0.00103

119 ->242 0.00116

120 ->141 -0.00220

120 ->143 -0.00283

120 ->149 -0.00632

120 ->153 0.00155

120 ->158 -0.00597

120 ->162 -0.00104

120 ->175 0.00101

120 ->178 -0.00360

120 ->179 0.00404

120 ->182 -0.00202

120 ->193 -0.00195

120 ->201 -0.00206

120 ->205 0.00315

120 ->207 -0.00221

120 ->211 -0.00296

120 ->229 0.00155

120 ->298 -0.00113

121 ->142 -0.00237

121 ->146 -0.00231

121 ->150 0.00139

121 ->157 -0.00155

121 ->170 -0.00180

121 ->183 0.00264

121 ->192 0.00140

121 ->214 -0.00106

121 ->260 0.00115

121 ->282 0.00104

122 ->141 -0.00543

122 ->143 -0.00559

122 ->153 0.00394

122 ->158 0.00332

122 ->168 0.00152

122 ->175 0.00125

122 ->178 0.00121

122 ->179 -0.00161

122 ->184 -0.00238

122 ->205 -0.00121

122 ->211 0.00100

122 ->230 -0.00230

123 ->142 -0.00392

123 ->146 -0.00577

123 ->150 0.00146

123 ->174 0.00171

123 ->183 -0.00115

123 ->240 -0.00153

123 ->246 0.00154

124 ->151 0.00132

124 ->172 -0.00106

124 ->181 0.00359

124 ->185 0.00109

124 ->190 0.00171

124 ->197 0.00221

124 ->204 0.00111

124 ->217 0.00137

124 ->252 -0.00100

125 ->149 -0.00393

125 ->158 -0.00449

125 ->169 0.00123

125 ->178 -0.00170

125 ->179 0.00466

125 ->182 0.00159

125 ->193 -0.00129

125 ->201 -0.00119

125 ->205 0.00179

125 ->207 -0.00125

125 ->211 -0.00310

125 ->229 0.00128

125 ->278 0.00115

126 ->170 0.00220

126 ->173 -0.00129

126 ->183 -0.00796

126 ->187 -0.00172

126 ->191 -0.00119

126 ->192 -0.00120

126 ->215 -0.00218

126 ->218 0.00147

126 ->226 0.00217

126 ->257 -0.00100

127 ->139 0.01459

127 ->145 -0.00761

127 ->147 -0.00165

127 ->164 -0.00112

127 ->177 -0.00173

127 ->242 0.00104

127 ->245 0.00260

128 ->139 0.00308

128 ->152 -0.00281

128 ->156 -0.00267

128 ->161 -0.00158

128 ->171 -0.00128

128 ->180 -0.00665

128 ->186 -0.00127

128 ->189 -0.00315

128 ->195 0.00281

128 ->200 -0.00268

128 ->203 -0.00135

128 ->208 0.00254

128 ->212 0.00190

128 ->216 0.00139

128 ->221 0.00205

128 ->224 0.00107

128 ->234 -0.00181

128 ->272 0.00121

128 ->277 0.00103

128 ->291 0.00144

128 ->294 -0.00138

128 ->301 -0.00125

129 ->148 0.00160

129 ->155 0.00219

129 ->172 -0.00288

129 ->181 0.00331

129 ->185 -0.00181

129 ->190 0.00310

129 ->194 0.00153

129 ->197 0.00369

129 ->204 0.00164

129 ->209 0.00120

129 ->213 0.00124

129 ->217 0.00201

129 ->280 -0.00137

130 ->140 -0.00635

130 ->144 0.00117

130 ->148 0.01102

130 ->165 0.00393

130 ->176 -0.00229

130 ->244 0.00225

131 ->141 -0.02370

131 ->143 0.00175

131 ->175 -0.00209

131 ->230 0.00103

131 ->253 0.00215

132 ->142 0.00526

132 ->146 0.01001

132 ->150 -0.01159

132 ->174 -0.00304

132 ->246 0.00246

133 ->140 0.01412

133 ->144 0.00437

133 ->148 0.00177

133 ->165 -0.00213

133 ->176 -0.00284

133 ->244 -0.00104

133 ->250 -0.00119

133 ->256 0.00132

134 ->140 -0.15135

134 ->148 0.01571

134 ->165 0.00186

134 ->176 -0.00224

134 ->433 -0.00120

135 ->143 0.00313

135 ->149 0.00718

135 ->153 -0.00383

135 ->154 -0.00111

135 ->158 -0.00239

135 ->168 -0.00536

135 ->175 -0.00295

135 ->184 0.00219

135 ->243 0.00136

135 ->263 -0.00142

136 ->142 0.00171

136 ->146 0.00869

136 ->150 0.00164

136 ->174 -0.00375

136 ->240 -0.00158

136 ->279 -0.00149

137 ->139 -0.00789

137 ->145 -0.00297

137 ->147 -0.00888

137 ->164 0.00419

137 ->177 -0.00267

137 ->249 -0.00164

137 ->255 -0.00151

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138 ->147 -0.00537

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138 ->177 -0.00199

138 ->208 0.00118

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138 ->249 0.00127

138 ->255 0.00158

138 ->261 0.00192

138 ->268 -0.00206

138 ->287 -0.00197

138 ->304 0.00117

138 ->313 -0.00102

45 <-185 0.00125

46 <-214 0.00112

47 <-207 0.00133

48 <-185 -0.00100

48 <-213 0.00111

61 <-180 -0.00148

62 <-183 0.00173

62 <-187 -0.00116

62 <-232 0.00117

63 <-179 -0.00111

64 <-186 -0.00149

68 <-197 0.00109

69 <-186 -0.00128

70 <-190 -0.00112

70 <-194 -0.00103

70 <-197 -0.00149

70 <-204 -0.00115

70 <-233 0.00103

71 <-182 0.00144

71 <-210 0.00104

72 <-183 -0.00144

73 <-180 0.00134

73 <-186 -0.00102

73 <-195 -0.00101

73 <-196 0.00117

78 <-190 0.00116

78 <-204 0.00111

79 <-179 0.00253

79 <-193 -0.00159

79 <-205 0.00137

79 <-211 -0.00159

80 <-183 -0.00206

80 <-187 0.00129

80 <-257 -0.00126

80 <-260 -0.00173

80 <-297 -0.00147

81 <-151 -0.00109

81 <-185 0.00110

82 <-157 0.00118

82 <-257 -0.00107

82 <-297 -0.00164

82 <-320 -0.00109

83 <-154 -0.00182

83 <-162 0.00111

83 <-178 0.00206

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83 <-205 0.00116

83 <-207 -0.00153

83 <-211 -0.00172

83 <-266 -0.00108

84 <-152 0.00158

84 <-156 -0.00148

84 <-189 -0.00122

85 <-152 -0.00167

85 <-167 0.00107

85 <-180 -0.00434

85 <-200 -0.00144

85 <-203 0.00102

85 <-208 0.00154

85 <-212 0.00128

85 <-249 -0.00145

85 <-251 0.00112

85 <-291 0.00141

85 <-301 -0.00112

86 <-185 0.00199

87 <-173 -0.00145

87 <-192 0.00108

87 <-214 -0.00119

88 <-154 0.00152

88 <-169 0.00120

88 <-178 -0.00170

88 <-182 0.00317

88 <-207 0.00108

88 <-258 0.00113

88 <-271 0.00127

89 <-155 -0.00135

89 <-194 0.00111

90 <-157 0.00160

91 <-154 -0.00150

91 <-162 -0.00102

91 <-179 0.00170

91 <-193 -0.00150

92 <-144 0.00242

92 <-165 0.00364

92 <-176 0.00161

92 <-217 0.00171

93 <-161 0.00124

93 <-171 -0.00209

93 <-186 0.00272

93 <-195 0.00166

94 <-156 -0.00105

94 <-180 0.00111

94 <-196 -0.00123

95 <-141 0.00235

95 <-143 0.00306

95 <-149 0.00253

95 <-153 -0.00272

95 <-158 -0.00121

95 <-168 -0.00298

95 <-175 -0.00145

95 <-220 -0.00112

95 <-243 -0.00131

96 <-142 -0.00304

96 <-150 0.00276

96 <-219 0.00123

97 <-155 -0.00200

97 <-160 -0.00109

97 <-185 0.00144

98 <-163 -0.00158

98 <-173 0.00192

99 <-154 -0.00161

99 <-159 0.00278

99 <-182 -0.00104

100 <-160 0.00223

100 <-172 -0.00183

101 <-152 0.00156

101 <-156 -0.00118

101 <-161 -0.00208

101 <-186 0.00275

101 <-195 0.00144

102 <-159 0.00124

102 <-162 0.00192

102 <-178 0.00233

102 <-188 0.00160

102 <-207 -0.00214

102 <-210 -0.00129

103 <-157 -0.00242

103 <-163 -0.00150

103 <-183 0.00100

103 <-192 0.00115

103 <-206 0.00123

103 <-226 0.00116

104 <-139 -0.00266

104 <-145 -0.00111

104 <-156 0.00178

104 <-167 -0.00100

104 <-189 -0.00131

104 <-212 -0.00138

104 <-216 0.00128

105 <-139 -0.00384

105 <-145 -0.00174

105 <-147 -0.00138

105 <-164 0.00132

105 <-189 0.00121

105 <-203 0.00114

105 <-216 0.00103

106 <-155 0.00109

107 <-140 -0.00721

107 <-148 0.00258

107 <-165 -0.00167

107 <-176 -0.00147

107 <-217 -0.00116

108 <-160 -0.00112

108 <-166 0.00191

108 <-172 -0.00112

108 <-185 -0.00190

108 <-194 -0.00127

109 <-142 -0.00142

109 <-150 0.00301

109 <-219 -0.00158

110 <-149 0.00162

110 <-153 -0.00195

110 <-168 -0.00219

110 <-220 0.00150

110 <-230 -0.00101

110 <-243 -0.00103

111 <-163 -0.00201

111 <-191 0.00184

111 <-192 -0.00145

112 <-169 -0.00222

112 <-178 -0.00107

112 <-182 0.00256

113 <-140 0.00447

113 <-165 -0.00246

113 <-223 -0.00164

114 <-161 0.00114

114 <-167 -0.00184

114 <-186 0.00311

114 <-189 0.00185

114 <-195 0.00169

115 <-166 0.00161

115 <-172 0.00248

115 <-185 0.00135

115 <-190 -0.00103

116 <-139 -0.00365

116 <-145 -0.00162

116 <-147 -0.00409

116 <-164 0.00209

116 <-224 0.00158

116 <-245 -0.00102

117 <-170 0.00273

117 <-192 -0.00191

118 <-149 -0.00162

118 <-154 -0.00121

118 <-158 -0.00157

118 <-162 0.00211

118 <-178 -0.00287

118 <-207 0.00202

119 <-161 0.00173

119 <-167 0.00169

119 <-171 0.00101

119 <-189 -0.00156

119 <-195 0.00211

119 <-221 -0.00146

120 <-143 -0.00158

120 <-149 -0.00400

120 <-158 -0.00386

120 <-178 -0.00258

120 <-179 0.00300

120 <-182 -0.00155

120 <-193 -0.00154

120 <-201 -0.00158

120 <-205 0.00243

120 <-207 -0.00178

120 <-211 -0.00233

120 <-229 0.00122

121 <-146 -0.00174

121 <-157 -0.00102

121 <-170 -0.00127

121 <-183 0.00194

121 <-192 0.00105

122 <-141 0.00128

122 <-143 -0.00314

122 <-158 0.00227

122 <-168 0.00125

122 <-179 -0.00113

122 <-184 -0.00192

122 <-230 -0.00167

123 <-146 -0.00444

123 <-174 0.00130

123 <-240 -0.00119

123 <-246 0.00136

124 <-181 0.00259

124 <-190 0.00128

124 <-197 0.00164

124 <-217 0.00110

125 <-149 -0.00225

125 <-158 -0.00279

125 <-178 -0.00114

125 <-179 0.00333

125 <-182 0.00111

125 <-193 -0.00101

125 <-205 0.00137

125 <-211 -0.00239

125 <-229 0.00102

126 <-170 0.00152

126 <-183 -0.00575

126 <-187 -0.00123

126 <-215 -0.00175

126 <-218 0.00115

126 <-226 0.00171

127 <-139 0.01115

127 <-145 -0.00372

127 <-147 0.00100

127 <-164 -0.00104

127 <-245 0.00214

128 <-152 -0.00166

128 <-156 -0.00160

128 <-180 -0.00468

128 <-189 -0.00227

128 <-195 0.00204

128 <-200 -0.00199

128 <-208 0.00196

128 <-212 0.00143

128 <-216 0.00106

128 <-221 0.00162

128 <-234 -0.00141

128 <-291 0.00121

128 <-294 -0.00115

128 <-301 -0.00106

129 <-155 0.00134

129 <-172 -0.00196

129 <-181 0.00237

129 <-185 -0.00129

129 <-190 0.00230

129 <-194 0.00113

129 <-197 0.00273

129 <-204 0.00125

129 <-217 0.00158

129 <-280 -0.00114

130 <-140 -0.00598

130 <-144 -0.00133

130 <-148 0.00502

130 <-165 0.00196

130 <-176 -0.00136

130 <-244 0.00169

131 <-141 -0.00502

131 <-143 0.00194

131 <-175 -0.00133

131 <-253 0.00176

132 <-142 0.00111

132 <-146 0.00494

132 <-150 -0.00616

132 <-174 -0.00180

132 <-246 0.00192

133 <-140 0.00641

133 <-144 0.00129

133 <-148 0.00132

133 <-165 -0.00154

133 <-176 -0.00231

133 <-256 0.00107

134 <-140 -0.05392

134 <-148 0.01116

134 <-165 0.00149

134 <-176 -0.00209

134 <-433 -0.00129

135 <-141 -0.00249

135 <-143 0.00199

135 <-149 0.00386

135 <-153 -0.00229

135 <-158 -0.00147

135 <-168 -0.00345

135 <-175 -0.00237

135 <-184 0.00154

135 <-243 0.00104

135 <-263 -0.00120

136 <-146 0.00596

136 <-150 0.00152

136 <-174 -0.00309

136 <-240 -0.00127

136 <-279 -0.00121

137 <-139 -0.00293

137 <-145 -0.00243

137 <-147 -0.00548

137 <-164 0.00281

137 <-177 -0.00218

137 <-249 -0.00129

137 <-255 -0.00122

138 <-139 -0.07206

138 <-145 0.00240

138 <-147 -0.00640

138 <-177 -0.00111

138 <-255 0.00118

138 <-261 0.00153

138 <-268 -0.00167

138 <-287 -0.00166

138 <-304 0.00101

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

56 ->189 -0.00113

57 ->188 0.00122

58 ->191 0.00104

66 ->207 -0.00145

67 ->231 -0.00104

69 ->222 0.00101

72 ->225 -0.00103

73 ->197 -0.00113

80 ->179 -0.00131

80 ->188 0.00127

81 ->180 -0.00118

83 ->187 -0.00103

84 ->185 0.00117

85 ->181 0.00159

85 ->213 -0.00127

86 ->161 -0.00115

86 ->186 -0.00134

87 ->154 -0.00101

87 ->162 -0.00131

87 ->182 -0.00170

88 ->187 -0.00108

88 ->192 -0.00142

88 ->215 -0.00108

92 ->139 -0.00632

92 ->177 0.00124

93 ->160 0.00119

93 ->166 0.00108

93 ->185 -0.00180

95 ->142 -0.00228

95 ->146 -0.00135

95 ->174 0.00164

96 ->141 0.00319

96 ->175 0.00104

97 ->180 -0.00152

97 ->196 0.00142

97 ->265 -0.00136

98 ->159 -0.00121

99 ->187 0.00132

101 ->185 -0.00130

102 ->157 -0.00117

102 ->187 -0.00139

102 ->191 -0.00102

102 ->226 -0.00117

102 ->257 0.00145

102 ->297 -0.00129

103 ->179 0.00183

103 ->182 -0.00117

103 ->198 -0.00150

103 ->207 0.00115

103 ->271 -0.00123

103 ->278 -0.00142

104 ->144 0.00141

104 ->181 -0.00140

104 ->204 0.00121

104 ->264 -0.00125

105 ->144 0.00218

105 ->148 0.00114

105 ->165 0.00115

105 ->176 -0.00151

106 ->208 0.00129

106 ->234 -0.00112

107 ->139 -0.00387

107 ->145 0.00110

107 ->147 -0.00146

108 ->156 0.00106

108 ->161 -0.00105

108 ->171 -0.00107

109 ->141 0.00669

109 ->153 -0.00327

109 ->175 -0.00292

110 ->174 -0.00193

111 ->162 -0.00131

111 ->182 0.00153

112 ->157 -0.00105

112 ->187 -0.00107

112 ->206 -0.00106

113 ->139 0.01639

113 ->145 -0.00103

113 ->147 0.00195

113 ->177 0.00235

114 ->166 -0.00108

114 ->181 0.00128

114 ->185 -0.00166

115 ->180 -0.00142

115 ->189 -0.00123

115 ->195 -0.00181

115 ->227 0.00135

116 ->140 0.02953

116 ->144 0.00287

116 ->148 -0.00183

116 ->165 0.00177

116 ->176 0.00233

117 ->179 -0.00229

117 ->188 0.00165

117 ->237 0.00108

118 ->163 0.00107

118 ->170 0.00111

118 ->187 0.00147

118 ->191 -0.00193

118 ->192 -0.00104

118 ->231 -0.00131

119 ->166 -0.00155

119 ->181 -0.00209

119 ->190 0.00180

119 ->228 -0.00110

119 ->264 -0.00113

120 ->142 0.00252

120 ->150 -0.00236

120 ->260 -0.00150

121 ->143 -0.00122

121 ->182 -0.00117

121 ->184 0.00111

121 ->207 0.00111

121 ->211 0.00159

121 ->225 0.00106

121 ->229 -0.00102

122 ->142 0.00432

122 ->150 -0.00358

123 ->141 -0.00761

123 ->143 -0.00358

123 ->168 0.00139

124 ->152 0.00114

124 ->161 -0.00129

124 ->180 -0.00101

124 ->189 -0.00130

124 ->265 -0.00131

125 ->183 -0.00158

125 ->187 -0.00135

125 ->191 0.00106

125 ->192 -0.00120

125 ->218 0.00119

125 ->226 -0.00100

126 ->141 0.00189

126 ->154 0.00111

126 ->159 -0.00140

126 ->188 -0.00102

126 ->207 0.00105

126 ->210 0.00158

126 ->271 -0.00143

127 ->140 -0.01533

127 ->144 0.00282

127 ->165 0.00161

127 ->176 0.00155

128 ->140 0.04742

128 ->148 -0.00222

128 ->185 -0.00180

128 ->222 0.00135

129 ->145 0.00108

129 ->152 0.00129

129 ->189 0.00140

129 ->196 -0.00219

130 ->139 0.02207

130 ->145 0.00745

130 ->164 -0.00257

131 ->142 -0.00568

131 ->146 0.00227

131 ->219 -0.00129

132 ->141 -0.00668

132 ->143 0.00991

132 ->153 0.00510

132 ->168 -0.00231

132 ->220 0.00143

133 ->139 0.20586

133 ->145 -0.00338

133 ->147 0.01284

133 ->164 0.00355

134 ->139 0.13849

134 ->145 0.00679

134 ->147 0.00249

134 ->164 -0.00452

134 ->177 -0.00144

135 ->142 0.00764

135 ->146 0.00921

135 ->150 -0.00145

135 ->174 0.00129

136 ->141 0.04985

136 ->143 0.00430

136 ->153 -0.01810

136 ->168 -0.00349

136 ->175 -0.00146

136 ->274 0.00158

137 ->140 0.65326

137 ->144 0.00264

137 ->148 -0.01878

137 ->165 0.00686

137 ->176 0.00162

138 ->140 -0.03424

138 ->144 0.04979

66 <-207 -0.00104

85 <-181 0.00121

87 <-182 -0.00101

92 <-139 -0.00235

92 <-177 0.00110

93 <-185 -0.00110

95 <-146 -0.00116

95 <-174 0.00145

96 <-141 0.00189

97 <-180 -0.00103

97 <-196 0.00101

97 <-265 -0.00108

102 <-257 0.00113

102 <-297 -0.00100

103 <-179 0.00119

103 <-198 -0.00109

103 <-278 -0.00111

105 <-144 0.00122

105 <-165 0.00103

105 <-176 -0.00127

107 <-139 -0.00175

109 <-175 -0.00211

110 <-174 -0.00173

113 <-139 0.00160

113 <-164 -0.00135

113 <-177 0.00174

115 <-195 -0.00118

116 <-148 0.00174

116 <-176 0.00156

117 <-179 -0.00142

117 <-188 0.00103

118 <-191 -0.00123

119 <-181 -0.00127

119 <-190 0.00111

120 <-260 -0.00111

121 <-211 0.00109

122 <-142 0.00250

122 <-150 -0.00166

123 <-141 -0.00107

123 <-153 -0.00170

123 <-168 0.00158

126 <-210 0.00105

126 <-271 -0.00103

127 <-140 -0.00385

127 <-144 0.00249

128 <-185 -0.00103

129 <-196 -0.00134

130 <-139 0.00238

130 <-145 0.00268

131 <-142 -0.00342

131 <-146 0.00165

132 <-141 0.00189

132 <-143 0.00277

132 <-153 0.00193

133 <-139 -0.00355

133 <-145 0.00298

133 <-147 0.00570

133 <-164 -0.00104

134 <-139 -0.00420

134 <-164 -0.00264

134 <-177 -0.00102

135 <-146 0.00551

135 <-150 0.00180

135 <-269 -0.00128

136 <-141 -0.00703

136 <-143 0.00224

136 <-153 -0.00220

136 <-168 -0.00214

136 <-274 0.00127

137 <-140 -0.00859

137 <-148 -0.00426

137 <-165 0.00186

137 <-176 0.00101

138 <-140 0.01554

138 <-144 0.00155

138 <-148 0.00106

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

56 ->190 0.00113

57 ->191 0.00104

58 ->188 0.00122

66 ->231 -0.00104

67 ->207 -0.00145

69 ->221 0.00101

71 ->225 -0.00103

73 ->196 0.00113

79 ->179 0.00131

79 ->188 -0.00127

81 ->181 -0.00118

82 ->187 0.00103

84 ->186 0.00117

85 ->180 -0.00159

85 ->212 0.00127

86 ->160 -0.00115

86 ->185 0.00134

87 ->187 -0.00108

87 ->192 0.00142

87 ->215 0.00108

88 ->154 0.00101

88 ->162 0.00131

88 ->182 0.00170

92 ->140 -0.00632

92 ->176 0.00124

93 ->161 0.00119

93 ->167 0.00108

93 ->186 0.00180

95 ->141 -0.00319

95 ->175 -0.00104

96 ->142 -0.00228

96 ->146 0.00135

96 ->174 -0.00164

97 ->181 -0.00152

97 ->197 0.00142

97 ->264 -0.00136

98 ->187 -0.00132

99 ->159 0.00121

101 ->186 0.00130

102 ->179 -0.00183

102 ->182 -0.00117

102 ->198 0.00150

102 ->207 -0.00115

102 ->271 0.00123

102 ->278 0.00142

103 ->157 -0.00117

103 ->187 0.00139

103 ->191 0.00102

103 ->226 0.00117

103 ->257 -0.00145

103 ->297 0.00129

104 ->145 -0.00141

104 ->180 -0.00140

104 ->203 -0.00121

104 ->265 -0.00125

105 ->145 -0.00218

105 ->147 -0.00114

105 ->164 0.00115

105 ->177 -0.00151

106 ->209 0.00129

106 ->233 -0.00112

107 ->140 0.00387

107 ->144 0.00110

107 ->148 -0.00146

108 ->155 -0.00106

108 ->160 -0.00105

108 ->172 -0.00107

109 ->174 0.00193

110 ->141 -0.00669

110 ->153 0.00327

110 ->175 0.00292

111 ->157 -0.00105

111 ->187 0.00107

111 ->206 -0.00106

112 ->162 -0.00131

112 ->182 0.00153

113 ->140 0.01639

113 ->144 0.00103

113 ->148 -0.00195

113 ->176 0.00235

114 ->167 -0.00108

114 ->180 -0.00128

114 ->186 0.00166

115 ->181 -0.00142

115 ->190 0.00123

115 ->194 0.00181

115 ->228 -0.00135

116 ->139 0.02953

116 ->145 -0.00287

116 ->147 0.00183

116 ->164 0.00177

116 ->177 0.00233

117 ->163 -0.00107

117 ->170 0.00111

117 ->187 -0.00147

117 ->191 0.00193

117 ->192 -0.00104

117 ->231 0.00131

118 ->179 0.00229

118 ->188 -0.00165

118 ->237 -0.00108

119 ->167 0.00155

119 ->180 -0.00209

119 ->189 -0.00180

119 ->227 0.00110

119 ->265 -0.00113

120 ->143 -0.00122

120 ->182 -0.00117

120 ->184 0.00111

120 ->207 -0.00111

120 ->211 -0.00159

120 ->225 0.00106

120 ->229 0.00102

121 ->142 0.00252

121 ->150 -0.00236

121 ->260 0.00150

122 ->141 0.00761

122 ->143 -0.00358

122 ->168 0.00139

123 ->142 0.00432

123 ->150 -0.00358

124 ->151 0.00114

124 ->160 0.00129

124 ->181 -0.00101

124 ->190 0.00130

124 ->264 -0.00131

125 ->141 -0.00189

125 ->154 0.00111

125 ->159 0.00140

125 ->188 0.00102

125 ->207 -0.00105

125 ->210 0.00158

125 ->271 0.00143

126 ->183 -0.00158

126 ->187 0.00135

126 ->191 -0.00106

126 ->192 -0.00120

126 ->218 0.00119

126 ->226 0.00100

127 ->139 0.01533

127 ->145 0.00282

127 ->164 -0.00161

127 ->177 -0.00155

128 ->139 0.04742

128 ->147 0.00222

128 ->186 -0.00180

128 ->221 0.00135

129 ->144 0.00108

129 ->151 -0.00129

129 ->190 0.00140

129 ->197 0.00219

130 ->140 -0.02207

130 ->144 0.00745

130 ->165 0.00257

131 ->141 -0.00668

131 ->143 -0.00991

131 ->153 0.00510

131 ->168 0.00231

131 ->220 -0.00143

132 ->142 0.00568

132 ->146 0.00227

132 ->219 0.00129

133 ->140 0.20586

133 ->144 0.00338

133 ->148 -0.01284

133 ->165 0.00355

134 ->140 0.13849

134 ->144 -0.00679

134 ->148 -0.00249

134 ->165 -0.00452

134 ->176 -0.00144

135 ->141 -0.04985

135 ->143 0.00430

135 ->153 0.01810

135 ->168 -0.00349

135 ->175 0.00146

135 ->274 -0.00158

136 ->142 0.00764

136 ->146 -0.00921

136 ->150 -0.00145

136 ->174 -0.00129

137 ->139 0.65326

137 ->145 -0.00264

137 ->147 0.01878

137 ->164 0.00686

137 ->177 0.00162

138 ->139 0.03424

138 ->145 0.04979

67 <-207 -0.00104

85 <-180 -0.00121

88 <-182 0.00101

92 <-140 -0.00235

92 <-176 0.00110

93 <-186 0.00110

95 <-141 -0.00189

96 <-146 0.00116

96 <-174 -0.00145

97 <-181 -0.00103

97 <-197 0.00101

97 <-264 -0.00108

102 <-179 -0.00119

102 <-198 0.00109

102 <-278 0.00111

103 <-257 -0.00113

103 <-297 0.00100

105 <-145 -0.00122

105 <-164 0.00103

105 <-177 -0.00127

107 <-140 0.00175

109 <-174 0.00173

110 <-175 0.00211

113 <-140 0.00160

113 <-165 -0.00135

113 <-176 0.00174

115 <-194 0.00118

116 <-147 -0.00174

116 <-177 0.00156

117 <-191 0.00123

118 <-179 0.00142

118 <-188 -0.00103

119 <-180 -0.00127

119 <-189 -0.00111

120 <-211 -0.00109

121 <-260 0.00111

122 <-141 0.00107

122 <-153 0.00170

122 <-168 0.00158

123 <-142 0.00250

123 <-150 -0.00166

125 <-210 0.00105

125 <-271 0.00103

127 <-139 0.00385

127 <-145 0.00249

128 <-186 -0.00103

129 <-197 0.00134

130 <-140 -0.00238

130 <-144 0.00268

131 <-141 0.00189

131 <-143 -0.00277

131 <-153 0.00193

132 <-142 0.00342

132 <-146 0.00165

133 <-140 -0.00355

133 <-144 -0.00298

133 <-148 -0.00570

133 <-165 -0.00104

134 <-140 -0.00420

134 <-165 -0.00264

134 <-176 -0.00102

135 <-141 0.00703

135 <-143 0.00224

135 <-153 0.00220

135 <-168 -0.00214

135 <-274 -0.00127

136 <-146 -0.00551

136 <-150 0.00180

136 <-269 0.00128

137 <-139 -0.00859

137 <-147 0.00426

137 <-164 0.00186

137 <-177 0.00101

138 <-139 -0.01554

138 <-145 0.00155

138 <-147 0.00106

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

56 ->191 -0.00127

56 ->239 0.00110

57 ->190 -0.00121

58 ->189 0.00121

59 ->188 -0.00155

64 ->198 -0.00120

65 ->231 0.00108

69 ->179 0.00123

69 ->207 -0.00176

71 ->196 -0.00102

71 ->221 -0.00110

72 ->197 0.00102

72 ->222 0.00110

73 ->225 0.00107

79 ->180 -0.00122

80 ->181 0.00122

81 ->163 0.00117

81 ->187 0.00163

84 ->188 -0.00137

86 ->192 0.00114

86 ->218 -0.00108

87 ->185 0.00140

88 ->186 0.00140

92 ->174 -0.00139

93 ->162 0.00143

93 ->182 0.00129

93 ->225 -0.00121

95 ->139 0.00575

95 ->177 -0.00129

96 ->140 -0.00575

96 ->176 0.00129

97 ->187 0.00265

97 ->191 0.00131

97 ->226 0.00113

97 ->239 -0.00100

97 ->257 -0.00231

97 ->297 0.00160

98 ->181 0.00109

99 ->180 -0.00109

101 ->259 0.00122

102 ->180 0.00193

102 ->189 -0.00116

102 ->203 0.00123

102 ->265 0.00174

103 ->181 -0.00193

103 ->190 -0.00116

103 ->204 0.00123

103 ->264 -0.00174

104 ->141 -0.00202

104 ->179 0.00205

104 ->198 -0.00187

104 ->271 -0.00133

104 ->278 -0.00152

105 ->141 -0.00322

105 ->175 -0.00178

105 ->179 -0.00120

105 ->198 0.00131

105 ->278 0.00104

106 ->187 -0.00139

107 ->150 -0.00142

108 ->157 -0.00136

108 ->170 0.00122

109 ->140 -0.01557

109 ->148 0.00237

109 ->176 -0.00273

110 ->139 0.01557

110 ->147 0.00237

110 ->177 0.00273

111 ->155 -0.00115

112 ->156 0.00115

113 ->146 0.00193

113 ->174 -0.00261

114 ->158 0.00117

114 ->162 -0.00114

114 ->182 0.00121

115 ->163 0.00106

115 ->187 0.00229

115 ->191 -0.00242

115 ->231 -0.00184

115 ->257 -0.00113

115 ->289 -0.00102

115 ->331 0.00103

116 ->141 -0.01238

116 ->153 0.00476

116 ->175 0.00265

117 ->181 0.00208

117 ->190 -0.00144

117 ->194 -0.00160

117 ->228 0.00147

117 ->264 0.00105

118 ->180 -0.00208

118 ->189 -0.00144

118 ->195 -0.00160

118 ->227 0.00147

118 ->265 -0.00105

119 ->169 0.00120

119 ->179 0.00318

119 ->188 -0.00192

119 ->207 -0.00119

119 ->237 -0.00123

119 ->258 0.00137

119 ->271 -0.00106

120 ->139 -0.00570

120 ->180 0.00164

121 ->140 0.00570

121 ->181 -0.00164

122 ->139 -0.03506

122 ->145 0.00125

122 ->147 -0.00236

123 ->140 0.03506

123 ->144 0.00125

123 ->148 -0.00236

124 ->187 0.00147

124 ->226 0.00118

124 ->257 -0.00148

125 ->139 0.00888

125 ->189 0.00127

125 ->196 -0.00105

126 ->140 -0.00888

126 ->190 0.00127

126 ->197 0.00105

127 ->143 -0.00498

127 ->220 -0.00156

128 ->141 -0.00427

128 ->179 -0.00149

128 ->188 0.00109

128 ->207 -0.00131

128 ->211 -0.00109

128 ->271 0.00125

129 ->142 -0.00227

129 ->218 0.00112

130 ->142 -0.00785

130 ->150 -0.00224

130 ->219 -0.00170

131 ->139 0.00460

131 ->145 0.00960

131 ->147 0.00146

131 ->224 -0.00112

132 ->140 0.00460

132 ->144 -0.00960

132 ->148 -0.00146

132 ->223 -0.00112

133 ->146 0.01226

135 ->139 0.49414

135 ->145 -0.00440

135 ->147 0.02042

135 ->164 0.00543

135 ->177 0.00219

136 ->140 -0.49414

136 ->144 -0.00440

136 ->148 0.02042

136 ->165 -0.00543

136 ->176 -0.00219

137 ->141 -0.05375

137 ->153 0.02308

137 ->175 0.00299

137 ->274 -0.00178

138 ->143 -0.05930

138 ->149 0.00252

56 <-191 -0.00100

59 <-188 -0.00112

69 <-207 -0.00133

81 <-187 0.00114

92 <-174 -0.00119

95 <-139 0.00128

95 <-177 -0.00115

96 <-140 -0.00128

96 <-176 0.00115

97 <-187 0.00184

97 <-257 -0.00178

97 <-297 0.00125

102 <-180 0.00129

102 <-265 0.00135

103 <-181 -0.00129

103 <-264 -0.00135

104 <-141 -0.00141

104 <-179 0.00130

104 <-198 -0.00131

104 <-278 -0.00117

105 <-141 -0.00202

105 <-175 -0.00143

109 <-176 -0.00196

110 <-177 0.00196

113 <-174 -0.00233

115 <-187 0.00144

115 <-191 -0.00155

115 <-231 -0.00135

116 <-141 -0.00114

116 <-175 0.00163

117 <-181 0.00130

117 <-194 -0.00103

117 <-228 0.00107

118 <-180 -0.00130

118 <-195 -0.00103

118 <-227 0.00107

119 <-179 0.00194

119 <-188 -0.00116

119 <-258 0.00106

122 <-139 -0.00282

122 <-147 0.00103

123 <-140 0.00282

123 <-148 0.00103

124 <-257 -0.00110

127 <-143 -0.00350

127 <-149 0.00137

130 <-142 -0.00421

130 <-219 -0.00102

131 <-145 0.00455

131 <-147 0.00146

132 <-144 -0.00455

132 <-148 -0.00146

133 <-146 0.00730

133 <-174 -0.00151

133 <-269 -0.00145

135 <-139 -0.00777

135 <-145 0.00126

135 <-147 0.00626

135 <-177 0.00149

136 <-140 0.00777

136 <-144 0.00126

136 <-148 0.00626

136 <-176 -0.00149

137 <-141 0.00921

137 <-153 0.00361

137 <-175 0.00132

137 <-274 -0.00147

138 <-143 -0.00215

138 <-149 -0.00200

138 <-168 0.00171

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

48 ->207 -0.00119

56 ->188 0.00158

57 ->186 0.00123

58 ->185 0.00123

59 ->191 0.00132

59 ->239 -0.00113

64 ->187 -0.00120

65 ->169 -0.00100

65 ->207 -0.00163

65 ->321 0.00112

66 ->221 -0.00106

67 ->222 -0.00106

68 ->193 0.00102

68 ->201 0.00106

69 ->187 -0.00120

69 ->231 0.00125

70 ->205 0.00103

71 ->181 -0.00105

72 ->180 0.00105

73 ->183 -0.00114

73 ->202 -0.00107

79 ->190 -0.00129

80 ->189 -0.00129

81 ->179 -0.00142

81 ->188 0.00126

84 ->191 0.00151

84 ->260 -0.00118

85 ->183 0.00153

85 ->218 -0.00131

86 ->162 0.00146

86 ->182 0.00184

87 ->161 0.00120

87 ->186 0.00153

87 ->189 0.00135

87 ->251 0.00106

88 ->160 -0.00120

88 ->185 0.00153

88 ->190 -0.00135

88 ->252 0.00106

89 ->179 -0.00118

92 ->141 -0.00319

92 ->175 -0.00132

93 ->157 -0.00132

93 ->192 0.00179

93 ->215 0.00150

95 ->140 -0.00448

95 ->176 0.00152

96 ->139 0.00448

96 ->177 -0.00152

97 ->179 -0.00199

97 ->198 0.00190

97 ->271 0.00153

97 ->278 0.00188

101 ->215 0.00106

102 ->181 -0.00133

102 ->197 0.00122

102 ->204 0.00107

102 ->264 -0.00114

103 ->180 0.00133

103 ->196 -0.00122

103 ->203 0.00107

103 ->265 0.00114

104 ->146 0.00110

104 ->174 -0.00139

104 ->187 -0.00178

104 ->226 -0.00157

104 ->231 -0.00105

104 ->257 0.00159

104 ->297 -0.00129

105 ->146 0.00182

105 ->174 -0.00216

105 ->187 0.00118

105 ->226 0.00102

105 ->257 -0.00110

106 ->141 0.00115

106 ->207 0.00139

106 ->211 0.00158

107 ->143 0.00167

108 ->162 0.00121

108 ->182 -0.00156

109 ->139 0.02009

109 ->145 -0.00144

109 ->147 0.00224

109 ->177 0.00276

110 ->140 -0.02009

110 ->144 -0.00144

110 ->148 0.00224

110 ->176 -0.00276

111 ->139 0.00141

111 ->156 -0.00105

111 ->186 -0.00139

112 ->140 -0.00141

112 ->155 0.00105

112 ->185 0.00139

113 ->141 0.00883

113 ->153 -0.00327

113 ->175 -0.00305

113 ->296 0.00106

114 ->170 -0.00152

114 ->192 0.00145

114 ->206 0.00130

115 ->169 -0.00114

115 ->179 -0.00222

115 ->188 0.00172

115 ->211 -0.00116

115 ->237 0.00153

116 ->174 0.00166

117 ->139 0.00170

117 ->180 -0.00190

117 ->189 -0.00201

117 ->195 -0.00134

117 ->227 0.00110

118 ->140 -0.00170

118 ->181 0.00190

118 ->190 -0.00201

118 ->194 -0.00134

118 ->228 0.00110

119 ->163 -0.00146

119 ->187 -0.00250

119 ->191 0.00243

119 ->231 0.00129

119 ->257 0.00126

119 ->260 -0.00113

119 ->331 -0.00119

120 ->197 0.00132

120 ->252 -0.00145

121 ->196 -0.00132

121 ->251 0.00145

122 ->140 0.01583

123 ->139 -0.01583

124 ->141 -0.00179

124 ->159 0.00218

124 ->188 0.00211

124 ->207 -0.00101

124 ->271 0.00124

125 ->140 -0.00668

125 ->151 0.00198

125 ->160 0.00114

125 ->181 -0.00111

125 ->185 0.00145

125 ->197 -0.00147

125 ->264 -0.00139

126 ->139 0.00668

126 ->152 -0.00198

126 ->161 0.00114

126 ->180 0.00111

126 ->186 -0.00145

126 ->196 0.00147

126 ->265 0.00139

127 ->142 0.00892

127 ->150 -0.00546

127 ->219 0.00121

128 ->226 0.00170

128 ->260 0.00214

129 ->143 0.00137

129 ->149 -0.00107

129 ->154 -0.00192

129 ->162 0.00109

129 ->182 -0.00139

129 ->205 -0.00106

129 ->210 -0.00178

129 ->225 0.00104

129 ->259 -0.00137

129 ->266 0.00111

130 ->143 0.00956

130 ->168 -0.00256

130 ->220 0.00150

131 ->140 -0.01171

131 ->144 -0.01007

131 ->148 0.00268

131 ->165 -0.00446

132 ->139 -0.01171

132 ->145 0.01007

132 ->147 -0.00268

132 ->164 -0.00446

133 ->141 0.04862

133 ->153 -0.01986

133 ->175 -0.00117

133 ->274 0.00194

134 ->141 0.00590

134 ->230 -0.00104

135 ->140 -0.49606

135 ->148 0.01711

135 ->165 -0.00456

136 ->139 0.49606

136 ->147 0.01711

136 ->164 0.00456

137 ->146 -0.01024

137 ->174 -0.00175

138 ->142 0.04491

138 ->150 0.00799

56 <-188 0.00114

59 <-191 0.00103

65 <-207 -0.00118

84 <-191 0.00103

85 <-183 0.00124

86 <-182 0.00111

92 <-141 -0.00189

92 <-175 -0.00122

93 <-192 0.00109

93 <-215 0.00109

95 <-140 -0.00136

95 <-176 0.00138

96 <-139 0.00136

96 <-177 -0.00138

97 <-179 -0.00134

97 <-198 0.00141

97 <-271 0.00115

97 <-278 0.00148

104 <-174 -0.00126

104 <-187 -0.00119

104 <-226 -0.00108

104 <-257 0.00121

104 <-297 -0.00102

105 <-146 0.00109

105 <-174 -0.00185

106 <-211 0.00112

109 <-139 0.00207

109 <-177 0.00206

110 <-140 -0.00207

110 <-176 -0.00206

113 <-175 -0.00214

115 <-179 -0.00137

115 <-188 0.00107

115 <-237 0.00113

116 <-146 0.00179

116 <-174 0.00158

117 <-180 -0.00117

117 <-189 -0.00125

118 <-181 0.00117

118 <-190 -0.00125

119 <-187 -0.00157

119 <-191 0.00152

120 <-140 -0.00141

120 <-252 -0.00103

121 <-139 0.00141

121 <-251 0.00103

122 <-140 -0.00280

122 <-148 0.00188

123 <-139 0.00280

123 <-147 0.00188

124 <-159 0.00103

124 <-188 0.00117

125 <-264 -0.00103

126 <-265 0.00103

127 <-142 0.00405

127 <-150 -0.00114

128 <-226 0.00109

128 <-260 0.00151

129 <-210 -0.00118

130 <-143 0.00300

131 <-140 0.00171

131 <-144 -0.00236

131 <-148 0.00221

131 <-165 -0.00120

132 <-139 0.00171

132 <-145 0.00236

132 <-147 -0.00221

132 <-164 -0.00120

133 <-141 -0.00777

133 <-153 -0.00319

133 <-274 0.00159

134 <-141 -0.00315

134 <-153 0.00292

135 <-140 0.00599

135 <-144 0.00351

135 <-148 0.00500

136 <-139 -0.00599

136 <-145 0.00351

136 <-147 0.00500

137 <-146 -0.00623

137 <-269 0.00152

138 <-142 -0.00270

138 <-150 0.00289

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

41 ->140 0.00138

43 ->141 0.00113

43 ->153 -0.00112

45 ->140 -0.00202

45 ->165 -0.00123

47 ->141 0.00126

47 ->153 -0.00113

47 ->168 -0.00134

48 ->140 0.00123

48 ->165 0.00124

68 ->140 0.00325

70 ->140 -0.00389

70 ->148 0.00164

71 ->168 -0.00102

73 ->164 -0.00103

78 ->140 0.00253

78 ->148 -0.00105

79 ->141 -0.00219

79 ->153 0.00205

80 ->142 0.00132

80 ->150 -0.00219

81 ->165 0.00101

82 ->150 -0.00104

83 ->168 -0.00143

85 ->139 0.00109

85 ->145 -0.00208

85 ->164 0.00337

86 ->165 0.00111

88 ->168 -0.00133

97 ->165 0.00166

98 ->146 0.00108

98 ->150 -0.00105

99 ->153 0.00115

100 ->140 -0.00281

100 ->148 0.00130

102 ->141 0.00154

103 ->150 0.00115

106 ->140 -0.00274

106 ->144 -0.00254

106 ->165 -0.00323

108 ->140 -0.00588

108 ->148 0.00213

111 ->146 -0.00179

111 ->150 0.00119

112 ->141 0.00122

112 ->143 0.00151

112 ->153 -0.00186

112 ->168 -0.00121

114 ->139 0.00188

114 ->145 -0.00207

114 ->147 -0.00148

114 ->164 0.00126

115 ->144 0.00213

115 ->165 0.00241

119 ->139 -0.00103

120 ->141 0.01625

120 ->143 0.00166

120 ->153 -0.00639

120 ->168 -0.00180

120 ->175 -0.00138

121 ->142 -0.00828

121 ->150 0.00696

122 ->141 -0.00896

122 ->153 0.00331

123 ->142 0.00458

123 ->150 -0.00352

124 ->140 0.00201

124 ->144 -0.01197

124 ->148 -0.00560

124 ->165 -0.01052

124 ->176 -0.00207

124 ->267 0.00101

124 ->327 0.00147

125 ->141 -0.05259

125 ->143 -0.00567

125 ->149 -0.00218

125 ->153 0.01526

125 ->168 0.00477

125 ->175 0.00260

125 ->315 0.00182

125 ->316 0.00109

125 ->337 0.00111

125 ->338 -0.00134

126 ->142 0.02883

126 ->146 0.00566

126 ->150 -0.02068

126 ->240 -0.00107

127 ->139 -0.00224

128 ->139 -0.10417

128 ->147 -0.00493

129 ->139 -0.00464

129 ->140 0.67681

129 ->144 0.00138

129 ->148 -0.02399

129 ->165 0.00171

129 ->176 0.00282

129 ->327 -0.00157

130 ->139 0.00108

130 ->140 -0.15767

130 ->148 0.00436

131 ->141 0.00394

132 ->142 0.00125

132 ->150 -0.00130

133 ->140 -0.00501

133 ->144 0.00123

134 ->140 -0.00859

134 ->160 -0.00109

134 ->166 -0.00100

134 ->185 -0.00105

135 ->141 -0.00111

135 ->143 -0.00181

136 ->142 0.00209

137 ->139 0.00671

137 ->145 0.00161

138 ->139 -0.00305

138 ->145 -0.00392

138 ->152 -0.00112

138 ->186 -0.00101

48 <-140 0.00105

68 <-140 0.00113

120 <-141 -0.00119

122 <-205 0.00135

122 <-210 0.00110

122 <-266 -0.00125

124 <-140 0.00386

124 <-144 0.00149

124 <-165 0.00280

124 <-176 0.00135

125 <-141 0.00408

125 <-143 0.00151

125 <-153 -0.00308

125 <-168 -0.00254

125 <-175 -0.00129

129 <-140 -0.00520

129 <-144 -0.00129

129 <-165 -0.00252

129 <-176 -0.00130

130 <-140 0.00137

134 <-181 -0.00242

134 <-197 -0.00204

138 <-139 0.00157

138 <-180 -0.00194

138 <-189 0.00117

138 <-196 -0.00210

138 <-203 0.00104

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

41 ->139 -0.00138

42 ->141 0.00113

42 ->153 -0.00112

45 ->139 -0.00202

45 ->164 -0.00123

46 ->141 0.00126

46 ->153 -0.00113

46 ->168 0.00134

48 ->139 -0.00123

48 ->164 -0.00124

68 ->139 0.00325

70 ->139 -0.00389

70 ->147 -0.00164

72 ->168 0.00102

73 ->165 -0.00103

78 ->139 0.00253

78 ->147 0.00105

79 ->142 -0.00132

79 ->150 0.00219

80 ->141 -0.00219

80 ->153 0.00205

81 ->164 -0.00101

82 ->168 0.00143

83 ->150 0.00104

85 ->140 0.00109

85 ->144 0.00208

85 ->165 0.00337

86 ->164 0.00111

87 ->168 -0.00133

97 ->164 -0.00166

98 ->153 0.00115

99 ->146 0.00108

99 ->150 0.00105

100 ->139 -0.00281

100 ->147 -0.00130

102 ->150 -0.00115

103 ->141 0.00154

106 ->139 0.00274

106 ->145 -0.00254

106 ->164 0.00323

108 ->139 -0.00588

108 ->147 -0.00213

111 ->141 0.00122

111 ->143 -0.00151

111 ->153 -0.00186

111 ->168 0.00121

112 ->146 -0.00179

112 ->150 -0.00119

114 ->140 0.00188

114 ->144 0.00207

114 ->148 0.00148

114 ->165 0.00126

115 ->145 0.00213

115 ->164 -0.00241

119 ->140 0.00103

120 ->142 0.00828

120 ->150 -0.00696

121 ->141 0.01625

121 ->143 -0.00166

121 ->153 -0.00639

121 ->168 0.00180

121 ->175 -0.00138

122 ->142 -0.00458

122 ->150 0.00352

123 ->141 -0.00896

123 ->153 0.00331

124 ->139 -0.00201

124 ->145 -0.01197

124 ->147 -0.00560

124 ->164 0.01052

124 ->177 0.00207

124 ->268 -0.00101

124 ->328 -0.00147

125 ->142 -0.02883

125 ->146 0.00566

125 ->150 0.02068

125 ->240 0.00107

126 ->141 -0.05259

126 ->143 0.00567

126 ->149 0.00218

126 ->153 0.01526

126 ->168 -0.00477

126 ->175 0.00260

126 ->315 -0.00182

126 ->316 -0.00109

126 ->337 0.00111

126 ->338 -0.00134

127 ->140 -0.00224

128 ->140 0.10417

128 ->148 -0.00493

129 ->139 0.67681

129 ->140 0.00464

129 ->145 -0.00138

129 ->147 0.02399

129 ->164 0.00171

129 ->177 0.00282

129 ->328 -0.00157

130 ->139 -0.15767

130 ->140 -0.00108

130 ->147 -0.00436

131 ->142 0.00125

131 ->150 -0.00130

132 ->141 -0.00394

133 ->139 0.00501

133 ->145 0.00123

134 ->139 0.00859

134 ->161 -0.00109

134 ->167 -0.00100

134 ->186 0.00105

135 ->142 -0.00209

136 ->141 -0.00111

136 ->143 0.00181

137 ->140 -0.00671

137 ->144 0.00161

138 ->140 -0.00305

138 ->144 0.00392

138 ->151 -0.00112

138 ->185 -0.00101

48 <-139 -0.00105

68 <-139 0.00113

121 <-141 -0.00119

123 <-205 -0.00135

123 <-210 -0.00110

123 <-266 0.00125

124 <-139 -0.00386

124 <-145 0.00149

124 <-164 -0.00280

124 <-177 -0.00135

126 <-141 0.00408

126 <-143 -0.00151

126 <-153 -0.00308

126 <-168 0.00254

126 <-175 -0.00129

129 <-139 -0.00520

129 <-145 0.00129

129 <-164 -0.00252

129 <-177 -0.00130

130 <-139 0.00137

134 <-180 0.00242

134 <-196 0.00204

138 <-140 0.00157

138 <-181 -0.00194

138 <-190 -0.00117

138 <-197 -0.00210

138 <-204 -0.00104

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

44 ->139 0.00134

87 ->142 0.00122

87 ->150 -0.00106

88 ->141 0.00108

89 ->148 -0.00124

89 ->165 0.00127

90 ->146 -0.00191

90 ->150 -0.00112

91 ->153 0.00193

93 ->145 0.00110

93 ->164 -0.00152

94 ->139 -0.00484

94 ->147 -0.00273

95 ->178 0.00106

104 ->139 0.00180

104 ->147 0.00132

105 ->139 -0.00213

105 ->147 -0.00110

106 ->140 0.00806

106 ->144 0.00441

106 ->165 0.00456

107 ->140 0.00133

110 ->141 0.00114

114 ->145 0.00113

115 ->140 -0.00188

116 ->139 -0.00560

117 ->142 0.00284

117 ->150 -0.00283

118 ->141 -0.00437

118 ->153 0.00229

118 ->184 0.00123

119 ->139 0.00626

119 ->147 0.00171

120 ->141 -0.02308

120 ->149 0.00162

120 ->153 0.00890

120 ->158 -0.00137

120 ->175 0.00178

120 ->184 0.00250

121 ->142 0.01258

121 ->146 -0.00214

121 ->150 -0.01046

122 ->141 0.00828

122 ->149 -0.00257

122 ->153 -0.00336

122 ->178 -0.00101

122 ->193 -0.00109

123 ->142 -0.00426

123 ->150 0.00326

124 ->140 -0.00513

124 ->144 -0.00585

124 ->148 -0.00181

124 ->165 -0.00519

124 ->176 -0.00105

125 ->141 -0.02562

125 ->143 -0.00350

125 ->153 0.00796

125 ->168 0.00253

125 ->175 0.00131

125 ->184 0.00208

126 ->142 0.01344

126 ->150 -0.00969

127 ->139 0.00411

128 ->139 0.69404

128 ->145 0.00567

128 ->147 0.02800

128 ->164 -0.00346

128 ->177 0.00221

128 ->313 -0.00115

129 ->140 0.10414

129 ->144 0.00115

129 ->148 -0.00357

129 ->165 0.00110

130 ->140 -0.00632

130 ->144 -0.00116

131 ->143 0.00145

133 ->140 -0.01220

133 ->148 0.00155

134 ->140 0.03176

134 ->181 -0.00110

135 ->141 0.00113

135 ->149 0.00255

135 ->153 -0.00122

135 ->158 0.00155

135 ->178 0.00149

135 ->193 0.00100

135 ->205 -0.00125

136 ->146 0.00154

137 ->139 -0.05251

137 ->147 -0.00150

137 ->180 0.00118

138 ->139 0.00364

138 ->145 -0.01330

138 ->147 -0.00322

106 <-140 0.00101

106 <-165 -0.00131

120 <-168 -0.00140

121 <-142 -0.00194

121 <-150 0.00178

124 <-140 0.00125

125 <-141 0.00127

128 <-139 -0.00402

128 <-145 -0.00160

128 <-164 0.00198

129 <-140 -0.00128

134 <-140 -0.00149

134 <-204 -0.00134

134 <-233 0.00117

138 <-139 -0.00244

138 <-147 -0.00103

138 <-180 0.00147

138 <-189 0.00124

138 <-203 0.00104

138 <-208 -0.00119

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

44 ->140 0.00134

87 ->141 0.00108

88 ->142 -0.00122

88 ->150 0.00106

89 ->147 0.00124

89 ->164 0.00127

90 ->153 -0.00193

91 ->146 0.00191

91 ->150 -0.00112

93 ->144 0.00110

93 ->165 0.00152

94 ->140 -0.00484

94 ->148 0.00273

96 ->178 0.00106

104 ->140 0.00180

104 ->148 -0.00132

105 ->140 -0.00213

105 ->148 0.00110

106 ->139 0.00806

106 ->145 -0.00441

106 ->164 0.00456

107 ->139 -0.00133

109 ->141 -0.00114

114 ->144 0.00113

115 ->139 -0.00188

116 ->140 -0.00560

117 ->141 0.00437

117 ->153 -0.00229

117 ->184 0.00123

118 ->142 0.00284

118 ->150 -0.00283

119 ->140 0.00626

119 ->148 -0.00171

120 ->142 0.01258

120 ->146 0.00214

120 ->150 -0.01046

121 ->141 0.02308

121 ->149 0.00162

121 ->153 -0.00890

121 ->158 -0.00137

121 ->175 -0.00178

121 ->184 0.00250

122 ->142 -0.00426

122 ->150 0.00326

123 ->141 -0.00828

123 ->149 -0.00257

123 ->153 0.00336

123 ->178 -0.00101

123 ->193 -0.00109

124 ->139 -0.00513

124 ->145 0.00585

124 ->147 0.00181

124 ->164 -0.00519

124 ->177 -0.00105

125 ->142 0.01344

125 ->150 -0.00969

126 ->141 0.02562

126 ->143 -0.00350

126 ->153 -0.00796

126 ->168 0.00253

126 ->175 -0.00131

126 ->184 0.00208

127 ->140 -0.00411

128 ->140 0.69404

128 ->144 -0.00567

128 ->148 -0.02800

128 ->165 -0.00346

128 ->176 0.00221

128 ->314 -0.00115

129 ->139 -0.10414

129 ->145 0.00115

129 ->147 -0.00357

129 ->164 -0.00110

130 ->139 0.00632

130 ->145 -0.00116

132 ->143 -0.00145

133 ->139 -0.01220

133 ->147 -0.00155

134 ->139 0.03176

134 ->180 -0.00110

135 ->146 -0.00154

136 ->141 -0.00113

136 ->149 0.00255

136 ->153 0.00122

136 ->158 0.00155

136 ->178 0.00149

136 ->193 0.00100

136 ->205 -0.00125

137 ->140 -0.05251

137 ->148 0.00150

137 ->181 0.00118

138 ->140 -0.00364

138 ->144 -0.01330

138 ->148 -0.00322

106 <-139 0.00101

106 <-164 -0.00131

120 <-142 -0.00194

120 <-150 0.00178

121 <-168 -0.00140

124 <-139 0.00125

126 <-141 -0.00127

128 <-140 -0.00402

128 <-144 0.00160

128 <-165 0.00198

129 <-139 0.00128

134 <-139 -0.00149

134 <-203 0.00134

134 <-234 0.00117

138 <-140 0.00244

138 <-148 -0.00103

138 <-181 -0.00147

138 <-190 0.00124

138 <-204 0.00104

138 <-209 0.00119

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

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

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

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

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Population analysis using the SCF density.

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

Orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The electronic state is 1-A1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Alpha virt. eigenvalues -- 0.02202 0.04724 0.04866 0.04866 0.05327

Alpha virt. eigenvalues -- 0.05534 0.06745 0.06745 0.06854 0.06937

Alpha virt. eigenvalues -- 0.07382 0.08784 0.08784 0.09724 0.10512

Alpha virt. eigenvalues -- 0.10712 0.10712 0.11804 0.11804 0.12159

Alpha virt. eigenvalues -- 0.12419 0.14372 0.15107 0.15107 0.16021

Alpha virt. eigenvalues -- 0.16775 0.17290 0.17381 0.17381 0.18513

Alpha virt. eigenvalues -- 0.19845 0.20176 0.20176 0.20642 0.21210

Alpha virt. eigenvalues -- 0.22390 0.22898 0.22898 0.23198 0.23844

Alpha virt. eigenvalues -- 0.24404 0.24404 0.25235 0.25817 0.26464

Alpha virt. eigenvalues -- 0.26779 0.26779 0.27231 0.27231 0.28057

Alpha virt. eigenvalues -- 0.28145 0.28145 0.28251 0.28825 0.29517

Alpha virt. eigenvalues -- 0.29517 0.30265 0.30368 0.31116 0.32284

Alpha virt. eigenvalues -- 0.32284 0.33460 0.33578 0.34646 0.34646

Alpha virt. eigenvalues -- 0.35448 0.35513 0.36297 0.36297 0.37176

Alpha virt. eigenvalues -- 0.37538 0.38145 0.38248 0.38248 0.38977

Alpha virt. eigenvalues -- 0.38977 0.39341 0.39901 0.40212 0.40212

Alpha virt. eigenvalues -- 0.40279 0.40525 0.41057 0.41145 0.41580

Alpha virt. eigenvalues -- 0.41580 0.42203 0.42203 0.42239 0.42280

Alpha virt. eigenvalues -- 0.42643 0.42854 0.42935 0.42935 0.43046

Alpha virt. eigenvalues -- 0.43104 0.43104 0.43255 0.43491 0.43527

Alpha virt. eigenvalues -- 0.44818 0.44818 0.46232 0.46232 0.46401

Alpha virt. eigenvalues -- 0.46513 0.46962 0.46962 0.47538 0.47680

Alpha virt. eigenvalues -- 0.47875 0.49632 0.49643 0.49643 0.50346

Alpha virt. eigenvalues -- 0.50637 0.50637 0.51129 0.51336 0.51336

Alpha virt. eigenvalues -- 0.51779 0.51855 0.52870 0.53574 0.53574

Alpha virt. eigenvalues -- 0.54090 0.54434 0.55224 0.55224 0.56392

Alpha virt. eigenvalues -- 0.58122 0.59182 0.59182 0.60043 0.60098

Alpha virt. eigenvalues -- 0.60153 0.60153 0.60208 0.60623 0.60623

Alpha virt. eigenvalues -- 0.60852 0.61319 0.61319 0.61383 0.62508

Alpha virt. eigenvalues -- 0.62667 0.62667 0.62814 0.63154 0.64290

Alpha virt. eigenvalues -- 0.64408 0.64429 0.64471 0.64471 0.65624

Alpha virt. eigenvalues -- 0.66463 0.66463 0.66818 0.67411 0.67411

Alpha virt. eigenvalues -- 0.69095 0.69573 0.69573 0.69771 0.70220

Alpha virt. eigenvalues -- 0.70220 0.70363 0.71507 0.72105 0.73316

Alpha virt. eigenvalues -- 0.73316 0.73460 0.74088 0.74489 0.74489

Alpha virt. eigenvalues -- 0.75869 0.76700 0.77134 0.77195 0.77195

Alpha virt. eigenvalues -- 0.77474 0.77474 0.77541 0.78684 0.79440

Alpha virt. eigenvalues -- 0.79440 0.79673 0.79763 0.79918 0.81388

Alpha virt. eigenvalues -- 0.81601 0.81781 0.81781 0.82652 0.83338

Alpha virt. eigenvalues -- 0.83931 0.83931 0.85036 0.86100 0.86568

Alpha virt. eigenvalues -- 0.86568 0.86637 0.88119 0.88663 0.88663

Alpha virt. eigenvalues -- 0.89360 0.90215 0.90215 0.90805 0.90805

Alpha virt. eigenvalues -- 0.91198 0.91342 0.91342 0.91778 0.93597

Alpha virt. eigenvalues -- 0.94404 0.95577 0.96911 0.98919 0.98919

Alpha virt. eigenvalues -- 0.98972 0.99369 0.99369 0.99692 0.99791

Alpha virt. eigenvalues -- 1.00188 1.01868 1.01868 1.02231 1.02561

Alpha virt. eigenvalues -- 1.02561 1.05092 1.05230 1.05230 1.06917

Alpha virt. eigenvalues -- 1.09538 1.10027 1.10027 1.10247 1.10255

Alpha virt. eigenvalues -- 1.10648 1.11628 1.11738 1.11738 1.13364

Alpha virt. eigenvalues -- 1.13462 1.14074 1.14074 1.14404 1.14448

Alpha virt. eigenvalues -- 1.15290 1.15290 1.17975 1.18947 1.20253

Alpha virt. eigenvalues -- 1.20253 1.20383 1.20495 1.20670 1.20762

Alpha virt. eigenvalues -- 1.20836 1.20836 1.22673 1.22673 1.25084

Alpha virt. eigenvalues -- 1.25084 1.25337 1.25896 1.26364 1.26801

Alpha virt. eigenvalues -- 1.26801 1.27799 1.28262 1.28578 1.28655

Alpha virt. eigenvalues -- 1.31596 1.32937 1.32937 1.33151 1.34024

Alpha virt. eigenvalues -- 1.34024 1.35216 1.37862 1.38082 1.40601

Alpha virt. eigenvalues -- 1.40601 1.40649 1.42072 1.42072 1.42413

Alpha virt. eigenvalues -- 1.44816 1.44816 1.45182 1.45206 1.45206

Alpha virt. eigenvalues -- 1.45321 1.48087 1.49368 1.50860 1.50860

Alpha virt. eigenvalues -- 1.51296 1.52273 1.52283 1.52500 1.52500

Alpha virt. eigenvalues -- 1.52587 1.53062 1.53062 1.54586 1.55280

Alpha virt. eigenvalues -- 1.57361 1.57361 1.58808 1.61525 1.61525

Alpha virt. eigenvalues -- 1.62336 1.62554 1.63044 1.64018 1.65160

Alpha virt. eigenvalues -- 1.65160 1.65481 1.67347 1.68281 1.68281

Alpha virt. eigenvalues -- 1.71929 1.71929 1.72134 1.73574 1.73725

Alpha virt. eigenvalues -- 1.73926 1.74588 1.74588 1.75795 1.76085

Alpha virt. eigenvalues -- 1.76085 1.79924 1.80627 1.80781 1.80781

Alpha virt. eigenvalues -- 1.81462 1.81503 1.81788 1.82173 1.82173

Alpha virt. eigenvalues -- 1.82691 1.83872 1.84075 1.84075 1.86248

Alpha virt. eigenvalues -- 1.86248 1.86562 1.88597 1.89342 1.90532

Alpha virt. eigenvalues -- 1.90532 1.90590 1.90637 1.90864 1.90864

Alpha virt. eigenvalues -- 1.91044 1.91119 1.91329 1.91329 1.92162

Alpha virt. eigenvalues -- 1.92162 1.92221 1.92760 1.93648 1.94590

Alpha virt. eigenvalues -- 1.94601 1.94601 1.95182 1.98256 1.98611

Alpha virt. eigenvalues -- 1.98611 1.99500 2.00458 2.02234 2.02234

Alpha virt. eigenvalues -- 2.02768 2.03595 2.03652 2.05624 2.05624

Alpha virt. eigenvalues -- 2.08209 2.10522 2.12875 2.12875 2.15268

Alpha virt. eigenvalues -- 2.15268 2.18130 2.19177 2.21333 2.22229

Alpha virt. eigenvalues -- 2.22605 2.23289 2.23289 2.24311 2.25080

Alpha virt. eigenvalues -- 2.25080 2.25931 2.26808 2.27362 2.27362

Alpha virt. eigenvalues -- 2.27723 2.27723 2.27878 2.28369 2.28726

Alpha virt. eigenvalues -- 2.30003 2.30389 2.30447 2.30447 2.32618

Alpha virt. eigenvalues -- 2.32954 2.32954 2.33554 2.36877 2.38447

Alpha virt. eigenvalues -- 2.38447 2.39415 2.39493 2.39601 2.39601

Alpha virt. eigenvalues -- 2.41428 2.43012 2.43012 2.43533 2.44865

Alpha virt. eigenvalues -- 2.45806 2.48400 2.48400 2.51302 2.52273

Alpha virt. eigenvalues -- 2.53193 2.53193 2.55029 2.55127 2.55127

Alpha virt. eigenvalues -- 2.56184 2.56575 2.57798 2.58113 2.58113

Alpha virt. eigenvalues -- 2.59315 2.60992 2.64100 2.64324 2.64324

Alpha virt. eigenvalues -- 2.65036 2.65619 2.65619 2.67804 2.68529

Alpha virt. eigenvalues -- 2.68563 2.68563 2.69939 2.73572 2.74057

Alpha virt. eigenvalues -- 2.74057 2.74101 2.74794 2.74968 2.74968

Alpha virt. eigenvalues -- 2.75972 2.77247 2.77620 2.78076 2.78076

Alpha virt. eigenvalues -- 2.78688 2.78991 2.78991 2.81223 2.81846

Alpha virt. eigenvalues -- 2.82180 2.82261 2.82261 2.84686 2.84686

Alpha virt. eigenvalues -- 2.85136 2.86455 2.87824 2.87824 2.88142

Alpha virt. eigenvalues -- 2.88725 2.91359 2.91382 2.91712 2.91716

Alpha virt. eigenvalues -- 2.91716 2.96836 2.96836 2.99743 3.03722

Alpha virt. eigenvalues -- 3.04501 3.04644 3.04644 3.07101 3.09169

Alpha virt. eigenvalues -- 3.09169 3.15919 3.16775 3.16826 3.16826

Alpha virt. eigenvalues -- 3.17720 3.18605 3.19086 3.19086 3.19925

Alpha virt. eigenvalues -- 3.21234 3.22072 3.22675 3.22675 3.25266

Alpha virt. eigenvalues -- 3.25686 3.25686 3.26838 3.27399 3.27424

Alpha virt. eigenvalues -- 3.27424 3.27648 3.30005 3.30446 3.30446

Alpha virt. eigenvalues -- 3.30510 3.31028 3.33012 3.33012 3.35867

Alpha virt. eigenvalues -- 3.37827 3.39959 3.39959 3.41504 3.45948

Alpha virt. eigenvalues -- 3.46862 3.46862 3.47565 3.47667 3.48191

Alpha virt. eigenvalues -- 3.48191 3.49669 3.55443 3.60743 3.60743

Alpha virt. eigenvalues -- 3.65006 3.65006 3.65012 3.65672 3.72516

Alpha virt. eigenvalues -- 3.72516 3.73163 3.74018 3.75762 3.76324

Alpha virt. eigenvalues -- 3.76602 3.76602 3.81925 3.83356 3.83356

Alpha virt. eigenvalues -- 3.84257 3.86940 3.87945 3.89589 3.89589

Alpha virt. eigenvalues -- 3.89946 3.95365 3.96186 3.96186 3.97166

Alpha virt. eigenvalues -- 4.10750 4.11744 4.11744 4.17354 4.17835

Alpha virt. eigenvalues -- 4.17835 4.20617 4.22966 4.33807 4.39313

Alpha virt. eigenvalues -- 4.39313 4.40260 4.46145 4.53110 4.53171

Alpha virt. eigenvalues -- 4.53171 4.78690 4.78832 4.78832 4.79132

Alpha virt. eigenvalues -- 5.12102 5.12102 5.13221 5.16329 5.20802

Alpha virt. eigenvalues -- 5.36052 5.36052 5.52397 7.83886 7.86323

Alpha virt. eigenvalues -- 7.86323 7.89915 8.12600 11.11816 23.27409

Alpha virt. eigenvalues -- 23.30383 23.30383 23.32110 23.76747 23.79126

Alpha virt. eigenvalues -- 23.79126 23.79265 23.79482 23.79482 23.79650

Alpha virt. eigenvalues -- 23.81081 23.88431 23.88431 23.88617 23.89182

Alpha virt. eigenvalues -- 23.89336 23.89623 23.90011 23.90011 24.03275

Alpha virt. eigenvalues -- 24.03605 24.03605 24.04220 24.05626 24.05640

Alpha virt. eigenvalues -- 24.05640 24.05724 24.13932 24.14084 24.14084

Alpha virt. eigenvalues -- 24.14438 35.56481 35.60200 35.60200 35.61455

Alpha virt. eigenvalues -- 35.68759 35.69653 35.69653 35.69731

Condensed to atoms (all electrons):

Mulliken charges:

1

1 C 0.383710

2 N -0.652760

3 C 0.383710

4 C -0.062491

5 C -0.062491

6 N -0.400169

7 C 0.383710

8 N -0.652760

9 C 0.383710

10 C -0.062491

11 C -0.062491

12 N -0.400169

13 C -0.062491

14 C -0.062491

15 C 0.383710

16 N -0.652760

17 C 0.383710

18 N -0.400169

19 N -0.652760

20 C 0.383710

21 C -0.062491

22 C -0.062491

23 C 0.383710

24 N -0.400169

25 Zn 1.408722

26 C -0.206140

27 C -0.223613

28 C -0.223613

29 C -0.206140

30 C -0.206140

31 C -0.223613

32 C -0.223613

33 C -0.206140

34 C -0.206140

35 C -0.223613

36 C -0.223613

37 C -0.206140

38 C -0.206140

39 C -0.223613

40 C -0.223613

41 C -0.206140

42 H 0.227431

43 H 0.227431

44 H 0.227431

45 H 0.227431

46 H 0.227431

47 H 0.227431

48 H 0.227431

49 H 0.227431

50 H 0.231478

51 H 0.231478

52 H 0.231478

53 H 0.231478

54 H 0.231478

55 H 0.231478

56 H 0.231478

57 H 0.231478

Sum of Mulliken charges = -0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 C 0.383710

2 N -0.652760

3 C 0.383710

4 C -0.062491

5 C -0.062491

6 N -0.400169

7 C 0.383710

8 N -0.652760

9 C 0.383710

10 C -0.062491

11 C -0.062491

12 N -0.400169

13 C -0.062491

14 C -0.062491

15 C 0.383710

16 N -0.652760

17 C 0.383710

18 N -0.400169

19 N -0.652760

20 C 0.383710

21 C -0.062491

22 C -0.062491

23 C 0.383710

24 N -0.400169

25 Zn 1.408722

26 C 0.021290

27 C 0.007865

28 C 0.007865

29 C 0.021290

30 C 0.021290

31 C 0.007865

32 C 0.007865

33 C 0.021290

34 C 0.021290

35 C 0.007865

36 C 0.007865

37 C 0.021290

38 C 0.021290

39 C 0.007865

40 C 0.007865

41 C 0.021290

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

Charge= -0.0000 electrons

Dipole moment (field-independent basis, Debye):

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

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

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

XY= -0.0000 XZ= 0.0000 YZ= 0.0000

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

XX= 12.5309 YY= 12.5309 ZZ= -25.0618

XY= -0.0000 XZ= 0.0000 YZ= 0.0000

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

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

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

YYZ= -9.0862 XYZ= 0.0000

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

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

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

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

XXYZ= -0.0000 YYXZ= -0.0000 ZZXY= 0.0000

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

Symmetry A1 KE= 5.103287750189D+02

Symmetry A2 KE= 3.909478542394D+02

Symmetry B1 KE= 4.376325044598D+02

Symmetry B2 KE= 4.376325044598D+02

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

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

Test job not archived.

1\1\ WCSS.PL-BEM-DHCP-129-94-98-136\SP\RB3LYP TD-FC\GenECP\C32H16N8Zn1

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

(C32H16)]\\@

VIRTUE IS LEARNED AT YOUR MOTHER'S KNEE,

VICES ARE PICKED UP AT SOME OTHER JOINT.

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

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

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